Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:25 PM GMT

PDB ID	:	4RS5
Title	:	Crystal structure of an uncoating intermediate of a EV71 recombinant virus
Authors	:	Chen, R.; Lyu, K.
Deposited on	:	2014-11-07
Resolution	:	3.81 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

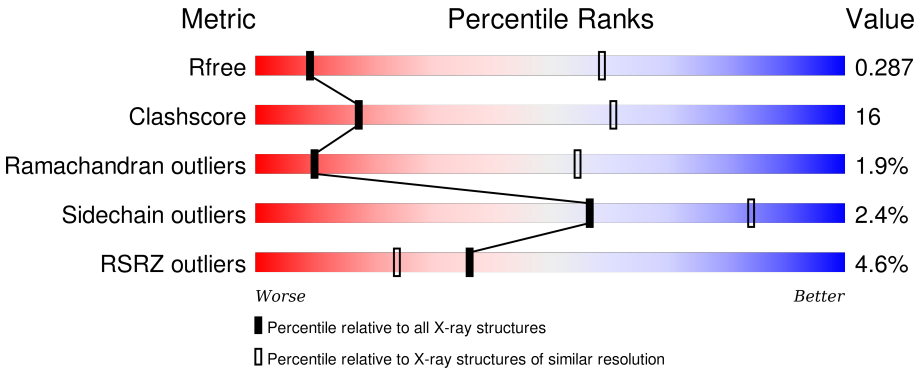
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.81 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	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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 <=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	B	242	3% 54% 38% • 8%
1	E	242	2% 61% 31% 8%
1	H	242	% 60% 31% • 8%
1	K	242	% 65% 26% • 8%
1	N	242	2% 63% 29% 8%

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Mol	Chain	Length	Quality of chain
2	C	323	6% 44% 27% 27%
2	F	323	6% 47% 26% 27%
2	I	323	6% 43% 29% 27%
2	L	323	6% 51% 21% 27%
2	O	323	4% 46% 25% 27%
3	A	313	3% 43% 25% 29%
3	D	313	4% 43% 25% 29%
3	G	313	3% 43% 24% 29%
3	J	313	4% 47% 21% 29%
3	M	313	2% 40% 28% 29%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26425 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 Capsid protein VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	223	Total	C	N	O	S	0	0	0
			1699	1093	279	316	11			
1	N	223	Total	C	N	O	S	0	0	0
			1699	1093	279	316	11			
1	B	223	Total	C	N	O	S	0	0	0
			1699	1093	279	316	11			
1	H	223	Total	C	N	O	S	0	0	0
			1699	1093	279	316	11			
1	K	223	Total	C	N	O	S	0	0	0
			1699	1093	279	316	11			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	227	GLN	LYS	engineered mutation	UNP F6KTB0
N	227	GLN	LYS	engineered mutation	UNP F6KTB0
B	227	GLN	LYS	engineered mutation	UNP F6KTB0
H	227	GLN	LYS	engineered mutation	UNP F6KTB0
K	227	GLN	LYS	engineered mutation	UNP F6KTB0

- Molecule 2 is a protein called Capsid protein VP0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	236	Total	C	N	O	S	0	0	0
			1829	1174	303	344	8			
2	O	236	Total	C	N	O	S	0	0	0
			1829	1174	303	344	8			
2	C	236	Total	C	N	O	S	0	0	0
			1829	1174	303	344	8			
2	I	236	Total	C	N	O	S	0	0	0
			1829	1174	303	344	8			
2	L	236	Total	C	N	O	S	0	0	0
			1829	1174	303	344	8			

- Molecule 3 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	221	Total	C	N	O	S	0	0	0
			1757	1128	295	323	11			
3	M	221	Total	C	N	O	S	0	0	0
			1757	1128	295	323	11			
3	A	221	Total	C	N	O	S	0	0	0
			1757	1128	295	323	11			
3	G	221	Total	C	N	O	S	0	0	0
			1757	1128	295	323	11			
3	J	221	Total	C	N	O	S	0	0	0
			1757	1128	295	323	11			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	101	SER	-	INSERTION	UNP F6KTB0
D	102	VAL	-	INSERTION	UNP F6KTB0
D	103	LYS	-	INSERTION	UNP F6KTB0
D	104	ARG	-	INSERTION	UNP F6KTB0
D	105	GLY	-	INSERTION	UNP F6KTB0
D	106	THR	-	INSERTION	UNP F6KTB0
D	107	SER	-	INSERTION	UNP F6KTB0
D	108	VAL	-	INSERTION	UNP F6KTB0
D	109	GLY	-	INSERTION	UNP F6KTB0
D	110	MET	-	INSERTION	UNP F6KTB0
D	111	LYS	-	INSERTION	UNP F6KTB0
D	112	PRO	-	INSERTION	UNP F6KTB0
D	113	SER	-	INSERTION	UNP F6KTB0
D	114	PRO	-	INSERTION	UNP F6KTB0
D	115	ARG	-	INSERTION	UNP F6KTB0
D	116	PRO	-	INSERTION	UNP F6KTB0
M	101	SER	-	INSERTION	UNP F6KTB0
M	102	VAL	-	INSERTION	UNP F6KTB0
M	103	LYS	-	INSERTION	UNP F6KTB0
M	104	ARG	-	INSERTION	UNP F6KTB0
M	105	GLY	-	INSERTION	UNP F6KTB0
M	106	THR	-	INSERTION	UNP F6KTB0
M	107	SER	-	INSERTION	UNP F6KTB0
M	108	VAL	-	INSERTION	UNP F6KTB0
M	109	GLY	-	INSERTION	UNP F6KTB0
M	110	MET	-	INSERTION	UNP F6KTB0
M	111	LYS	-	INSERTION	UNP F6KTB0
M	112	PRO	-	INSERTION	UNP F6KTB0

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Chain	Residue	Modelled	Actual	Comment	Reference
M	113	SER	-	INSERTION	UNP F6KTB0
M	114	PRO	-	INSERTION	UNP F6KTB0
M	115	ARG	-	INSERTION	UNP F6KTB0
M	116	PRO	-	INSERTION	UNP F6KTB0
A	101	SER	-	INSERTION	UNP F6KTB0
A	102	VAL	-	INSERTION	UNP F6KTB0
A	103	LYS	-	INSERTION	UNP F6KTB0
A	104	ARG	-	INSERTION	UNP F6KTB0
A	105	GLY	-	INSERTION	UNP F6KTB0
A	106	THR	-	INSERTION	UNP F6KTB0
A	107	SER	-	INSERTION	UNP F6KTB0
A	108	VAL	-	INSERTION	UNP F6KTB0
A	109	GLY	-	INSERTION	UNP F6KTB0
A	110	MET	-	INSERTION	UNP F6KTB0
A	111	LYS	-	INSERTION	UNP F6KTB0
A	112	PRO	-	INSERTION	UNP F6KTB0
A	113	SER	-	INSERTION	UNP F6KTB0
A	114	PRO	-	INSERTION	UNP F6KTB0
A	115	ARG	-	INSERTION	UNP F6KTB0
A	116	PRO	-	INSERTION	UNP F6KTB0
G	101	SER	-	INSERTION	UNP F6KTB0
G	102	VAL	-	INSERTION	UNP F6KTB0
G	103	LYS	-	INSERTION	UNP F6KTB0
G	104	ARG	-	INSERTION	UNP F6KTB0
G	105	GLY	-	INSERTION	UNP F6KTB0
G	106	THR	-	INSERTION	UNP F6KTB0
G	107	SER	-	INSERTION	UNP F6KTB0
G	108	VAL	-	INSERTION	UNP F6KTB0
G	109	GLY	-	INSERTION	UNP F6KTB0
G	110	MET	-	INSERTION	UNP F6KTB0
G	111	LYS	-	INSERTION	UNP F6KTB0
G	112	PRO	-	INSERTION	UNP F6KTB0
G	113	SER	-	INSERTION	UNP F6KTB0
G	114	PRO	-	INSERTION	UNP F6KTB0
G	115	ARG	-	INSERTION	UNP F6KTB0
G	116	PRO	-	INSERTION	UNP F6KTB0
J	101	SER	-	INSERTION	UNP F6KTB0
J	102	VAL	-	INSERTION	UNP F6KTB0
J	103	LYS	-	INSERTION	UNP F6KTB0
J	104	ARG	-	INSERTION	UNP F6KTB0
J	105	GLY	-	INSERTION	UNP F6KTB0
J	106	THR	-	INSERTION	UNP F6KTB0

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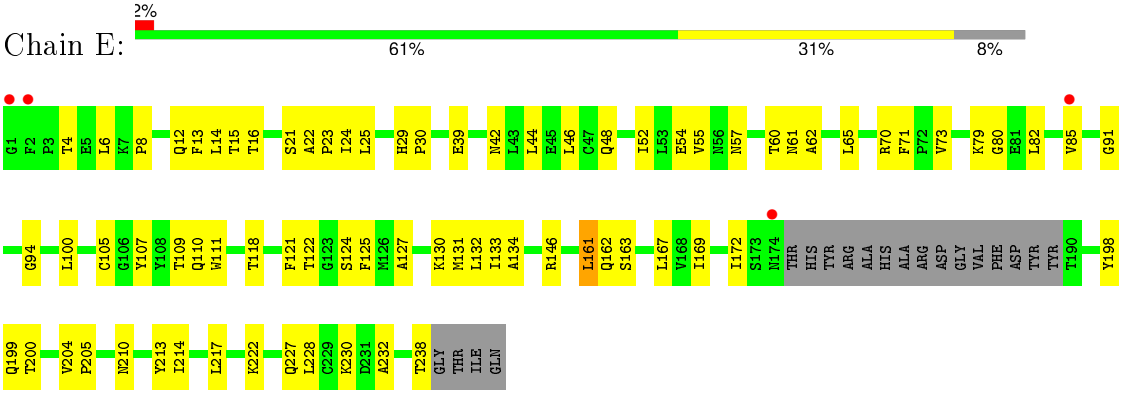
Chain	Residue	Modelled	Actual	Comment	Reference
J	107	SER	-	INSERTION	UNP F6KTB0
J	108	VAL	-	INSERTION	UNP F6KTB0
J	109	GLY	-	INSERTION	UNP F6KTB0
J	110	MET	-	INSERTION	UNP F6KTB0
J	111	LYS	-	INSERTION	UNP F6KTB0
J	112	PRO	-	INSERTION	UNP F6KTB0
J	113	SER	-	INSERTION	UNP F6KTB0
J	114	PRO	-	INSERTION	UNP F6KTB0
J	115	ARG	-	INSERTION	UNP F6KTB0
J	116	PRO	-	INSERTION	UNP F6KTB0

3 Residue-property plots (i)

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.

