



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:46 PM GMT

PDB ID : 4D0M
Title : Phosphatidylinositol 4-kinase III beta in a complex with Rab11a-GTP-gamma-S and the Rab-binding domain of FIP3
Authors : Burke, J.E.; Inglis, A.J.; Perisic, O.; Masson, G.R.; McLaughlin, S.H.; Rutaganira, F.; Shokat, K.M.; Williams, R.L.
Deposited on : 2014-04-27
Resolution : 6.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

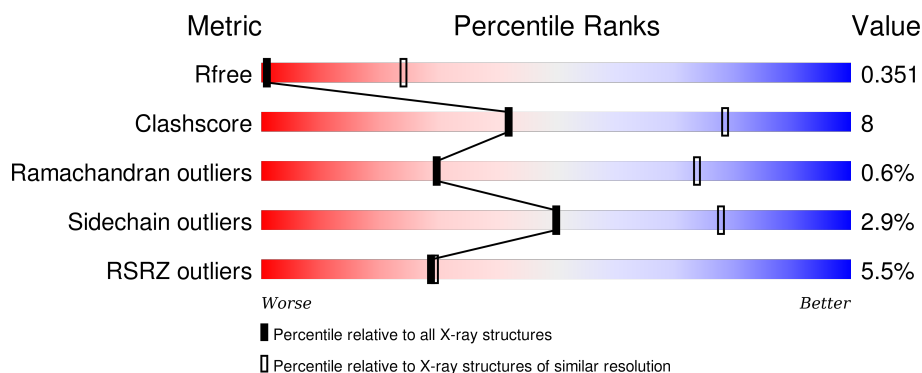
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1002 (8.30-3.66)
Clashscore	102246	1050 (8.30-3.70)
Ramachandran outliers	100387	1023 (8.30-3.66)
Sidechain outliers	100360	1012 (8.30-3.64)
RSRZ outliers	91569	1001 (8.30-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	566	<div> <div>70%</div> <div>11%</div> <div>17%</div> </div>
1	C	566	<div>9%</div> <div>69%</div> <div>13%</div> <div>17%</div>
1	G	566	<div>2%</div> <div>69%</div> <div>13%</div> <div>17%</div>
1	I	566	<div>11%</div> <div>69%</div> <div>12%</div> <div>17%</div>
1	M	566	<div>2%</div> <div>69%</div> <div>12%</div> <div>17%</div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	O	566	
1	Q	566	
1	S	566	
1	W	566	
1	Y	566	
1	c	566	
1	g	566	
2	B	219	
2	D	219	
2	H	219	
2	J	219	
2	N	219	
2	P	219	
2	R	219	
2	T	219	
2	X	219	
2	Z	219	
2	d	219	
2	h	219	
3	E	48	
3	F	48	
3	K	48	
3	L	48	
3	U	48	
3	V	48	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	a	48	 81% • 15%
3	b	48	 67% 33%
3	e	48	 83% • 15%
3	f	48	 67% 33%
3	i	48	 83% • 15%
3	j	48	 67% 33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GSP	D	2000	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 65970 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL 4-KINASE BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	C	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	G	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	I	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	M	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	O	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	Q	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	S	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	W	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	Y	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	c	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	g	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	GLY	-	EXPRESSION TAG	UNP Q9UBF8
A	120	SER	-	EXPRESSION TAG	UNP Q9UBF8
A	294	ALA	SER	ENGINEERED MUTATION	UNP Q9UBF8
A	507	ARG	LYS	CONFLICT	UNP Q9UBF8
C	119	GLY	-	EXPRESSION TAG	UNP Q9UBF8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	120	SER	-	EXPRESSION TAG	UNP Q9UBF8
C	294	ALA	SER	ENGINEERED MUTATION	UNP Q9UBF8
C	507	ARG	LYS	CONFLICT	UNP Q9UBF8
G	119	GLY	-	EXPRESSION TAG	UNP Q9UBF8
G	120	SER	-	EXPRESSION TAG	UNP Q9UBF8
G	294	ALA	SER	ENGINEERED MUTATION	UNP Q9UBF8
G	507	ARG	LYS	CONFLICT	UNP Q9UBF8
I	119	GLY	-	EXPRESSION TAG	UNP Q9UBF8
I	120	SER	-	EXPRESSION TAG	UNP Q9UBF8
I	294	ALA	SER	ENGINEERED MUTATION	UNP Q9UBF8
I	507	ARG	LYS	CONFLICT	UNP Q9UBF8
M	119	GLY	-	EXPRESSION TAG	UNP Q9UBF8
M	120	SER	-	EXPRESSION TAG	UNP Q9UBF8
M	294	ALA	SER	ENGINEERED MUTATION	UNP Q9UBF8
M	507	ARG	LYS	CONFLICT	UNP Q9UBF8
O	119	GLY	-	EXPRESSION TAG	UNP Q9UBF8
O	120	SER	-	EXPRESSION TAG	UNP Q9UBF8
O	294	ALA	SER	ENGINEERED MUTATION	UNP Q9UBF8
O	507	ARG	LYS	CONFLICT	UNP Q9UBF8
Q	119	GLY	-	EXPRESSION TAG	UNP Q9UBF8
Q	120	SER	-	EXPRESSION TAG	UNP Q9UBF8
Q	294	ALA	SER	ENGINEERED MUTATION	UNP Q9UBF8
Q	507	ARG	LYS	CONFLICT	UNP Q9UBF8
S	119	GLY	-	EXPRESSION TAG	UNP Q9UBF8
S	120	SER	-	EXPRESSION TAG	UNP Q9UBF8
S	294	ALA	SER	ENGINEERED MUTATION	UNP Q9UBF8
S	507	ARG	LYS	CONFLICT	UNP Q9UBF8
W	119	GLY	-	EXPRESSION TAG	UNP Q9UBF8
W	120	SER	-	EXPRESSION TAG	UNP Q9UBF8
W	294	ALA	SER	ENGINEERED MUTATION	UNP Q9UBF8
W	507	ARG	LYS	CONFLICT	UNP Q9UBF8
Y	119	GLY	-	EXPRESSION TAG	UNP Q9UBF8
Y	120	SER	-	EXPRESSION TAG	UNP Q9UBF8
Y	294	ALA	SER	ENGINEERED MUTATION	UNP Q9UBF8
Y	507	ARG	LYS	CONFLICT	UNP Q9UBF8
c	119	GLY	-	EXPRESSION TAG	UNP Q9UBF8
c	120	SER	-	EXPRESSION TAG	UNP Q9UBF8
c	294	ALA	SER	ENGINEERED MUTATION	UNP Q9UBF8
c	507	ARG	LYS	CONFLICT	UNP Q9UBF8
g	119	GLY	-	EXPRESSION TAG	UNP Q9UBF8
g	120	SER	-	EXPRESSION TAG	UNP Q9UBF8
g	294	ALA	SER	ENGINEERED MUTATION	UNP Q9UBF8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
g	507	ARG	LYS	CONFLICT	UNP Q9UBF8

- Molecule 2 is a protein called RAS-RELATED PROTEIN RAB-11A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	D	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	H	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	J	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	N	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	P	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	R	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	T	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	X	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	Z	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	d	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	h	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	EXPRESSION TAG	UNP P62491
B	-1	SER	-	EXPRESSION TAG	UNP P62491
B	0	HIS	-	EXPRESSION TAG	UNP P62491
B	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
D	-2	GLY	-	EXPRESSION TAG	UNP P62491
D	-1	SER	-	EXPRESSION TAG	UNP P62491
D	0	HIS	-	EXPRESSION TAG	UNP P62491
D	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
H	-2	GLY	-	EXPRESSION TAG	UNP P62491

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	SER	-	EXPRESSION TAG	UNP P62491
H	0	HIS	-	EXPRESSION TAG	UNP P62491
H	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
J	-2	GLY	-	EXPRESSION TAG	UNP P62491
J	-1	SER	-	EXPRESSION TAG	UNP P62491
J	0	HIS	-	EXPRESSION TAG	UNP P62491
J	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
N	-2	GLY	-	EXPRESSION TAG	UNP P62491
N	-1	SER	-	EXPRESSION TAG	UNP P62491
N	0	HIS	-	EXPRESSION TAG	UNP P62491
N	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
P	-2	GLY	-	EXPRESSION TAG	UNP P62491
P	-1	SER	-	EXPRESSION TAG	UNP P62491
P	0	HIS	-	EXPRESSION TAG	UNP P62491
P	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
R	-2	GLY	-	EXPRESSION TAG	UNP P62491
R	-1	SER	-	EXPRESSION TAG	UNP P62491
R	0	HIS	-	EXPRESSION TAG	UNP P62491
R	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
T	-2	GLY	-	EXPRESSION TAG	UNP P62491
T	-1	SER	-	EXPRESSION TAG	UNP P62491
T	0	HIS	-	EXPRESSION TAG	UNP P62491
T	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
X	-2	GLY	-	EXPRESSION TAG	UNP P62491
X	-1	SER	-	EXPRESSION TAG	UNP P62491
X	0	HIS	-	EXPRESSION TAG	UNP P62491
X	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
Z	-2	GLY	-	EXPRESSION TAG	UNP P62491
Z	-1	SER	-	EXPRESSION TAG	UNP P62491
Z	0	HIS	-	EXPRESSION TAG	UNP P62491
Z	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
d	-2	GLY	-	EXPRESSION TAG	UNP P62491
d	-1	SER	-	EXPRESSION TAG	UNP P62491
d	0	HIS	-	EXPRESSION TAG	UNP P62491
d	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
h	-2	GLY	-	EXPRESSION TAG	UNP P62491
h	-1	SER	-	EXPRESSION TAG	UNP P62491
h	0	HIS	-	EXPRESSION TAG	UNP P62491
h	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491

- Molecule 3 is a protein called RAB11 FAMILY-INTERACTING PROTEIN 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	41	Total	C	N	O	S	0	0	0
			314	199	54	60	1			
3	F	32	Total	C	N	O	S	0	0	0
			237	153	41	42	1			
3	K	41	Total	C	N	O	S	0	0	0
			314	199	54	60	1			
3	L	32	Total	C	N	O	S	0	0	0
			237	153	41	42	1			
3	U	41	Total	C	N	O	S	0	0	0
			314	199	54	60	1			
3	V	32	Total	C	N	O	S	0	0	0
			237	153	41	42	1			
3	a	41	Total	C	N	O	S	0	0	0
			314	199	54	60	1			
3	b	32	Total	C	N	O	S	0	0	0
			237	153	41	42	1			
3	e	41	Total	C	N	O	S	0	0	0
			314	199	54	60	1			
3	f	32	Total	C	N	O	S	0	0	0
			237	153	41	42	1			
3	i	41	Total	C	N	O	S	0	0	0
			314	199	54	60	1			
3	j	32	Total	C	N	O	S	0	0	0
			237	153	41	42	1			

There are 48 discrepancies between the modelled and reference sequences:

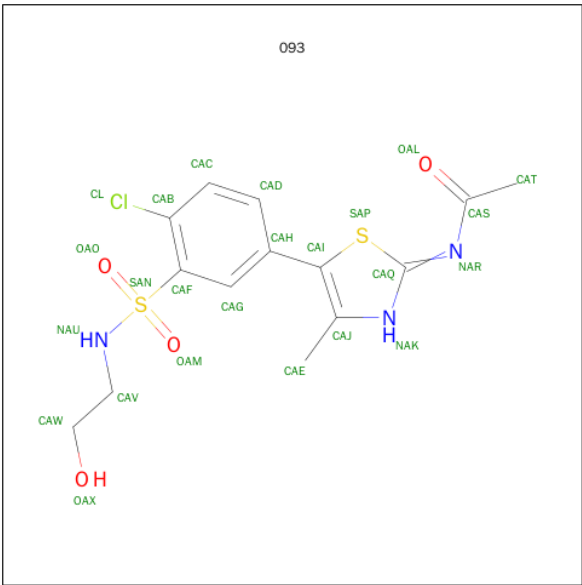
Chain	Residue	Modelled	Actual	Comment	Reference
E	709	GLY	-	EXPRESSION TAG	UNP O75154
E	710	SER	-	EXPRESSION TAG	UNP O75154
E	711	HIS	-	EXPRESSION TAG	UNP O75154
E	712	MET	-	EXPRESSION TAG	UNP O75154
F	709	GLY	-	EXPRESSION TAG	UNP O75154
F	710	SER	-	EXPRESSION TAG	UNP O75154
F	711	HIS	-	EXPRESSION TAG	UNP O75154
F	712	MET	-	EXPRESSION TAG	UNP O75154
K	709	GLY	-	EXPRESSION TAG	UNP O75154
K	710	SER	-	EXPRESSION TAG	UNP O75154
K	711	HIS	-	EXPRESSION TAG	UNP O75154
K	712	MET	-	EXPRESSION TAG	UNP O75154
L	709	GLY	-	EXPRESSION TAG	UNP O75154
L	710	SER	-	EXPRESSION TAG	UNP O75154
L	711	HIS	-	EXPRESSION TAG	UNP O75154
L	712	MET	-	EXPRESSION TAG	UNP O75154

Continued on next page...

Continued from previous page...

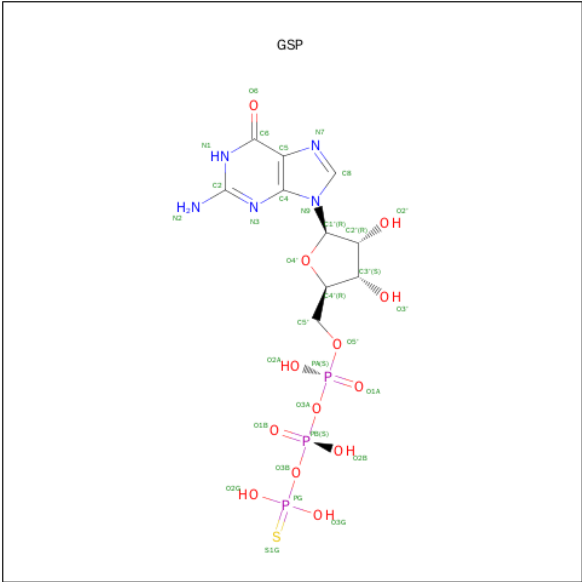
Chain	Residue	Modelled	Actual	Comment	Reference
U	709	GLY	-	EXPRESSION TAG	UNP O75154
U	710	SER	-	EXPRESSION TAG	UNP O75154
U	711	HIS	-	EXPRESSION TAG	UNP O75154
U	712	MET	-	EXPRESSION TAG	UNP O75154
V	709	GLY	-	EXPRESSION TAG	UNP O75154
V	710	SER	-	EXPRESSION TAG	UNP O75154
V	711	HIS	-	EXPRESSION TAG	UNP O75154
V	712	MET	-	EXPRESSION TAG	UNP O75154
a	709	GLY	-	EXPRESSION TAG	UNP O75154
a	710	SER	-	EXPRESSION TAG	UNP O75154
a	711	HIS	-	EXPRESSION TAG	UNP O75154
a	712	MET	-	EXPRESSION TAG	UNP O75154
b	709	GLY	-	EXPRESSION TAG	UNP O75154
b	710	SER	-	EXPRESSION TAG	UNP O75154
b	711	HIS	-	EXPRESSION TAG	UNP O75154
b	712	MET	-	EXPRESSION TAG	UNP O75154
e	709	GLY	-	EXPRESSION TAG	UNP O75154
e	710	SER	-	EXPRESSION TAG	UNP O75154
e	711	HIS	-	EXPRESSION TAG	UNP O75154
e	712	MET	-	EXPRESSION TAG	UNP O75154
f	709	GLY	-	EXPRESSION TAG	UNP O75154
f	710	SER	-	EXPRESSION TAG	UNP O75154
f	711	HIS	-	EXPRESSION TAG	UNP O75154
f	712	MET	-	EXPRESSION TAG	UNP O75154
i	709	GLY	-	EXPRESSION TAG	UNP O75154
i	710	SER	-	EXPRESSION TAG	UNP O75154
i	711	HIS	-	EXPRESSION TAG	UNP O75154
i	712	MET	-	EXPRESSION TAG	UNP O75154
j	709	GLY	-	EXPRESSION TAG	UNP O75154
j	710	SER	-	EXPRESSION TAG	UNP O75154
j	711	HIS	-	EXPRESSION TAG	UNP O75154
j	712	MET	-	EXPRESSION TAG	UNP O75154

- Molecule 4 is N-(5-(4-CHLORO-3-(2-HYDROXY-ETHYLSULFAMOYL)- PHENYLTHIA ZOLE-2-YL)-ACETAMIDE (three-letter code: 093) (formula: C₁₄H₁₆ClN₃O₄S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	24	0
4	C	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	24	0
4	G	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	24	0
4	I	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	24	0
4	M	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	24	0
4	O	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	24	0
4	Q	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	24	0
4	S	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	24	0
4	W	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	24	0
4	Y	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	24	0
4	c	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	24	0
4	g	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	24	0

- Molecule 5 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: C₁₀H₁₆N₅O₁₃P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	D	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	H	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	J	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	N	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	P	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	R	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	T	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	X	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	Z	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	d	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	h	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		

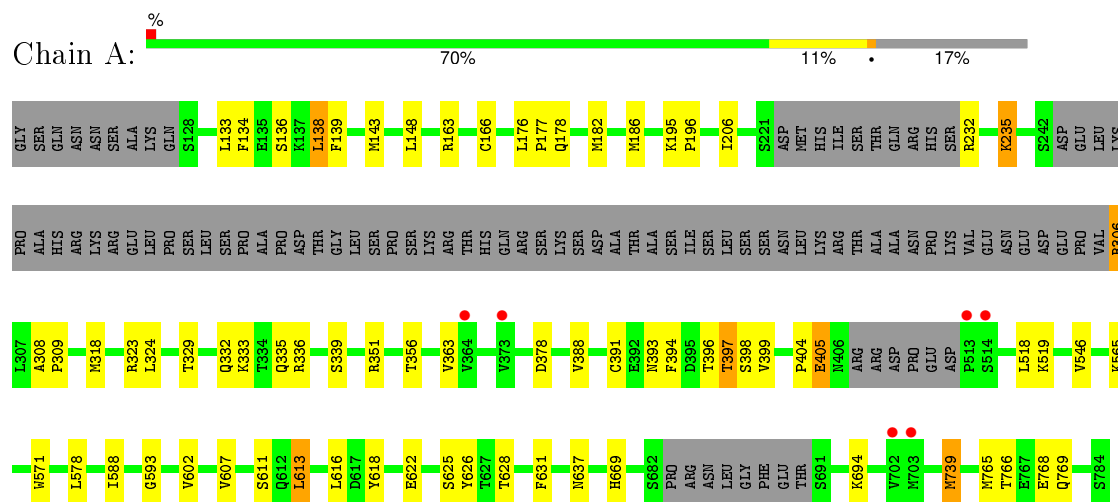
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	1	Total	Mg	0	0
			1	1		
6	J	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	H	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	h	1	Total	Mg	0	0
			1	1		
6	Z	1	Total	Mg	0	0
			1	1		
6	T	1	Total	Mg	0	0
			1	1		
6	N	1	Total	Mg	0	0
			1	1		
6	X	1	Total	Mg	0	0
			1	1		
6	d	1	Total	Mg	0	0
			1	1		
6	R	1	Total	Mg	0	0
			1	1		

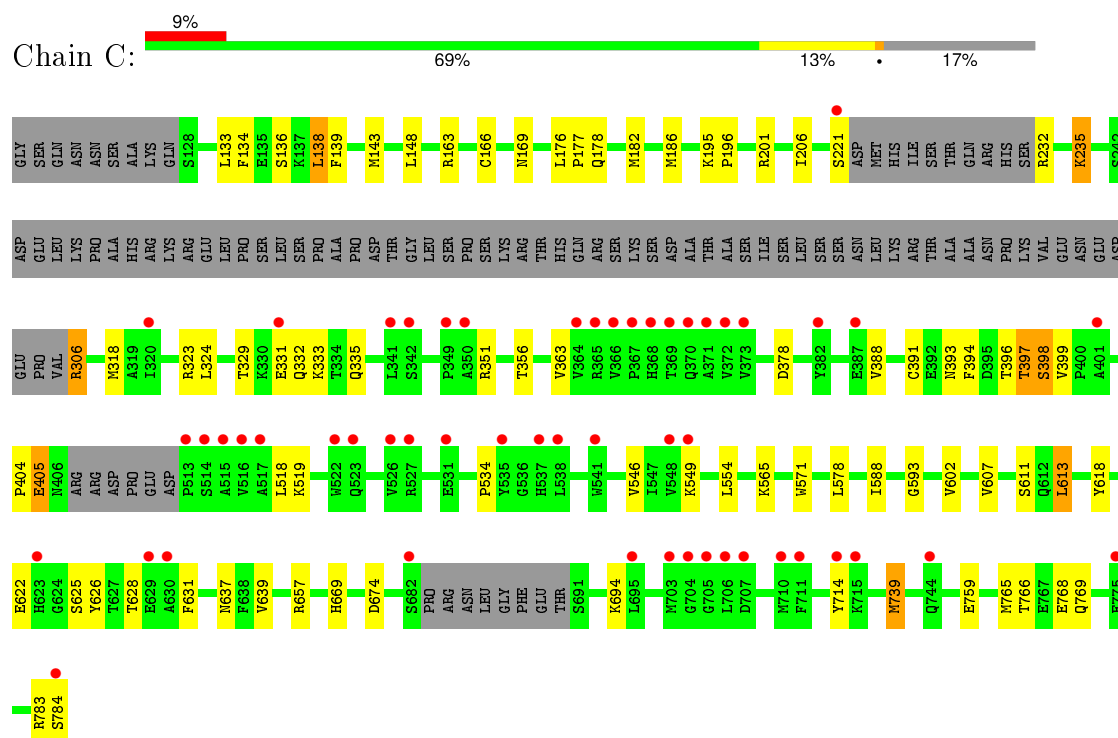
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

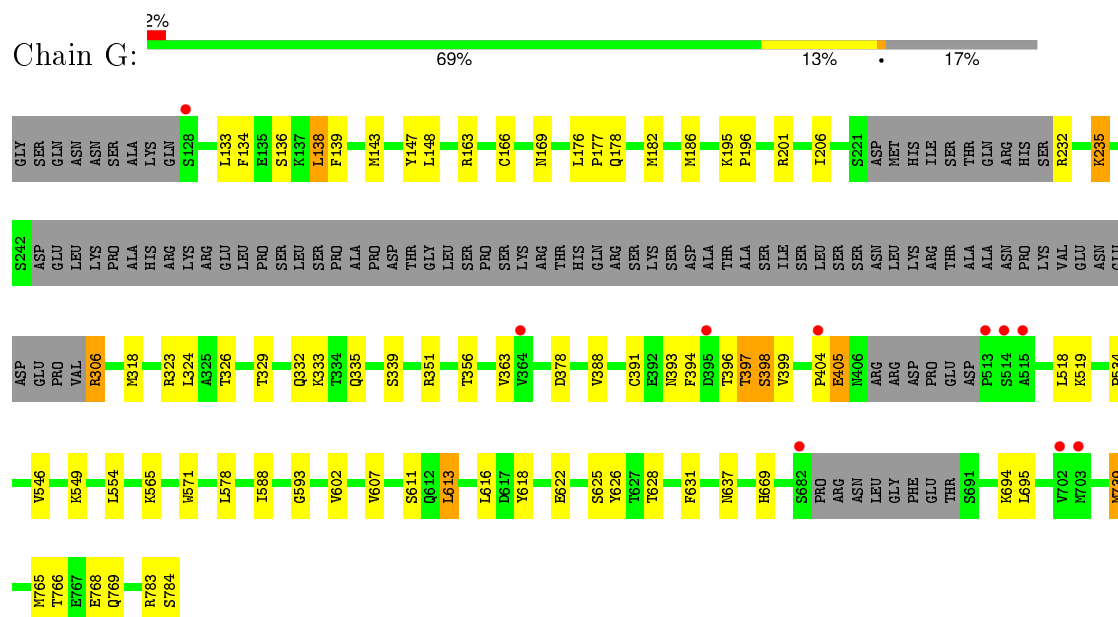
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA



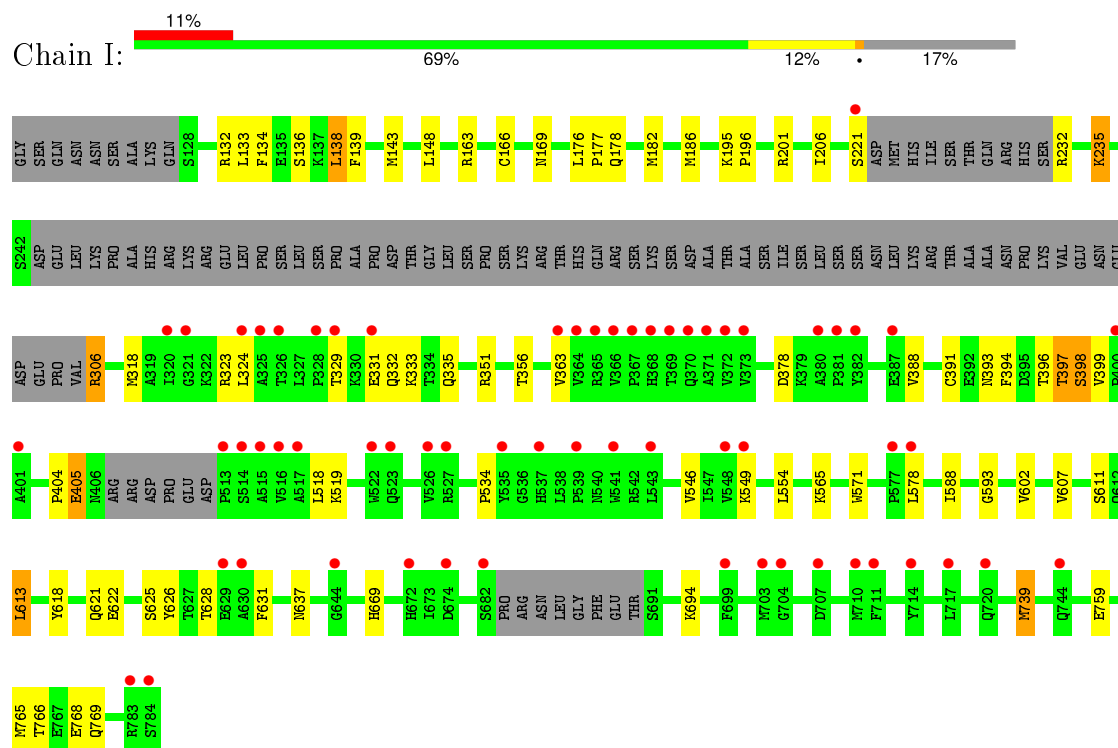
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA