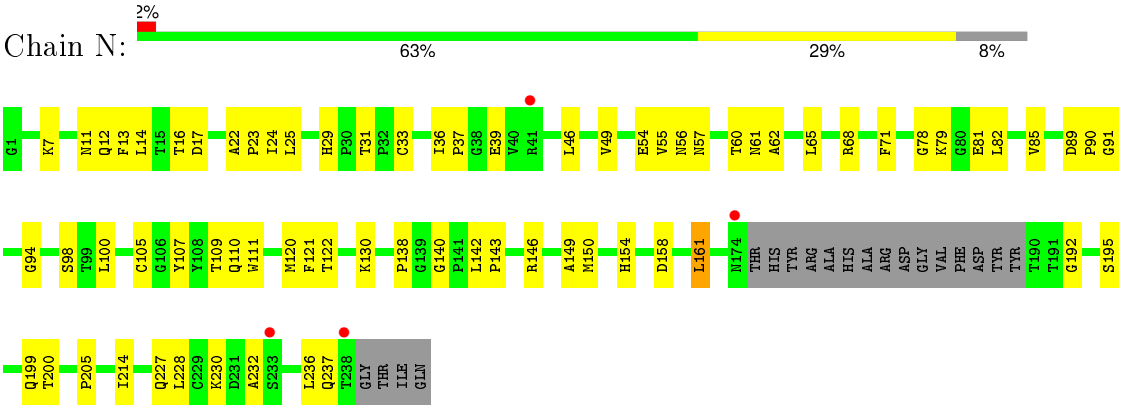
- Molecule 1: Capsid protein VP3

Chain E:



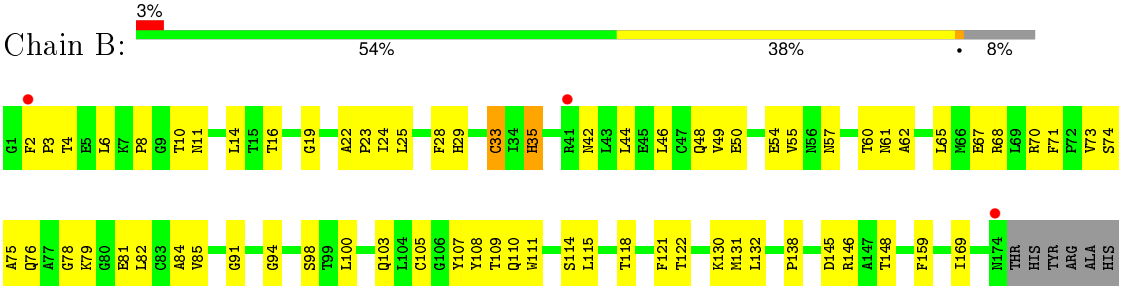
- Molecule 1: Capsid protein VP3

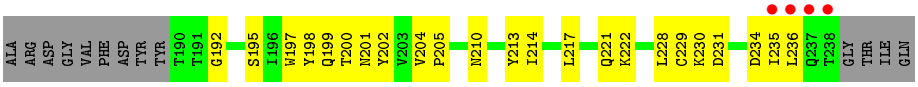
Chain N:



- Molecule 1: Capsid protein VP3

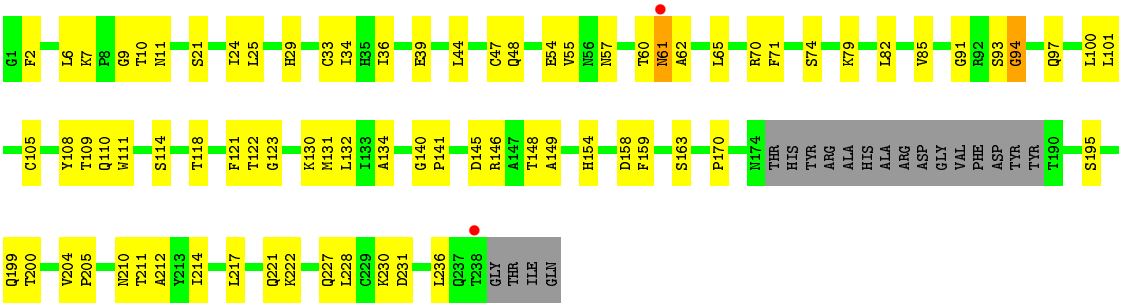
Chain B:





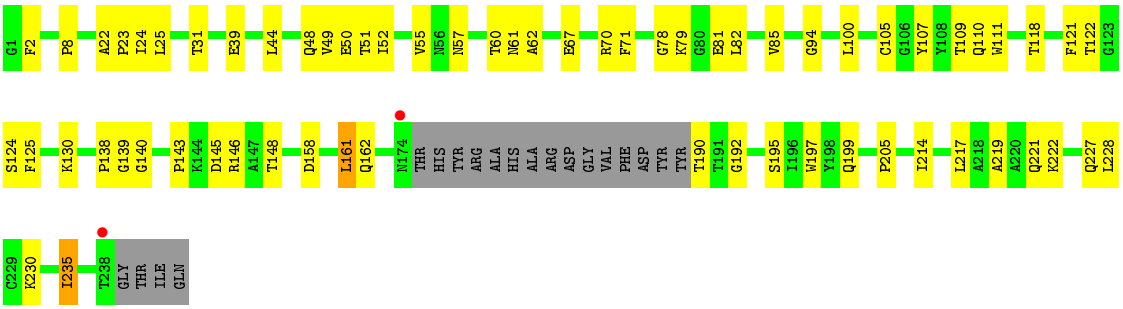
• Molecule 1: Capsid protein VP3

Chain H:



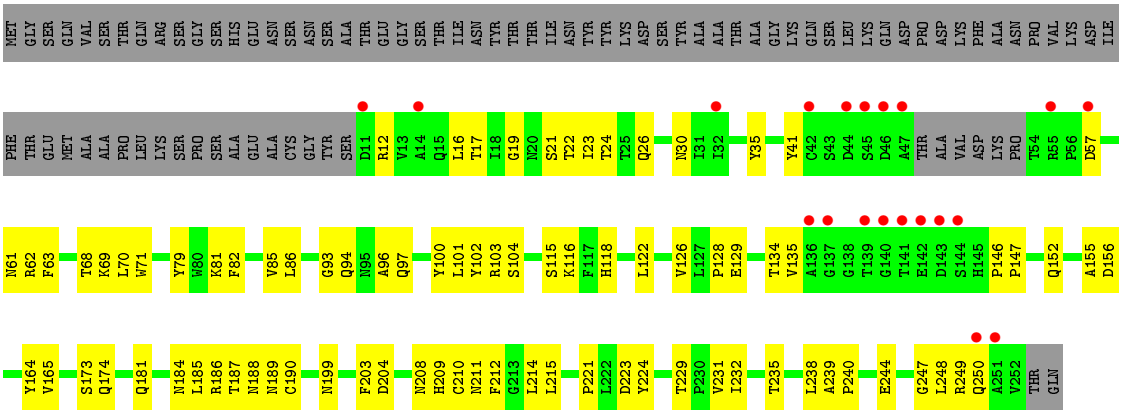
• Molecule 1: Capsid protein VP3

Chain K:



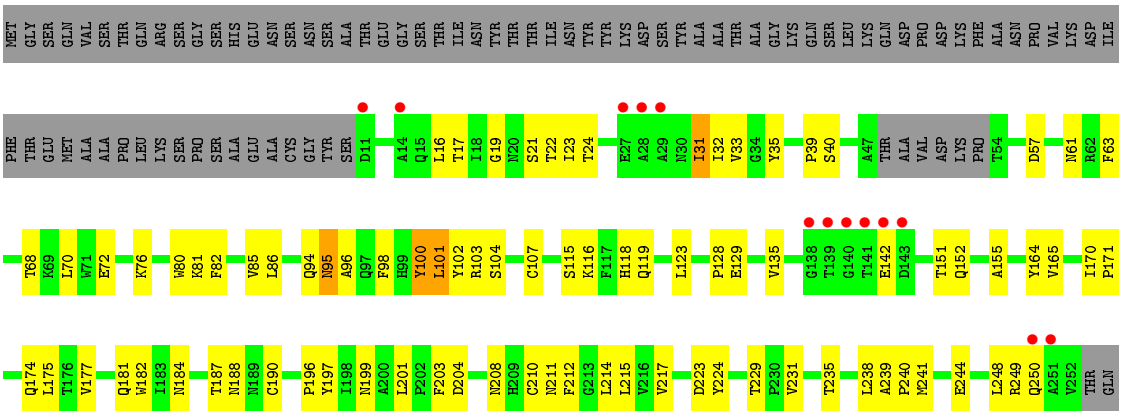
• Molecule 2: Capsid protein VP0

Chain F:

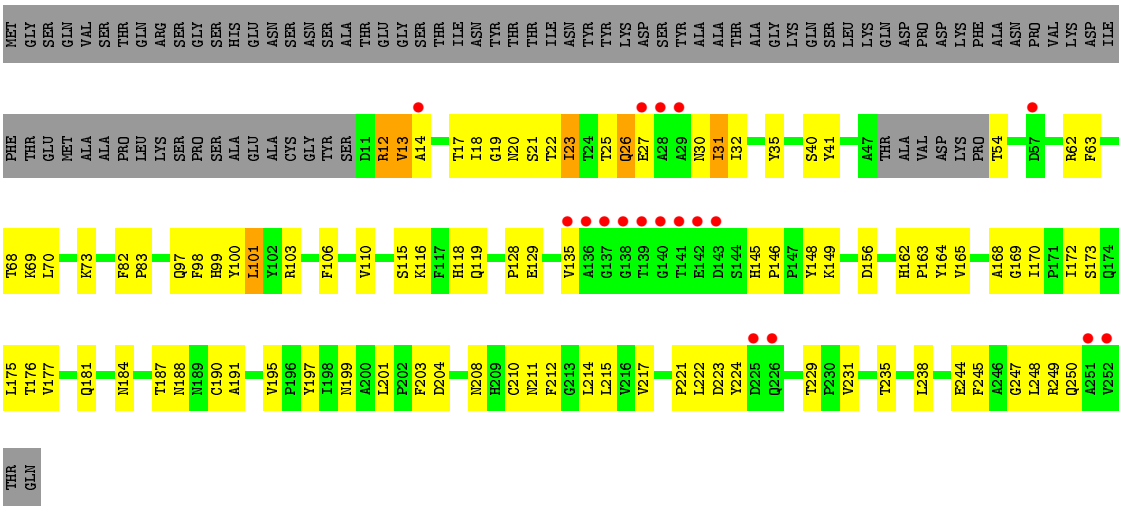


• Molecule 2: Capsid protein VP0

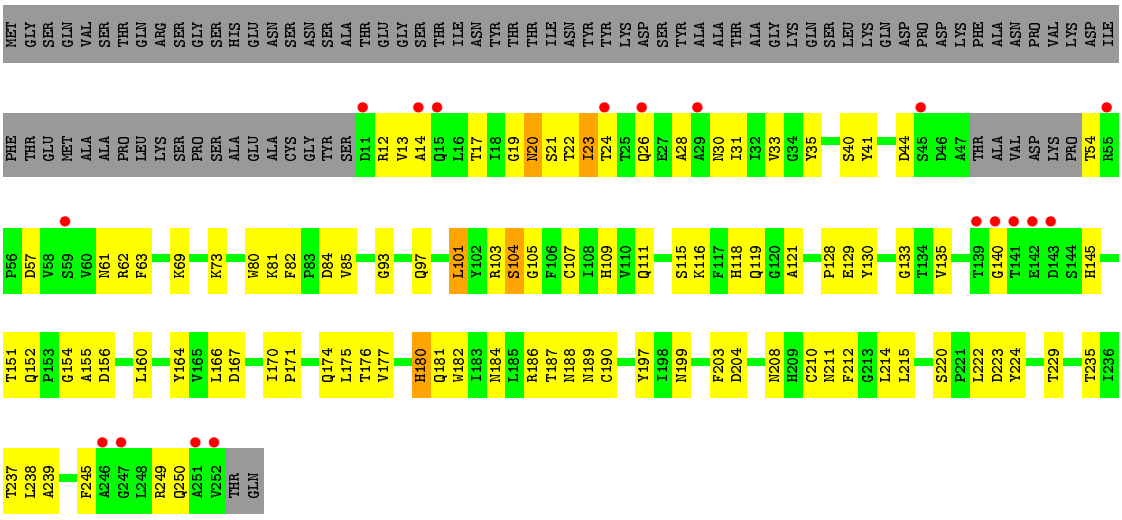
Chain O:



• Molecule 2: Capsid protein VP0

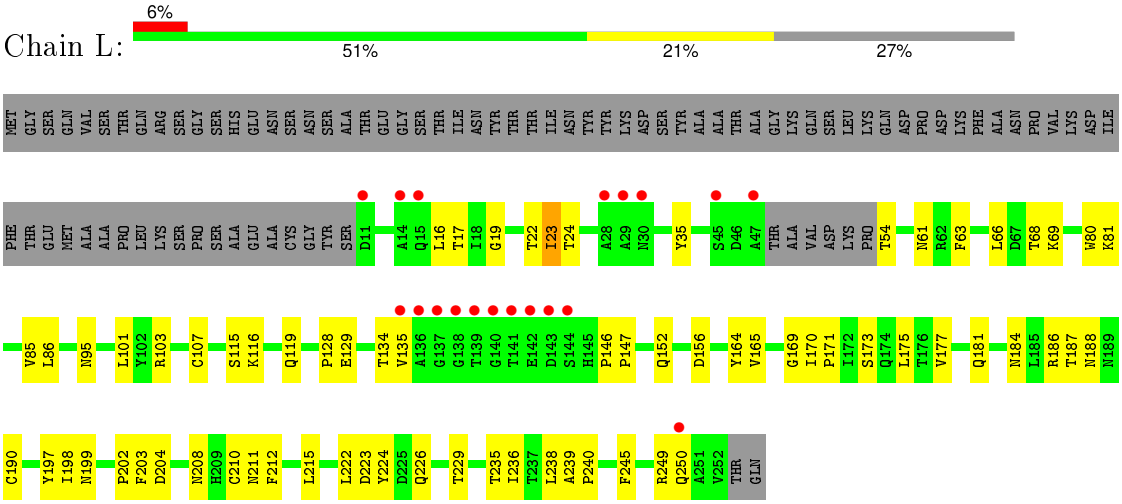


• Molecule 2: Capsid protein VP0



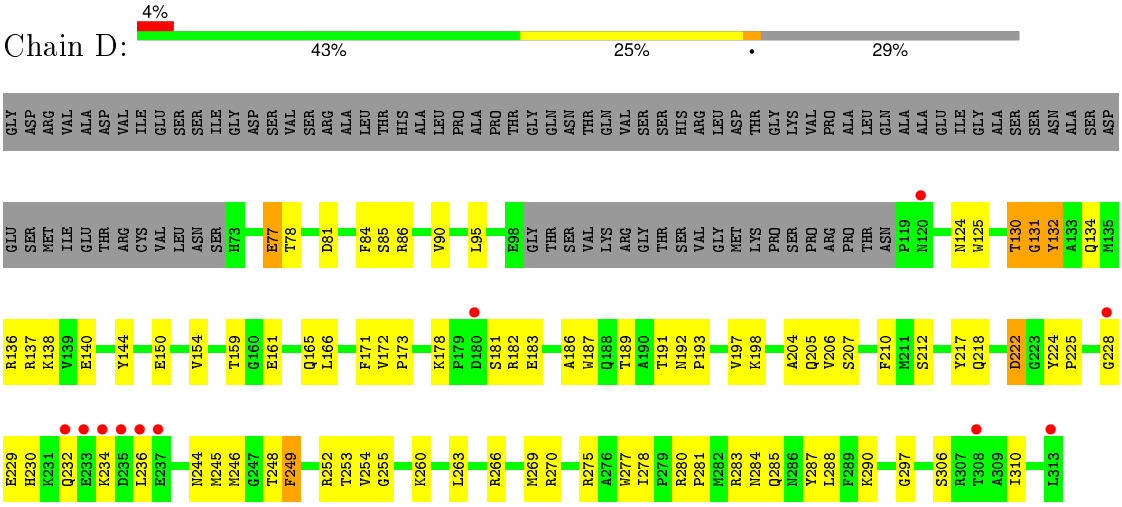
• Molecule 2: Capsid protein VP0

Chain L:



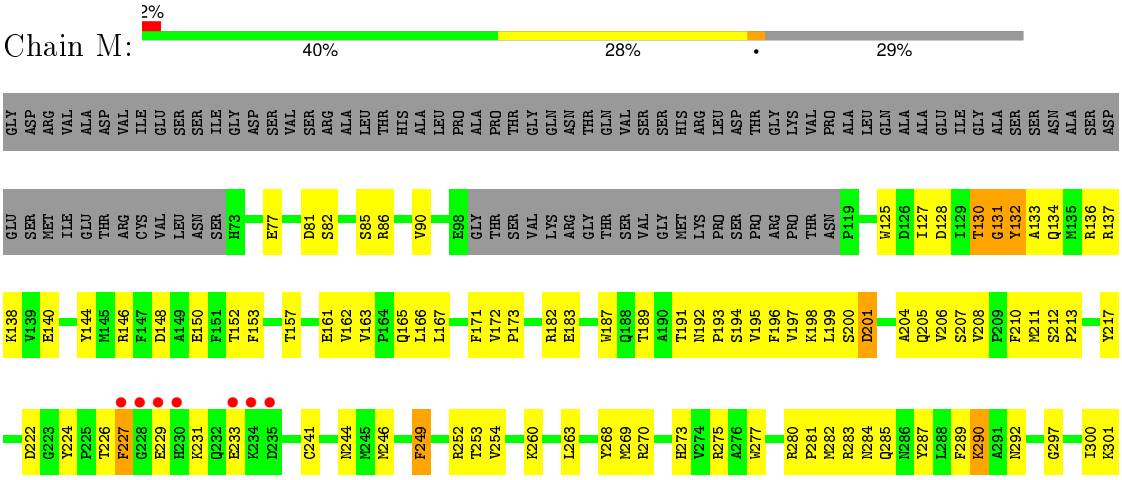
• Molecule 3: Capsid protein VP1

Chain D:



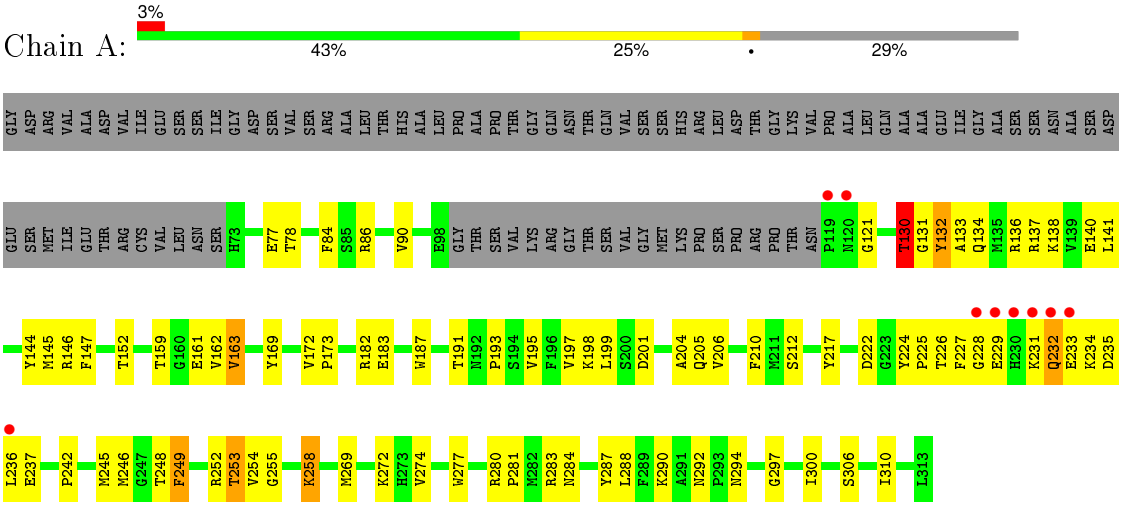
• Molecule 3: Capsid protein VP1

Chain M:



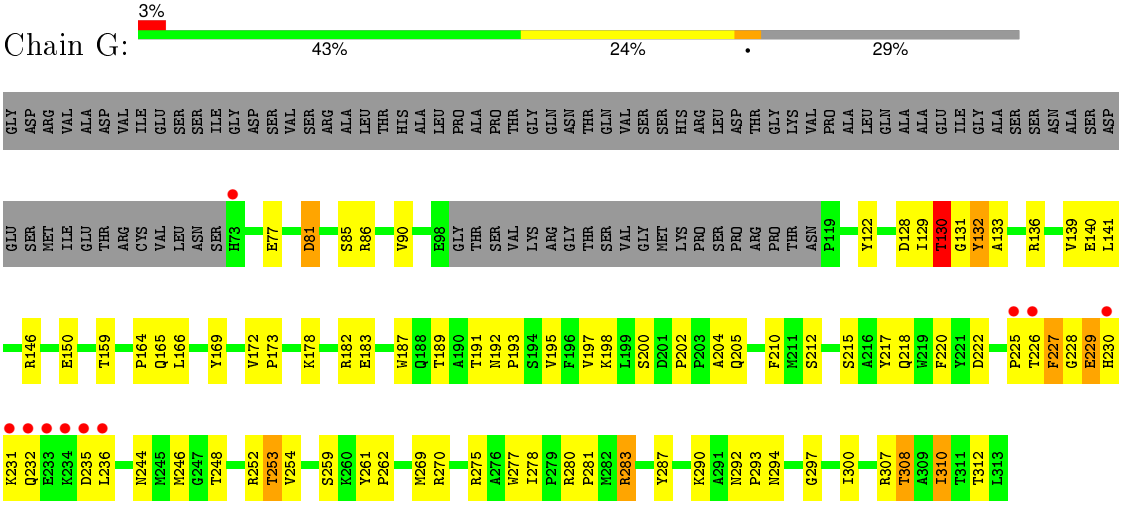
• Molecule 3: Capsid protein VP1

Chain A:



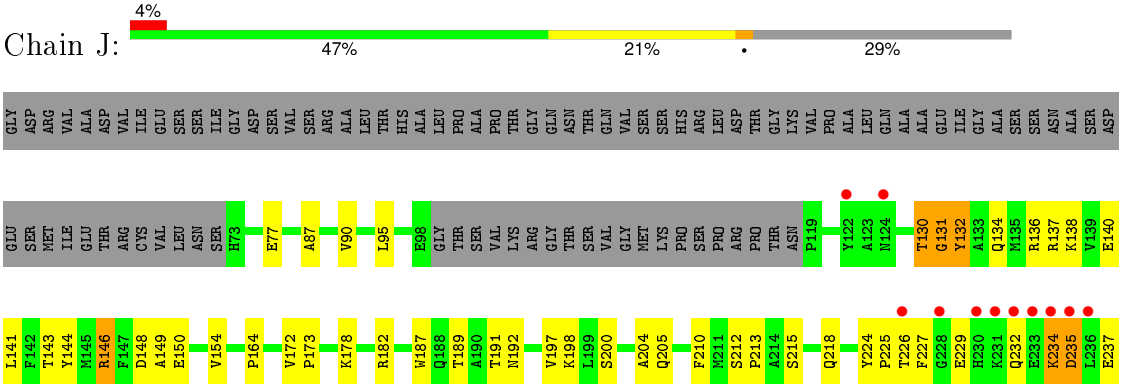
• Molecule 3: Capsid protein VP1

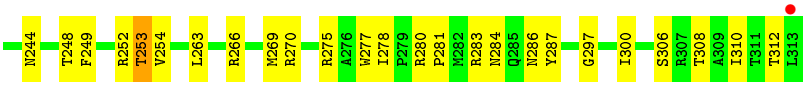
Chain G:



• Molecule 3: Capsid protein VP1

Chain J:




N244
T248
F249
R252
T253
V254
L263
R266
M269
R270
R275
A276
W277
I278
P279
R280
P281
M282
R283
N284
Q285
N286
Y287
G297
I300
S306
R307
T308
A309
I310
T311
T312
L313

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 3 2	Depositor
Cell constants a, b, c, α, β, γ	350.15Å 350.15Å 350.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.79 – 3.81 46.79 – 3.81	Depositor EDS
% Data completeness (in resolution range)	(Not available) (46.79-3.81) 77.3 (46.79-3.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 3.77Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.271 , 0.299 0.261 , 0.287	Depositor DCC
R_{free} test set	1673 reflections (3.01%)	DCC
Wilson B-factor (Å^2)	103.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 38.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 66730 reflections	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	26425	wwPDB-VP
Average B, all atoms (Å^2)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	B	0.29	0/1744	0.51	0/2387
1	E	0.28	0/1744	0.50	0/2387
1	H	0.30	0/1744	0.54	1/2387 (0.0%)
1	K	0.28	0/1744	0.50	0/2387
1	N	0.28	0/1744	0.50	0/2387
2	C	0.29	0/1882	0.51	0/2580
2	F	0.28	0/1882	0.48	0/2580
2	I	0.30	0/1882	0.52	0/2580
2	L	0.30	0/1882	0.51	0/2580
2	O	0.28	0/1882	0.52	0/2580
3	A	0.29	0/1811	0.50	0/2464
3	D	0.30	0/1811	0.49	0/2464
3	G	0.29	0/1811	0.50	0/2464
3	J	0.29	0/1811	0.51	0/2464
3	M	0.29	0/1811	0.51	0/2464
All	All	0.29	0/27185	0.51	1/37155 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	61	ASN	N-CA-C	-5.29	96.72	111.00

There are no chirality outliers.

There are no planarity outliers.

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	B	1699	0	1691	73	0
1	E	1699	0	1691	65	0
1	H	1699	0	1691	73	0
1	K	1699	0	1691	51	0
1	N	1699	0	1691	63	0
2	C	1829	0	1765	67	0
2	F	1829	0	1765	62	0
2	I	1829	0	1765	80	0
2	L	1829	0	1765	53	0
2	O	1829	0	1765	65	0
3	A	1757	0	1707	82	0
3	D	1757	0	1707	73	0
3	G	1757	0	1707	77	0
3	J	1757	0	1707	64	0
3	M	1757	0	1707	95	0
All	All	26425	0	25815	838	0

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 16.