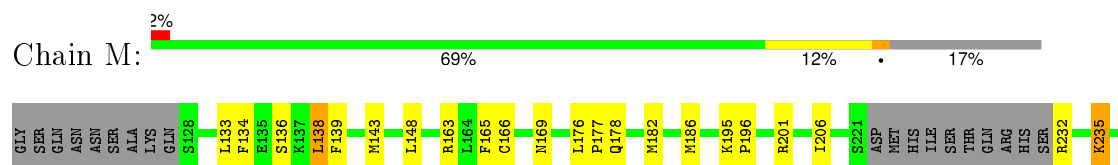
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA



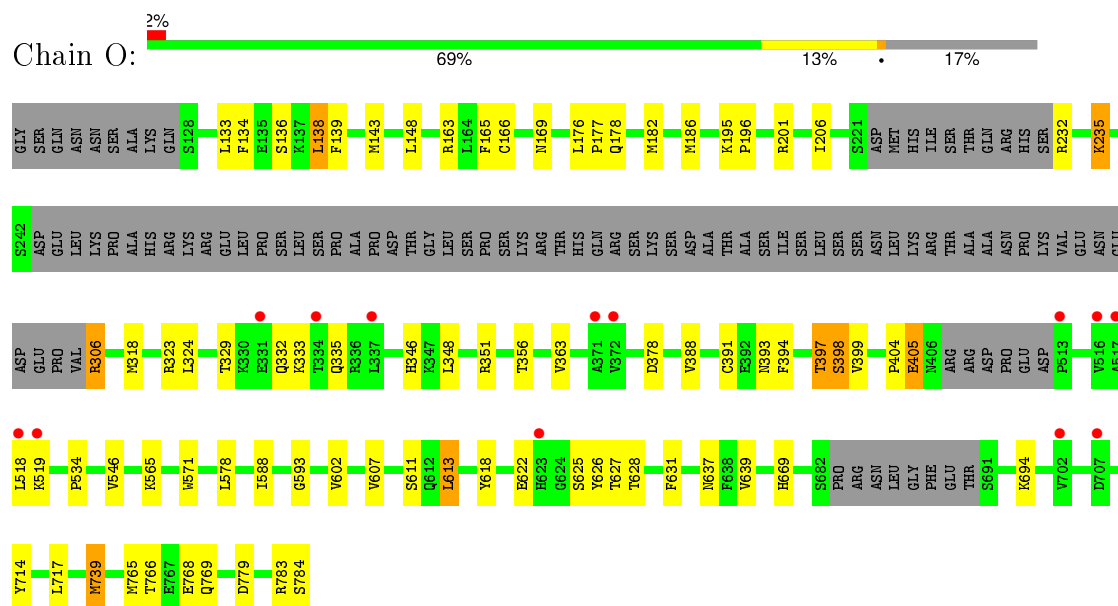
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA



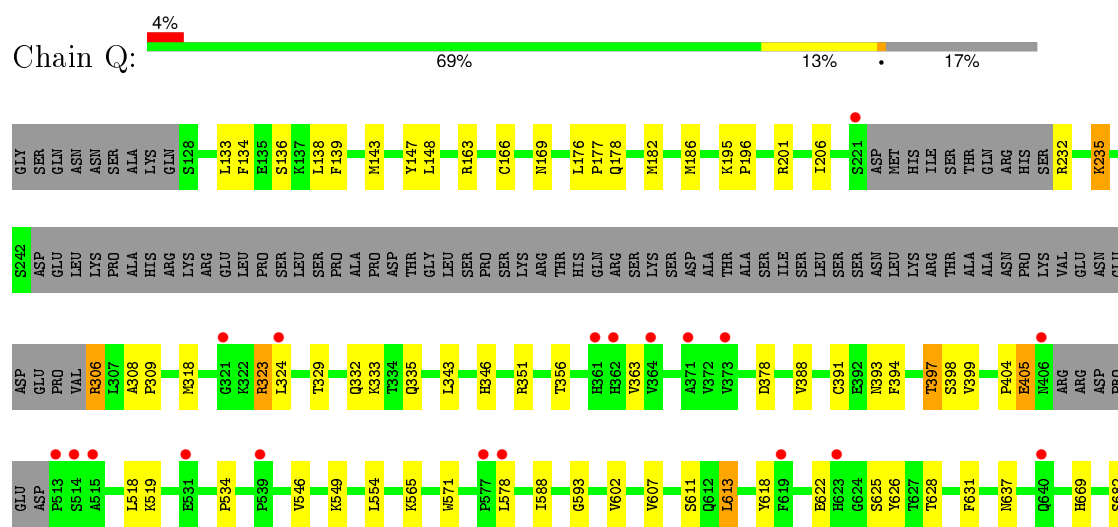
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

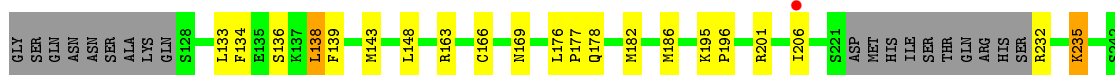


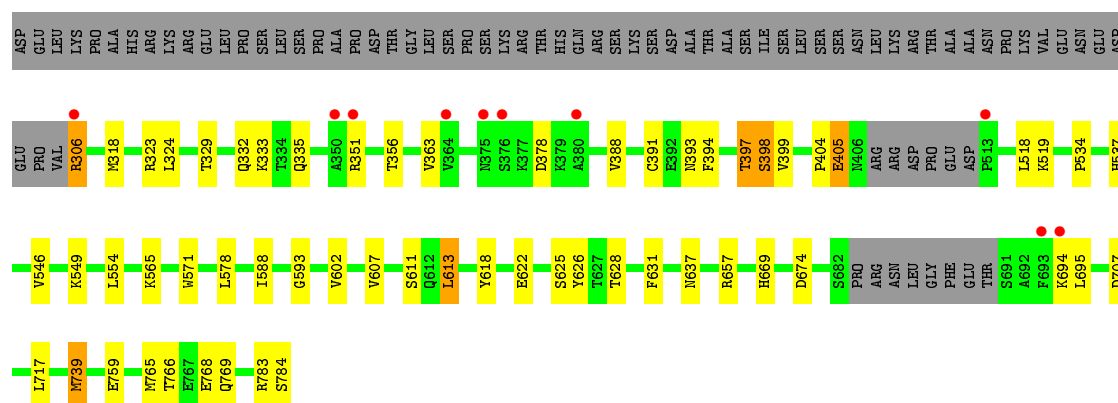
- Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA



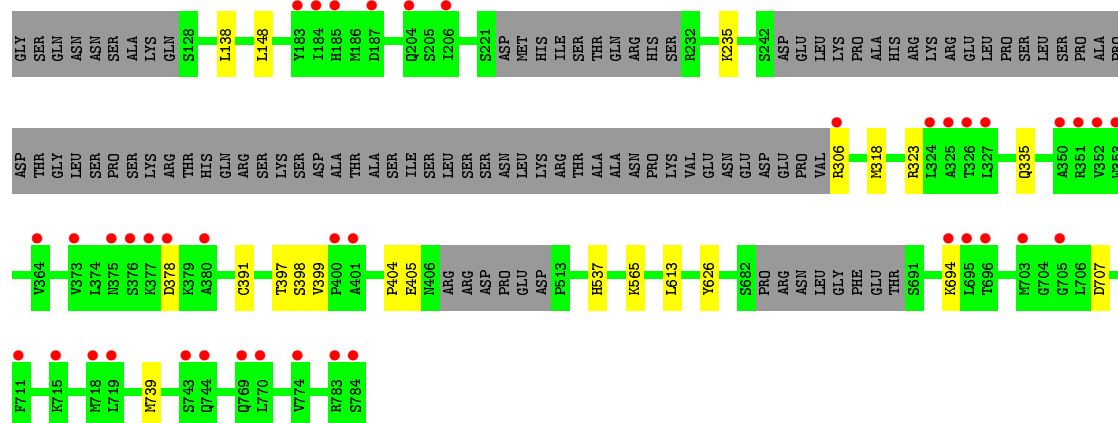
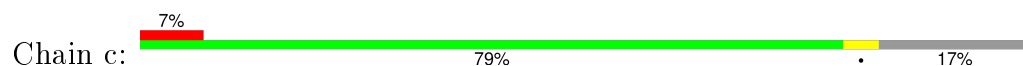
- Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA



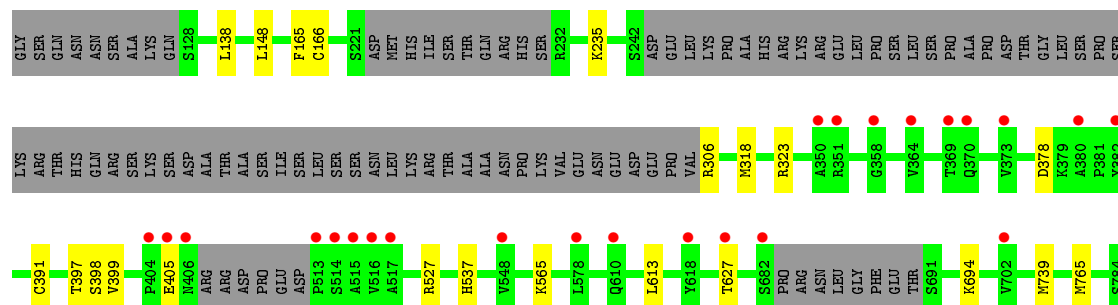
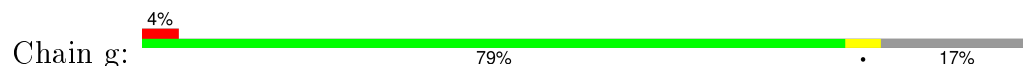




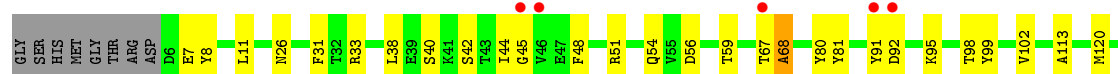
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

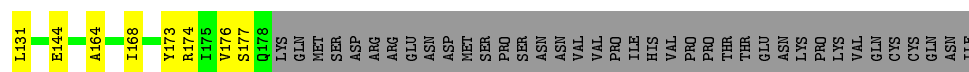


• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

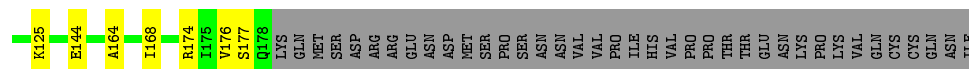
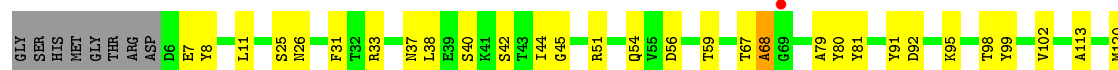


• Molecule 2: RAS-RELATED PROTEIN RAB-11A

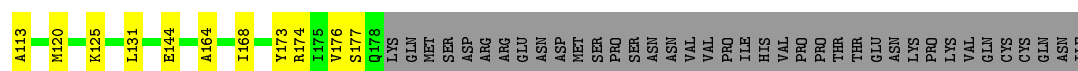
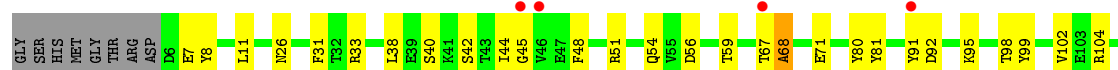




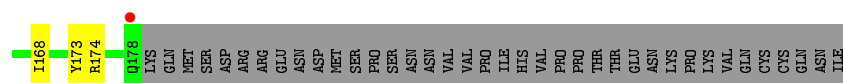
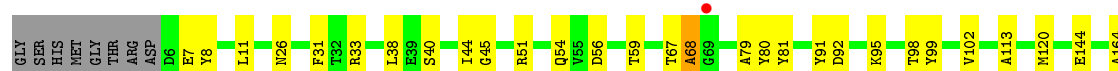
• Molecule 2: RAS-RELATED PROTEIN RAB-11A



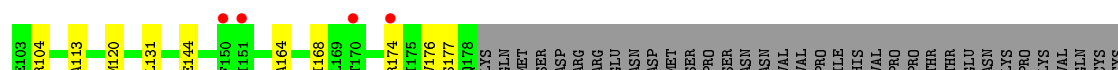
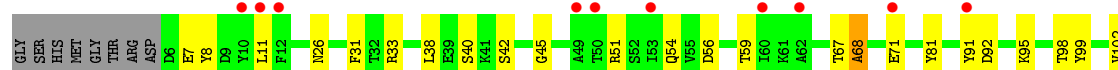
• Molecule 2: RAS-RELATED PROTEIN RAB-11A



• Molecule 2: RAS-RELATED PROTEIN RAB-11A

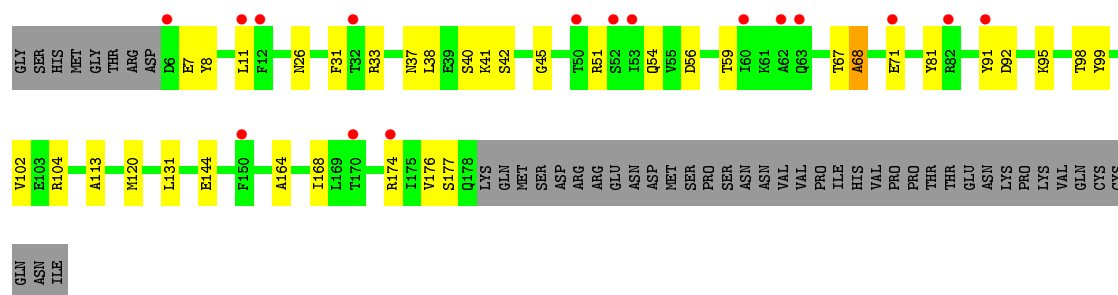


• Molecule 2: RAS-RELATED PROTEIN RAB-11A

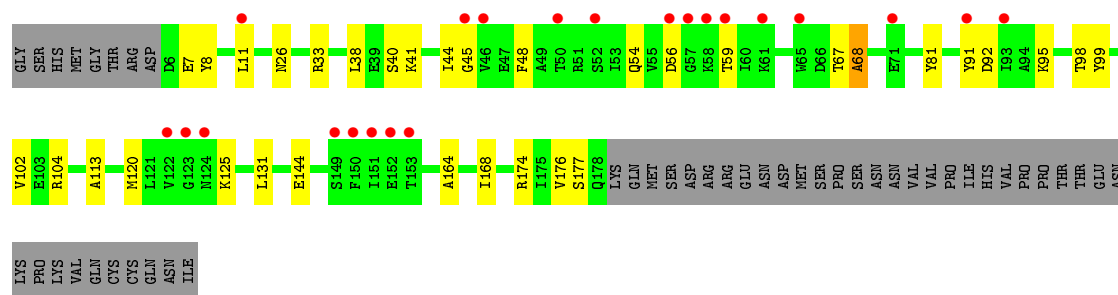


• Molecule 2: RAS-RELATED PROTEIN RAB-11A

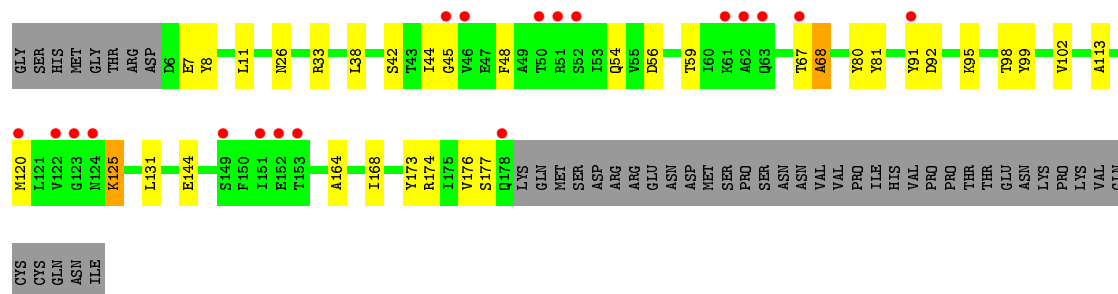




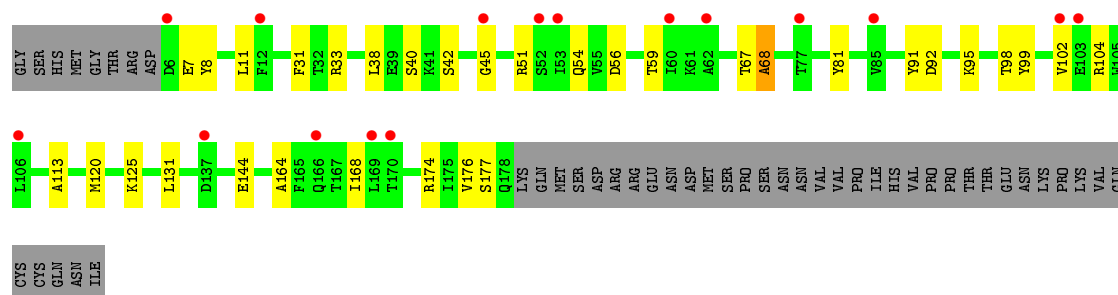
- Molecule 2: RAS-RELATED PROTEIN RAB-11A



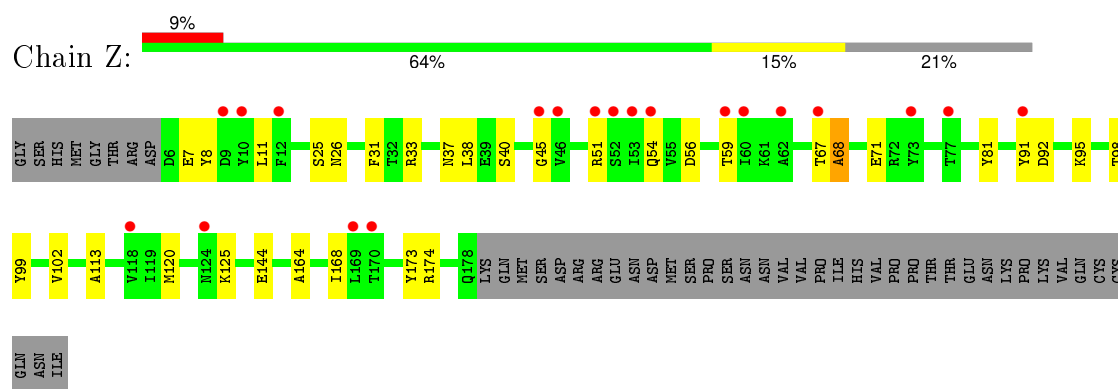
- Molecule 2: RAS-RELATED PROTEIN RAB-11A



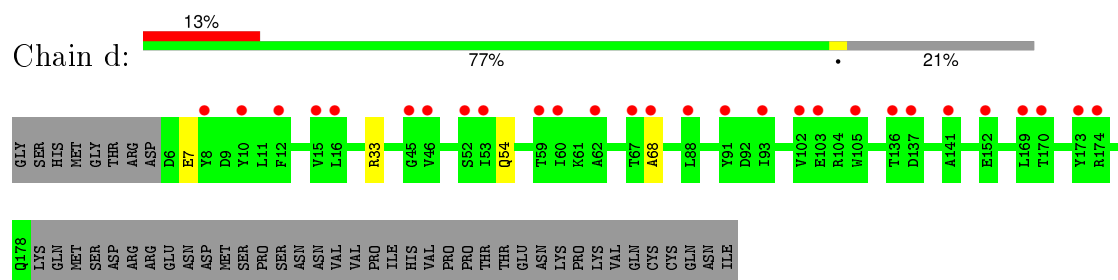
- Molecule 2: RAS-RELATED PROTEIN RAB-11A



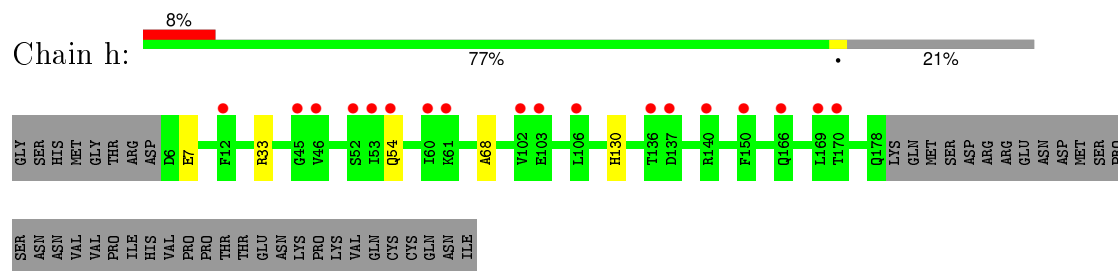
- Molecule 2: RAS-RELATED PROTEIN RAB-11A



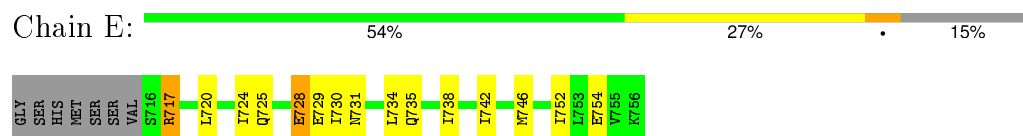
- Molecule 2: RAS-RELATED PROTEIN RAB-11A



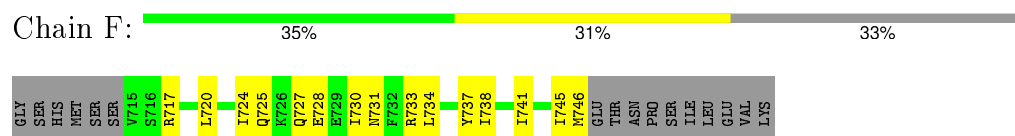
- Molecule 2: RAS-RELATED PROTEIN RAB-11A



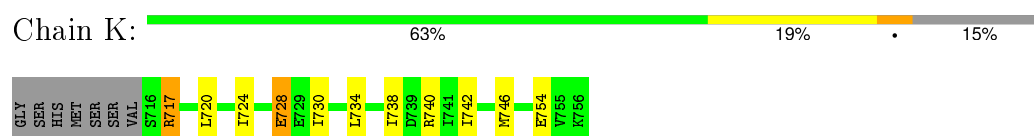
- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3



- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

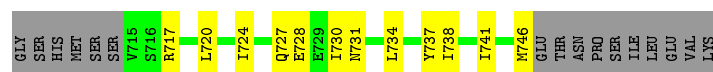


- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3



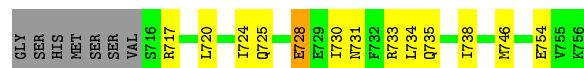
- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain L: 



- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain U: 




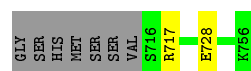
- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain V: 



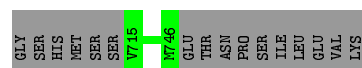
- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain a: 




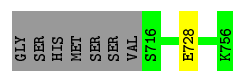
- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain b: 



- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain e: 




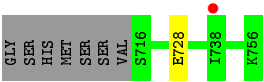
- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain f: 



- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain i: 



● Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	199.50Å 134.47Å 294.33Å 90.00° 90.33° 90.00°	Depositor
Resolution (Å)	294.32 – 6.00 49.88 – 6.00	Depositor EDS
% Data completeness (in resolution range)	94.3 (294.32-6.00) 94.5 (49.88-6.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 6.15Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.253 , 0.359 0.252 , 0.351	Depositor DCC
R_{free} test set	2048 reflections (5.78%)	DCC
Wilson B-factor (Å ²)	248.6	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 207.4	EDS
Estimated twinning fraction	0.389 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 37330 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	65970	wwPDB-VP
Average B, all atoms (Å ²)	264.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GSP, MG, 093

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.59	0/3866	0.72	0/5219
1	C	0.56	0/3866	0.70	0/5219
1	G	0.59	0/3866	0.72	0/5219
1	I	0.56	0/3866	0.69	1/5219 (0.0%)
1	M	0.59	0/3866	0.71	1/5219 (0.0%)
1	O	0.59	0/3866	0.71	0/5219
1	Q	0.57	0/3866	0.70	0/5219
1	S	0.57	0/3866	0.70	0/5219
1	W	0.58	0/3866	0.70	1/5219 (0.0%)
1	Y	0.59	0/3866	0.70	0/5219
1	c	0.60	0/3866	0.71	0/5219
1	g	0.59	0/3866	0.70	2/5219 (0.0%)
2	B	0.64	0/1399	0.76	0/1892
2	D	0.61	0/1399	0.75	0/1892
2	H	0.63	0/1399	0.74	0/1892
2	J	0.63	0/1399	0.75	0/1892
2	N	0.58	0/1399	0.73	0/1892
2	P	0.59	0/1399	0.73	0/1892
2	R	0.59	0/1399	0.72	0/1892
2	T	0.58	0/1399	0.73	0/1892
2	X	0.58	0/1399	0.72	0/1892
2	Z	0.58	0/1399	0.73	0/1892
2	d	0.58	0/1399	0.73	0/1892
2	h	0.59	0/1399	0.72	0/1892
3	E	0.94	1/316 (0.3%)	0.98	1/429 (0.2%)
3	F	0.83	0/238	0.87	0/323
3	K	0.94	1/316 (0.3%)	0.97	1/429 (0.2%)
3	L	0.84	0/238	0.89	0/323
3	U	0.83	0/316	0.82	0/429
3	V	0.90	0/238	0.89	0/323
3	a	0.94	1/316 (0.3%)	0.96	1/429 (0.2%)
3	b	0.86	0/238	0.88	0/323

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	e	0.85	0/316	0.86	0/429
3	f	0.88	0/238	0.89	0/323
3	i	0.85	0/316	0.81	0/429
3	j	0.88	0/238	0.87	0/323
All	All	0.60	3/66504 (0.0%)	0.72	8/89844 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	G	0	1
1	I	0	1
1	M	0	1
1	O	0	1
1	Q	0	1
1	S	0	1
1	W	0	1
1	Y	0	1
1	c	0	1
1	g	0	1
All	All	0	12

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	717	ARG	CD-NE	5.41	1.55	1.46
3	E	717	ARG	CD-NE	5.12	1.55	1.46
3	K	717	ARG	CD-NE	5.07	1.55	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	717	ARG	NE-CZ-NH1	7.64	124.12	120.30
3	a	717	ARG	NE-CZ-NH1	7.64	124.12	120.30
3	E	717	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	g	527	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	I	132	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	M	765	MET	CG-SD-CE	5.09	108.35	100.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	g	765	MET	CG-SD-CE	5.05	108.28	100.20
1	W	765	MET	CG-SD-CE	5.03	108.25	100.20

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	398	SER	Peptide
1	C	398	SER	Peptide
1	G	398	SER	Peptide
1	I	398	SER	Peptide
1	M	398	SER	Peptide
1	O	398	SER	Peptide
1	Q	398	SER	Peptide
1	S	398	SER	Peptide
1	W	398	SER	Peptide
1	Y	398	SER	Peptide
1	c	398	SER	Peptide
1	g	398	SER	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3788	0	3838	55	8
1	C	3788	0	3839	100	2
1	G	3788	0	3839	70	9
1	I	3788	0	3839	80	2
1	M	3788	0	3839	56	12
1	O	3788	0	3839	56	17
1	Q	3788	0	3839	62	4
1	S	3788	0	3839	65	12
1	W	3788	0	3838	56	4
1	Y	3788	0	3839	57	12
1	c	3788	0	3839	0	6
1	g	3788	0	3839	0	13
2	B	1377	0	1370	44	9

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1377	0	1370	43	4
2	H	1377	0	1370	39	3
2	J	1377	0	1370	34	4
2	N	1377	0	1370	26	0
2	P	1377	0	1371	29	0
2	R	1377	0	1370	29	0
2	T	1377	0	1370	28	0
2	X	1377	0	1370	23	0
2	Z	1377	0	1371	24	0
2	d	1377	0	1370	0	0
2	h	1377	0	1370	0	1
3	E	314	0	298	89	0
3	F	237	0	222	78	0
3	K	314	0	298	52	0
3	L	237	0	222	35	0
3	U	314	0	298	23	0
3	V	237	0	222	47	0
3	a	314	0	298	0	0
3	b	237	0	222	0	0
3	e	314	0	298	0	0
3	f	237	0	222	0	0
3	i	314	0	298	0	0
3	j	237	0	222	0	0
4	A	24	0	16	0	0
4	C	24	0	16	0	0
4	G	24	0	16	0	0
4	I	24	0	16	0	0
4	M	24	0	16	0	0
4	O	24	0	16	0	0
4	Q	24	0	16	0	0
4	S	24	0	16	0	0
4	W	24	0	16	0	0
4	Y	24	0	16	0	0
4	c	24	0	16	0	0
4	g	24	0	16	0	0
5	B	32	0	12	6	0
5	D	32	0	12	11	0
5	H	32	0	12	7	0
5	J	32	0	12	4	0
5	N	32	0	12	6	0
5	P	32	0	12	7	0
5	R	32	0	12	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	T	32	0	12	5	0
5	X	32	0	12	6	0
5	Z	32	0	12	6	0
5	d	32	0	12	0	0
5	h	32	0	12	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	H	1	0	0	0	0
6	J	1	0	0	0	0
6	N	1	0	0	0	0
6	P	1	0	0	0	0
6	R	1	0	0	0	0
6	T	1	0	0	0	0
6	X	1	0	0	0	0
6	Z	1	0	0	1	0
6	d	1	0	0	0	0
6	h	1	0	0	0	0
All	All	65970	0	65964	993	61