All (838) 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:C:12:ARG:O	2:C:26:GLN:NE2	2.10	0.84
3:J:191:THR:HG21	1:N:230:LYS:HA	1.61	0.82
3:A:136:ARG:HD3	1:B:236:LEU:HD12	1.60	0.82
3:A:253:THR:H	3:A:254:VAL:HA	1.44	0.81
1:E:121:PHE:O	2:F:184:ASN:ND2	2.13	0.81
3:A:146:ARG:NH2	1:B:33:CYS:SG	2.53	0.81
2:O:101:LEU:HG	2:O:203:PHE:HB3	1.60	0.81
3:D:136:ARG:HH22	3:D:290:LYS:HG2	1.46	0.81
1:K:121:PHE:O	2:L:184:ASN:ND2	2.14	0.80
1:B:82:LEU:HD11	1:B:85:VAL:HG13	1.62	0.80
3:M:134:GLN:NE2	1:N:232:ALA:O	2.15	0.78
2:I:12:ARG:O	2:I:26:GLN:NE2	2.15	0.78
1:E:24:ILE:HG22	1:E:25:LEU:HG	1.65	0.78
3:A:280:ARG:NH2	2:C:129:GLU:O	2.16	0.78
3:G:146:ARG:NH2	1:H:33:CYS:SG	2.56	0.78
3:D:191:THR:HG21	1:H:230:LYS:HA	1.65	0.78
1:K:138:PRO:HA	1:K:192:GLY:H	1.50	0.76
1:H:82:LEU:HD11	1:H:85:VAL:HG13	1.67	0.76
1:B:49:VAL:HG11	2:C:177:VAL:HA	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:90:VAL:HG21	3:M:269:MET:HB3	1.68	0.76
3:J:232:GLN:HG3	3:J:234:LYS:HB2	1.68	0.76
2:C:25:THR:OG1	2:C:26:GLN:N	2.19	0.75
2:I:54:THR:N	2:I:245:PHE:O	2.20	0.75
1:B:24:ILE:HG22	1:B:25:LEU:HG	1.68	0.75
1:E:4:THR:HG22	1:H:2:PHE:HB3	1.68	0.75
3:D:205:GLN:OE1	1:H:7:LYS:NZ	2.20	0.74
1:H:71:PHE:HB2	1:H:214:ILE:HB	1.69	0.74
3:G:228:GLY:O	2:I:208:ASN:ND2	2.20	0.74
2:C:97:GLN:O	2:C:249:ARG:NH1	2.19	0.74
3:A:137:ARG:NH1	3:A:283:ARG:O	2.17	0.74
3:D:197:VAL:HG11	3:D:204:ALA:HB2	1.69	0.74
2:I:101:LEU:HG	2:I:203:PHE:HB3	1.69	0.74
3:G:308:THR:HG23	3:G:312:THR:HG21	1.70	0.74
1:N:121:PHE:O	2:O:184:ASN:ND2	2.21	0.74
1:H:121:PHE:O	2:I:184:ASN:ND2	2.19	0.73
2:F:208:ASN:ND2	3:D:228:GLY:O	2.21	0.73
1:N:24:ILE:HG22	1:N:25:LEU:HG	1.71	0.73
3:J:178:LYS:HE2	3:J:248:THR:HG21	1.70	0.73
1:E:79:LYS:HD2	1:E:80:GLY:N	2.03	0.73
2:C:101:LEU:HG	2:C:203:PHE:HB3	1.70	0.73
1:E:82:LEU:HD11	1:E:85:VAL:HG13	1.71	0.73
1:N:122:THR:HA	2:O:184:ASN:HD21	1.53	0.73
2:I:21:SER:HB2	2:I:62:ARG:HG3	1.71	0.72
1:K:24:ILE:HG22	1:K:25:LEU:HG	1.71	0.72
3:G:140:GLU:HG3	3:G:220:PHE:HZ	1.55	0.72
3:G:191:THR:HG21	1:B:230:LYS:HA	1.72	0.71
1:E:230:LYS:HA	3:M:191:THR:HG21	1.73	0.71
1:B:48:GLN:HE22	1:B:222:LYS:HA	1.55	0.71
1:B:121:PHE:O	2:C:184:ASN:ND2	2.23	0.71
3:M:287:TYR:HB3	1:N:237:GLN:HE22	1.54	0.71
2:O:187:THR:OG1	2:O:188:ASN:N	2.24	0.70
2:O:188:ASN:ND2	2:O:190:CYS:O	2.21	0.70
2:C:26:GLN:HG3	2:C:27:GLU:H	1.56	0.70
3:D:218:GLN:O	3:D:244:ASN:ND2	2.23	0.70
3:A:191:THR:HG21	1:K:230:LYS:HA	1.72	0.70
1:E:232:ALA:O	3:D:134:GLN:NE2	2.24	0.70
3:J:253:THR:H	3:J:254:VAL:HA	1.55	0.70
3:G:197:VAL:HG11	3:G:204:ALA:HB2	1.72	0.70
3:G:218:GLN:O	3:G:244:ASN:ND2	2.24	0.70
3:J:197:VAL:HG11	3:J:204:ALA:HB2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:137:ARG:NH1	3:M:283:ARG:O	2.25	0.70
1:K:122:THR:HA	2:L:184:ASN:HD21	1.57	0.70
3:G:280:ARG:NH2	2:I:129:GLU:O	2.25	0.70
1:K:71:PHE:HB2	1:K:214:ILE:HB	1.73	0.69
1:H:122:THR:HA	2:I:184:ASN:HD21	1.57	0.69
1:E:8:PRO:O	3:M:205:GLN:NE2	2.22	0.69
3:A:197:VAL:HG11	3:A:204:ALA:HB2	1.73	0.69
2:C:31:ILE:HD12	2:C:32:ILE:H	1.58	0.69
1:B:105:CYS:HB3	1:B:111:TRP:HE1	1.58	0.69
2:C:99:HIS:O	2:C:249:ARG:NH1	2.25	0.68
1:N:82:LEU:HD11	1:N:85:VAL:HG13	1.75	0.68
2:L:101:LEU:HG	2:L:203:PHE:HB3	1.75	0.68
1:H:24:ILE:HG22	1:H:25:LEU:HG	1.73	0.68
2:C:199:ASN:ND2	2:C:204:ASP:OD2	2.27	0.68
1:H:48:GLN:HE22	1:H:222:LYS:HA	1.56	0.68
2:C:13:VAL:O	2:C:26:GLN:NE2	2.26	0.68
3:J:90:VAL:HG21	3:J:269:MET:HB3	1.76	0.68
3:M:193:PRO:HG2	1:N:24:ILE:HG23	1.76	0.68
1:K:82:LEU:HD11	1:K:85:VAL:HG13	1.76	0.68
2:L:187:THR:OG1	2:L:188:ASN:N	2.27	0.67
2:L:128:PRO:HA	2:L:212:PHE:HA	1.75	0.67
2:O:82:PHE:HE2	2:O:214:LEU:HB2	1.59	0.67
2:L:68:THR:HG22	2:L:235:THR:HA	1.76	0.67
2:L:69:LYS:NZ	2:L:156:ASP:O	2.27	0.67
3:D:204:ALA:HA	1:H:9:GLY:HA2	1.74	0.67
3:A:283:ARG:NH1	2:C:168:ALA:O	2.28	0.67
1:K:105:CYS:HB3	1:K:111:TRP:HE1	1.59	0.67
3:A:199:LEU:O	3:G:198:LYS:NZ	2.27	0.67
2:I:188:ASN:OD1	2:I:190:CYS:N	2.27	0.67
3:M:182:ARG:NH2	3:M:253:THR:OG1	2.27	0.67
3:J:150:GLU:OE1	3:J:270:ARG:NH2	2.28	0.67
3:M:136:ARG:HH12	3:M:290:LYS:HG3	1.60	0.66
3:J:136:ARG:NH1	3:J:140:GLU:OE2	2.27	0.66
1:B:138:PRO:HA	1:B:192:GLY:H	1.60	0.66
2:F:103:ARG:NH1	2:F:244:GLU:OE1	2.27	0.66
3:A:90:VAL:HG21	3:A:269:MET:HB3	1.75	0.66
2:I:20:ASN:OD1	2:I:20:ASN:N	2.28	0.66
3:G:205:GLN:OE1	1:H:21:SER:OG	2.12	0.66
3:G:253:THR:H	3:G:254:VAL:HA	1.60	0.66
3:D:186:ALA:O	3:D:192:ASN:ND2	2.28	0.66
2:I:121:ALA:H	2:I:220:SER:HB3	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:188:ASN:ND2	2:F:190:CYS:O	2.24	0.66
3:G:130:THR:HG21	3:G:290:LYS:HE3	1.77	0.66
2:O:128:PRO:HA	2:O:212:PHE:HA	1.76	0.66
2:F:21:SER:HB2	2:F:62:ARG:HG3	1.77	0.66
2:L:197:TYR:OH	2:L:204:ASP:OD2	2.10	0.66
3:A:253:THR:N	3:A:254:VAL:HA	2.08	0.65
1:B:204:VAL:HG11	1:B:210:ASN:HA	1.78	0.65
1:K:143:PRO:HB3	2:C:250:GLN:HG3	1.78	0.65
2:F:187:THR:OG1	2:F:188:ASN:N	2.28	0.65
1:N:100:LEU:HD22	2:O:177:VAL:HG11	1.78	0.65
3:M:198:LYS:HG3	3:M:201:ASP:HB3	1.78	0.65
1:E:71:PHE:HB2	1:E:214:ILE:HB	1.77	0.65
3:M:82:SER:O	3:M:86:ARG:NH1	2.27	0.64
3:A:182:ARG:HH22	3:A:253:THR:HG22	1.63	0.64
2:I:30:ASN:ND2	2:I:181:GLN:OE1	2.30	0.64
3:D:161:GLU:OE1	3:M:260:LYS:NZ	2.26	0.64
3:A:134:GLN:NE2	1:B:231:ASP:OD2	2.30	0.64
2:C:187:THR:OG1	2:C:188:ASN:N	2.31	0.64
3:M:146:ARG:NH2	1:N:31:THR:O	2.31	0.64
2:F:57:ASP:O	2:F:61:ASN:ND2	2.30	0.63
3:M:162:VAL:HB	3:J:164:PRO:HB2	1.80	0.63
3:A:77:GLU:OE2	1:H:29:HIS:N	2.31	0.63
3:M:253:THR:H	3:M:254:VAL:HA	1.63	0.63
3:M:229:GLU:OE2	2:O:208:ASN:ND2	2.30	0.63
3:G:210:PHE:CZ	3:G:212:SER:HB3	2.33	0.63
3:J:137:ARG:HH21	1:K:107:TYR:HE1	1.46	0.63
2:O:80:TRP:NE1	2:O:155:ALA:O	2.28	0.63
3:M:138:LYS:HG2	1:N:107:TYR:CE2	2.33	0.63
1:H:44:LEU:O	1:H:48:GLN:HG2	1.98	0.63