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (993) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:44:ILE:HD11	3:K:734:LEU:CD2	1.30	1.59
2:J:44:ILE:CD1	3:K:734:LEU:HD22	1.30	1.59
2:D:44:ILE:HD11	3:E:734:LEU:CD2	1.41	1.50
1:C:138:LEU:HG	1:S:769:GLN:CG	1.41	1.48
2:D:44:ILE:CD1	3:E:734:LEU:HD22	1.44	1.47
1:C:138:LEU:CG	1:S:769:GLN:HG2	1.45	1.42
1:I:138:LEU:HG	1:Q:769:GLN:CG	1.52	1.38
1:I:138:LEU:CG	1:Q:769:GLN:HG2	1.53	1.34
1:G:138:LEU:HD21	1:M:765:MET:CE	1.59	1.30
1:A:138:LEU:HD21	1:O:765:MET:CE	1.63	1.27
3:F:728:GLU:CD	3:K:717:ARG:HD3	120.84	1.22
1:A:138:LEU:HD21	1:O:765:MET:HE3	1.23	1.18
2:B:80:TYR:OH	3:E:746:MET:CG	1.94	1.15
2:B:80:TYR:OH	3:E:746:MET:HG2	1.45	1.14
1:G:138:LEU:HD21	1:M:765:MET:HE2	1.23	1.13
2:H:80:TYR:OH	3:K:746:MET:HG2	1.48	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:731:ASN:HD21	3:F:731:ASN:CG	4.33	1.09
1:C:138:LEU:HD21	1:S:769:GLN:HB3	1.29	1.09
3:F:728:GLU:CD	3:K:717:ARG:CD	121.14	1.06
2:D:56:ASP:OD2	2:D:174:ARG:NH1	1.90	1.05
2:X:56:ASP:OD2	2:X:174:ARG:NH1	1.89	1.04
2:R:56:ASP:OD2	2:R:174:ARG:NH1	1.90	1.04
3:U:738:ILE:HD13	3:V:738:ILE:HD13	1.40	1.04
1:I:138:LEU:HD21	1:Q:769:GLN:HB3	1.34	1.04
2:T:56:ASP:OD2	2:T:174:ARG:NH1	1.90	1.04
2:H:56:ASP:OD2	2:H:174:ARG:NH1	1.91	1.04
3:E:717:ARG:CG	3:V:728:GLU:OE2	2.06	1.04
2:J:56:ASP:OD2	2:J:174:ARG:NH1	1.90	1.04
2:N:56:ASP:OD2	2:N:174:ARG:NH1	1.90	1.03
2:P:56:ASP:OD2	2:P:174:ARG:NH1	1.90	1.03
3:F:728:GLU:OE1	3:K:717:ARG:CD	121.62	1.03
1:G:769:GLN:HG2	1:Y:138:LEU:HG	182.13	1.02
3:E:738:ILE:HG21	3:F:738:ILE:HD11	3.82	1.02
2:Z:56:ASP:OD2	2:Z:174:ARG:NH1	1.90	1.02
3:E:717:ARG:HD3	3:V:728:GLU:CD	1.80	1.01
3:K:738:ILE:HD13	3:L:738:ILE:CD1	1.90	1.01
1:C:765:MET:HE3	1:W:138:LEU:HD21	140.06	1.01
2:B:56:ASP:OD2	2:B:174:ARG:NH1	1.92	1.01
1:C:138:LEU:HD21	1:W:765:MET:CE	142.94	1.01
2:J:44:ILE:HD11	3:K:734:LEU:HD21	1.43	1.00
2:J:44:ILE:HD13	3:K:734:LEU:HD22	1.43	0.99
2:H:48:PHE:HD2	3:K:754:GLU:HA	1.26	0.99
1:C:138:LEU:CG	1:S:769:GLN:CG	2.20	0.99
3:F:728:GLU:OE2	3:K:717:ARG:CG	119.50	0.98
3:F:728:GLU:OE2	3:K:717:ARG:HD3	119.80	0.97
2:D:44:ILE:HD11	3:E:734:LEU:HD21	1.46	0.97
2:J:79:ALA:CB	3:L:746:MET:CE	2.43	0.97
3:E:731:ASN:ND2	3:F:731:ASN:CG	4.24	0.96
2:B:48:PHE:HD2	3:E:754:GLU:HA	1.29	0.96
2:H:80:TYR:OH	3:K:746:MET:CG	2.13	0.95
1:G:138:LEU:CD2	1:M:765:MET:HE2	1.98	0.94
2:D:38:LEU:O	5:D:2000:GSP:O3'	2.20	0.93
1:A:138:LEU:CD2	1:O:765:MET:HE3	1.98	0.93
2:J:79:ALA:CB	3:L:746:MET:HE1	1.99	0.93
3:F:728:GLU:OE2	3:K:717:ARG:CD	120.10	0.93
3:U:738:ILE:HG21	3:V:738:ILE:HD11	1.51	0.92
2:J:79:ALA:HB3	3:L:746:MET:HE1	1.50	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:SER:O	2:Z:71:GLU:OE2	125.74	0.92
3:E:738:ILE:HD13	3:F:738:ILE:HD13	2.19	0.92
3:E:717:ARG:CD	3:V:728:GLU:CD	2.37	0.92
2:D:79:ALA:CB	3:F:746:MET:CE	2.48	0.91
1:C:138:LEU:HD23	1:S:769:GLN:CD	1.92	0.91
1:C:332:GLN:HE22	1:I:331:GLU:HG3	1.35	0.91
3:E:717:ARG:CD	3:V:724:ILE:HG22	2.01	0.90
1:G:138:LEU:HD21	1:M:765:MET:HE3	1.52	0.89
2:T:44:ILE:HD11	3:V:734:LEU:CD2	2.01	0.89
1:C:138:LEU:HD21	1:S:765:MET:HG2	1.55	0.89
3:E:738:ILE:HD13	3:F:738:ILE:HG12	1.54	0.88
1:G:765:MET:HG2	1:Y:138:LEU:HD21	179.51	0.88
2:B:48:PHE:CD2	3:E:754:GLU:HA	2.08	0.87
1:G:147:TYR:OH	1:Y:759:GLU:OE2	164.25	0.87
2:H:48:PHE:CD2	3:K:754:GLU:HA	2.09	0.87
3:E:717:ARG:HG3	3:V:728:GLU:CD	1.95	0.87
3:F:734:LEU:CD2	2:R:44:ILE:HD11	120.85	0.86
2:D:79:ALA:CB	3:F:746:MET:HE3	2.04	0.86
3:E:717:ARG:HG3	3:V:728:GLU:OE2	1.72	0.86
3:E:717:ARG:CD	3:V:728:GLU:OE1	2.24	0.86
1:C:138:LEU:CD2	1:S:769:GLN:HB3	2.06	0.86
1:G:138:LEU:CD2	1:M:765:MET:CE	2.49	0.85
1:G:769:GLN:CG	1:Y:138:LEU:HG	182.34	0.85
1:A:138:LEU:CD2	1:O:765:MET:CE	2.51	0.85
1:A:339:SER:OG	1:Y:537:HIS:HB2	1.75	0.85
3:F:734:LEU:HD21	2:R:44:ILE:HD11	120.57	0.84
1:C:138:LEU:CD2	1:S:769:GLN:CG	2.54	0.84
1:I:138:LEU:CG	1:Q:769:GLN:CG	2.30	0.84
1:C:138:LEU:HD21	1:S:769:GLN:CB	2.05	0.84
1:I:138:LEU:HD23	1:Q:769:GLN:CD	1.98	0.84
2:H:95:LYS:O	2:H:98:THR:HG22	1.78	0.84
2:B:95:LYS:O	2:B:98:THR:HG22	1.78	0.83
2:D:37:ASN:O	5:D:2000:GSP:O2'	2.38	0.83
2:R:95:LYS:O	2:R:98:THR:HG22	1.78	0.83
2:T:95:LYS:O	2:T:98:THR:HG22	1.78	0.83
2:N:95:LYS:O	2:N:98:THR:HG22	1.79	0.83
1:A:138:LEU:HD21	1:O:765:MET:HE2	1.61	0.83
2:P:95:LYS:O	2:P:98:THR:HG22	1.79	0.83
2:B:44:ILE:HB	3:F:737:TYR:CZ	2.14	0.82
2:Z:95:LYS:O	2:Z:98:THR:HG22	1.78	0.82
3:K:738:ILE:HD13	3:L:738:ILE:CG1	2.09	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:95:LYS:O	2:X:98:THR:HG22	1.79	0.82
1:C:138:LEU:HD21	1:W:765:MET:HE3	142.62	0.82
3:U:738:ILE:HG21	3:V:738:ILE:CD1	2.09	0.82
2:J:79:ALA:HB3	3:L:746:MET:CE	2.09	0.82
3:U:731:ASN:HD21	3:V:731:ASN:CG	1.83	0.82
2:D:44:ILE:HD11	3:E:734:LEU:HD22	0.87	0.81
2:J:95:LYS:O	2:J:98:THR:HG22	1.79	0.81
1:M:163:ARG:O	1:M:166:CYS:SG	2.38	0.81
2:D:95:LYS:O	2:D:98:THR:HG22	1.79	0.81
1:A:163:ARG:O	1:A:166:CYS:SG	2.39	0.81
2:D:44:ILE:HD13	3:E:734:LEU:HD22	1.59	0.81
3:F:728:GLU:OE1	3:K:717:ARG:NE	121.26	0.81
1:G:163:ARG:O	1:G:166:CYS:SG	2.39	0.81
1:A:138:LEU:HD11	1:O:765:MET:HE2	1.63	0.80
1:O:163:ARG:O	1:O:166:CYS:SG	2.39	0.80
1:I:138:LEU:HD21	1:Q:765:MET:HG2	1.61	0.80
3:E:724:ILE:CG2	3:V:717:ARG:CZ	2.59	0.80
1:W:163:ARG:O	1:W:166:CYS:SG	2.39	0.80
3:K:738:ILE:HD13	3:L:738:ILE:HG12	1.61	0.80
1:C:163:ARG:O	1:C:166:CYS:SG	2.39	0.80
2:T:44:ILE:CD1	3:V:734:LEU:HD22	2.11	0.80
3:E:717:ARG:NH2	3:V:725:GLN:CB	2.45	0.79
1:G:769:GLN:HB3	1:Y:138:LEU:HD21	181.18	0.79
3:E:717:ARG:HD3	3:V:728:GLU:OE2	1.83	0.79
1:C:138:LEU:CD2	1:S:769:GLN:CD	2.50	0.79
3:E:717:ARG:HG3	3:V:728:GLU:OE1	1.82	0.79
3:F:728:GLU:OE1	3:K:717:ARG:CG	121.02	0.79
1:G:765:MET:HG2	1:Y:138:LEU:CD2	178.73	0.79
1:I:138:LEU:CD2	1:Q:769:GLN:CG	2.60	0.79
1:I:163:ARG:O	1:I:166:CYS:SG	2.39	0.79
3:F:728:GLU:CD	3:K:717:ARG:CG	120.54	0.79
3:E:717:ARG:CG	3:V:728:GLU:CD	2.48	0.79
1:Y:163:ARG:O	1:Y:166:CYS:SG	2.39	0.79
2:D:79:ALA:HB3	3:F:746:MET:CE	2.12	0.79
1:S:163:ARG:O	1:S:166:CYS:SG	2.39	0.79
1:Q:163:ARG:O	1:Q:166:CYS:SG	2.39	0.78
1:I:138:LEU:HD21	1:Q:769:GLN:CB	2.12	0.78
3:E:738:ILE:HG21	3:F:738:ILE:CD1	4.20	0.78
2:D:42:SER:HA	5:D:2000:GSP:S1G	2.78	0.77
3:E:717:ARG:CG	3:V:728:GLU:OE1	2.32	0.77
1:C:331:GLU:CG	1:I:332:GLN:HE22	1.98	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:738:ILE:CD1	3:L:738:ILE:CD1	2.62	0.77
1:M:232:ARG:O	1:M:235:LYS:NZ	2.18	0.77
3:E:717:ARG:CD	3:V:728:GLU:OE2	2.32	0.77
1:O:232:ARG:O	1:O:235:LYS:NZ	2.19	0.76
1:Q:232:ARG:O	1:Q:235:LYS:NZ	2.18	0.76
1:S:232:ARG:O	1:S:235:LYS:NZ	2.18	0.75
1:I:138:LEU:CD2	1:Q:769:GLN:HB3	2.13	0.75
3:E:724:ILE:HG23	3:V:717:ARG:CZ	2.16	0.75
2:T:44:ILE:HD11	3:V:734:LEU:HD21	1.67	0.75
1:C:332:GLN:HE22	1:I:331:GLU:CG	2.00	0.75
1:I:178:GLN:HA	1:I:739:MET:HE1	1.69	0.75
1:Q:178:GLN:HA	1:Q:739:MET:HE1	1.69	0.75
2:B:80:TYR:OH	3:E:746:MET:SD	2.45	0.74
2:B:80:TYR:HH	3:E:746:MET:HG2	1.51	0.74
3:F:734:LEU:HD22	2:R:44:ILE:CD1	120.88	0.74
1:S:178:GLN:HA	1:S:739:MET:HE1	1.70	0.74
2:Z:37:ASN:O	5:Z:2000:GSP:O2'	2.05	0.74
2:D:38:LEU:HA	5:D:2000:GSP:O2'	2.00	0.74
2:B:44:ILE:O	3:F:737:TYR:OH	2.05	0.74
1:I:232:ARG:O	1:I:235:LYS:NZ	2.19	0.74
1:M:178:GLN:HA	1:M:739:MET:HE1	1.70	0.74
3:E:738:ILE:HD13	3:F:738:ILE:CG1	2.18	0.74
2:D:44:ILE:CD1	3:E:734:LEU:CD2	2.27	0.73
1:C:232:ARG:O	1:C:235:LYS:NZ	2.19	0.73
1:C:178:GLN:HA	1:C:739:MET:HE1	1.70	0.73
2:J:79:ALA:CB	3:L:746:MET:HE3	2.17	0.73
1:W:232:ARG:O	1:W:235:LYS:NZ	2.19	0.73
1:O:178:GLN:HA	1:O:739:MET:HE1	1.70	0.73
1:S:393:ASN:O	1:S:397:THR:OG1	2.07	0.73
3:E:735:GLN:NE2	3:F:734:LEU:CD1	3.83	0.73
1:G:178:GLN:HA	1:G:739:MET:HE1	1.70	0.73
3:F:728:GLU:CD	3:K:717:ARG:HG3	119.60	0.73
3:E:735:GLN:NE2	3:F:734:LEU:HD12	4.28	0.73
1:Q:393:ASN:O	1:Q:397:THR:OG1	2.07	0.73
3:E:717:ARG:HD2	3:V:724:ILE:HG22	1.71	0.73
1:Y:178:GLN:HA	1:Y:739:MET:HE1	1.69	0.73
1:Y:232:ARG:O	1:Y:235:LYS:NZ	2.19	0.73
1:C:332:GLN:HE21	1:I:332:GLN:HG3	1.53	0.73
1:G:769:GLN:HB3	1:Y:138:LEU:CD2	180.40	0.73
1:I:138:LEU:CD2	1:Q:769:GLN:CD	2.57	0.72
1:G:232:ARG:O	1:G:235:LYS:NZ	2.19	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:ILE:HD12	3:F:737:TYR:CD2	2.24	0.72
1:C:393:ASN:O	1:C:397:THR:OG1	2.07	0.72
1:W:393:ASN:O	1:W:397:THR:OG1	2.08	0.72
1:O:393:ASN:O	1:O:397:THR:OG1	2.07	0.72
1:G:393:ASN:O	1:G:397:THR:OG1	2.07	0.72
1:A:393:ASN:O	1:A:397:THR:OG1	2.07	0.72
1:W:178:GLN:HA	1:W:739:MET:HE1	1.72	0.72
1:M:393:ASN:O	1:M:397:THR:OG1	2.07	0.72
3:E:717:ARG:HD2	3:V:724:ILE:CG2	2.20	0.72
1:I:393:ASN:O	1:I:397:THR:OG1	2.07	0.72
2:D:40:SER:HB3	5:D:2000:GSP:H3'	1.99	0.71
1:A:178:GLN:HA	1:A:739:MET:HE1	1.71	0.71
1:Y:393:ASN:O	1:Y:397:THR:OG1	2.07	0.71
3:F:728:GLU:OE1	3:K:717:ARG:HG3	120.08	0.71
2:T:44:ILE:CD1	3:V:734:LEU:CD2	2.69	0.71
1:A:232:ARG:O	1:A:235:LYS:NZ	2.19	0.71
2:J:44:ILE:HD11	3:K:734:LEU:HD22	0.73	0.71
1:C:138:LEU:HD21	1:W:765:MET:HE2	142.50	0.71
2:T:44:ILE:HD13	3:V:734:LEU:HD22	1.73	0.70
3:E:724:ILE:O	3:V:717:ARG:NH1	2.24	0.70
1:C:138:LEU:CD2	1:S:769:GLN:CB	2.68	0.70
2:H:44:ILE:HB	3:L:737:TYR:CZ	2.26	0.70
3:F:728:GLU:OE2	3:K:717:ARG:HG3	118.56	0.70
3:U:731:ASN:ND2	3:V:731:ASN:CG	2.45	0.70
2:P:38:LEU:O	5:P:2000:GSP:O3'	2.10	0.70
3:E:738:ILE:HD13	3:F:738:ILE:CD1	2.21	0.70
3:K:738:ILE:CD1	3:L:738:ILE:HD13	2.22	0.69
2:D:79:ALA:CB	3:F:746:MET:HE1	2.20	0.69
2:B:80:TYR:OH	3:E:746:MET:CB	2.41	0.69
3:E:717:ARG:NH2	3:L:731:ASN:HD22	123.12	0.69
2:J:44:ILE:CD1	3:K:734:LEU:CD2	2.17	0.69
1:C:139:PHE:HA	1:C:143:MET:HE2	1.76	0.69
3:F:734:LEU:CD2	2:R:44:ILE:CD1	120.43	0.68
1:Q:139:PHE:HA	1:Q:143:MET:HE2	1.75	0.68
2:B:38:LEU:HA	5:B:2000:GSP:O2'	1.94	0.68
1:C:332:GLN:HG3	1:I:332:GLN:CG	2.24	0.68
1:S:139:PHE:HA	1:S:143:MET:HE2	1.76	0.68
2:J:79:ALA:HB1	3:L:746:MET:HE3	1.76	0.67
1:C:221:SER:C	2:Z:71:GLU:OE2	125.72	0.67
1:O:139:PHE:HA	1:O:143:MET:HE2	1.74	0.67
1:A:139:PHE:HA	1:A:143:MET:HE2	1.75	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:139:PHE:HA	1:Y:143:MET:HE2	1.75	0.67
1:G:139:PHE:HA	1:G:143:MET:HE2	1.75	0.67
2:J:38:LEU:HA	5:J:2000:GSP:O2'	1.94	0.67
3:E:717:ARG:HH21	3:V:725:GLN:CB	2.04	0.67
3:F:717:ARG:NH1	3:K:724:ILE:O	120.35	0.67
3:F:717:ARG:NH1	3:K:728:GLU:HB2	123.05	0.67
1:I:139:PHE:HA	1:I:143:MET:HE2	1.76	0.67
1:M:139:PHE:HA	1:M:143:MET:HE2	1.76	0.67
1:W:139:PHE:HA	1:W:143:MET:HE2	1.76	0.67
2:D:79:ALA:HB1	3:F:746:MET:HE3	1.77	0.66
2:N:38:LEU:O	5:N:2000:GSP:O3'	2.13	0.66
1:C:138:LEU:CG	1:S:769:GLN:CB	2.73	0.66
3:U:738:ILE:HD13	3:V:738:ILE:CD1	2.22	0.66
1:C:138:LEU:HD23	1:S:769:GLN:OE1	1.95	0.66
2:D:79:ALA:HB3	3:F:746:MET:HE3	1.72	0.66
3:E:752:ILE:HG21	3:F:745:ILE:HD11	3.84	0.65
3:K:738:ILE:HD13	3:L:738:ILE:HD11	1.73	0.65
3:E:742:ILE:HD11	3:F:741:ILE:HG21	1.79	0.65
1:C:138:LEU:HD11	1:W:765:MET:HE2	144.78	0.65
2:H:44:ILE:O	3:L:737:TYR:OH	2.15	0.65
2:N:38:LEU:HA	5:N:2000:GSP:O2'	1.96	0.65
2:T:26:ASN:ND2	5:T:2000:GSP:O1A	2.29	0.65
1:G:769:GLN:CB	1:Y:138:LEU:HG	181.93	0.64
3:F:725:GLN:CB	3:K:717:ARG:NH2	122.43	0.64
3:E:738:ILE:CD1	3:F:738:ILE:HD13	2.56	0.64
2:Z:45:GLY:O	2:Z:67:THR:O	2.16	0.64
2:H:45:GLY:O	2:H:67:THR:O	2.16	0.64
2:P:40:SER:HB3	5:P:2000:GSP:H3'	1.79	0.64
2:N:45:GLY:O	2:N:67:THR:O	2.16	0.64
2:P:45:GLY:O	2:P:67:THR:O	2.16	0.64
2:X:45:GLY:O	2:X:67:THR:O	2.16	0.64
2:T:80:TYR:OH	3:U:746:MET:HB3	1.98	0.64
2:R:45:GLY:O	2:R:67:THR:O	2.16	0.63
2:D:79:ALA:HB3	3:F:746:MET:HE1	1.78	0.63
2:B:80:TYR:CE1	3:E:746:MET:HE1	2.33	0.63
2:T:45:GLY:O	2:T:67:THR:O	2.16	0.63
1:Y:618:TYR:CZ	1:Y:622:GLU:HG3	2.33	0.63
2:D:45:GLY:O	2:D:67:THR:O	2.16	0.63
2:J:45:GLY:O	2:J:67:THR:O	2.16	0.63
3:F:724:ILE:HG22	3:K:717:ARG:CD	118.88	0.63
2:B:45:GLY:O	2:B:67:THR:O	2.16	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:SER:HA	2:P:71:GLU:OE2	1.99	0.62
2:B:81:TYR:HB3	2:B:113:ALA:HB2	1.82	0.62
2:H:67:THR:O	2:H:68:ALA:HB3	2.00	0.62
1:S:618:TYR:CZ	1:S:622:GLU:HG3	2.35	0.62
1:Q:618:TYR:CZ	1:Q:622:GLU:HG3	2.35	0.62
1:I:138:LEU:CD2	1:Q:769:GLN:CB	2.75	0.62
1:A:138:LEU:CD1	1:O:765:MET:HE2	2.30	0.62
1:G:765:MET:HA	1:G:769:GLN:OE1	1.99	0.62
2:Z:67:THR:O	2:Z:68:ALA:HB3	2.00	0.62
1:C:221:SER:C	2:P:71:GLU:OE2	2.37	0.62
2:D:81:TYR:HB3	2:D:113:ALA:HB2	1.82	0.62
1:I:221:SER:HA	2:N:71:GLU:OE2	1.99	0.62
1:Q:765:MET:HA	1:Q:769:GLN:OE1	1.99	0.62
3:F:731:ASN:HD22	3:U:717:ARG:NH2	1.98	0.62
2:D:26:ASN:ND2	5:D:2000:GSP:O1A	2.36	0.62
2:B:67:THR:O	2:B:68:ALA:HB3	2.00	0.62
2:H:44:ILE:HD12	3:L:737:TYR:CD2	2.35	0.61
2:P:67:THR:O	2:P:68:ALA:HB3	2.00	0.61
1:O:765:MET:HA	1:O:769:GLN:OE1	1.99	0.61
1:Y:626:TYR:HA	1:Y:631:PHE:CD1	2.35	0.61
2:X:81:TYR:HB3	2:X:113:ALA:HB2	1.82	0.61
2:R:67:THR:O	2:R:68:ALA:HB3	2.00	0.61
3:E:731:ASN:ND2	3:F:731:ASN:ND2	5.29	0.61
2:D:67:THR:O	2:D:68:ALA:HB3	2.01	0.61
2:J:67:THR:O	2:J:68:ALA:HB3	2.01	0.61
1:C:765:MET:HE2	1:W:138:LEU:HD11	141.92	0.61
2:N:67:THR:O	2:N:68:ALA:HB3	2.00	0.61
1:W:765:MET:HA	1:W:769:GLN:OE1	2.00	0.61
1:M:765:MET:HA	1:M:769:GLN:OE1	2.00	0.61
2:Z:38:LEU:O	5:Z:2000:GSP:O3'	2.16	0.61
2:T:67:THR:O	2:T:68:ALA:HB3	2.00	0.61
2:H:71:GLU:OE2	1:W:221:SER:C	118.62	0.61
1:Y:765:MET:HA	1:Y:769:GLN:OE1	2.01	0.61
3:F:734:LEU:HD22	2:R:44:ILE:HD13	120.79	0.61
2:H:81:TYR:HB3	2:H:113:ALA:HB2	1.83	0.61
2:P:38:LEU:HA	5:P:2000:GSP:O2'	2.01	0.61
1:G:618:TYR:CZ	1:G:622:GLU:HG3	2.36	0.61
2:J:81:TYR:HB3	2:J:113:ALA:HB2	1.82	0.61
1:A:626:TYR:HA	1:A:631:PHE:CD1	2.35	0.61
2:R:81:TYR:HB3	2:R:113:ALA:HB2	1.82	0.61
2:B:80:TYR:CE1	3:E:746:MET:SD	2.94	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:134:PHE:O	1:I:163:ARG:NH1	2.34	0.61
1:Y:134:PHE:O	1:Y:163:ARG:NH1	2.34	0.61
1:G:626:TYR:HA	1:G:631:PHE:CD2	2.35	0.61
1:W:618:TYR:CZ	1:W:622:GLU:HG3	2.35	0.61
1:S:765:MET:HA	1:S:769:GLN:OE1	2.00	0.61
2:T:81:TYR:HB3	2:T:113:ALA:HB2	1.82	0.61
1:C:134:PHE:O	1:C:163:ARG:NH1	2.34	0.60
1:C:637:ASN:HB3	1:C:669:HIS:CD2	2.37	0.60
2:X:67:THR:O	2:X:68:ALA:HB3	2.01	0.60
2:D:80:TYR:CE1	3:F:746:MET:HG2	2.36	0.60
1:M:637:ASN:HB3	1:M:669:HIS:CD2	2.37	0.60
1:A:765:MET:HA	1:A:769:GLN:OE1	2.01	0.60
1:A:618:TYR:CZ	1:A:622:GLU:HG3	2.36	0.60
1:Y:637:ASN:HB3	1:Y:669:HIS:CD2	2.37	0.60
1:W:637:ASN:HB3	1:W:669:HIS:CD2	2.36	0.60
1:I:637:ASN:HB3	1:I:669:HIS:CD2	2.37	0.60
1:C:759:GLU:OE2	1:S:147:TYR:OH	2.19	0.60
3:E:717:ARG:NE	3:V:728:GLU:OE1	2.35	0.60
1:C:765:MET:HA	1:C:769:GLN:OE1	2.01	0.60
2:N:81:TYR:HB3	2:N:113:ALA:HB2	1.82	0.60
1:A:134:PHE:O	1:A:163:ARG:NH1	2.35	0.60
1:A:765:MET:CE	1:O:138:LEU:HD21	2.32	0.60
1:I:765:MET:HA	1:I:769:GLN:OE1	2.01	0.60
2:Z:25:SER:HG	6:Z:2001:MG:MG	1.10	0.60
2:Z:81:TYR:HB3	2:Z:113:ALA:HB2	1.82	0.60
3:K:742:ILE:HD11	3:L:741:ILE:HG21	1.82	0.60
1:C:618:TYR:CZ	1:C:622:GLU:HG3	2.39	0.60
1:G:765:MET:CE	1:M:138:LEU:HD21	2.32	0.60
3:E:724:ILE:HG22	3:V:717:ARG:CZ	2.31	0.60
1:Q:637:ASN:HB3	1:Q:669:HIS:CD2	2.37	0.60
2:H:38:LEU:HA	5:H:2000:GSP:O2'	2.01	0.60
1:M:134:PHE:O	1:M:163:ARG:NH1	2.35	0.60
1:G:637:ASN:HB3	1:G:669:HIS:CD2	2.37	0.60
1:G:134:PHE:O	1:G:163:ARG:NH1	2.35	0.59
1:A:637:ASN:HB3	1:A:669:HIS:CD2	2.36	0.59
1:G:765:MET:CG	1:Y:138:LEU:HD21	179.02	0.59
2:P:42:SER:HA	5:P:2000:GSP:S1G	2.43	0.59
2:X:40:SER:HB3	5:X:2000:GSP:H3'	1.83	0.59
1:C:138:LEU:CD2	1:S:765:MET:HG2	2.27	0.59
2:P:81:TYR:HB3	2:P:113:ALA:HB2	1.83	0.59
1:O:637:ASN:HB3	1:O:669:HIS:CD2	2.38	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:GLN:NE2	1:I:331:GLU:HG3	2.15	0.59
2:X:38:LEU:O	5:X:2000:GSP:O3'	2.18	0.59
1:I:618:TYR:CZ	1:I:622:GLU:HG3	2.38	0.59
1:G:138:LEU:HD11	1:M:765:MET:HE2	1.83	0.58
2:B:80:TYR:OH	3:E:746:MET:HB3	2.04	0.58
1:Q:134:PHE:O	1:Q:163:ARG:NH1	2.36	0.58
1:S:637:ASN:HB3	1:S:669:HIS:CD2	2.38	0.58
1:C:332:GLN:CG	1:I:332:GLN:HG2	2.33	0.58
1:O:134:PHE:O	1:O:163:ARG:NH1	2.36	0.58
2:T:38:LEU:HA	5:T:2000:GSP:O2'	2.03	0.58
1:Q:626:TYR:HA	1:Q:631:PHE:CD2	2.38	0.58
2:B:42:SER:HA	5:B:2000:GSP:S1G	2.43	0.58
2:N:40:SER:HB3	5:N:2000:GSP:H3'	1.85	0.58
1:C:332:GLN:CG	1:I:332:GLN:CG	2.82	0.58
1:C:765:MET:CE	1:W:138:LEU:HD11	142.46	0.58
1:C:332:GLN:HG3	1:I:332:GLN:HG3	1.85	0.58
1:S:626:TYR:HA	1:S:631:PHE:CD1	2.38	0.58
1:G:769:GLN:HB3	1:Y:138:LEU:CG	180.73	0.58
1:S:134:PHE:O	1:S:163:ARG:NH1	2.37	0.58
1:Y:625:SER:O	1:Y:628:THR:HG22	2.03	0.58
1:A:625:SER:O	1:A:628:THR:HG22	2.04	0.58
1:C:625:SER:O	1:C:628:THR:HG22	2.05	0.58
1:M:618:TYR:CZ	1:M:622:GLU:HG3	2.40	0.57
1:W:134:PHE:O	1:W:163:ARG:NH1	2.37	0.57
1:S:625:SER:O	1:S:628:THR:HG22	2.04	0.57
1:G:625:SER:O	1:G:628:THR:HG22	2.04	0.57
1:O:618:TYR:CZ	1:O:622:GLU:HG3	2.40	0.57
1:G:138:LEU:CD2	1:M:765:MET:HE3	2.26	0.57
2:J:26:ASN:ND2	5:J:2000:GSP:O1A	2.37	0.57
1:Q:625:SER:O	1:Q:628:THR:HG22	2.04	0.57
1:C:138:LEU:HG	1:S:769:GLN:CB	2.28	0.57
1:G:626:TYR:HA	1:G:631:PHE:CD1	3.46	0.57
2:N:42:SER:HA	5:N:2000:GSP:S1G	2.45	0.57
2:H:40:SER:HB3	5:H:2000:GSP:H3'	2.03	0.57
1:M:626:TYR:HA	1:M:631:PHE:CD1	2.40	0.57
1:C:765:MET:CE	1:W:138:LEU:HD21	140.02	0.57
1:M:625:SER:O	1:M:628:THR:HG22	2.04	0.57
1:G:611:SER:HB2	1:G:613:LEU:HD22	1.87	0.57
1:W:626:TYR:HA	1:W:631:PHE:CD1	2.40	0.57
2:H:42:SER:HA	5:H:2000:GSP:S1G	2.56	0.57
1:W:625:SER:O	1:W:628:THR:HG22	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:THR:HG21	1:I:329:THR:HG21	1.86	0.56
1:C:221:SER:CA	2:P:71:GLU:OE2	2.53	0.56
3:E:735:GLN:NE2	3:F:734:LEU:HD13	2.86	0.56
1:C:332:GLN:HG2	1:I:332:GLN:HG2	1.87	0.56
1:O:625:SER:O	1:O:628:THR:HG22	2.04	0.56
1:I:625:SER:O	1:I:628:THR:HG22	2.05	0.56
1:I:138:LEU:CG	1:Q:769:GLN:CB	2.84	0.56
1:I:611:SER:HB2	1:I:613:LEU:HD22	1.88	0.56
1:O:626:TYR:HA	1:O:631:PHE:CD1	2.41	0.56
1:C:611:SER:HB2	1:C:613:LEU:HD22	1.88	0.56
2:X:38:LEU:HA	5:X:2000:GSP:O2'	2.05	0.56
1:M:611:SER:HB2	1:M:613:LEU:HD22	1.88	0.56
1:A:611:SER:HB2	1:A:613:LEU:HD22	1.88	0.56
2:J:80:TYR:CE1	3:L:746:MET:HG2	2.40	0.56
2:H:38:LEU:O	5:H:2000:GSP:O3'	2.20	0.56
2:P:144:GLU:OE1	2:P:144:GLU:HA	2.06	0.56
2:D:144:GLU:OE1	2:D:144:GLU:HA	2.07	0.56
2:N:144:GLU:OE1	2:N:144:GLU:HA	2.06	0.56
3:E:731:ASN:ND2	3:F:731:ASN:OD1	3.21	0.55
2:D:25:SER:OG	5:D:2000:GSP:O2B	2.74	0.55
1:Y:611:SER:HB2	1:Y:613:LEU:HD22	1.88	0.55
1:I:626:TYR:HA	1:I:631:PHE:CD1	2.40	0.55
3:E:725:GLN:HA	3:L:717:ARG:NH2	119.09	0.55
2:J:144:GLU:HA	2:J:144:GLU:OE1	2.06	0.55
2:X:144:GLU:OE1	2:X:144:GLU:HA	2.07	0.55
2:Z:40:SER:HB3	5:Z:2000:GSP:H3'	1.87	0.55
1:W:611:SER:HB2	1:W:613:LEU:HD22	1.87	0.55
2:B:144:GLU:HA	2:B:144:GLU:OE1	2.07	0.55
1:G:138:LEU:CD1	1:M:765:MET:HE2	2.37	0.55
1:O:611:SER:HB2	1:O:613:LEU:HD22	1.89	0.55
2:B:80:TYR:HE1	3:E:746:MET:SD	2.30	0.55
3:E:717:ARG:HD3	3:V:724:ILE:HG22	1.85	0.55
2:H:144:GLU:HA	2:H:144:GLU:OE1	2.07	0.55
1:S:611:SER:HB2	1:S:613:LEU:HD22	1.88	0.55
1:I:138:LEU:HD23	1:Q:769:GLN:OE1	2.06	0.55
1:C:607:VAL:O	1:C:611:SER:OG	2.20	0.55
1:Q:611:SER:HB2	1:Q:613:LEU:HD22	1.88	0.55
3:E:717:ARG:CD	3:V:724:ILE:CG2	2.77	0.54
1:O:196:PRO:HG2	2:P:131:LEU:HD22	1.89	0.54
2:Z:144:GLU:HA	2:Z:144:GLU:OE1	2.07	0.54
2:T:144:GLU:HA	2:T:144:GLU:OE1	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:717:ARG:NH2	3:V:725:GLN:CA	2.71	0.54
3:E:717:ARG:NH2	3:L:728:GLU:CG	122.08	0.54
1:O:133:LEU:O	1:O:136:SER:OG	2.21	0.54
2:B:38:LEU:O	5:B:2000:GSP:O3'	2.14	0.54
2:R:125:LYS:HG2	5:R:2000:GSP:C6	2.42	0.54
2:B:40:SER:HB3	5:B:2000:GSP:H3'	1.89	0.54
2:H:125:LYS:HG2	5:H:2000:GSP:C6	2.58	0.54
2:R:144:GLU:OE1	2:R:144:GLU:HA	2.07	0.54
1:M:133:LEU:O	1:M:136:SER:OG	2.21	0.54
1:C:626:TYR:HA	1:C:631:PHE:CD1	2.43	0.54
3:F:717:ARG:CZ	3:K:724:ILE:CG2	119.60	0.53
3:E:717:ARG:NH2	3:L:728:GLU:HG2	122.21	0.53
1:M:196:PRO:HG2	2:N:131:LEU:HD22	1.89	0.53
2:H:80:TYR:OH	3:K:746:MET:CB	2.56	0.53
1:M:306:ARG:O	1:M:351:ARG:NH1	2.41	0.53
1:O:306:ARG:O	1:O:351:ARG:NH1	2.41	0.53
1:Q:602:VAL:HG23	1:Q:607:VAL:HG23	1.90	0.53
2:X:8:TYR:HA	2:X:59:THR:OG1	2.08	0.53
2:H:8:TYR:HA	2:H:59:THR:OG1	2.10	0.53
3:E:724:ILE:HG23	3:V:717:ARG:NH2	2.23	0.53
1:C:602:VAL:HG23	1:C:607:VAL:HG23	1.92	0.53
1:C:331:GLU:HG3	1:I:332:GLN:HE22	1.73	0.53
2:Z:67:THR:O	2:Z:68:ALA:CB	2.57	0.53
1:I:602:VAL:HG23	1:I:607:VAL:HG23	1.91	0.53
2:D:8:TYR:CE2	2:D:11:LEU:HB2	2.47	0.53
1:M:602:VAL:HG23	1:M:607:VAL:HG23	1.91	0.53
2:R:8:TYR:HA	2:R:59:THR:OG1	2.09	0.53
2:H:67:THR:O	2:H:68:ALA:CB	2.57	0.53
1:S:306:ARG:O	1:S:351:ARG:NH1	2.42	0.53
5:X:2000:GSP:O2B	5:X:2000:GSP:O3G	2.27	0.52
1:S:602:VAL:HG23	1:S:607:VAL:HG23	1.90	0.52
2:R:40:SER:HB3	5:R:2000:GSP:H3'	1.91	0.52
5:D:2000:GSP:O2B	5:D:2000:GSP:O3G	2.29	0.52
2:R:92:ASP:H	2:R:98:THR:HG21	1.74	0.52
5:T:2000:GSP:O2B	5:T:2000:GSP:O3G	2.27	0.52
2:P:8:TYR:CE2	2:P:11:LEU:HB2	2.44	0.52
1:A:306:ARG:O	1:A:351:ARG:NH1	2.42	0.52
2:N:8:TYR:CE2	2:N:11:LEU:HB2	2.44	0.52
2:D:92:ASP:H	2:D:98:THR:HG21	1.74	0.52
2:X:67:THR:O	2:X:68:ALA:CB	2.58	0.52
2:H:26:ASN:ND2	5:H:2000:GSP:O1A	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:602:VAL:HG23	1:O:607:VAL:HG23	1.92	0.52
1:G:306:ARG:O	1:G:351:ARG:NH1	2.42	0.52
2:T:8:TYR:HA	2:T:59:THR:OG1	2.10	0.52
3:U:735:GLN:NE2	3:V:734:LEU:CD1	2.72	0.52
1:A:765:MET:HE3	1:O:138:LEU:HD21	1.91	0.52
1:W:306:ARG:O	1:W:351:ARG:NH1	2.43	0.52
2:Z:8:TYR:CE2	2:Z:11:LEU:HB2	2.45	0.52
1:G:133:LEU:O	1:G:136:SER:OG	2.21	0.52
1:C:138:LEU:CD2	1:W:765:MET:CE	143.28	0.52
1:A:138:LEU:CD2	1:O:765:MET:HE2	2.31	0.52
2:D:67:THR:O	2:D:68:ALA:CB	2.57	0.52
1:A:602:VAL:HG23	1:A:607:VAL:HG23	1.92	0.52
2:P:26:ASN:ND2	5:P:2000:GSP:O1A	2.39	0.52
1:Q:628:THR:HG23	1:Q:631:PHE:H	1.75	0.52
1:Q:306:ARG:O	1:Q:351:ARG:NH1	2.42	0.52
1:C:138:LEU:CG	1:S:769:GLN:CD	2.79	0.52
5:Z:2000:GSP:O2B	5:Z:2000:GSP:O3G	2.27	0.52
2:R:67:THR:O	2:R:68:ALA:CB	2.57	0.52
1:A:133:LEU:O	1:A:136:SER:OG	2.21	0.52
1:C:138:LEU:CD2	1:W:765:MET:HE3	142.95	0.52
1:I:138:LEU:CD2	1:Q:765:MET:HG2	2.35	0.52
2:H:92:ASP:H	2:H:98:THR:HG21	1.75	0.52
2:N:8:TYR:HA	2:N:59:THR:OG1	2.09	0.52
1:Y:306:ARG:O	1:Y:351:ARG:NH1	2.43	0.52
3:U:738:ILE:CD1	3:V:738:ILE:HD13	2.26	0.52
1:G:765:MET:HE3	1:M:138:LEU:HD21	1.91	0.52
2:T:67:THR:O	2:T:68:ALA:CB	2.57	0.52
5:H:2000:GSP:O3G	5:H:2000:GSP:O2B	2.27	0.52
2:D:8:TYR:HA	2:D:59:THR:OG1	2.11	0.52
1:Y:602:VAL:HG23	1:Y:607:VAL:HG23	1.92	0.52
1:I:306:ARG:O	1:I:351:ARG:NH1	2.43	0.52
1:C:306:ARG:O	1:C:351:ARG:NH1	2.43	0.52
3:E:738:ILE:CD1	3:F:738:ILE:CD1	2.88	0.51
2:N:26:ASN:ND2	5:N:2000:GSP:O1A	2.41	0.51
2:B:67:THR:O	2:B:68:ALA:CB	2.57	0.51
2:P:8:TYR:HA	2:P:59:THR:OG1	2.09	0.51
1:S:196:PRO:HG2	2:T:131:LEU:HD22	1.92	0.51
2:J:8:TYR:HA	2:J:59:THR:OG1	2.09	0.51
1:S:628:THR:HG23	1:S:631:PHE:H	1.75	0.51
2:H:8:TYR:CE2	2:H:11:LEU:HB2	2.47	0.51
1:G:602:VAL:HG23	1:G:607:VAL:HG23	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:92:ASP:H	2:Z:98:THR:HG21	1.75	0.51
1:W:602:VAL:HG23	1:W:607:VAL:HG23	1.91	0.51
2:J:67:THR:O	2:J:68:ALA:CB	2.58	0.51
1:A:765:MET:HE2	1:O:138:LEU:HD11	1.92	0.51
2:P:67:THR:O	2:P:68:ALA:CB	2.57	0.51
1:W:628:THR:HG23	1:W:631:PHE:H	1.75	0.51
1:I:206:ILE:HD11	1:I:394:PHE:HE2	1.75	0.51
1:C:138:LEU:CG	1:S:769:GLN:HB3	2.40	0.51
2:Z:26:ASN:ND2	5:Z:2000:GSP:O1A	2.43	0.51
2:Z:8:TYR:HA	2:Z:59:THR:OG1	2.10	0.51
1:Q:133:LEU:O	1:Q:136:SER:OG	2.21	0.51
3:E:738:ILE:CD1	3:F:738:ILE:HG12	2.33	0.51
2:P:92:ASP:H	2:P:98:THR:HG21	1.76	0.51
2:X:92:ASP:H	2:X:98:THR:HG21	1.74	0.51
2:X:8:TYR:CE2	2:X:11:LEU:HB2	2.46	0.51
1:S:133:LEU:O	1:S:136:SER:OG	2.21	0.51
1:G:628:THR:HG23	1:G:631:PHE:H	1.75	0.51
2:B:8:TYR:HA	2:B:59:THR:OG1	2.10	0.51
3:E:717:ARG:HH21	3:L:728:GLU:HG2	121.37	0.51
3:K:738:ILE:CD1	3:L:738:ILE:HG12	2.35	0.51
1:C:331:GLU:CB	1:I:332:GLN:HE22	2.23	0.51
2:B:92:ASP:H	2:B:98:THR:HG21	1.76	0.51
2:N:92:ASP:H	2:N:98:THR:HG21	1.76	0.51
2:N:67:THR:O	2:N:68:ALA:CB	2.57	0.51
2:X:125:LYS:HG2	5:X:2000:GSP:C6	2.46	0.51
1:A:178:GLN:CD	1:A:739:MET:CE	2.79	0.51
1:Y:628:THR:HG23	1:Y:631:PHE:H	1.77	0.51
2:X:42:SER:HA	5:X:2000:GSP:S1G	2.51	0.51
1:M:607:VAL:O	1:M:611:SER:OG	2.20	0.51
2:T:8:TYR:CE2	2:T:11:LEU:HB2	2.45	0.50
1:W:133:LEU:O	1:W:136:SER:OG	2.21	0.50
3:F:717:ARG:CZ	3:K:724:ILE:HG22	119.79	0.50
5:N:2000:GSP:O2B	5:N:2000:GSP:O3G	2.28	0.50
1:A:628:THR:HG23	1:A:631:PHE:H	1.76	0.50
1:O:607:VAL:O	1:O:611:SER:OG	2.20	0.50
1:W:356:THR:HG21	1:W:546:VAL:HG12	1.93	0.50
1:C:206:ILE:HD11	1:C:394:PHE:HE2	1.75	0.50
3:E:717:ARG:NH2	3:L:728:GLU:HA	123.77	0.50
2:D:91:TYR:HB2	2:D:98:THR:HG23	1.94	0.50
2:T:92:ASP:H	2:T:98:THR:HG21	1.76	0.50
2:R:8:TYR:CE2	2:R:11:LEU:HB2	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:196:PRO:HG2	2:H:131:LEU:HD22	1.98	0.50
1:Q:356:THR:HG21	1:Q:546:VAL:HG12	1.93	0.50
5:B:2000:GSP:O2B	5:B:2000:GSP:O3G	2.29	0.49
3:K:720:LEU:O	3:K:724:ILE:HG12	2.11	0.49
5:P:2000:GSP:O3G	5:P:2000:GSP:O2B	2.29	0.49
1:O:628:THR:HG23	1:O:631:PHE:H	1.77	0.49
5:R:2000:GSP:O2B	5:R:2000:GSP:O3G	2.30	0.49
1:I:628:THR:HG23	1:I:631:PHE:H	1.76	0.49
3:E:728:GLU:CB	3:L:717:ARG:NH2	123.87	0.49
1:S:356:THR:HG21	1:S:546:VAL:HG12	1.94	0.49
1:M:628:THR:HG23	1:M:631:PHE:H	1.78	0.49
1:M:518:LEU:HG	1:M:519:LYS:H	1.77	0.49
3:F:724:ILE:HG22	3:K:717:ARG:HD2	119.85	0.49
3:E:717:ARG:HH21	3:L:728:GLU:HA	122.93	0.49
2:N:120:MET:HE3	2:N:164:ALA:HB1	1.95	0.49
1:O:356:THR:HG21	1:O:546:VAL:HG12	1.95	0.49
2:B:91:TYR:HB2	2:B:98:THR:HG23	1.95	0.49
2:J:91:TYR:HB2	2:J:98:THR:HG23	1.95	0.49
1:C:628:THR:HG23	1:C:631:PHE:H	1.76	0.49
1:W:611:SER:HB2	1:W:613:LEU:CD2	2.43	0.49
1:G:518:LEU:HG	1:G:519:LYS:H	1.80	0.49
1:G:356:THR:HG21	1:G:546:VAL:HG12	1.95	0.49
1:A:138:LEU:HD21	1:O:765:MET:SD	2.50	0.49
1:I:356:THR:HG21	1:I:546:VAL:HG12	1.95	0.49
1:G:769:GLN:HB3	1:Y:138:LEU:HG	181.02	0.49
2:H:91:TYR:HB2	2:H:98:THR:HG23	1.95	0.49
3:F:725:GLN:CB	3:K:717:ARG:HH21	121.58	0.48
1:Q:607:VAL:O	1:Q:611:SER:OG	2.20	0.48
2:D:120:MET:HB2	2:D:168:ILE:HD12	1.95	0.48
1:S:766:THR:HG22	1:S:769:GLN:HG3	1.95	0.48
3:E:717:ARG:HD2	3:V:724:ILE:HG21	1.94	0.48
3:U:735:GLN:NE2	3:V:734:LEU:HD12	2.27	0.48
2:J:92:ASP:H	2:J:98:THR:HG21	1.78	0.48
1:M:178:GLN:CD	1:M:739:MET:CE	2.81	0.48
1:I:611:SER:HB2	1:I:613:LEU:CD2	2.43	0.48
1:M:768:GLU:CD	1:M:768:GLU:H	2.17	0.48
1:G:611:SER:HB2	1:G:613:LEU:CD2	2.43	0.48
1:M:206:ILE:HD11	1:M:394:PHE:HE2	1.77	0.48
2:P:120:MET:HE3	2:P:164:ALA:HB1	1.95	0.48
1:Q:766:THR:HG22	1:Q:769:GLN:HG3	1.95	0.48
3:E:752:ILE:HG21	3:F:745:ILE:CD1	3.88	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:42:SER:HA	5:T:2000:GSP:S1G	2.53	0.48
1:I:221:SER:CA	2:N:71:GLU:OE2	2.61	0.48
1:C:611:SER:HB2	1:C:613:LEU:CD2	2.44	0.48
2:B:8:TYR:CE2	2:B:11:LEU:HB2	2.48	0.48
1:M:518:LEU:HG	1:M:519:LYS:N	2.29	0.48
1:A:356:THR:HG21	1:A:546:VAL:HG12	1.95	0.48
1:I:518:LEU:HG	1:I:519:LYS:H	1.79	0.48
3:E:729:GLU:HG3	1:S:751:SER:OG	2.13	0.48
2:R:91:TYR:HB2	2:R:98:THR:HG23	1.94	0.48
2:P:91:TYR:HB2	2:P:98:THR:HG23	1.95	0.48
3:E:720:LEU:O	3:E:724:ILE:HG12	2.12	0.48
2:J:38:LEU:O	5:J:2000:GSP:O3'	2.22	0.48
2:N:91:TYR:HB2	2:N:98:THR:HG23	1.95	0.48
1:C:206:ILE:HD11	1:C:394:PHE:HE1	5.52	0.48
1:W:206:ILE:HD11	1:W:394:PHE:HE2	1.79	0.48
3:E:717:ARG:NH2	3:L:731:ASN:ND2	123.23	0.48
2:X:91:TYR:HB2	2:X:98:THR:HG23	1.95	0.48
1:S:607:VAL:O	1:S:611:SER:OG	2.20	0.48
1:S:611:SER:HB2	1:S:613:LEU:CD2	2.43	0.48
1:Y:206:ILE:HD11	1:Y:394:PHE:HE1	1.79	0.48
1:O:768:GLU:H	1:O:768:GLU:CD	2.17	0.48
2:B:120:MET:HB2	2:B:168:ILE:HD12	1.96	0.48
3:L:720:LEU:O	3:L:724:ILE:HG13	2.14	0.48
1:Y:356:THR:HG21	1:Y:546:VAL:HG12	1.96	0.48
1:M:356:THR:HG21	1:M:546:VAL:HG12	1.96	0.48
1:S:588:ILE:HD12	1:S:593:GLY:HA2	1.95	0.48
1:G:138:LEU:CG	1:M:765:MET:HE2	2.44	0.48
1:I:178:GLN:CA	1:I:739:MET:HE1	2.42	0.48
2:J:8:TYR:CE2	2:J:11:LEU:HB2	2.48	0.48
2:B:120:MET:HE1	2:B:164:ALA:HB1	1.95	0.48
2:Z:120:MET:HE1	2:Z:164:ALA:HB1	1.96	0.48
1:G:182:MET:HA	1:G:186:MET:HG3	1.97	0.48
1:C:518:LEU:HG	1:C:519:LYS:H	1.79	0.48
3:U:720:LEU:O	3:U:724:ILE:HG12	2.14	0.48
2:P:41:LYS:HD2	3:U:733:ARG:NH2	2.29	0.48
3:F:733:ARG:HD2	2:R:41:LYS:HD2	120.96	0.48
1:C:356:THR:HG21	1:C:546:VAL:HG12	1.96	0.48
1:W:768:GLU:CD	1:W:768:GLU:H	2.17	0.48
2:J:120:MET:HB2	2:J:168:ILE:HD12	1.95	0.47
1:G:206:ILE:HD11	1:G:394:PHE:HE1	5.54	0.47
1:C:768:GLU:H	1:C:768:GLU:CD	2.19	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:768:GLU:CD	1:G:768:GLU:H	2.19	0.47
3:F:717:ARG:NH2	3:U:728:GLU:HB3	2.29	0.47
2:X:31:PHE:O	2:X:51:ARG:NH1	2.46	0.47
3:F:720:LEU:O	3:F:724:ILE:HG13	2.15	0.47
1:S:768:GLU:H	1:S:768:GLU:CD	2.17	0.47
2:H:120:MET:HE1	2:H:164:ALA:HB1	1.95	0.47
1:O:766:THR:HG22	1:O:769:GLN:HG3	1.97	0.47
2:T:91:TYR:HB2	2:T:98:THR:HG23	1.95	0.47
1:A:611:SER:HB2	1:A:613:LEU:CD2	2.44	0.47
1:Y:611:SER:HB2	1:Y:613:LEU:CD2	2.43	0.47
1:Q:611:SER:HB2	1:Q:613:LEU:CD2	2.44	0.47
2:D:120:MET:HE3	2:D:164:ALA:HB1	2.96	0.47
1:S:518:LEU:HG	1:S:519:LYS:H	1.78	0.47
2:Z:120:MET:HB2	2:Z:168:ILE:HD12	1.96	0.47
2:H:120:MET:HB2	2:H:168:ILE:HD12	1.97	0.47
1:Q:206:ILE:HD11	1:Q:394:PHE:HE2	1.79	0.47
2:R:120:MET:HE1	2:R:164:ALA:HB1	1.96	0.47
2:D:31:PHE:O	2:D:51:ARG:NH1	2.45	0.47
3:F:717:ARG:NH2	3:U:725:GLN:HA	2.29	0.47
1:I:138:LEU:HG	1:Q:769:GLN:CB	2.37	0.47
2:Z:91:TYR:HB2	2:Z:98:THR:HG23	1.95	0.47
2:P:120:MET:HB2	2:P:168:ILE:HD12	1.96	0.47
1:A:324:LEU:O	1:A:333:LYS:HE3	2.15	0.47
2:J:31:PHE:O	2:J:51:ARG:NH1	2.46	0.47
1:O:518:LEU:HG	1:O:519:LYS:H	1.80	0.47
1:W:518:LEU:HG	1:W:519:LYS:H	1.80	0.47
1:Q:768:GLU:CD	1:Q:768:GLU:H	2.17	0.47
3:V:720:LEU:O	3:V:724:ILE:HG13	2.15	0.47
1:C:331:GLU:HB3	1:I:332:GLN:HE22	1.79	0.47
1:G:178:GLN:CD	1:G:739:MET:CE	2.83	0.47
1:G:324:LEU:O	1:G:333:LYS:HE3	2.15	0.47
1:G:765:MET:HE2	1:M:138:LEU:HD11	1.97	0.47
1:Q:602:VAL:HG23	1:Q:607:VAL:CG2	2.45	0.47
1:Q:195:LYS:HB3	1:Q:196:PRO:HD3	1.97	0.47
3:F:728:GLU:HG2	3:U:717:ARG:HH21	1.80	0.47
1:C:178:GLN:CA	1:C:739:MET:HE1	2.44	0.47
1:M:611:SER:HB2	1:M:613:LEU:CD2	2.44	0.47
1:Q:329:THR:HG23	1:Q:332:GLN:H	1.80	0.47
2:B:80:TYR:CZ	3:E:746:MET:CE	2.99	0.46
2:R:120:MET:HB2	2:R:168:ILE:HD12	1.97	0.46
1:O:206:ILE:HD11	1:O:394:PHE:HE2	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:363:VAL:HA	1:G:388:VAL:HG12	1.99	0.46
2:T:120:MET:HE1	2:T:164:ALA:HB1	1.97	0.46
1:C:766:THR:HG22	1:C:769:GLN:HG3	1.98	0.46
2:N:120:MET:HB2	2:N:168:ILE:HD12	1.96	0.46
2:T:120:MET:HB2	2:T:168:ILE:HD12	1.97	0.46
1:C:324:LEU:O	1:C:333:LYS:HE3	2.16	0.46
1:Y:178:GLN:CD	1:Y:739:MET:CE	2.84	0.46
1:S:602:VAL:HG23	1:S:607:VAL:CG2	2.45	0.46
1:O:324:LEU:O	1:O:333:LYS:HE3	2.15	0.46
1:A:182:MET:HA	1:A:186:MET:HG3	1.98	0.46
2:P:31:PHE:O	2:P:51:ARG:NH1	2.45	0.46
1:Y:324:LEU:O	1:Y:333:LYS:HE3	2.15	0.46
1:M:324:LEU:O	1:M:333:LYS:HE3	2.15	0.46
3:E:717:ARG:NH1	3:V:724:ILE:HB	2.31	0.46
1:G:766:THR:HG22	1:G:769:GLN:HG3	1.98	0.46
1:I:766:THR:HG22	1:I:769:GLN:HG3	1.98	0.46
1:A:195:LYS:HB3	1:A:196:PRO:HD3	1.98	0.46
1:M:404:PRO:O	1:M:405:GLU:CB	2.64	0.46
1:W:324:LEU:O	1:W:333:LYS:HE3	2.16	0.46
1:O:178:GLN:CD	1:O:739:MET:CE	2.83	0.46
1:G:518:LEU:HG	1:G:519:LYS:N	2.32	0.46
2:P:99:TYR:O	2:P:102:VAL:HG22	2.16	0.46
2:D:99:TYR:O	2:D:102:VAL:HG22	2.16	0.46
1:A:176:LEU:N	1:A:177:PRO:CD	2.78	0.46
1:Q:518:LEU:HG	1:Q:519:LYS:H	1.79	0.46
2:X:120:MET:HB2	2:X:168:ILE:HD12	1.96	0.46
1:C:133:LEU:O	1:C:136:SER:OG	2.21	0.46
1:G:138:LEU:HD21	1:M:765:MET:SD	2.53	0.46
2:H:80:TYR:HE1	3:K:746:MET:SD	2.39	0.46
1:C:178:GLN:CD	1:C:739:MET:CE	2.84	0.46
1:C:602:VAL:HG23	1:C:607:VAL:CG2	2.46	0.46
2:J:120:MET:HE1	2:J:164:ALA:HB1	1.97	0.46
1:S:329:THR:HG23	1:S:332:GLN:H	1.81	0.46
1:Y:133:LEU:O	1:Y:136:SER:OG	2.21	0.46
1:C:182:MET:HA	1:C:186:MET:HG3	1.97	0.46
2:N:99:TYR:O	2:N:102:VAL:HG22	2.16	0.46
1:Y:768:GLU:H	1:Y:768:GLU:CD	2.18	0.46
3:F:725:GLN:CA	3:K:717:ARG:NH2	122.10	0.46
1:O:611:SER:HB2	1:O:613:LEU:CD2	2.45	0.46
1:O:404:PRO:O	1:O:405:GLU:CB	2.64	0.46
1:Y:182:MET:HA	1:Y:186:MET:HG3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:182:MET:HA	1:S:186:MET:HG3	1.98	0.46
1:M:182:MET:HA	1:M:186:MET:HG3	1.98	0.46
2:H:176:VAL:HG23	2:H:177:SER:N	2.31	0.46
1:S:206:ILE:HD11	1:S:394:PHE:HE2	1.80	0.46
1:W:182:MET:HA	1:W:186:MET:HG3	1.98	0.46
1:I:133:LEU:O	1:I:136:SER:OG	2.21	0.46
2:B:99:TYR:O	2:B:102:VAL:HG22	2.16	0.46
2:H:99:TYR:O	2:H:102:VAL:HG22	2.16	0.46
1:M:766:THR:HG22	1:M:769:GLN:HG3	1.98	0.46
3:E:724:ILE:HG22	3:V:717:ARG:NE	2.31	0.46
1:G:195:LYS:HB3	1:G:196:PRO:HD3	1.98	0.46
2:B:176:VAL:HG23	2:B:177:SER:N	2.31	0.46
2:B:80:TYR:OH	3:E:746:MET:CE	2.64	0.45
3:E:724:ILE:CG2	3:V:717:ARG:NE	2.78	0.45
1:Q:178:GLN:CD	1:Q:739:MET:CE	2.84	0.45
1:A:518:LEU:HG	1:A:519:LYS:H	1.81	0.45
2:N:31:PHE:O	2:N:51:ARG:NH1	2.46	0.45
3:F:728:GLU:CG	3:U:717:ARG:NH2	2.78	0.45
2:B:80:TYR:CZ	3:E:746:MET:SD	3.09	0.45
2:D:120:MET:HE1	2:D:164:ALA:HB1	1.98	0.45
2:J:99:TYR:O	2:J:102:VAL:HG22	2.17	0.45
1:Q:324:LEU:O	1:Q:333:LYS:HE3	2.17	0.45
1:M:329:THR:HG23	1:M:332:GLN:H	1.81	0.45
1:C:138:LEU:CD2	1:S:769:GLN:OE1	2.61	0.45
1:I:178:GLN:CD	1:I:739:MET:CE	2.84	0.45
1:Q:178:GLN:CA	1:Q:739:MET:HE1	2.44	0.45
1:O:195:LYS:HB3	1:O:196:PRO:HD3	1.97	0.45
1:Y:602:VAL:HG23	1:Y:607:VAL:CG2	2.47	0.45
1:O:518:LEU:HG	1:O:519:LYS:N	2.32	0.45
1:M:588:ILE:HD12	1:M:593:GLY:HA2	1.98	0.45
1:Q:363:VAL:HA	1:Q:388:VAL:HG12	1.98	0.45
1:A:363:VAL:HA	1:A:388:VAL:HG12	1.98	0.45
3:F:728:GLU:HG2	3:U:717:ARG:NH2	2.31	0.45
2:J:79:ALA:HB2	3:L:746:MET:HE1	1.94	0.45
1:I:404:PRO:O	1:I:405:GLU:CB	2.65	0.45
1:O:329:THR:HG23	1:O:332:GLN:H	1.81	0.45
1:I:768:GLU:H	1:I:768:GLU:CD	2.19	0.45
1:A:178:GLN:CA	1:A:739:MET:HE1	2.43	0.45
1:W:602:VAL:HG23	1:W:607:VAL:CG2	2.46	0.45
1:S:195:LYS:HB3	1:S:196:PRO:HD3	1.99	0.45
1:S:518:LEU:HG	1:S:519:LYS:N	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:99:TYR:O	2:X:102:VAL:HG22	2.16	0.45
1:C:404:PRO:O	1:C:405:GLU:CB	2.65	0.45
1:I:182:MET:HA	1:I:186:MET:HG3	1.97	0.45
1:Q:404:PRO:O	1:Q:405:GLU:CB	2.64	0.45
2:Z:38:LEU:HA	5:Z:2000:GSP:O2'	2.16	0.45
1:I:607:VAL:O	1:I:611:SER:OG	2.20	0.45
2:R:38:LEU:HA	5:R:2000:GSP:O2'	2.16	0.45
1:I:206:ILE:HD11	1:I:394:PHE:CE2	2.51	0.45
2:X:120:MET:HE3	2:X:164:ALA:HB1	1.97	0.45
1:S:404:PRO:O	1:S:405:GLU:CB	2.64	0.45
1:C:195:LYS:HB3	1:C:196:PRO:HD3	1.99	0.45
2:R:99:TYR:O	2:R:102:VAL:HG22	2.16	0.45
3:F:724:ILE:CG2	3:K:717:ARG:HD2	118.99	0.45
2:B:80:TYR:CE1	3:E:746:MET:CE	2.98	0.45
2:D:80:TYR:HE1	3:F:746:MET:HG2	1.82	0.45
1:S:178:GLN:CA	1:S:739:MET:HE1	2.44	0.45
1:I:602:VAL:HG23	1:I:607:VAL:CG2	2.47	0.45
1:M:602:VAL:HG23	1:M:607:VAL:CG2	2.46	0.45
1:G:602:VAL:HG23	1:G:607:VAL:CG2	2.48	0.45
1:C:206:ILE:HD11	1:C:394:PHE:CE2	2.51	0.45
1:S:324:LEU:O	1:S:333:LYS:HE3	2.17	0.45
1:Y:363:VAL:HA	1:Y:388:VAL:HG12	1.99	0.45
1:A:768:GLU:H	1:A:768:GLU:CD	2.18	0.45
1:G:178:GLN:CA	1:G:739:MET:HE1	2.46	0.45
1:O:588:ILE:HD12	1:O:593:GLY:HA2	1.99	0.45
1:Q:588:ILE:HD12	1:Q:593:GLY:HA2	1.98	0.45
1:W:404:PRO:O	1:W:405:GLU:CB	2.65	0.45
1:G:404:PRO:O	1:G:405:GLU:CB	2.65	0.45
1:I:329:THR:HG23	1:I:332:GLN:H	1.82	0.45
1:I:518:LEU:HG	1:I:519:LYS:N	2.31	0.45
1:Q:196:PRO:HG2	2:R:131:LEU:HD22	1.98	0.45
1:Q:182:MET:HA	1:Q:186:MET:HG3	1.99	0.45
1:G:329:THR:HG23	1:G:332:GLN:H	1.82	0.45
1:M:176:LEU:N	1:M:177:PRO:CD	2.80	0.45
1:M:363:VAL:HA	1:M:388:VAL:HG12	1.99	0.45
2:T:99:TYR:O	2:T:102:VAL:HG22	2.16	0.45
1:Y:766:THR:HG22	1:Y:769:GLN:HG3	1.99	0.45
1:C:518:LEU:HG	1:C:519:LYS:N	2.31	0.45
1:A:329:THR:HG23	1:A:332:GLN:H	1.82	0.45
1:Y:588:ILE:HD12	1:Y:593:GLY:HA2	1.99	0.45
1:C:363:VAL:HA	1:C:388:VAL:HG12	2.01	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:717:ARG:HG2	3:V:728:GLU:OE2	2.12	0.44
2:D:38:LEU:CA	5:D:2000:GSP:O2'	2.86	0.44
1:S:405:GLU:HA	1:S:534:PRO:HG3	1.99	0.44
1:Y:518:LEU:HG	1:Y:519:LYS:H	1.83	0.44
1:S:363:VAL:HA	1:S:388:VAL:HG12	1.99	0.44
1:Y:195:LYS:HB3	1:Y:196:PRO:HD3	1.99	0.44
1:M:178:GLN:CA	1:M:739:MET:HE1	2.44	0.44
1:O:178:GLN:CA	1:O:739:MET:HE1	2.44	0.44
1:W:178:GLN:CD	1:W:739:MET:CE	2.85	0.44
1:A:766:THR:HG22	1:A:769:GLN:HG3	2.00	0.44
1:O:602:VAL:HG23	1:O:607:VAL:CG2	2.47	0.44
1:M:195:LYS:HB3	1:M:196:PRO:HD3	1.98	0.44
1:Q:518:LEU:HG	1:Q:519:LYS:N	2.31	0.44
1:C:588:ILE:HD12	1:C:593:GLY:HA2	1.98	0.44
1:I:324:LEU:O	1:I:333:LYS:HE3	2.16	0.44
1:A:336:ARG:HA	1:Y:537:HIS:CD2	2.53	0.44
2:T:125:LYS:HG2	5:T:2000:GSP:C6	2.53	0.44
1:W:518:LEU:HG	1:W:519:LYS:N	2.32	0.44
1:I:195:LYS:HB3	1:I:196:PRO:HD3	1.99	0.44
1:G:176:LEU:N	1:G:177:PRO:CD	2.80	0.44
1:W:607:VAL:O	1:W:611:SER:OG	2.20	0.44
2:R:26:ASN:ND2	5:R:2000:GSP:O1A	2.50	0.44
1:G:206:ILE:HD11	1:G:394:PHE:HE2	1.81	0.44
2:Z:99:TYR:O	2:Z:102:VAL:HG22	2.17	0.44
1:I:759:GLU:OE2	1:Q:147:TYR:OH	2.33	0.44
1:C:176:LEU:N	1:C:177:PRO:CD	2.81	0.44
1:A:206:ILE:HD11	1:A:394:PHE:HE1	1.81	0.44
1:C:329:THR:HG23	1:C:332:GLN:H	1.83	0.44
2:B:44:ILE:HD12	3:F:737:TYR:CE2	2.51	0.44
1:S:178:GLN:CD	1:S:739:MET:CE	2.85	0.44
3:K:740:ARG:HH22	1:Q:682:SER:HB3	1.83	0.44
2:H:104:ARG:HD2	2:H:104:ARG:HA	1.79	0.44
1:W:766:THR:HG22	1:W:769:GLN:HG3	1.98	0.44
1:W:178:GLN:CA	1:W:739:MET:HE1	2.44	0.44
3:F:733:ARG:CZ	2:R:41:LYS:HB3	122.00	0.44
1:Y:329:THR:HG23	1:Y:332:GLN:H	1.83	0.44
1:Y:404:PRO:O	1:Y:405:GLU:CB	2.65	0.44
2:T:176:VAL:HG23	2:T:177:SER:N	2.33	0.44
3:K:738:ILE:HD11	3:L:738:ILE:HD13	1.99	0.44
1:Y:178:GLN:CA	1:Y:739:MET:HE1	2.45	0.44
3:F:717:ARG:HH11	3:K:728:GLU:HB2	123.26	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:588:ILE:HD12	1:I:593:GLY:HA2	1.98	0.44
3:E:735:GLN:HE22	3:F:734:LEU:CD1	3.85	0.44
2:B:26:ASN:ND2	5:B:2000:GSP:O1A	2.48	0.44
1:C:206:ILE:HD11	1:C:394:PHE:CE1	4.76	0.44
1:M:206:ILE:HD11	1:M:394:PHE:CE2	2.53	0.44
1:A:588:ILE:HD12	1:A:593:GLY:HA2	1.99	0.44
1:O:363:VAL:HA	1:O:388:VAL:HG12	2.00	0.44
1:A:178:GLN:CD	1:A:739:MET:HE3	2.39	0.43
1:O:169:ASN:OD1	1:O:201:ARG:CZ	2.66	0.43
2:R:176:VAL:HG23	2:R:177:SER:N	2.34	0.43
1:G:588:ILE:HD12	1:G:593:GLY:HA2	1.99	0.43
1:W:176:LEU:N	1:W:177:PRO:CD	2.81	0.43
1:A:404:PRO:O	1:A:405:GLU:CB	2.65	0.43
1:W:363:VAL:HA	1:W:388:VAL:HG12	2.00	0.43
1:I:405:GLU:HA	1:I:534:PRO:HG3	2.00	0.43
1:C:571:TRP:CE2	1:C:578:LEU:HD12	2.55	0.43
2:R:104:ARG:HD2	2:R:104:ARG:HA	1.79	0.43
2:B:80:TYR:CZ	3:E:746:MET:HE1	2.53	0.43
2:J:40:SER:HB3	5:J:2000:GSP:H3'	2.00	0.43
3:E:752:ILE:HD13	3:F:745:ILE:CD1	4.40	0.43
1:C:405:GLU:HA	1:C:534:PRO:HG3	2.00	0.43
1:C:331:GLU:HG3	1:I:332:GLN:NE2	2.32	0.43
1:Y:518:LEU:HG	1:Y:519:LYS:N	2.34	0.43
1:A:571:TRP:CE2	1:A:578:LEU:HD12	2.53	0.43
2:N:104:ARG:HD2	2:N:104:ARG:HA	1.77	0.43
3:F:731:ASN:ND2	3:U:717:ARG:NH2	2.64	0.43
1:I:221:SER:C	2:N:71:GLU:OE2	2.56	0.43
1:Y:206:ILE:HD11	1:Y:394:PHE:CE1	2.54	0.43
1:A:518:LEU:HG	1:A:519:LYS:N	2.33	0.43
1:Y:176:LEU:N	1:Y:177:PRO:CD	2.81	0.43
1:O:176:LEU:N	1:O:177:PRO:CD	2.82	0.43
1:W:195:LYS:HB3	1:W:196:PRO:HD3	1.99	0.43
1:C:138:LEU:HA	1:S:769:GLN:HE21	1.84	0.43
1:G:206:ILE:HD11	1:G:394:PHE:CE1	4.79	0.43
3:F:730:ILE:O	3:F:734:LEU:HG	2.20	0.43
1:C:549:LYS:HD3	1:C:554:LEU:HD21	2.02	0.43
1:M:169:ASN:OD1	1:M:201:ARG:CZ	2.67	0.43
1:Q:206:ILE:HD11	1:Q:394:PHE:CE2	2.54	0.43
1:O:405:GLU:HA	1:O:534:PRO:HG3	1.99	0.43
1:Q:405:GLU:HA	1:Q:534:PRO:HG3	2.01	0.43
1:W:588:ILE:HD12	1:W:593:GLY:HA2	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:176:VAL:HG23	2:P:177:SER:N	2.34	0.42
1:C:138:LEU:CD1	1:W:765:MET:HE2	145.12	0.42
2:H:80:TYR:CE1	3:K:746:MET:SD	3.12	0.42
2:P:37:ASN:O	5:P:2000:GSP:O2'	2.21	0.42
1:Q:308:ALA:N	1:Q:309:PRO:CD	2.81	0.42
1:M:571:TRP:CE2	1:M:578:LEU:HD12	2.54	0.42
1:G:571:TRP:CE2	1:G:578:LEU:HD12	2.54	0.42
1:W:329:THR:HG23	1:W:332:GLN:H	1.82	0.42
2:D:125:LYS:HG2	5:D:2000:GSP:C6	2.55	0.42
3:V:730:ILE:O	3:V:734:LEU:HG	2.20	0.42
1:A:602:VAL:HG23	1:A:607:VAL:CG2	2.48	0.42
1:I:363:VAL:HA	1:I:388:VAL:HG12	2.01	0.42
1:I:138:LEU:CG	1:Q:769:GLN:HB3	2.49	0.42
2:D:40:SER:HB3	5:D:2000:GSP:C3'	2.82	0.42
3:F:717:ARG:NH2	3:U:728:GLU:CB	2.82	0.42
3:E:728:GLU:HB3	3:L:717:ARG:CZ	123.85	0.42
1:W:206:ILE:HD11	1:W:394:PHE:CE2	2.53	0.42
1:I:176:LEU:N	1:I:177:PRO:CD	2.82	0.42
1:O:182:MET:HA	1:O:186:MET:HG3	2.02	0.42
3:E:730:ILE:O	3:E:734:LEU:HG	2.20	0.42
1:M:405:GLU:HA	1:M:534:PRO:HG3	2.00	0.42
2:X:176:VAL:HG23	2:X:177:SER:N	2.34	0.42
2:N:176:VAL:HG23	2:N:177:SER:N	2.34	0.42
1:I:571:TRP:CE2	1:I:578:LEU:HD12	2.54	0.42
1:S:206:ILE:HD11	1:S:394:PHE:CE2	2.55	0.42
2:H:80:TYR:CE1	3:K:746:MET:HE1	2.54	0.42
1:O:206:ILE:HD11	1:O:394:PHE:CE2	2.54	0.42
3:E:728:GLU:HB3	3:L:717:ARG:NH2	123.54	0.42
1:C:657:ARG:NH2	1:C:674:ASP:O	2.57	0.42
1:Y:405:GLU:HA	1:Y:534:PRO:HG3	2.02	0.42
2:D:176:VAL:HG23	2:D:177:SER:N	2.36	0.42
3:K:730:ILE:O	3:K:734:LEU:HG	2.20	0.42
3:E:754:GLU:HA	2:R:48:PHE:HD2	125.19	0.42
1:A:206:ILE:HD11	1:A:394:PHE:CE1	2.55	0.42
1:Y:571:TRP:CE2	1:Y:578:LEU:HD12	2.55	0.42
2:Z:173:TYR:O	2:Z:173:TYR:CG	2.73	0.42
1:Q:176:LEU:N	1:Q:177:PRO:CD	2.83	0.42
1:W:405:GLU:HA	1:W:534:PRO:HG3	2.02	0.41
1:W:196:PRO:HG2	2:X:131:LEU:HD22	2.02	0.41
1:G:549:LYS:HD3	1:G:554:LEU:HD21	2.03	0.41
1:S:169:ASN:OD1	1:S:201:ARG:CZ	2.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:724:ILE:HA	3:F:727:GLN:HE21	1.85	0.41
2:P:41:LYS:HB3	3:U:733:ARG:HH22	1.83	0.41
1:C:571:TRP:CD2	1:C:578:LEU:HD12	2.56	0.41
1:I:169:ASN:OD1	1:I:201:ARG:CZ	2.68	0.41
1:S:176:LEU:N	1:S:177:PRO:CD	2.83	0.41
2:B:173:TYR:CG	2:B:173:TYR:O	2.72	0.41
2:J:173:TYR:CG	2:J:173:TYR:O	2.73	0.41
2:H:80:TYR:OH	3:K:746:MET:HB3	2.19	0.41
1:M:308:ALA:N	1:M:309:PRO:CD	2.83	0.41
1:G:169:ASN:OD1	1:G:201:ARG:CZ	2.68	0.41
2:B:44:ILE:HD13	3:F:737:TYR:CD1	2.56	0.41
1:G:405:GLU:HA	1:G:534:PRO:HG3	2.02	0.41
2:P:104:ARG:HA	2:P:104:ARG:HD2	1.79	0.41
1:G:206:ILE:HD11	1:G:394:PHE:CE2	2.55	0.41
1:C:169:ASN:OD1	1:C:201:ARG:CZ	2.68	0.41
1:A:308:ALA:N	1:A:309:PRO:CD	2.83	0.41
1:W:169:ASN:OD1	1:W:201:ARG:CZ	2.68	0.41
3:E:731:ASN:HD21	3:F:731:ASN:CB	4.72	0.41
2:H:80:TYR:CE1	3:K:746:MET:CE	3.04	0.41
1:A:571:TRP:CD2	1:A:578:LEU:HD12	2.56	0.41
1:Q:169:ASN:OD1	1:Q:201:ARG:CZ	2.68	0.41
2:Z:31:PHE:O	2:Z:51:ARG:NH1	2.46	0.41
1:I:549:LYS:HD3	1:I:554:LEU:HD21	2.02	0.41
3:V:724:ILE:HA	3:V:727:GLN:HE21	1.85	0.41
1:C:332:GLN:NE2	1:I:332:GLN:HG3	2.30	0.41
1:A:336:ARG:HE	1:Y:537:HIS:CE1	2.37	0.41
1:Y:578:LEU:CD2	1:Y:717:LEU:HB3	2.50	0.41
1:Y:549:LYS:HD3	1:Y:554:LEU:HD21	2.02	0.41
1:S:549:LYS:HD3	1:S:554:LEU:HD21	2.02	0.41
2:H:31:PHE:O	2:H:51:ARG:NH1	2.46	0.41
1:S:578:LEU:CD2	1:S:717:LEU:HB3	2.51	0.41
1:G:695:LEU:HD12	1:G:695:LEU:HA	1.97	0.41
1:S:766:THR:O	1:S:769:GLN:HB2	2.21	0.41
1:A:196:PRO:HG2	2:B:131:LEU:HD22	2.01	0.41
1:Q:571:TRP:CE2	1:Q:578:LEU:HD12	2.55	0.41
1:W:308:ALA:N	1:W:309:PRO:CD	2.84	0.41
2:B:31:PHE:O	2:B:51:ARG:NH1	2.46	0.41
1:Y:695:LEU:HA	1:Y:695:LEU:HD12	1.96	0.41
1:O:571:TRP:CE2	1:O:578:LEU:HD12	2.56	0.41
3:L:730:ILE:O	3:L:734:LEU:HG	2.19	0.41
1:I:133:LEU:HD11	1:I:138:LEU:HD22	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:GLN:HG3	1:I:332:GLN:HE21	1.85	0.41
1:Q:578:LEU:CD2	1:Q:717:LEU:HB3	2.52	0.41
1:W:571:TRP:CE2	1:W:578:LEU:HD12	2.56	0.41
1:W:783:ARG:O	1:W:784:SER:CB	2.69	0.41
1:Y:657:ARG:NH2	1:Y:674:ASP:O	2.54	0.41
3:U:730:ILE:O	3:U:734:LEU:HG	2.21	0.41
1:I:621:GLN:NE2	1:I:622:GLU:OE2	2.53	0.40
1:O:578:LEU:HD21	1:O:717:LEU:HB3	2.03	0.40
1:C:783:ARG:O	1:C:784:SER:CB	2.70	0.40
1:O:639:VAL:HG13	1:O:714:TYR:HB2	2.03	0.40
1:C:639:VAL:HG13	1:C:714:TYR:HB2	2.04	0.40
1:Q:549:LYS:HD3	1:Q:554:LEU:HD21	2.03	0.40
1:M:571:TRP:CD2	1:M:578:LEU:HD12	2.55	0.40
1:G:571:TRP:CD2	1:G:578:LEU:HD12	2.57	0.40
1:S:571:TRP:CE2	1:S:578:LEU:HD12	2.55	0.40
1:O:783:ARG:O	1:O:784:SER:CB	2.69	0.40
1:Y:783:ARG:O	1:Y:784:SER:CB	2.70	0.40
2:X:104:ARG:HD2	2:X:104:ARG:HA	1.78	0.40
2:T:173:TYR:O	2:T:173:TYR:CG	2.74	0.40
2:H:173:TYR:O	2:H:173:TYR:CG	2.73	0.40
1:M:783:ARG:O	1:M:784:SER:CB	2.70	0.40
2:T:48:PHE:HD2	3:U:754:GLU:HA	1.86	0.40
1:W:549:LYS:HD3	1:W:554:LEU:HD21	2.03	0.40
1:Q:766:THR:O	1:Q:769:GLN:HB2	2.22	0.40
2:D:79:ALA:HB2	3:F:746:MET:HE1	2.01	0.40
1:S:783:ARG:O	1:S:784:SER:CB	2.69	0.40
1:G:783:ARG:O	1:G:784:SER:CB	2.70	0.40
3:K:742:ILE:HD11	3:L:741:ILE:HD13	2.04	0.40
3:L:724:ILE:HA	3:L:727:GLN:HE21	1.86	0.40
1:O:578:LEU:CD2	1:O:717:LEU:HB3	2.51	0.40
1:W:657:ARG:NH2	1:W:674:ASP:O	2.54	0.40
1:Y:169:ASN:OD1	1:Y:201:ARG:CZ	2.69	0.40
1:C:133:LEU:HD11	1:C:138:LEU:HD22	2.04	0.40
1:I:139:PHE:HD1	1:I:143:MET:CE	2.34	0.40

All (61) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:174:ARG:NH2	1:M:166:CYS:O[2_545]	0.72	1.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:174:ARG:NH2	1:O:166:CYS:O[2_556]	0.76	1.44
2:B:174:ARG:NH2	1:g:166:CYS:O[2_656]	0.78	1.42
1:I:396:THR:OG1	1:M:627:THR:OG1[2_545]	0.85	1.35
1:S:346:HIS:O	1:Y:626:TYR:CE1[2_656]	1.08	1.12
1:C:396:THR:OG1	1:O:627:THR:OG1[2_556]	1.08	1.12
2:H:174:ARG:NH2	1:W:166:CYS:O[2_655]	1.08	1.12
1:S:346:HIS:CA	1:Y:626:TYR:OH[2_656]	1.20	1.00
1:Q:343:LEU:O	1:c:626:TYR:OH[2_655]	1.29	0.91
1:O:779:ASP:OD2	1:g:537:HIS:CD2[2_656]	1.37	0.83
2:D:174:ARG:CZ	1:O:166:CYS:O[2_556]	1.41	0.79
2:J:56:ASP:OD1	1:M:165:PHE:O[2_545]	1.44	0.76
2:B:56:ASP:OD1	1:g:165:PHE:O[2_656]	1.47	0.73
2:D:56:ASP:OD1	1:O:165:PHE:O[2_556]	1.47	0.73
2:J:174:ARG:CZ	1:M:166:CYS:O[2_545]	1.51	0.69
1:A:626:TYR:CD2	1:O:346:HIS:O[2_546]	1.53	0.67
1:G:626:TYR:OH	1:M:348:LEU:N[2_555]	1.55	0.65
1:G:626:TYR:CD2	1:M:346:HIS:O[2_555]	1.56	0.64
1:S:346:HIS:C	1:Y:626:TYR:OH[2_656]	1.61	0.59
1:S:346:HIS:O	1:Y:626:TYR:CZ[2_656]	1.61	0.59
1:A:626:TYR:OH	1:O:348:LEU:N[2_546]	1.63	0.57
1:G:626:TYR:CE2	1:M:346:HIS:O[2_555]	1.69	0.51
1:A:626:TYR:OH	1:O:348:LEU:O[2_546]	1.72	0.48
1:S:346:HIS:CA	1:Y:626:TYR:CZ[2_656]	1.75	0.45
1:A:626:TYR:CE2	1:O:346:HIS:O[2_546]	1.76	0.44
1:G:626:TYR:OH	1:M:348:LEU:O[2_555]	1.80	0.40
1:S:323:ARG:NH1	1:Y:707:ASP:OD2[2_656]	1.81	0.39
1:A:396:THR:OG1	1:g:627:THR:OG1[2_656]	1.81	0.39
2:B:174:ARG:CZ	1:g:166:CYS:O[2_656]	1.84	0.36
1:Q:346:HIS:CB	1:c:626:TYR:CZ[2_655]	1.84	0.36
1:I:396:THR:CB	1:M:627:THR:OG1[2_545]	1.87	0.33
2:H:56:ASP:OD1	1:W:165:PHE:O[2_655]	1.87	0.33
2:B:174:ARG:NH2	1:g:166:CYS:C[2_656]	1.87	0.33
1:S:346:HIS:C	1:Y:626:TYR:CZ[2_656]	1.88	0.32
2:H:174:ARG:CZ	1:W:166:CYS:O[2_655]	1.88	0.32
2:B:56:ASP:OD2	1:g:166:CYS:CA[2_656]	1.89	0.31
2:J:174:ARG:NH2	1:M:166:CYS:C[2_545]	1.93	0.27
1:G:339:SER:OG	1:c:537:HIS:CG[1_565]	1.94	0.26
2:D:174:ARG:NH2	1:O:166:CYS:C[2_556]	1.97	0.23
1:S:346:HIS:O	1:Y:626:TYR:OH[2_656]	1.98	0.22
1:S:346:HIS:CB	1:Y:626:TYR:CE2[2_656]	2.00	0.20
2:B:56:ASP:CG	1:g:166:CYS:CA[2_656]	2.01	0.19