2:O:199:ASN:ND2	2:O:204:ASP:OD2	2.31	0.63
3:M:150:GLU:OE1	3:M:270:ARG:NH2	2.32	0.62
2:I:187:THR:OG1	2:I:188:ASN:N	2.31	0.62
3:M:280:ARG:NH2	2:O:129:GLU:O	2.33	0.62
3:J:144:TYR:HB2	3:J:277:TRP:HB2	1.81	0.62
1:B:85:VAL:HG12	1:B:195:SER:HA	1.80	0.62
1:N:62:ALA:HA	1:N:65:LEU:HB2	1.80	0.62
3:G:130:THR:OG1	3:G:131:GLY:N	2.32	0.62
3:J:280:ARG:NH2	2:L:129:GLU:O	2.33	0.62
2:I:12:ARG:HG3	2:I:28:ALA:HB2	1.80	0.62
3:D:253:THR:H	3:D:254:VAL:HA	1.65	0.62
1:E:48:GLN:HE22	1:E:222:LYS:HA	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:139:GLY:C	2:C:249:ARG:HE	2.02	0.62
3:J:77:GLU:OE2	1:B:29:HIS:N	2.27	0.62
3:J:95:LEU:HB2	3:J:263:LEU:HB2	1.82	0.62
2:F:12:ARG:HD3	2:F:26:GLN:HA	1.82	0.62
2:O:115:SER:OG	2:O:116:LYS:N	2.32	0.62
1:N:130:LYS:N	1:N:200:THR:OG1	2.29	0.62
3:D:182:ARG:NH2	3:D:253:THR:OG1	2.17	0.61
3:M:208:VAL:HG13	3:M:211:MET:HE3	1.82	0.61
3:A:121:GLY:O	3:A:182:ARG:NH1	2.33	0.61
2:C:98:PHE:O	2:C:249:ARG:N	2.29	0.61
2:L:188:ASN:ND2	2:L:190:CYS:O	2.29	0.61
3:M:133:ALA:HA	1:N:236:LEU:HD12	1.82	0.61
3:A:234:LYS:HE2	3:A:237:GLU:H	1.65	0.61
2:F:128:PRO:HA	2:F:212:PHE:HA	1.83	0.61
3:G:307:ARG:H	1:H:57:ASN:HB3	1.63	0.61
2:L:134:THR:HG23	2:L:146:PRO:HG3	1.82	0.61
2:F:101:LEU:HG	2:F:203:PHE:HB3	1.82	0.61
3:M:307:ARG:HG3	1:N:57:ASN:HD22	1.64	0.61
1:E:122:THR:HA	2:F:184:ASN:HD21	1.66	0.61
2:O:115:SER:HB3	2:O:118:HIS:CE1	2.36	0.61
1:N:61:ASN:OD1	1:N:62:ALA:N	2.34	0.61
3:M:138:LYS:HG2	1:N:107:TYR:HE2	1.65	0.60
3:J:154:VAL:HB	3:J:266:ARG:HB2	1.83	0.60
3:D:229:GLU:HG3	3:D:230:HIS:H	1.66	0.60
3:M:241:CYS:O	3:M:244:ASN:ND2	2.30	0.60
2:C:40:SER:O	2:C:103:ARG:NH2	2.35	0.60
3:A:161:GLU:OE1	3:A:163:VAL:HG13	2.01	0.60
3:M:81:ASP:OD1	3:M:85:SER:OG	2.19	0.60
3:A:258:LYS:HD3	3:A:258:LYS:H	1.66	0.60
2:F:69:LYS:NZ	2:F:156:ASP:O	2.22	0.60
2:F:86:LEU:HD11	2:F:238:LEU:HD11	1.84	0.60
2:I:69:LYS:NZ	2:I:156:ASP:O	2.28	0.59
1:H:204:VAL:HG11	1:H:210:ASN:HA	1.84	0.59
3:A:193:PRO:HG2	1:B:24:ILE:HG23	1.82	0.59
3:D:81:ASP:OD1	3:D:85:SER:OG	2.19	0.59
3:D:198:LYS:NZ	3:G:200:SER:O	2.36	0.59
1:K:44:LEU:O	1:K:48:GLN:HG2	2.01	0.59
1:E:24:ILE:HG23	3:D:193:PRO:HG2	1.84	0.59
3:J:150:GLU:OE2	3:J:205:GLN:NE2	2.35	0.59
2:L:199:ASN:ND2	2:L:204:ASP:OD2	2.35	0.59
1:E:55:VAL:HB	1:E:71:PHE:HE1	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:300:ILE:HB	1:H:62:ALA:HB2	1.84	0.59
3:A:130:THR:OG1	3:A:131:GLY:N	2.34	0.59
1:E:44:LEU:O	1:E:48:GLN:HG2	2.03	0.59
3:G:297:GLY:HA2	3:G:300:ILE:HD11	1.85	0.59
3:J:210:PHE:CZ	3:J:212:SER:HB3	2.38	0.59
3:G:226:THR:HG23	3:G:227:PHE:CD1	2.37	0.59
3:M:130:THR:O	3:M:132:TYR:N	2.35	0.59
3:J:187:TRP:CD2	3:J:252:ARG:HD2	2.37	0.58
2:F:134:THR:HG23	2:F:146:PRO:HG3	1.85	0.58
3:D:187:TRP:CD2	3:D:252:ARG:HD2	2.38	0.58
3:G:253:THR:N	3:G:254:VAL:HA	2.19	0.58
1:K:161:LEU:HD12	1:K:162:GLN:H	1.68	0.58
3:M:297:GLY:H	2:O:135:VAL:HG13	1.68	0.58
2:C:25:THR:O	2:C:26:GLN:HB2	2.03	0.58
3:M:197:VAL:HG11	3:M:204:ALA:HB2	1.86	0.58
1:H:54:GLU:OE2	2:I:164:TYR:OH	2.11	0.58
2:C:172:ILE:HD13	2:C:217:VAL:HG11	1.86	0.58
1:B:100:LEU:HD22	2:C:177:VAL:HG11	1.84	0.58
2:F:26:GLN:NE2	2:F:190:CYS:SG	2.75	0.58
3:J:297:GLY:HA3	2:L:135:VAL:HG22	1.86	0.58
2:I:23:ILE:HD13	2:I:237:THR:HG21	1.85	0.58
2:O:17:THR:HB	2:O:22:THR:HG23	1.84	0.58
3:J:253:THR:N	3:J:254:VAL:HA	2.17	0.58
2:L:175:LEU:HD21	2:L:215:LEU:HD11	1.86	0.58
2:F:115:SER:OG	2:F:116:LYS:N	2.37	0.58
1:K:50:GLU:HA	1:K:219:ALA:HB2	1.86	0.58
3:A:297:GLY:HA2	3:A:300:ILE:HD11	1.85	0.58
3:G:90:VAL:HG21	3:G:269:MET:HB3	1.85	0.58
1:E:161:LEU:HD12	1:E:162:GLN:H	1.69	0.58
3:M:152:THR:N	3:M:268:TYR:O	2.33	0.57
1:N:105:CYS:HB3	1:N:111:TRP:HE1	1.69	0.57
3:J:224:TYR:HD2	3:J:237:GLU:HB3	1.70	0.57
2:F:199:ASN:HD21	2:F:209:HIS:CD2	2.23	0.57
2:L:226:GLN:OE1	2:L:226:GLN:N	2.38	0.57
2:O:175:LEU:HD21	2:O:215:LEU:HD11	1.87	0.57
3:A:86:ARG:NH1	1:B:229:CYS:SG	2.78	0.57
2:F:223:ASP:OD1	2:F:224:TYR:N	2.38	0.57
1:E:46:LEU:HB3	1:E:100:LEU:HD23	1.84	0.57
1:B:62:ALA:HA	1:B:65:LEU:HB2	1.85	0.57
1:B:55:VAL:HB	1:B:71:PHE:HE1	1.70	0.57
2:C:115:SER:OG	2:C:116:LYS:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:THR:OG1	3:M:194:SER:N	2.37	0.57
3:G:140:GLU:HG3	3:G:220:PHE:CZ	2.39	0.57
3:D:130:THR:O	3:D:132:TYR:N	2.38	0.57
1:K:109:THR:OG1	1:K:110:GLN:N	2.38	0.57
3:M:136:ARG:HH22	3:M:290:LYS:HG3	1.70	0.57
3:J:226:THR:HA	3:J:227:PHE:HD1	1.70	0.57
2:I:130:TYR:OH	2:I:166:LEU:O	2.17	0.57
2:I:41:TYR:HA	2:I:103:ARG:HH12	1.69	0.57
1:B:78:GLY:N	1:B:81:GLU:OE2	2.38	0.57
2:F:129:GLU:O	3:D:280:ARG:NH2	2.38	0.57
1:H:109:THR:HG21	1:H:228:LEU:HD23	1.87	0.56
3:G:141:LEU:O	3:G:280:ARG:N	2.35	0.56
3:G:130:THR:O	3:G:132:TYR:N	2.37	0.56
2:C:223:ASP:OD1	2:C:224:TYR:N	2.39	0.56
1:E:24:ILE:HG12	3:D:206:VAL:HG11	1.87	0.56
2:I:115:SER:OG	2:I:116:LYS:N	2.36	0.56
3:A:224:TYR:N	2:C:208:ASN:O	2.35	0.56
3:A:217:TYR:OH	3:A:246:MET:SD	2.50	0.56
2:O:103:ARG:HG3	2:O:197:TYR:CG	2.41	0.56
2:C:41:TYR:HA	2:C:103:ARG:HH12	1.71	0.56
2:I:23:ILE:HD11	2:I:63:PHE:CG	2.41	0.56
2:F:199:ASN:ND2	2:F:204:ASP:OD2	2.39	0.56
2:C:83:PRO:HD2	2:C:210:CYS:HA	1.85	0.56
2:O:86:LEU:HD11	2:O:238:LEU:HD11	1.87	0.56
3:G:132:TYR:OH	1:H:231:ASP:OD2	2.23	0.56
3:G:277:TRP:NE1	1:H:36:ILE:O	2.38	0.56
2:I:249:ARG:HG2	2:I:250:GLN:H	1.71	0.56
3:J:87:ALA:HA	3:J:270:ARG:HB2	1.88	0.56
2:F:26:GLN:NE2	2:F:189:ASN:OD1	2.39	0.56
2:O:102:TYR:OH	2:O:104:SER:OG	2.24	0.56
2:F:41:TYR:HA	2:F:103:ARG:HH12	1.71	0.55
2:I:249:ARG:HG2	2:I:250:GLN:N	2.21	0.55
3:A:205:GLN:NE2	1:K:8:PRO:O	2.26	0.55
1:N:54:GLU:OE2	2:O:164:TYR:OH	2.19	0.55
2:C:30:ASN:ND2	2:C:181:GLN:OE1	2.38	0.55
2:L:54:THR:N	2:L:245:PHE:O	2.40	0.55
2:L:16:LEU:O	2:L:23:ILE:N	2.39	0.55