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:346:HIS:CB	1:c:626:TYR:OH[2_655]	2.03	0.17
1:A:616:LEU:CD2	1:O:346:HIS:CD2[2_546]	2.03	0.17
1:G:616:LEU:CD2	1:M:346:HIS:CD2[2_555]	2.07	0.13
1:S:346:HIS:C	1:Y:626:TYR:CE1[2_656]	2.07	0.13
1:C:396:THR:CB	1:O:627:THR:OG1[2_556]	2.08	0.12
1:Q:323:ARG:NH1	1:c:707:ASP:OD2[2_655]	2.09	0.11
2:B:56:ASP:O	2:h:130:HIS:CE1[2_656]	2.09	0.11
2:B:56:ASP:OD1	1:g:166:CYS:C[2_656]	2.10	0.10
1:G:326:THR:O	1:c:404:PRO:CD[1_565]	2.10	0.10
1:O:779:ASP:OD2	1:g:537:HIS:NE2[2_656]	2.10	0.10
2:B:56:ASP:OD1	1:g:166:CYS:CA[2_656]	2.10	0.10
1:G:396:THR:OG1	1:W:627:THR:OG1[2_655]	2.11	0.09
1:O:779:ASP:CG	1:g:537:HIS:CD2[2_656]	2.14	0.06
1:O:779:ASP:OD2	1:g:537:HIS:CG[2_656]	2.15	0.05
1:S:346:HIS:CB	1:Y:626:TYR:CZ[2_656]	2.17	0.03
1:S:346:HIS:N	1:Y:626:TYR:OH[2_656]	2.18	0.02
1:A:626:TYR:CG	1:O:346:HIS:O[2_546]	2.18	0.02
1:G:626:TYR:OH	1:M:348:LEU:CA[2_555]	2.19	0.01
1:A:626:TYR:OH	1:O:348:LEU:C[2_546]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	460/566 (81%)	442 (96%)	16 (4%)	2 (0%)	39	80
1	C	460/566 (81%)	439 (95%)	18 (4%)	3 (1%)	26	71
1	G	460/566 (81%)	439 (95%)	18 (4%)	3 (1%)	26	71
1	I	460/566 (81%)	440 (96%)	17 (4%)	3 (1%)	26	71
1	M	460/566 (81%)	441 (96%)	16 (4%)	3 (1%)	26	71
1	O	460/566 (81%)	442 (96%)	15 (3%)	3 (1%)	26	71
1	Q	460/566 (81%)	439 (95%)	19 (4%)	2 (0%)	39	80

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	460/566 (81%)	439 (95%)	18 (4%)	3 (1%)	26	71
1	W	460/566 (81%)	442 (96%)	15 (3%)	3 (1%)	26	71
1	Y	460/566 (81%)	439 (95%)	18 (4%)	3 (1%)	26	71
1	c	460/566 (81%)	440 (96%)	18 (4%)	2 (0%)	39	80
1	g	460/566 (81%)	440 (96%)	18 (4%)	2 (0%)	39	80
2	B	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	30	74
2	D	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	30	74
2	H	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	30	74
2	J	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	30	74
2	N	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	30	74
2	P	171/219 (78%)	162 (95%)	8 (5%)	1 (1%)	30	74
2	R	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	30	74
2	T	171/219 (78%)	163 (95%)	6 (4%)	2 (1%)	16	61
2	X	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	30	74
2	Z	171/219 (78%)	163 (95%)	6 (4%)	2 (1%)	16	61
2	d	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	30	74
2	h	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	30	74
3	E	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	F	30/48 (62%)	30 (100%)	0	0	100	100
3	K	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	L	30/48 (62%)	30 (100%)	0	0	100	100
3	U	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	V	30/48 (62%)	30 (100%)	0	0	100	100
3	a	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	b	30/48 (62%)	30 (100%)	0	0	100	100
3	e	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	f	30/48 (62%)	30 (100%)	0	0	100	100
3	i	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	j	30/48 (62%)	30 (100%)	0	0	100	100
All	All	7986/9996 (80%)	7645 (96%)	295 (4%)	46 (1%)	30	74

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	405	GLU
2	B	68	ALA
1	C	405	GLU
2	D	68	ALA
1	G	405	GLU
2	H	68	ALA
1	I	405	GLU
2	J	68	ALA
1	M	405	GLU
2	N	68	ALA
1	O	405	GLU
2	P	68	ALA
1	Q	405	GLU
2	R	68	ALA
1	S	405	GLU
2	T	68	ALA
1	W	405	GLU
2	X	68	ALA
1	Y	405	GLU
2	Z	68	ALA
1	c	405	GLU
2	d	68	ALA
1	g	405	GLU
2	h	68	ALA
1	W	398	SER
1	C	398	SER
1	G	398	SER
1	I	398	SER
1	M	398	SER
1	O	398	SER
1	S	398	SER
2	T	125	LYS
1	Y	398	SER
2	Z	125	LYS
1	A	399	VAL
1	O	399	VAL
1	W	399	VAL
1	g	399	VAL
1	C	399	VAL
1	G	399	VAL
1	I	399	VAL
1	M	399	VAL
1	Q	399	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Y	399	VAL
1	c	399	VAL
1	S	399	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	422/508 (83%)	408 (97%)	14 (3%)	45	76
1	C	422/508 (83%)	408 (97%)	14 (3%)	45	76
1	G	422/508 (83%)	408 (97%)	14 (3%)	45	76
1	I	422/508 (83%)	408 (97%)	14 (3%)	45	76
1	M	422/508 (83%)	408 (97%)	14 (3%)	45	76
1	O	422/508 (83%)	408 (97%)	14 (3%)	45	76
1	Q	422/508 (83%)	408 (97%)	14 (3%)	45	76
1	S	422/508 (83%)	408 (97%)	14 (3%)	45	76
1	W	422/508 (83%)	408 (97%)	14 (3%)	45	76
1	Y	422/508 (83%)	408 (97%)	14 (3%)	45	76
1	c	422/508 (83%)	408 (97%)	14 (3%)	45	76
1	g	422/508 (83%)	409 (97%)	13 (3%)	47	77
2	B	147/191 (77%)	144 (98%)	3 (2%)	63	85
2	D	147/191 (77%)	144 (98%)	3 (2%)	63	85
2	H	147/191 (77%)	144 (98%)	3 (2%)	63	85
2	J	147/191 (77%)	144 (98%)	3 (2%)	63	85
2	N	147/191 (77%)	144 (98%)	3 (2%)	63	85
2	P	147/191 (77%)	144 (98%)	3 (2%)	63	85
2	R	147/191 (77%)	144 (98%)	3 (2%)	63	85
2	T	147/191 (77%)	144 (98%)	3 (2%)	63	85
2	X	147/191 (77%)	144 (98%)	3 (2%)	63	85

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Z	147/191 (77%)	144 (98%)	3 (2%)	63	85
2	d	147/191 (77%)	144 (98%)	3 (2%)	63	85
2	h	147/191 (77%)	144 (98%)	3 (2%)	63	85
3	E	31/45 (69%)	30 (97%)	1 (3%)	46	76
3	F	21/45 (47%)	21 (100%)	0	100	100
3	K	31/45 (69%)	30 (97%)	1 (3%)	46	76
3	L	21/45 (47%)	21 (100%)	0	100	100
3	U	31/45 (69%)	30 (97%)	1 (3%)	46	76
3	V	21/45 (47%)	21 (100%)	0	100	100
3	a	31/45 (69%)	30 (97%)	1 (3%)	46	76
3	b	21/45 (47%)	21 (100%)	0	100	100
3	e	31/45 (69%)	30 (97%)	1 (3%)	46	76
3	f	21/45 (47%)	21 (100%)	0	100	100
3	i	31/45 (69%)	30 (97%)	1 (3%)	46	76
3	j	21/45 (47%)	21 (100%)	0	100	100
All	All	7140/8928 (80%)	6931 (97%)	209 (3%)	50	78

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	LEU
1	A	148	LEU
1	A	235	LYS
1	A	306	ARG
1	A	318	MET
1	A	323	ARG
1	A	335	GLN
1	A	378	ASP
1	A	391	CYS
1	A	397	THR
1	A	565	LYS
1	A	613	LEU
1	A	694	LYS
1	A	739	MET
2	B	7	GLU
2	B	33	ARG
2	B	54	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	138	LEU
1	C	148	LEU
1	C	235	LYS
1	C	306	ARG
1	C	318	MET
1	C	323	ARG
1	C	335	GLN
1	C	378	ASP
1	C	391	CYS
1	C	397	THR
1	C	565	LYS
1	C	613	LEU
1	C	694	LYS
1	C	739	MET
2	D	7	GLU
2	D	33	ARG
2	D	54	GLN
3	E	728	GLU
1	G	138	LEU
1	G	148	LEU
1	G	235	LYS
1	G	306	ARG
1	G	318	MET
1	G	323	ARG
1	G	335	GLN
1	G	378	ASP
1	G	391	CYS
1	G	397	THR
1	G	565	LYS
1	G	613	LEU
1	G	694	LYS
1	G	739	MET
2	H	7	GLU
2	H	33	ARG
2	H	54	GLN
1	I	138	LEU
1	I	148	LEU
1	I	235	LYS
1	I	306	ARG
1	I	318	MET
1	I	323	ARG
1	I	335	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	378	ASP
1	I	391	CYS
1	I	397	THR
1	I	565	LYS
1	I	613	LEU
1	I	694	LYS
1	I	739	MET
2	J	7	GLU
2	J	33	ARG
2	J	54	GLN
3	K	728	GLU
1	M	138	LEU
1	M	148	LEU
1	M	235	LYS
1	M	306	ARG
1	M	318	MET
1	M	323	ARG
1	M	335	GLN
1	M	378	ASP
1	M	391	CYS
1	M	397	THR
1	M	565	LYS
1	M	613	LEU
1	M	694	LYS
1	M	739	MET
2	N	7	GLU
2	N	33	ARG
2	N	54	GLN
1	O	138	LEU
1	O	148	LEU
1	O	235	LYS
1	O	306	ARG
1	O	318	MET
1	O	323	ARG
1	O	335	GLN
1	O	378	ASP
1	O	391	CYS
1	O	397	THR
1	O	565	LYS
1	O	613	LEU
1	O	694	LYS
1	O	739	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	7	GLU
2	P	33	ARG
2	P	54	GLN
1	Q	138	LEU
1	Q	148	LEU
1	Q	235	LYS
1	Q	306	ARG
1	Q	318	MET
1	Q	323	ARG
1	Q	335	GLN
1	Q	378	ASP
1	Q	391	CYS
1	Q	397	THR
1	Q	565	LYS
1	Q	613	LEU
1	Q	694	LYS
1	Q	739	MET
2	R	7	GLU
2	R	33	ARG
2	R	54	GLN
1	S	138	LEU
1	S	148	LEU
1	S	235	LYS
1	S	306	ARG
1	S	318	MET
1	S	323	ARG
1	S	335	GLN
1	S	378	ASP
1	S	391	CYS
1	S	397	THR
1	S	565	LYS
1	S	613	LEU
1	S	694	LYS
1	S	739	MET
2	T	7	GLU
2	T	33	ARG
2	T	54	GLN
3	U	728	GLU
1	W	138	LEU
1	W	148	LEU
1	W	235	LYS
1	W	306	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	W	318	MET
1	W	323	ARG
1	W	335	GLN
1	W	378	ASP
1	W	391	CYS
1	W	397	THR
1	W	565	LYS
1	W	613	LEU
1	W	694	LYS
1	W	739	MET
2	X	7	GLU
2	X	33	ARG
2	X	54	GLN
1	Y	138	LEU
1	Y	148	LEU
1	Y	235	LYS
1	Y	306	ARG
1	Y	318	MET
1	Y	323	ARG
1	Y	335	GLN
1	Y	378	ASP
1	Y	391	CYS
1	Y	397	THR
1	Y	565	LYS
1	Y	613	LEU
1	Y	694	LYS
1	Y	739	MET
2	Z	7	GLU
2	Z	33	ARG
2	Z	54	GLN
3	a	728	GLU
1	c	138	LEU
1	c	148	LEU
1	c	235	LYS
1	c	306	ARG
1	c	318	MET
1	c	323	ARG
1	c	335	GLN
1	c	378	ASP
1	c	391	CYS
1	c	397	THR
1	c	565	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	c	613	LEU
1	c	694	LYS
1	c	739	MET
2	d	7	GLU
2	d	33	ARG
2	d	54	GLN
3	e	728	GLU
1	g	138	LEU
1	g	148	LEU
1	g	235	LYS
1	g	306	ARG
1	g	318	MET
1	g	323	ARG
1	g	378	ASP
1	g	391	CYS
1	g	397	THR
1	g	565	LYS
1	g	613	LEU
1	g	694	LYS
1	g	739	MET
2	h	7	GLU
2	h	33	ARG
2	h	54	GLN
3	i	728	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	540	ASN
1	A	606	GLN
1	C	332	GLN
1	C	540	ASN
1	C	606	GLN
3	F	727	GLN
3	F	731	ASN
1	G	540	ASN
1	G	606	GLN
1	I	332	GLN
1	I	540	ASN
1	I	606	GLN
1	I	776	GLN
3	K	731	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	K	735	GLN
3	L	727	GLN
3	L	731	ASN
1	M	540	ASN
1	M	606	GLN
1	O	393	ASN
1	O	540	ASN
1	O	606	GLN
1	Q	540	ASN
1	Q	606	GLN
1	S	393	ASN
1	S	540	ASN
1	S	606	GLN
3	U	731	ASN
3	U	735	GLN
3	V	727	GLN
1	W	540	ASN
1	W	606	GLN
1	W	776	GLN
1	Y	540	ASN
1	Y	606	GLN
3	b	727	GLN
1	c	540	ASN
1	c	606	GLN
3	e	731	ASN
3	e	735	GLN
3	f	727	GLN
1	g	540	ASN
1	g	606	GLN
1	g	776	GLN
3	i	735	GLN
3	j	727	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	093	A	2002	-	21,25,25	2.00	6 (28%)	24,36,36	4.52	11 (45%)
5	GSP	B	2000	6	25,34,34	1.49	4 (16%)	31,54,54	2.00	7 (22%)
4	093	C	2002	-	21,25,25	2.02	6 (28%)	24,36,36	4.52	10 (41%)
5	GSP	D	2000	6	25,34,34	1.59	5 (20%)	31,54,54	2.18	10 (32%)
4	093	G	2002	1	21,25,25	2.01	6 (28%)	24,36,36	4.53	11 (45%)
5	GSP	H	2000	6	25,34,34	1.39	4 (16%)	31,54,54	2.10	8 (25%)
4	093	I	2002	-	21,25,25	2.01	6 (28%)	24,36,36	4.52	11 (45%)
5	GSP	J	2000	6	25,34,34	1.62	5 (20%)	31,54,54	2.28	10 (32%)
4	093	M	2002	-	21,25,25	2.03	6 (28%)	24,36,36	4.52	11 (45%)
5	GSP	N	2000	6	25,34,34	1.32	4 (16%)	31,54,54	2.27	11 (35%)
4	093	O	2002	1	21,25,25	2.04	6 (28%)	24,36,36	4.52	11 (45%)
5	GSP	P	2000	6	25,34,34	1.36	5 (20%)	31,54,54	2.16	10 (32%)
4	093	Q	2002	1	21,25,25	2.02	6 (28%)	24,36,36	4.53	11 (45%)
5	GSP	R	2000	6	25,34,34	1.43	4 (16%)	31,54,54	2.17	8 (25%)
4	093	S	2002	1	21,25,25	2.02	6 (28%)	24,36,36	4.54	11 (45%)
5	GSP	T	2000	6	25,34,34	1.33	4 (16%)	31,54,54	2.14	8 (25%)
4	093	W	2002	1	21,25,25	2.01	6 (28%)	24,36,36	4.52	11 (45%)
5	GSP	X	2000	6	25,34,34	1.52	5 (20%)	31,54,54	2.07	10 (32%)
4	093	Y	2002	1	21,25,25	2.02	6 (28%)	24,36,36	4.52	11 (45%)
5	GSP	Z	2000	6	25,34,34	1.47	5 (20%)	31,54,54	2.08	8 (25%)
4	093	c	2002	1	21,25,25	2.04	6 (28%)	24,36,36	4.52	11 (45%)
5	GSP	d	2000	6	25,34,34	1.49	5 (20%)	31,54,54	2.25	11 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	093	g	2002	1	21,25,25	2.02	6 (28%)	24,36,36	4.53	11 (45%)
5	GSP	h	2000	6	25,34,34	1.64	6 (24%)	31,54,54	2.08	10 (32%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	093	A	2002	-	-	0/17/19/19	0/2/2/2
5	GSP	B	2000	6	-	0/15/38/38	0/3/3/3
4	093	C	2002	-	-	0/17/19/19	0/2/2/2
5	GSP	D	2000	6	-	0/15/38/38	0/3/3/3
4	093	G	2002	1	-	0/17/19/19	0/2/2/2
5	GSP	H	2000	6	-	0/15/38/38	0/3/3/3
4	093	I	2002	-	-	0/17/19/19	0/2/2/2
5	GSP	J	2000	6	-	0/15/38/38	0/3/3/3
4	093	M	2002	-	-	0/17/19/19	0/2/2/2
5	GSP	N	2000	6	-	0/15/38/38	0/3/3/3
4	093	O	2002	1	-	0/17/19/19	0/2/2/2
5	GSP	P	2000	6	-	0/15/38/38	0/3/3/3
4	093	Q	2002	1	-	0/17/19/19	0/2/2/2
5	GSP	R	2000	6	-	0/15/38/38	0/3/3/3
4	093	S	2002	1	-	0/17/19/19	0/2/2/2
5	GSP	T	2000	6	-	0/15/38/38	0/3/3/3
4	093	W	2002	1	-	0/17/19/19	0/2/2/2
5	GSP	X	2000	6	-	0/15/38/38	0/3/3/3
4	093	Y	2002	1	-	0/17/19/19	0/2/2/2
5	GSP	Z	2000	6	-	0/15/38/38	0/3/3/3
4	093	c	2002	1	-	0/17/19/19	0/2/2/2
5	GSP	d	2000	6	-	0/15/38/38	0/3/3/3
4	093	g	2002	1	-	0/17/19/19	0/2/2/2
5	GSP	h	2000	6	-	0/15/38/38	0/3/3/3

All (128) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	c	2002	093	OAM-SAN	-3.20	1.40	1.43
4	O	2002	093	OAM-SAN	-3.16	1.40	1.43
4	M	2002	093	OAM-SAN	-3.14	1.40	1.43
4	g	2002	093	OAM-SAN	-3.12	1.40	1.43
4	W	2002	093	OAM-SAN	-3.11	1.40	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2002	093	OAM-SAN	-3.07	1.40	1.43
4	S	2002	093	OAM-SAN	-3.07	1.40	1.43
4	A	2002	093	OAM-SAN	-3.06	1.40	1.43
4	Q	2002	093	OAM-SAN	-3.05	1.40	1.43
4	I	2002	093	OAM-SAN	-3.02	1.40	1.43
4	G	2002	093	OAM-SAN	-3.01	1.40	1.43
4	Y	2002	093	OAM-SAN	-2.99	1.40	1.43
4	I	2002	093	CAV-CAW	-2.34	1.41	1.50
4	G	2002	093	CAV-CAW	-2.32	1.42	1.50
4	C	2002	093	CAV-CAW	-2.32	1.42	1.50
4	Y	2002	093	CAV-CAW	-2.32	1.42	1.50
4	g	2002	093	CAV-CAW	-2.32	1.42	1.50
4	S	2002	093	CAV-CAW	-2.31	1.42	1.50
4	Q	2002	093	CAV-CAW	-2.31	1.42	1.50
4	W	2002	093	CAV-CAW	-2.31	1.42	1.50
4	c	2002	093	CAV-CAW	-2.31	1.42	1.50
4	A	2002	093	CAV-CAW	-2.30	1.42	1.50
4	M	2002	093	CAV-CAW	-2.30	1.42	1.50
4	O	2002	093	CAV-CAW	-2.28	1.42	1.50
5	J	2000	GSP	O4'-C1'	2.01	1.43	1.41
5	h	2000	GSP	PG-O3G	2.05	1.62	1.55
5	P	2000	GSP	PG-O3G	2.13	1.62	1.55
5	T	2000	GSP	PG-O2G	2.17	1.62	1.55
5	Z	2000	GSP	O4'-C1'	2.19	1.44	1.41
5	D	2000	GSP	O4'-C1'	2.20	1.44	1.41
5	T	2000	GSP	O4'-C1'	2.20	1.44	1.41
5	X	2000	GSP	PG-O2G	2.22	1.62	1.55
5	d	2000	GSP	PG-O3G	2.23	1.63	1.55
5	X	2000	GSP	PG-S1G	2.33	1.95	1.90
5	R	2000	GSP	PG-S1G	2.37	1.95	1.90
5	P	2000	GSP	PG-O2G	2.42	1.63	1.55
5	N	2000	GSP	PG-S1G	2.43	1.95	1.90
5	H	2000	GSP	PG-S1G	2.47	1.95	1.90
5	N	2000	GSP	C5-C4	2.49	1.46	1.40
5	P	2000	GSP	C5-C4	2.50	1.46	1.40
4	S	2002	093	CAT-CAS	2.54	1.53	1.49
4	W	2002	093	CAT-CAS	2.54	1.53	1.49
4	c	2002	093	CAT-CAS	2.54	1.53	1.49
5	D	2000	GSP	PG-O2G	2.55	1.64	1.55
5	Z	2000	GSP	PG-S1G	2.55	1.95	1.90
4	G	2002	093	CAT-CAS	2.57	1.53	1.49
4	M	2002	093	CAT-CAS	2.59	1.53	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	g	2002	093	CAT-CAS	2.59	1.53	1.49
4	A	2002	093	CAT-CAS	2.59	1.53	1.49
5	H	2000	GSP	PG-O2G	2.61	1.64	1.55
4	O	2002	093	CAT-CAS	2.62	1.53	1.49
4	Q	2002	093	CAT-CAS	2.62	1.53	1.49
5	d	2000	GSP	PG-S1G	2.63	1.95	1.90
4	C	2002	093	CAT-CAS	2.65	1.53	1.49
5	R	2000	GSP	PG-O2G	2.67	1.64	1.55
4	Y	2002	093	CAT-CAS	2.67	1.53	1.49
4	I	2002	093	CAT-CAS	2.67	1.53	1.49
5	N	2000	GSP	PG-O2G	2.73	1.64	1.55
4	Y	2002	093	CAS-NAR	2.75	1.44	1.37
4	W	2002	093	CAS-NAR	2.75	1.44	1.37
4	Q	2002	093	CAS-NAR	2.76	1.44	1.37
4	g	2002	093	CAS-NAR	2.76	1.44	1.37
4	S	2002	093	CAS-NAR	2.77	1.44	1.37
4	I	2002	093	CAS-NAR	2.77	1.44	1.37
5	d	2000	GSP	PG-O2G	2.78	1.64	1.55
4	A	2002	093	CAS-NAR	2.78	1.44	1.37
4	O	2002	093	CAS-NAR	2.80	1.44	1.37
5	h	2000	GSP	PG-O2G	2.80	1.65	1.55
5	J	2000	GSP	PG-O2G	2.81	1.65	1.55
4	c	2002	093	CAS-NAR	2.82	1.44	1.37
4	M	2002	093	CAS-NAR	2.82	1.44	1.37
4	C	2002	093	CAS-NAR	2.83	1.44	1.37
4	G	2002	093	CAS-NAR	2.84	1.44	1.37
5	H	2000	GSP	C5-C4	2.87	1.47	1.40
5	Z	2000	GSP	PG-O2G	2.91	1.65	1.55
5	B	2000	GSP	C5-C4	2.95	1.47	1.40
5	d	2000	GSP	C5-C4	2.97	1.47	1.40
5	P	2000	GSP	PG-S1G	2.99	1.96	1.90
5	B	2000	GSP	PG-O2G	3.00	1.65	1.55
5	X	2000	GSP	C5-C4	3.00	1.47	1.40
5	Z	2000	GSP	C5-C4	3.00	1.47	1.40
5	h	2000	GSP	C5-C4	3.11	1.47	1.40
5	h	2000	GSP	PG-S1G	3.12	1.96	1.90
5	T	2000	GSP	C5-C4	3.15	1.47	1.40
5	D	2000	GSP	PG-S1G	3.17	1.96	1.90
5	R	2000	GSP	C5-C4	3.20	1.47	1.40
5	J	2000	GSP	C5-C4	3.35	1.48	1.40
5	B	2000	GSP	PG-S1G	3.39	1.97	1.90
5	D	2000	GSP	C5-C4	3.40	1.48	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	2000	GSP	PG-S1G	3.44	1.97	1.90
5	X	2000	GSP	O4'-C1'	3.48	1.45	1.41
5	N	2000	GSP	C6-C5	3.49	1.48	1.41
5	d	2000	GSP	C6-C5	3.68	1.48	1.41
5	P	2000	GSP	C6-C5	3.70	1.48	1.41
5	R	2000	GSP	C6-C5	3.71	1.48	1.41
5	h	2000	GSP	O4'-C1'	3.72	1.45	1.41
5	Z	2000	GSP	C6-C5	3.78	1.48	1.41
5	h	2000	GSP	C6-C5	3.85	1.48	1.41
5	T	2000	GSP	C6-C5	3.89	1.49	1.41
5	X	2000	GSP	C6-C5	3.89	1.49	1.41
5	B	2000	GSP	C6-C5	3.99	1.49	1.41
5	H	2000	GSP	C6-C5	4.03	1.49	1.41
4	C	2002	093	CAQ-NAR	4.11	1.45	1.33
5	J	2000	GSP	C6-C5	4.11	1.49	1.41
4	I	2002	093	CAQ-NAR	4.13	1.45	1.33
4	A	2002	093	CAQ-NAR	4.14	1.45	1.33
4	Y	2002	093	CAQ-NAR	4.14	1.45	1.33
4	G	2002	093	CAQ-NAR	4.15	1.45	1.33
4	c	2002	093	CAQ-NAR	4.16	1.45	1.33
4	M	2002	093	CAQ-NAR	4.16	1.45	1.33
4	g	2002	093	CAQ-NAR	4.16	1.45	1.33
4	O	2002	093	CAQ-NAR	4.17	1.45	1.33
4	W	2002	093	CAQ-NAR	4.17	1.45	1.33
4	S	2002	093	CAQ-NAR	4.18	1.45	1.33
4	Q	2002	093	CAQ-NAR	4.19	1.45	1.33
5	D	2000	GSP	C6-C5	4.20	1.49	1.41
4	g	2002	093	SAN-NAU	4.66	1.67	1.61
4	A	2002	093	SAN-NAU	4.69	1.67	1.61
4	S	2002	093	SAN-NAU	4.71	1.67	1.61
4	I	2002	093	SAN-NAU	4.72	1.67	1.61
4	C	2002	093	SAN-NAU	4.75	1.67	1.61
4	Q	2002	093	SAN-NAU	4.76	1.67	1.61
4	W	2002	093	SAN-NAU	4.77	1.67	1.61
4	O	2002	093	SAN-NAU	4.78	1.67	1.61
4	M	2002	093	SAN-NAU	4.78	1.67	1.61
4	Y	2002	093	SAN-NAU	4.78	1.67	1.61
4	G	2002	093	SAN-NAU	4.78	1.67	1.61
4	c	2002	093	SAN-NAU	4.81	1.67	1.61

All (242) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	2002	093	OAQ-SAN-OAM	-18.87	94.51	119.54
4	g	2002	093	OAQ-SAN-OAM	-18.85	94.53	119.54
4	Q	2002	093	OAQ-SAN-OAM	-18.84	94.55	119.54
4	G	2002	093	OAQ-SAN-OAM	-18.83	94.56	119.54
4	C	2002	093	OAQ-SAN-OAM	-18.83	94.56	119.54
4	A	2002	093	OAQ-SAN-OAM	-18.83	94.57	119.54
4	I	2002	093	OAQ-SAN-OAM	-18.82	94.57	119.54
4	Y	2002	093	OAQ-SAN-OAM	-18.82	94.58	119.54
4	M	2002	093	OAQ-SAN-OAM	-18.82	94.58	119.54
4	W	2002	093	OAQ-SAN-OAM	-18.81	94.59	119.54
4	O	2002	093	OAQ-SAN-OAM	-18.80	94.60	119.54
4	c	2002	093	OAQ-SAN-OAM	-18.79	94.61	119.54
5	T	2000	GSP	PB-O3B-PG	-5.77	113.31	132.67
5	H	2000	GSP	PB-O3B-PG	-5.50	114.24	132.67
5	N	2000	GSP	PB-O3B-PG	-5.46	114.37	132.67
5	d	2000	GSP	PB-O3B-PG	-5.42	114.48	132.67
5	R	2000	GSP	PB-O3B-PG	-5.42	114.50	132.67
5	J	2000	GSP	PB-O3B-PG	-5.35	114.73	132.67
5	Z	2000	GSP	PB-O3B-PG	-5.29	114.93	132.67
5	D	2000	GSP	PB-O3B-PG	-5.22	115.17	132.67
5	B	2000	GSP	PB-O3B-PG	-5.20	115.24	132.67
5	X	2000	GSP	PB-O3B-PG	-5.09	115.60	132.67
5	P	2000	GSP	PB-O3B-PG	-5.05	115.73	132.67
5	J	2000	GSP	C4-C5-N7	-4.95	104.93	109.48
5	J	2000	GSP	C5-C6-N1	-4.90	116.89	123.59
5	h	2000	GSP	PB-O3B-PG	-4.87	116.34	132.67
5	D	2000	GSP	C4-C5-N7	-4.62	105.22	109.48
5	B	2000	GSP	C4-C5-N7	-4.59	105.26	109.48
5	N	2000	GSP	PA-O3A-PB	-4.48	120.16	132.73
5	T	2000	GSP	C5-C6-N1	-4.46	117.49	123.59
5	N	2000	GSP	C5-C6-N1	-4.44	117.52	123.59
5	Z	2000	GSP	C5-C6-N1	-4.43	117.53	123.59
5	D	2000	GSP	C5-C6-N1	-4.37	117.61	123.59
5	H	2000	GSP	PA-O3A-PB	-4.30	120.64	132.73
5	B	2000	GSP	PA-O3A-PB	-4.28	120.71	132.73
5	R	2000	GSP	C5-C6-N1	-4.26	117.76	123.59
5	H	2000	GSP	C4-C5-N7	-4.25	105.57	109.48
5	P	2000	GSP	PA-O3A-PB	-4.12	121.16	132.73
5	P	2000	GSP	C5-C6-N1	-4.01	118.11	123.59
5	H	2000	GSP	C5-C6-N1	-4.00	118.11	123.59
5	D	2000	GSP	PA-O3A-PB	-4.00	121.49	132.73
5	d	2000	GSP	PA-O3A-PB	-4.00	121.49	132.73
5	R	2000	GSP	PA-O3A-PB	-3.87	121.87	132.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	h	2000	GSP	C4-C5-N7	-3.87	105.92	109.48
5	X	2000	GSP	PA-O3A-PB	-3.85	121.92	132.73
5	T	2000	GSP	PA-O3A-PB	-3.83	121.97	132.73
5	h	2000	GSP	PA-O3A-PB	-3.79	122.09	132.73
5	Z	2000	GSP	PA-O3A-PB	-3.73	122.25	132.73
5	d	2000	GSP	C5-C6-N1	-3.73	118.49	123.59
5	J	2000	GSP	PA-O3A-PB	-3.72	122.28	132.73
5	d	2000	GSP	C6-C5-C4	-3.69	116.48	120.90
5	B	2000	GSP	C5-C6-N1	-3.61	118.65	123.59
5	d	2000	GSP	C2'-C1'-N9	-3.61	108.78	114.29
5	Z	2000	GSP	C4-C5-N7	-3.54	106.22	109.48
5	X	2000	GSP	C6-C5-C4	-3.48	116.74	120.90
5	R	2000	GSP	O3A-PA-O5'	-3.45	93.78	102.94
5	X	2000	GSP	C5-C6-N1	-3.41	118.92	123.59
5	T	2000	GSP	C4-C5-N7	-3.40	106.35	109.48
5	X	2000	GSP	C4-C5-N7	-3.40	106.35	109.48
5	h	2000	GSP	C5-C6-N1	-3.34	119.02	123.59
5	P	2000	GSP	C2'-C1'-N9	-3.32	109.21	114.29
5	P	2000	GSP	C6-C5-C4	-3.31	116.95	120.90
5	h	2000	GSP	C6-C5-C4	-3.30	116.95	120.90
5	N	2000	GSP	C6-C5-C4	-3.28	116.98	120.90
5	P	2000	GSP	C4-C5-N7	-3.27	106.47	109.48
5	d	2000	GSP	C4-C5-N7	-3.23	106.51	109.48
4	g	2002	093	OAX-CAW-CAV	-3.09	99.44	111.64
4	A	2002	093	OAX-CAW-CAV	-3.09	99.45	111.64
4	G	2002	093	OAX-CAW-CAV	-3.08	99.46	111.64
4	W	2002	093	OAX-CAW-CAV	-3.08	99.47	111.64
4	c	2002	093	OAX-CAW-CAV	-3.08	99.47	111.64
4	O	2002	093	OAX-CAW-CAV	-3.08	99.49	111.64
4	Q	2002	093	OAX-CAW-CAV	-3.08	99.49	111.64
4	M	2002	093	OAX-CAW-CAV	-3.08	99.49	111.64
4	S	2002	093	OAX-CAW-CAV	-3.07	99.51	111.64
4	C	2002	093	OAX-CAW-CAV	-3.07	99.52	111.64
4	Y	2002	093	OAX-CAW-CAV	-3.07	99.53	111.64
4	I	2002	093	OAX-CAW-CAV	-3.05	99.60	111.64
5	d	2000	GSP	O3A-PA-O5'	-3.02	94.92	102.94
5	h	2000	GSP	N3-C2-N1	-2.99	122.89	127.44
5	R	2000	GSP	C6-C5-C4	-2.97	117.35	120.90
5	N	2000	GSP	C1'-N9-C4	-2.90	122.56	126.94
5	Z	2000	GSP	C6-C5-C4	-2.90	117.43	120.90
5	R	2000	GSP	N3-C2-N1	-2.88	123.05	127.44
5	d	2000	GSP	C1'-N9-C4	-2.81	122.71	126.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	2000	GSP	C4-C5-N7	-2.80	106.91	109.48
5	B	2000	GSP	C6-C5-C4	-2.80	117.56	120.90
4	c	2002	093	OAL-CAS-NAR	-2.79	118.23	123.68
5	D	2000	GSP	O3A-PA-O5'	-2.79	95.54	102.94
5	P	2000	GSP	C1'-N9-C4	-2.79	122.73	126.94
4	G	2002	093	OAL-CAS-NAR	-2.79	118.25	123.68
4	S	2002	093	OAL-CAS-NAR	-2.79	118.25	123.68
4	O	2002	093	OAL-CAS-NAR	-2.78	118.26	123.68
4	g	2002	093	OAL-CAS-NAR	-2.77	118.27	123.68
4	C	2002	093	OAL-CAS-NAR	-2.77	118.28	123.68
4	A	2002	093	OAL-CAS-NAR	-2.77	118.28	123.68
4	W	2002	093	OAL-CAS-NAR	-2.76	118.29	123.68
4	I	2002	093	OAL-CAS-NAR	-2.76	118.30	123.68
4	M	2002	093	OAL-CAS-NAR	-2.76	118.30	123.68
4	Q	2002	093	OAL-CAS-NAR	-2.74	118.33	123.68
4	Y	2002	093	OAL-CAS-NAR	-2.74	118.33	123.68
5	N	2000	GSP	C2'-C1'-N9	-2.74	110.11	114.29
5	H	2000	GSP	O3A-PA-O5'	-2.73	95.69	102.94
5	d	2000	GSP	N3-C2-N1	-2.64	123.42	127.44
5	T	2000	GSP	C6-C5-C4	-2.57	117.83	120.90
5	H	2000	GSP	C6-C5-C4	-2.57	117.83	120.90
5	J	2000	GSP	C2'-C1'-N9	-2.56	110.38	114.29
5	Z	2000	GSP	C2'-C1'-N9	-2.53	110.42	114.29
5	X	2000	GSP	C2'-C1'-N9	-2.53	110.43	114.29
5	T	2000	GSP	C2'-C1'-N9	-2.50	110.48	114.29
5	X	2000	GSP	N3-C2-N1	-2.49	123.65	127.44
5	D	2000	GSP	N3-C2-N1	-2.48	123.66	127.44
5	R	2000	GSP	C4-C5-N7	-2.48	107.19	109.48
5	D	2000	GSP	C6-C5-C4	-2.44	117.98	120.90
5	J	2000	GSP	N3-C2-N1	-2.33	123.90	127.44
5	N	2000	GSP	C4'-O4'-C1'	-2.32	107.17	109.72
5	J	2000	GSP	O3A-PA-O5'	-2.26	96.95	102.94
5	J	2000	GSP	C6-C5-C4	-2.22	118.25	120.90
5	N	2000	GSP	N3-C2-N1	-2.19	124.11	127.44
5	B	2000	GSP	O3A-PA-O5'	-2.15	97.22	102.94
5	H	2000	GSP	N3-C2-N1	-2.14	124.19	127.44
4	Q	2002	093	CAF-SAN-NAU	-2.13	105.07	107.92
4	S	2002	093	CAF-SAN-NAU	-2.12	105.08	107.92
4	c	2002	093	CAF-SAN-NAU	-2.12	105.08	107.92
4	Y	2002	093	CAF-SAN-NAU	-2.12	105.08	107.92
4	C	2002	093	CAF-SAN-NAU	-2.11	105.09	107.92
4	O	2002	093	CAF-SAN-NAU	-2.11	105.10	107.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	W	2002	093	CAF-SAN-NAU	-2.11	105.10	107.92
4	W	2002	093	CAH-CAG-CAF	-2.10	118.24	120.77
4	M	2002	093	CAF-SAN-NAU	-2.10	105.11	107.92
4	S	2002	093	CAH-CAG-CAF	-2.09	118.25	120.77
4	G	2002	093	CAF-SAN-NAU	-2.09	105.12	107.92
4	g	2002	093	CAF-SAN-NAU	-2.09	105.13	107.92
4	A	2002	093	CAH-CAG-CAF	-2.08	118.25	120.77
4	I	2002	093	CAF-SAN-NAU	-2.08	105.13	107.92
4	G	2002	093	CAH-CAG-CAF	-2.08	118.26	120.77
4	A	2002	093	CAF-SAN-NAU	-2.08	105.14	107.92
4	Q	2002	093	CAH-CAG-CAF	-2.06	118.28	120.77
4	O	2002	093	CAH-CAG-CAF	-2.06	118.29	120.77
4	I	2002	093	CAH-CAG-CAF	-2.05	118.29	120.77
4	g	2002	093	CAH-CAG-CAF	-2.05	118.30	120.77
4	M	2002	093	CAH-CAG-CAF	-2.05	118.30	120.77
4	Y	2002	093	CAH-CAG-CAF	-2.04	118.31	120.77
4	c	2002	093	CAH-CAG-CAF	-2.02	118.33	120.77
5	P	2000	GSP	N3-C2-N1	-2.02	124.37	127.44
5	h	2000	GSP	C2'-C1'-N9	-2.02	111.21	114.29
5	T	2000	GSP	C2'-C3'-C4'	2.01	106.75	102.61
5	h	2000	GSP	O2B-PB-O1B	2.02	123.50	112.53
5	Z	2000	GSP	C2'-C3'-C4'	2.03	106.79	102.61
5	D	2000	GSP	O2B-PB-O1B	2.05	123.64	112.53
5	X	2000	GSP	O2B-PB-O1B	2.06	123.67	112.53
5	P	2000	GSP	O2B-PB-O1B	2.07	123.72	112.53
5	J	2000	GSP	O2B-PB-O1B	2.08	123.78	112.53
5	N	2000	GSP	O2B-PB-O1B	2.09	123.86	112.53
5	d	2000	GSP	C2'-C3'-C4'	2.21	107.15	102.61
5	D	2000	GSP	C2'-C3'-C4'	2.22	107.17	102.61
5	h	2000	GSP	C2'-C3'-C4'	2.72	108.19	102.61
5	X	2000	GSP	C2'-C3'-C4'	2.93	108.63	102.61
4	A	2002	093	CAD-CAH-CAG	2.99	122.13	118.17
4	G	2002	093	CAD-CAH-CAG	2.99	122.14	118.17
4	Q	2002	093	CAD-CAH-CAG	3.01	122.16	118.17
4	W	2002	093	CAD-CAH-CAG	3.02	122.18	118.17
4	S	2002	093	CAD-CAH-CAG	3.04	122.19	118.17
4	Y	2002	093	CAD-CAH-CAG	3.04	122.20	118.17
4	I	2002	093	CAD-CAH-CAG	3.04	122.20	118.17
4	O	2002	093	CAD-CAH-CAG	3.04	122.21	118.17
4	C	2002	093	CAD-CAH-CAG	3.05	122.21	118.17
4	g	2002	093	CAD-CAH-CAG	3.05	122.22	118.17
4	c	2002	093	CAD-CAH-CAG	3.06	122.23	118.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	2002	093	CAD-CAH-CAG	3.08	122.25	118.17
5	B	2000	GSP	C6-N1-C2	3.34	120.58	115.94
4	O	2002	093	CAT-CAS-NAR	3.80	120.90	114.91
4	M	2002	093	CAT-CAS-NAR	3.80	120.90	114.91
5	H	2000	GSP	C6-N1-C2	3.80	121.22	115.94
4	Q	2002	093	CAT-CAS-NAR	3.81	120.91	114.91
4	c	2002	093	CAT-CAS-NAR	3.83	120.94	114.91
4	S	2002	093	CAT-CAS-NAR	3.83	120.94	114.91
4	g	2002	093	CAT-CAS-NAR	3.83	120.95	114.91
4	Y	2002	093	CAT-CAS-NAR	3.84	120.96	114.91
4	I	2002	093	CAT-CAS-NAR	3.85	120.98	114.91
4	A	2002	093	OAO-SAN-CAF	3.85	113.98	107.63
4	W	2002	093	CAT-CAS-NAR	3.85	120.98	114.91
4	A	2002	093	CAT-CAS-NAR	3.85	120.98	114.91
4	c	2002	093	OAO-SAN-CAF	3.85	113.98	107.63
4	I	2002	093	OAO-SAN-CAF	3.86	113.99	107.63
4	g	2002	093	OAO-SAN-CAF	3.86	114.00	107.63
4	G	2002	093	CAT-CAS-NAR	3.86	121.00	114.91
4	C	2002	093	CAT-CAS-NAR	3.87	121.00	114.91
4	G	2002	093	OAO-SAN-CAF	3.87	114.01	107.63
4	S	2002	093	OAM-SAN-CAF	3.87	114.01	107.63
4	Q	2002	093	OAM-SAN-CAF	3.87	114.02	107.63
4	W	2002	093	OAO-SAN-CAF	3.88	114.02	107.63
5	X	2000	GSP	C6-N1-C2	3.89	121.33	115.94
4	M	2002	093	OAO-SAN-CAF	3.89	114.03	107.63
4	A	2002	093	OAM-SAN-CAF	3.89	114.03	107.63
4	W	2002	093	OAM-SAN-CAF	3.89	114.04	107.63
4	g	2002	093	OAM-SAN-CAF	3.89	114.04	107.63
4	C	2002	093	OAO-SAN-CAF	3.89	114.05	107.63
4	O	2002	093	OAM-SAN-CAF	3.89	114.05	107.63
4	Y	2002	093	OAO-SAN-CAF	3.90	114.05	107.63
4	O	2002	093	OAO-SAN-CAF	3.90	114.05	107.63
4	S	2002	093	OAO-SAN-CAF	3.90	114.05	107.63
4	Q	2002	093	OAO-SAN-CAF	3.90	114.05	107.63
5	P	2000	GSP	C6-N1-C2	3.90	121.35	115.94
4	G	2002	093	OAM-SAN-CAF	3.90	114.06	107.63
4	Y	2002	093	OAM-SAN-CAF	3.91	114.07	107.63
4	I	2002	093	OAM-SAN-CAF	3.91	114.08	107.63
4	M	2002	093	OAM-SAN-CAF	3.92	114.09	107.63
4	c	2002	093	OAM-SAN-CAF	3.94	114.13	107.63
4	C	2002	093	OAM-SAN-CAF	3.95	114.14	107.63
5	Z	2000	GSP	C6-N1-C2	3.99	121.48	115.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	h	2000	GSP	C6-N1-C2	4.07	121.58	115.94
5	d	2000	GSP	C6-N1-C2	4.15	121.69	115.94
5	T	2000	GSP	C6-N1-C2	4.16	121.72	115.94
5	D	2000	GSP	C6-N1-C2	4.26	121.85	115.94
5	N	2000	GSP	C6-N1-C2	4.33	121.94	115.94
4	O	2002	093	OAM-SAN-NAU	4.45	114.18	107.03
4	Y	2002	093	OAM-SAN-NAU	4.45	114.18	107.03
4	C	2002	093	OAM-SAN-NAU	4.46	114.20	107.03
4	c	2002	093	OAM-SAN-NAU	4.46	114.20	107.03
5	J	2000	GSP	C6-N1-C2	4.47	122.14	115.94
4	M	2002	093	OAM-SAN-NAU	4.47	114.21	107.03
4	G	2002	093	OAM-SAN-NAU	4.49	114.24	107.03
4	W	2002	093	OAM-SAN-NAU	4.49	114.25	107.03
4	I	2002	093	OAM-SAN-NAU	4.50	114.26	107.03
4	A	2002	093	OAM-SAN-NAU	4.50	114.26	107.03
4	Q	2002	093	OAM-SAN-NAU	4.51	114.27	107.03
4	S	2002	093	OAM-SAN-NAU	4.51	114.28	107.03
4	g	2002	093	OAM-SAN-NAU	4.54	114.32	107.03
5	R	2000	GSP	C6-N1-C2	4.69	122.44	115.94
4	I	2002	093	OAO-SAN-NAU	5.00	115.07	107.03
4	C	2002	093	OAO-SAN-NAU	5.00	115.07	107.03
4	M	2002	093	OAO-SAN-NAU	5.01	115.08	107.03
4	g	2002	093	OAO-SAN-NAU	5.01	115.08	107.03
4	c	2002	093	OAO-SAN-NAU	5.02	115.10	107.03
4	G	2002	093	OAO-SAN-NAU	5.03	115.11	107.03
4	W	2002	093	OAO-SAN-NAU	5.03	115.11	107.03
4	A	2002	093	OAO-SAN-NAU	5.04	115.12	107.03
4	O	2002	093	OAO-SAN-NAU	5.04	115.13	107.03
4	Y	2002	093	OAO-SAN-NAU	5.05	115.15	107.03
4	Q	2002	093	OAO-SAN-NAU	5.05	115.15	107.03
4	S	2002	093	OAO-SAN-NAU	5.07	115.18	107.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2000	GSP	6	0
5	D	2000	GSP	11	0
5	H	2000	GSP	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	2000	GSP	4	0
5	N	2000	GSP	6	0
5	P	2000	GSP	7	0
5	R	2000	GSP	5	0
5	T	2000	GSP	5	0
5	X	2000	GSP	6	0
5	Z	2000	GSP	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	470/566 (83%)	-0.07	6 (1%) 79 73	95, 212, 331, 500	0
1	C	470/566 (83%)	0.58	53 (11%) 7 12	126, 300, 456, 500	0
1	G	470/566 (83%)	-0.05	10 (2%) 67 62	98, 214, 342, 500	0
1	I	470/566 (83%)	0.65	62 (13%) 4 10	124, 306, 474, 500	0
1	M	470/566 (83%)	-0.02	13 (2%) 56 52	95, 217, 341, 500	0
1	O	470/566 (83%)	-0.03	13 (2%) 56 52	102, 208, 335, 500	0
1	Q	470/566 (83%)	0.10	21 (4%) 37 36	102, 247, 364, 498	0
1	S	470/566 (83%)	0.11	17 (3%) 46 43	114, 251, 389, 500	0
1	W	470/566 (83%)	0.14	11 (2%) 64 59	99, 253, 387, 500	0
1	Y	470/566 (83%)	-0.07	11 (2%) 64 59	115, 250, 365, 474	0
1	c	470/566 (83%)	0.38	40 (8%) 13 17	119, 305, 478, 500	0
1	g	470/566 (83%)	0.27	24 (5%) 32 31	126, 268, 416, 500	0
2	B	173/219 (78%)	0.12	5 (2%) 55 50	94, 201, 375, 493	0
2	D	173/219 (78%)	0.05	1 (0%) 90 87	95, 220, 341, 488	0
2	H	173/219 (78%)	0.15	4 (2%) 64 59	94, 207, 382, 499	0
2	J	173/219 (78%)	0.05	2 (1%) 81 75	92, 198, 338, 500	0
2	N	173/219 (78%)	0.59	14 (8%) 15 18	137, 282, 424, 496	0
2	P	173/219 (78%)	0.65	16 (9%) 11 15	132, 277, 432, 496	0
2	R	173/219 (78%)	0.74	22 (12%) 5 10	139, 269, 415, 496	0
2	T	173/219 (78%)	0.61	19 (10%) 7 12	136, 266, 407, 493	0
2	X	173/219 (78%)	0.45	16 (9%) 11 15	146, 282, 453, 500	0
2	Z	173/219 (78%)	0.62	20 (11%) 6 11	165, 262, 362, 494	0
2	d	173/219 (78%)	0.91	28 (16%) 3 8	146, 308, 447, 500	0
2	h	173/219 (78%)	0.55	18 (10%) 8 13	158, 294, 440, 500	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
3	E	41/48 (85%)	0.02	0	100	100	153, 251, 365, 489	0
3	F	32/48 (66%)	-0.46	0	100	100	169, 285, 399, 466	0
3	K	41/48 (85%)	0.05	0	100	100	131, 240, 410, 465	0
3	L	32/48 (66%)	-0.45	0	100	100	170, 263, 384, 436	0
3	U	41/48 (85%)	0.19	0	100	100	175, 284, 408, 494	0
3	V	32/48 (66%)	-0.47	0	100	100	170, 260, 403, 435	0
3	a	41/48 (85%)	-0.08	0	100	100	195, 318, 423, 476	0
3	b	32/48 (66%)	-0.22	0	100	100	213, 309, 428, 479	0
3	e	41/48 (85%)	0.09	0	100	100	175, 255, 384, 478	0
3	f	32/48 (66%)	-0.48	0	100	100	194, 288, 337, 363	0
3	i	41/48 (85%)	0.08	1 (2%)	62	57	202, 325, 441, 500	0
3	j	32/48 (66%)	-0.20	0	100	100	194, 282, 404, 462	0
All	All	8154/9996 (81%)	0.22	447 (5%)	29	29	92, 255, 416, 500	0