2:O:40:SER:O	2:O:103:ARG:NH2	2.38	0.55
2:L:23:ILE:HD11	2:L:63:PHE:CG	2.41	0.55
1:K:61:ASN:OD1	1:K:62:ALA:N	2.39	0.55
1:K:109:THR:OG1	1:K:228:LEU:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:103:ARG:O	2:F:244:GLU:N	2.39	0.55
1:B:50:GLU:O	2:C:176:THR:OG1	2.11	0.55
1:H:62:ALA:HA	1:H:65:LEU:HB2	1.89	0.55
1:H:85:VAL:HG12	1:H:195:SER:HA	1.88	0.55
1:N:56:ASN:HB3	1:N:68:ARG:HA	1.88	0.55
1:N:49:VAL:HG11	2:O:177:VAL:HA	1.89	0.54
1:E:213:TYR:HD2	2:F:221:PRO:HD2	1.72	0.54
2:C:68:THR:HG22	2:C:235:THR:HA	1.89	0.54
3:A:162:VAL:HB	3:G:164:PRO:HB2	1.89	0.54
1:K:130:LYS:HG2	1:K:158:ASP:HA	1.89	0.54
2:I:33:VAL:HG21	2:I:181:GLN:HE21	1.71	0.54
3:J:144:TYR:HE2	2:L:198:ILE:HG22	1.73	0.54
3:J:130:THR:O	3:J:132:TYR:N	2.41	0.54
2:F:93:GLY:O	2:F:97:GLN:HG2	2.08	0.54
3:J:138:LYS:HG2	1:K:107:TYR:CE2	2.43	0.54
2:F:16:LEU:O	2:F:23:ILE:N	2.37	0.54
3:A:187:TRP:CD2	3:A:252:ARG:HD2	2.42	0.54
3:G:182:ARG:O	3:G:187:TRP:NE1	2.41	0.54
3:J:297:GLY:HA2	3:J:300:ILE:HD11	1.89	0.54
1:E:61:ASN:OD1	1:E:62:ALA:N	2.40	0.54
3:A:198:LYS:NZ	3:J:200:SER:O	2.41	0.54
2:I:160:LEU:HB2	2:I:167:ASP:OD2	2.08	0.54
1:B:130:LYS:N	1:B:200:THR:OG1	2.30	0.54
3:M:290:LYS:N	3:M:290:LYS:HD2	2.23	0.53
3:G:146:ARG:HG3	3:G:210:PHE:CD1	2.43	0.53
3:M:171:PHE:O	3:M:192:ASN:HB2	2.08	0.53
2:F:135:VAL:HG13	3:D:297:GLY:H	1.74	0.53
3:M:253:THR:N	3:M:254:VAL:HA	2.23	0.53
1:H:105:CYS:HB3	1:H:111:TRP:HE1	1.73	0.53
1:H:100:LEU:HD22	2:I:177:VAL:HG11	1.89	0.53
3:D:136:ARG:O	3:D:140:GLU:N	2.35	0.53
3:M:182:ARG:O	3:M:187:TRP:NE1	2.42	0.53
3:D:159:THR:HG21	3:M:260:LYS:HZ2	1.73	0.53
3:J:132:TYR:O	3:J:134:GLN:N	2.37	0.53
3:G:225:PRO:O	3:G:228:GLY:N	2.41	0.53
2:F:208:ASN:O	3:D:224:TYR:N	2.32	0.53
3:D:132:TYR:OH	3:M:189:THR:O	2.15	0.53
1:E:8:PRO:C	3:M:205:GLN:HE21	2.10	0.53
3:M:152:THR:HG21	1:N:13:PHE:CE1	2.44	0.53
2:F:128:PRO:HB2	3:D:278:ILE:HD13	1.91	0.53
2:I:250:GLN:N	2:I:250:GLN:OE1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:LEU:HD22	3:G:86:ARG:HH21	1.73	0.53
3:G:136:ARG:O	3:G:140:GLU:N	2.36	0.53
3:D:181:SER:OG	3:D:182:ARG:N	2.37	0.53
3:D:182:ARG:HH22	3:D:253:THR:HG1	1.50	0.53
2:L:115:SER:OG	2:L:116:LYS:N	2.41	0.53
1:K:78:GLY:N	1:K:81:GLU:OE2	2.42	0.53
3:M:77:GLU:HG3	1:N:227:GLN:HA	1.91	0.53
3:M:140:GLU:OE1	3:M:287:TYR:OH	2.22	0.52
3:A:201:ASP:O	3:G:198:LYS:NZ	2.41	0.52
3:D:253:THR:N	3:D:254:VAL:HA	2.24	0.52
2:I:199:ASN:ND2	2:I:204:ASP:OD2	2.43	0.52
2:I:128:PRO:HA	2:I:212:PHE:HA	1.91	0.52
2:I:40:SER:O	2:I:103:ARG:NH2	2.43	0.52
3:D:140:GLU:OE1	3:D:287:TYR:OH	2.21	0.52
3:J:237:GLU:OE1	3:J:237:GLU:N	2.41	0.52
3:A:140:GLU:OE1	3:A:287:TYR:OH	2.20	0.52
3:D:234:LYS:HZ1	3:D:236:LEU:HD12	1.74	0.52
1:N:46:LEU:HB3	1:N:100:LEU:HD23	1.89	0.52
3:D:124:ASN:HB3	3:D:178:LYS:HZ1	1.75	0.52
3:J:146:ARG:NE	3:J:215:SER:O	2.35	0.52
3:D:144:TYR:HB2	3:D:277:TRP:HB2	1.91	0.52
1:E:12:GLN:HA	3:M:197:VAL:HG12	1.92	0.52
1:K:125:PHE:HB3	2:L:116:LYS:HB3	1.90	0.52
3:J:130:THR:OG1	3:J:131:GLY:N	2.42	0.52
2:C:69:LYS:NZ	2:C:156:ASP:O	2.28	0.52
1:H:105:CYS:HB3	1:H:111:TRP:NE1	2.24	0.52
2:C:82:PHE:HE2	2:C:214:LEU:HB2	1.75	0.52
3:A:169:TYR:HB2	3:A:195:VAL:HB	1.91	0.52
1:N:130:LYS:H	1:N:200:THR:HG1	1.51	0.52
1:B:61:ASN:OD1	1:B:62:ALA:N	2.43	0.52
3:A:169:TYR:O	3:A:195:VAL:N	2.37	0.52
2:I:184:ASN:O	2:I:188:ASN:N	2.42	0.52
1:E:204:VAL:HG11	1:E:210:ASN:HA	1.92	0.52
3:G:193:PRO:HG2	1:H:24:ILE:HG23	1.92	0.51
3:A:134:GLN:O	3:A:138:LYS:HG3	2.10	0.51
1:E:21:SER:OG	1:H:7:LYS:NZ	2.34	0.51
1:K:55:VAL:HB	1:K:71:PHE:HE1	1.75	0.51
2:O:223:ASP:OD1	2:O:224:TYR:N	2.42	0.51
3:A:306:SER:OG	1:B:68:ARG:NH2	2.43	0.51
1:B:46:LEU:HB3	1:B:100:LEU:HD23	1.92	0.51
3:A:77:GLU:O	1:B:108:TYR:OH	2.16	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:297:GLY:HA3	2:I:135:VAL:HG13	1.93	0.51
3:G:292:ASN:OD1	3:G:294:ASN:ND2	2.24	0.51
1:E:227:GLN:NE2	1:N:29:HIS:O	2.44	0.51
2:O:16:LEU:O	2:O:23:ILE:N	2.40	0.51
1:N:237:GLN:CD	1:N:237:GLN:H	2.14	0.51
1:B:109:THR:OG1	1:B:110:GLN:N	2.44	0.51
2:C:188:ASN:ND2	2:C:190:CYS:O	2.40	0.51
1:N:130:LYS:HG2	1:N:158:ASP:HA	1.93	0.51
1:E:107:TYR:OH	3:D:137:ARG:NE	2.44	0.51
2:F:165:VAL:HG12	3:D:284:ASN:HD21	1.75	0.51
2:O:250:GLN:OE1	2:O:250:GLN:N	2.39	0.50
1:E:14:LEU:HG	1:E:16:THR:H	1.76	0.50
1:K:109:THR:HG22	1:K:230:LYS:HD3	1.93	0.50
2:O:23:ILE:HG22	2:O:24:THR:H	1.77	0.50
1:N:14:LEU:HG	1:N:16:THR:H	1.76	0.50
2:C:175:LEU:HD21	2:C:215:LEU:HD11	1.93	0.50
3:D:165:GLN:OE1	3:D:166:LEU:N	2.41	0.50
1:N:109:THR:OG1	1:N:110:GLN:N	2.44	0.50
1:E:109:THR:OG1	1:E:110:GLN:N	2.43	0.50
1:B:91:GLY:HA3	1:B:111:TRP:CZ2	2.46	0.50
3:D:90:VAL:HG21	3:D:269:MET:HB3	1.93	0.50
3:A:290:LYS:HE2	1:B:236:LEU:HD11	1.93	0.50
3:J:148:ASP:OD1	3:J:149:ALA:N	2.44	0.50
2:F:250:GLN:N	2:F:250:GLN:OE1	2.40	0.50
2:L:119:GLN:O	2:L:222:LEU:HA	2.11	0.50
3:M:152:THR:HG23	3:M:205:GLN:HB3	1.93	0.50
1:H:130:LYS:N	1:H:200:THR:OG1	2.38	0.50
1:E:109:THR:OG1	1:E:228:LEU:HB3	2.12	0.50
3:J:278:ILE:HD13	2:L:128:PRO:HG2	1.93	0.50
3:A:138:LYS:HG2	1:B:107:TYR:CE2	2.46	0.50
1:H:61:ASN:OD1	1:H:62:ALA:N	2.45	0.50
3:M:217:TYR:OH	3:M:246:MET:SD	2.52	0.50
3:M:157:THR:HG1	3:M:161:GLU:N	2.09	0.50
2:I:80:TRP:NE1	2:I:155:ALA:O	2.42	0.50
2:L:66:LEU:HD12	2:L:236:ILE:HG21	1.93	0.50
1:N:85:VAL:HG12	1:N:195:SER:HA	1.91	0.50
3:J:146:ARG:NH2	1:K:31:THR:O	2.45	0.50
3:M:163:VAL:H	3:M:199:LEU:HD11	1.77	0.50
3:D:95:LEU:HB2	3:D:263:LEU:HB2	1.92	0.50
1:N:109:THR:HG22	1:N:230:LYS:HD3	1.93	0.50
3:M:297:GLY:HA2	3:M:300:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:ASN:HB3	3:D:306:SER:HB3	1.93	0.50
2:O:70:LEU:HD13	2:O:231:VAL:HG11	1.93	0.50
1:H:118:THR:N	1:H:217:LEU:O	2.39	0.50
3:D:234:LYS:NZ	3:D:236:LEU:HB2	2.27	0.50
1:B:115:LEU:HB2	1:B:169:ILE:HB	1.94	0.50