All (447) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	382	TYR	6.1
1	g	515	ALA	6.0
2	H	46	VAL	5.7
1	I	513	PRO	5.5
1	M	513	PRO	5.4
2	B	45	GLY	5.4
1	W	515	ALA	5.3
1	c	375	ASN	5.3
1	c	306	ARG	5.2
2	h	102	VAL	5.0
1	I	514	SER	5.0
1	O	517	ALA	4.9
2	X	102	VAL	4.9
1	I	515	ALA	4.9
1	W	350	ALA	4.8
1	A	513	PRO	4.8
1	G	513	PRO	4.8
2	B	46	VAL	4.7
2	H	45	GLY	4.6
1	C	367	PRO	4.6
1	C	513	PRO	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	T	152	GLU	4.5
1	I	367	PRO	4.5
1	C	526	VAL	4.5
2	P	12	PHE	4.5
1	G	514	SER	4.4
1	c	695	LEU	4.4
2	d	102	VAL	4.4
2	R	123	GLY	4.4
1	I	784	SER	4.3
2	X	6	ASP	4.3
1	I	381	PRO	4.3
1	C	514	SER	4.3
1	c	376	SER	4.3
2	N	170	THR	4.3
2	h	103	GLU	4.2
1	g	380	ALA	4.2
1	I	703	MET	4.2
2	R	124	ASN	4.2
1	I	526	VAL	4.2
1	g	350	ALA	4.1
2	Z	73	TYR	4.1
1	W	514	SER	4.1
1	g	405	GLU	4.1
1	A	514	SER	4.1
1	C	366	VAL	4.1
2	R	152	GLU	4.1
2	d	170	THR	4.0
2	T	123	GLY	4.0
1	I	523	GLN	4.0
1	g	682	SER	4.0
2	Z	52	SER	4.0
2	X	103	GLU	3.9
1	g	382	TYR	3.9
1	I	366	VAL	3.9
2	d	45	GLY	3.9
1	g	516	VAL	3.9
1	C	703	MET	3.9
1	C	401	ALA	3.9
1	C	517	ALA	3.9
2	d	91	TYR	3.9
1	C	387	GLU	3.8
1	S	513	PRO	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	d	67	THR	3.8
1	I	372	VAL	3.8
1	I	401	ALA	3.8
1	I	371	ALA	3.7
1	I	387	GLU	3.7
1	M	515	ALA	3.7
2	Z	45	GLY	3.7
2	d	137	ASP	3.7
2	R	52	SER	3.7
2	T	52	SER	3.6
2	T	50	THR	3.6
1	c	378	ASP	3.6
2	h	166	GLN	3.6
1	W	513	PRO	3.6
1	c	351	ARG	3.6
1	I	682	SER	3.6
1	S	703	MET	3.5
2	X	52	SER	3.5
1	O	516	VAL	3.5
2	T	46	VAL	3.5
1	C	382	TYR	3.5
1	C	523	GLN	3.5
2	R	91	TYR	3.5
1	c	353	TRP	3.5
1	c	206	ILE	3.5
2	R	46	VAL	3.4
1	I	577	PRO	3.4
1	I	539	PRO	3.4
1	C	535	TYR	3.4
2	P	62	ALA	3.4
1	G	702	VAL	3.4
1	C	784	SER	3.4
1	g	517	ALA	3.4
1	I	548	VAL	3.4
2	D	69	GLY	3.4
2	d	62	ALA	3.4
1	C	515	ALA	3.4
1	C	373	VAL	3.3
1	I	324	LEU	3.4
2	N	150	PHE	3.3
1	Q	703	MET	3.3
1	W	682	SER	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	537	HIS	3.3
1	g	548	VAL	3.3
2	N	50	THR	3.2
2	h	170	THR	3.2
1	M	517	ALA	3.2
1	M	516	VAL	3.2
1	G	703	MET	3.2
1	M	514	SER	3.2
1	S	221	SER	3.2
1	S	514	SER	3.2
2	R	50	THR	3.1
1	c	696	THR	3.1
1	g	610	GLN	3.1
2	R	56	ASP	3.1
2	N	49	ALA	3.1
1	O	513	PRO	3.1
1	Y	375	ASN	3.1
2	X	12	PHE	3.1
1	Q	702	VAL	3.1
2	Z	51	ARG	3.1
1	I	370	GLN	3.0
1	W	516	VAL	3.0
1	G	682	SER	3.0
1	C	522	TRP	3.0
1	C	516	VAL	3.0
2	Z	77	THR	3.0
1	I	672	HIS	3.0
1	c	326	THR	3.0
1	Y	306	ARG	3.0
1	C	349	PRO	3.0
1	Q	513	PRO	3.0
2	T	124	ASN	3.0
1	c	705	GLY	2.9
2	d	60	ILE	2.9
2	Z	53	ILE	2.9
1	O	519	LYS	2.9
1	g	370	GLN	2.9
2	R	122	VAL	2.9
1	I	516	VAL	2.9
1	I	380	ALA	2.9
1	Q	514	SER	2.9
1	Q	577	PRO	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	g	513	PRO	2.9
2	N	12	PHE	2.9
1	C	707	ASP	2.9
1	c	718	MET	2.9
1	W	373	VAL	2.9
1	C	682	SER	2.9
1	I	522	TRP	2.9
1	I	541	TRP	2.8
2	T	153	THR	2.8
1	M	334	THR	2.8
1	S	373	VAL	2.8
1	Y	693	PHE	2.8
2	d	46	VAL	2.8
1	I	369	THR	2.8
1	I	578	LEU	2.8
1	I	629	GLU	2.8
1	g	373	VAL	2.8
1	c	183	TYR	2.8
1	I	537	HIS	2.8
1	S	635	GLN	2.8
1	g	358	GLY	2.8
1	I	783	ARG	2.8
2	X	77	THR	2.8
2	Z	9	ASP	2.8
2	d	136	THR	2.8
2	B	67	THR	2.8
1	g	514	SER	2.8
2	H	91	TYR	2.8
2	Z	46	VAL	2.7
1	Q	364	VAL	2.7
1	C	704	GLY	2.7
2	T	120	MET	2.7
1	g	406	ASN	2.7
2	X	45	GLY	2.7
1	C	372	VAL	2.7
2	Z	170	THR	2.7
2	h	169	LEU	2.7
1	S	364	VAL	2.7
2	X	85	VAL	2.7
2	d	52	SER	2.7
2	T	122	VAL	2.7
1	I	535	TYR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	c	350	ALA	2.7
1	Y	694	LYS	2.7
2	R	71	GLU	2.7
1	S	371	ALA	2.7
1	c	694	LYS	2.7
1	A	364	VAL	2.7
1	C	711	PHE	2.7
2	R	57	GLY	2.7
1	c	364	VAL	2.7
1	I	517	ALA	2.7
1	I	373	VAL	2.7
2	R	153	THR	2.7
1	I	326	THR	2.6
1	W	351	ARG	2.6
1	C	548	VAL	2.6
1	g	369	THR	2.6
2	T	91	TYR	2.6
1	c	400	PRO	2.6
2	X	106	LEU	2.6
2	d	173	TYR	2.6
1	Q	578	LEU	2.6
1	O	518	LEU	2.6
1	M	371	ALA	2.6
2	h	12	PHE	2.6
2	J	69	GLY	2.6
1	c	711	PHE	2.6
2	P	174	ARG	2.6
1	W	358	GLY	2.6
1	g	578	LEU	2.6
2	h	150	PHE	2.6
1	c	204	GLN	2.6
2	R	151	ILE	2.6
2	d	174	ARG	2.6
1	S	623	HIS	2.6
2	B	92	ASP	2.6
2	h	137	ASP	2.6
1	C	527	ARG	2.5
1	I	674	ASP	2.5
2	d	12	PHE	2.5
2	d	16	LEU	2.5
2	T	62	ALA	2.5
1	C	368	HIS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	d	15	VAL	2.5
1	Q	531	GLU	2.5
1	c	719	LEU	2.5
2	T	51	ARG	2.5
1	S	515	ALA	2.5
1	I	363	VAL	2.5
1	I	720	GLN	2.5
1	I	699	PHE	2.5
1	I	644	GLY	2.5
2	Z	91	TYR	2.5
1	c	325	ALA	2.5
1	C	371	ALA	2.5
1	O	702	VAL	2.5
1	c	352	VAL	2.5
1	c	774	VAL	2.5
2	Z	169	LEU	2.5
2	Z	12	PHE	2.5
1	W	578	LEU	2.4
2	h	53	ILE	2.4
2	h	52	SER	2.4
1	G	395	ASP	2.4
2	Z	67	THR	2.4
1	I	325	ALA	2.4
2	h	106	LEU	2.4
1	Q	324	LEU	2.4
1	c	327	LEU	2.4
2	P	52	SER	2.4
1	S	324	LEU	2.4
1	g	351	ARG	2.4
2	h	46	VAL	2.4
1	Y	350	ALA	2.4
1	C	531	GLU	2.4
1	c	377	LYS	2.4
1	I	707	ASP	2.4
2	h	61	LYS	2.4
1	C	629	GLU	2.4
1	I	704	GLY	2.4
1	Y	376	SER	2.4
1	M	370	GLN	2.4
2	d	53	ILE	2.4
2	N	10	TYR	2.4
1	C	630	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	364	VAL	2.4
1	I	630	ALA	2.4
1	Q	623	HIS	2.4
1	c	373	VAL	2.4
1	C	549	LYS	2.4
1	O	372	VAL	2.4
1	c	184	ILE	2.4
2	Z	59	THR	2.4
2	P	53	ILE	2.4
1	Q	362	HIS	2.4
1	I	717	LEU	2.3
1	Q	371	ALA	2.3
2	d	88	LEU	2.3
2	h	136	THR	2.3
1	I	368	HIS	2.3
1	C	365	ARG	2.3
1	c	401	ALA	2.3
2	N	53	ILE	2.3
1	I	549	LYS	2.3
2	d	105	TRP	2.3
1	I	714	TYR	2.3
1	Q	361	HIS	2.3
2	X	170	THR	2.3
1	G	404	PRO	2.3
2	d	10	TYR	2.3
2	P	6	ASP	2.3
2	P	82	ARG	2.3
1	C	695	LEU	2.3
1	W	382	TYR	2.3
2	P	60	ILE	2.3
1	c	743	SER	2.3
2	P	63	GLN	2.3
2	N	174	ARG	2.3
1	g	702	VAL	2.3
2	R	58	LYS	2.3
1	c	324	LEU	2.3
2	P	170	THR	2.3
2	h	45	GLY	2.3
1	I	711	PHE	2.3
1	C	623	HIS	2.3
2	Z	10	TYR	2.3
1	C	710	MET	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	R	150	PHE	2.3
2	X	169	LEU	2.3
1	C	370	GLN	2.2
1	S	702	VAL	2.2
1	M	518	LEU	2.2
1	c	784	SER	2.2
1	I	400	PRO	2.2
2	Z	62	ALA	2.2
1	I	365	ARG	2.2
1	C	320	ILE	2.2
2	R	59	THR	2.2
1	C	221	SER	2.2
1	Y	351	ARG	2.2
2	R	149	SER	2.2
2	Z	54	GLN	2.2
1	O	331	GLU	2.2
1	C	342	SER	2.2
1	c	783	ARG	2.2
2	T	151	ILE	2.2
1	A	702	VAL	2.2
1	C	341	LEU	2.2
1	c	187	ASP	2.2
1	Q	539	PRO	2.2
1	Y	513	PRO	2.2
2	B	91	TYR	2.2
1	Q	406	ASN	2.2
2	h	60	ILE	2.2
1	Y	364	VAL	2.2
1	O	334	THR	2.2
1	M	702	VAL	2.2
1	c	744	GLN	2.2
2	T	63	GLN	2.2
2	R	61	LYS	2.2
2	Z	60	ILE	2.2
1	S	578	LEU	2.2
2	N	11	LEU	2.2
2	d	68	ALA	2.2
1	Q	640	GLN	2.2
2	Z	118	VAL	2.2
2	N	91	TYR	2.2
2	d	93	ILE	2.2
1	I	321	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	h	54	GLN	2.2
1	C	364	VAL	2.2
1	I	329	THR	2.2
2	X	53	ILE	2.2
1	g	627	THR	2.2
2	P	71	GLU	2.2
1	Y	380	ALA	2.1
2	T	61	LYS	2.1
1	C	744	GLN	2.1
1	C	706	LEU	2.1
2	N	151	ILE	2.1
1	I	710	MET	2.1
1	c	703	MET	2.1
1	c	715	LYS	2.1
1	C	350	ALA	2.1
2	P	150	PHE	2.1
2	R	93	ILE	2.1
1	O	623	HIS	2.1
2	X	166	GLN	2.1
1	I	331	GLU	2.1
2	X	62	ALA	2.1
1	C	538	LEU	2.1
1	Q	221	SER	2.1
1	S	363	VAL	2.1
2	d	59	THR	2.1
1	Y	206	ILE	2.1
2	R	65	TRP	2.1
1	g	364	VAL	2.1
2	Z	124	ASN	2.1
1	I	320	ILE	2.1
2	P	11	LEU	2.1
1	G	515	ALA	2.1
1	M	519	LYS	2.1
1	c	380	ALA	2.1
1	C	775	GLU	2.1
1	g	404	PRO	2.1
2	P	91	TYR	2.1
1	O	707	ASP	2.1
2	T	67	THR	2.1
1	c	185	HIS	2.1
2	T	178	GLN	2.1
1	C	369	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	128	SER	2.1
1	S	352	VAL	2.1
1	g	618	TYR	2.1
1	I	221	SER	2.1
1	C	715	LYS	2.1
1	C	331	GLU	2.1
1	Q	619	PHE	2.1
1	S	321	GLY	2.1
2	d	169	LEU	2.1
1	C	714	TYR	2.1
2	d	103	GLU	2.1
1	Q	321	GLY	2.1
1	Q	373	VAL	2.1
2	P	32	THR	2.1
1	C	705	GLY	2.1
1	I	364	VAL	2.1
1	I	543	LEU	2.1
2	T	45	GLY	2.1
2	N	62	ALA	2.1
1	c	769	GLN	2.1
1	O	337	LEU	2.1
2	H	67	THR	2.1
1	A	703	MET	2.1
2	N	71	GLU	2.1
2	X	137	ASP	2.1
1	M	703	MET	2.0
2	R	45	GLY	2.0
2	N	60	ILE	2.0
2	T	149	SER	2.0
2	d	141	ALA	2.0
2	h	140	ARG	2.0
2	J	178	GLN	2.0
2	d	8	TYR	2.0
1	M	682	SER	2.0
1	I	328	PRO	2.0
2	P	50	THR	2.0
2	X	60	ILE	2.0
1	c	770	LEU	2.0
2	R	11	LEU	2.0
1	I	527	ARG	2.0
1	I	744	GLN	2.0
1	O	371	ALA	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	i	738	ILE	2.0
1	A	373	VAL	2.0
1	Q	515	ALA	2.0
1	S	365	ARG	2.0
2	d	152	GLU	2.0
1	C	541	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	GSP	N	2000	32/32	0.95	0.23	-0.49	97,151,255,301	0
5	GSP	J	2000	32/32	0.94	0.27	-0.50	94,165,285,323	0
5	GSP	h	2000	32/32	0.94	0.24	-0.55	123,249,350,363	0
5	GSP	D	2000	32/32	0.95	0.24	-0.69	110,193,250,272	0
5	GSP	T	2000	32/32	0.93	0.23	-0.71	123,205,238,264	0
5	GSP	R	2000	32/32	0.88	0.22	-0.72	108,197,262,274	0
5	GSP	Z	2000	32/32	0.90	0.21	-0.73	176,212,274,298	0
6	MG	d	2001	1/1	0.76	0.23	-0.77	167,167,167,167	0
5	GSP	P	2000	32/32	0.94	0.22	-0.78	111,168,247,275	0
5	GSP	B	2000	32/32	0.93	0.20	-0.81	141,197,232,249	0
5	GSP	d	2000	32/32	0.83	0.23	-0.88	174,212,349,391	0
5	GSP	H	2000	32/32	0.92	0.18	-0.89	141,183,247,282	0
6	MG	P	2001	1/1	0.93	0.16	-1.16	244,244,244,244	0
5	GSP	X	2000	32/32	0.95	0.20	-1.21	134,226,322,330	0
6	MG	T	2001	1/1	0.99	0.13	-1.24	127,127,127,127	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	J	2001	1/1	0.93	0.13	-1.24	142,142,142,142	0
6	MG	H	2001	1/1	0.94	0.12	-1.25	139,139,139,139	0
6	MG	B	2001	1/1	0.95	0.13	-1.27	159,159,159,159	0
6	MG	N	2001	1/1	0.91	0.12	-1.39	240,240,240,240	0
6	MG	Z	2001	1/1	0.85	0.10	-1.43	178,178,178,178	0
6	MG	R	2001	1/1	0.97	0.09	-1.49	106,106,106,106	0
6	MG	X	2001	1/1	0.89	0.12	-1.60	255,255,255,255	0
6	MG	D	2001	1/1	0.92	0.11	-1.92	64,64,64,64	0
6	MG	h	2001	1/1	0.75	0.12	-1.97	190,190,190,190	0
4	093	I	2002	24/24	-	-	-	60,76,105,130	24
4	093	S	2002	24/24	-	-	-	60,76,105,130	24
4	093	Q	2002	24/24	-	-	-	60,76,105,130	24
4	093	W	2002	24/24	-	-	-	60,76,105,130	24
4	093	G	2002	24/24	-	-	-	60,76,105,130	24
4	093	Y	2002	24/24	-	-	-	60,76,105,130	24
4	093	g	2002	24/24	-	-	-	60,76,105,130	24
4	093	O	2002	24/24	-	-	-	60,76,105,130	24
4	093	A	2002	24/24	-	-	-	60,76,105,130	24
4	093	c	2002	24/24	-	-	-	60,76,105,130	24
4	093	M	2002	24/24	-	-	-	60,76,105,130	24
4	093	C	2002	24/24	-	-	-	60,76,105,130	24

6.5 Other polymers

There are no such residues in this entry.