1:N:138:PRO:HA	1:N:192:GLY:H	1.77	0.50
1:H:109:THR:OG1	1:H:110:GLN:N	2.45	0.49
2:C:199:ASN:HB3	2:C:201:LEU:O	2.12	0.49
2:I:57:ASP:O	2:I:61:ASN:ND2	2.45	0.49
2:I:12:ARG:HB2	2:I:26:GLN:HG3	1.93	0.49
1:K:146:ARG:HD2	1:K:199:GLN:OE1	2.12	0.49
3:D:183:GLU:N	3:D:183:GLU:OE1	2.45	0.49
3:A:310:ILE:HD12	1:B:84:ALA:HB2	1.92	0.49
1:E:122:THR:HA	2:F:184:ASN:ND2	2.28	0.49
1:B:4:THR:HG22	1:K:2:PHE:HB3	1.94	0.49
3:D:217:TYR:OH	3:D:246:MET:SD	2.58	0.49
2:F:21:SER:OG	2:F:63:PHE:HB2	2.12	0.49
3:A:234:LYS:HD2	3:A:235:ASP:N	2.28	0.49
2:I:115:SER:HB3	2:I:118:HIS:ND1	2.27	0.49
3:A:152:THR:HG23	3:A:205:GLN:HB3	1.95	0.49
3:J:136:ARG:HB3	3:J:287:TYR:HE2	1.77	0.49
3:A:130:THR:O	3:A:132:TYR:N	2.45	0.49
3:M:144:TYR:HB2	3:M:277:TRP:HB2	1.94	0.49
3:A:272:LYS:NZ	1:B:19:GLY:O	2.30	0.49
3:A:182:ARG:O	3:A:187:TRP:NE1	2.46	0.49
1:B:44:LEU:O	1:B:48:GLN:HG2	2.11	0.49
1:K:85:VAL:HG12	1:K:195:SER:HA	1.92	0.49
3:D:225:PRO:O	3:D:228:GLY:N	2.45	0.49
3:J:218:GLN:O	3:J:244:ASN:ND2	2.46	0.49
1:H:74:SER:HB3	1:H:211:THR:HG23	1.95	0.49
1:H:55:VAL:HB	1:H:71:PHE:HE1	1.78	0.49
1:N:55:VAL:HB	1:N:71:PHE:HE1	1.78	0.49
1:N:109:THR:HG21	1:N:228:LEU:HD23	1.94	0.49
2:I:30:ASN:HD21	2:I:181:GLN:CD	2.15	0.49
3:A:242:PRO:O	3:A:245:MET:HG2	2.13	0.49
3:G:129:ILE:HD12	3:G:139:VAL:HG21	1.94	0.49
3:M:189:THR:HG23	3:M:192:ASN:OD1	2.13	0.49
1:E:13:PHE:HB3	3:M:196:PHE:HB2	1.95	0.49
3:J:197:VAL:HG12	1:N:12:GLN:HA	1.95	0.48
1:E:227:GLN:HA	3:D:77:GLU:OE1	2.12	0.48
2:O:68:THR:HG22	2:O:235:THR:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:146:ARG:NH1	1:N:33:CYS:SG	2.81	0.48
3:G:165:GLN:OE1	3:G:166:LEU:N	2.37	0.48
1:E:91:GLY:HA3	1:E:111:TRP:CZ2	2.49	0.48
3:G:205:GLN:NE2	1:B:8:PRO:HG2	2.29	0.48
3:G:150:GLU:OE1	1:H:21:SER:OG	2.31	0.48
2:F:17:THR:HB	2:F:22:THR:HG23	1.95	0.48
3:J:284:ASN:HD21	2:L:165:VAL:HG12	1.78	0.48
3:D:86:ARG:NH1	3:M:191:THR:OG1	2.45	0.48
3:G:283:ARG:NH2	3:G:293:PRO:O	2.46	0.48
1:E:24:ILE:HG12	3:D:206:VAL:CG1	2.43	0.48
3:M:224:TYR:O	2:O:208:ASN:HB3	2.13	0.48
1:K:118:THR:N	1:K:217:LEU:O	2.37	0.48
3:J:234:LYS:O	3:J:235:ASP:HB2	2.13	0.48
1:E:118:THR:N	1:E:217:LEU:O	2.46	0.48
1:H:221:GLN:HG3	1:H:222:LYS:H	1.79	0.48
1:B:6:LEU:H	1:H:10:THR:HB	1.79	0.48
3:M:153:PHE:HZ	3:M:249:PHE:CE2	2.31	0.48
3:G:226:THR:HA	3:G:227:PHE:HD1	1.79	0.48
1:H:91:GLY:HA3	1:H:111:TRP:CZ2	2.49	0.48
2:C:70:LEU:HD13	2:C:231:VAL:HG11	1.96	0.48
2:C:128:PRO:HA	2:C:212:PHE:HA	1.95	0.48
2:L:107:CYS:N	2:L:239:ALA:O	2.39	0.48
2:L:223:ASP:OD1	2:L:224:TYR:N	2.46	0.48
2:I:152:GLN:HG2	2:I:210:CYS:SG	2.54	0.48
1:B:71:PHE:HB2	1:B:214:ILE:HB	1.95	0.47
1:B:146:ARG:HD2	1:B:199:GLN:OE1	2.14	0.47
3:D:150:GLU:HG2	3:D:270:ARG:HB3	1.94	0.47
3:M:290:LYS:HE2	1:N:236:LEU:HD22	1.96	0.47
1:B:132:LEU:HB3	1:B:197:TRP:HB2	1.95	0.47
3:A:144:TYR:HB2	3:A:277:TRP:HB2	1.96	0.47
1:K:51:THR:HG21	1:K:100:LEU:HB2	1.97	0.47
2:O:39:PRO:HB3	2:O:196:PRO:HA	1.96	0.47
3:J:284:ASN:HB3	2:L:171:PRO:HD3	1.96	0.47
3:D:150:GLU:HA	3:D:207:SER:HA	1.96	0.47
3:A:133:ALA:C	3:A:136:ARG:HE	2.17	0.47
3:D:154:VAL:HB	3:D:266:ARG:HB2	1.97	0.47
2:I:107:CYS:N	2:I:239:ALA:O	2.41	0.47
3:G:178:LYS:HE3	3:G:248:THR:HG21	1.97	0.47
3:M:167:LEU:HD21	3:M:263:LEU:HD13	1.96	0.47
1:B:131:MET:HG3	1:B:159:PHE:CZ	2.50	0.47
2:I:17:THR:HB	2:I:22:THR:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:100:TYR:HE2	2:C:247:GLY:HA3	1.80	0.47
1:E:109:THR:HG22	1:E:230:LYS:HD3	1.96	0.47
2:L:250:GLN:OE1	2:L:250:GLN:N	2.45	0.47
3:J:182:ARG:HH22	3:J:253:THR:HG22	1.80	0.47
1:E:105:CYS:HB3	1:E:111:TRP:HE1	1.79	0.47
3:M:183:GLU:OE1	3:M:183:GLU:N	2.48	0.47
3:M:222:ASP:OD1	2:O:81:LYS:NZ	2.45	0.47
1:B:48:GLN:NE2	1:B:222:LYS:HA	2.26	0.47
3:A:234:LYS:HD2	3:A:236:LEU:H	1.80	0.47
2:L:146:PRO:HA	2:L:147:PRO:HD3	1.82	0.47
1:N:91:GLY:HA3	1:N:111:TRP:CZ2	2.50	0.47
1:B:132:LEU:HD13	1:B:146:ARG:HG3	1.95	0.47
3:A:159:THR:HG23	3:G:259:SER:HA	1.96	0.47
3:G:281:PRO:HB3	2:I:174:GLN:HB2	1.96	0.47
2:F:85:VAL:HG13	2:F:155:ALA:HA	1.96	0.47
2:F:115:SER:HB3	2:F:118:HIS:ND1	2.30	0.47
3:J:224:TYR:HA	3:J:225:PRO:HD3	1.83	0.47
3:G:222:ASP:OD1	2:I:81:LYS:NZ	2.35	0.47
3:A:226:THR:HA	3:A:227:PHE:HA	1.52	0.47
3:J:286:ASN:ND2	1:K:235:ILE:HD11	2.30	0.47
1:E:127:ALA:O	2:F:186:ARG:NH2	2.48	0.46
2:I:223:ASP:OD1	2:I:224:TYR:N	2.47	0.46
2:I:30:ASN:HD22	2:I:188:ASN:ND2	2.12	0.46
2:F:115:SER:HB3	2:F:118:HIS:CE1	2.49	0.46
3:D:210:PHE:CZ	3:D:212:SER:HB3	2.50	0.46
3:A:210:PHE:CZ	3:A:212:SER:HB3	2.49	0.46
1:E:131:MET:HA	1:E:199:GLN:H	1.80	0.46
1:E:169:ILE:HG21	1:E:172:ILE:HD11	1.98	0.46
1:E:163:SER:OG	2:F:186:ARG:HD3	2.16	0.46
3:A:136:ARG:NH1	1:B:236:LEU:HB2	2.31	0.46
2:O:82:PHE:CE1	2:O:238:LEU:HD22	2.51	0.46
3:J:137:ARG:NH1	3:J:283:ARG:O	2.48	0.46
2:F:82:PHE:CE1	2:F:238:LEU:HD22	2.50	0.46
3:M:284:ASN:HB3	2:O:171:PRO:HG3	1.98	0.46
3:M:226:THR:HA	3:M:227:PHE:HA	1.68	0.46
2:C:26:GLN:HG3	2:C:27:GLU:N	2.28	0.46
2:I:73:LYS:HG3	2:I:222:LEU:O	2.16	0.46
3:G:290:LYS:NZ	1:H:236:LEU:HD11	2.29	0.46
2:O:103:ARG:O	2:O:244:GLU:N	2.48	0.46
3:J:141:LEU:O	3:J:280:ARG:N	2.44	0.46
2:O:81:LYS:HD2	2:O:151:THR:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:98:PHE:HA	2:O:249:ARG:HG2	1.96	0.46
2:O:82:PHE:HE1	2:O:238:LEU:HD22	1.80	0.46
3:G:281:PRO:HG2	2:I:170:ILE:CG2	2.46	0.46
1:B:54:GLU:OE2	2:C:164:TYR:OH	2.19	0.46
1:E:130:LYS:N	1:E:200:THR:OG1	2.27	0.46
3:J:275:ARG:HH21	1:K:39:GLU:CD	2.19	0.46
2:O:72:GLU:HG2	2:O:72:GLU:H	1.56	0.46
1:B:74:SER:OG	1:B:76:GLN:HG2	2.16	0.46
2:O:123:LEU:N	2:O:217:VAL:O	2.48	0.46
2:I:82:PHE:HE1	2:I:238:LEU:HD22	1.80	0.46
3:G:290:LYS:HZ3	1:H:236:LEU:HD21	1.81	0.46
2:O:103:ARG:HG3	2:O:197:TYR:CD1	2.50	0.46
2:O:197:TYR:OH	2:O:204:ASP:OD2	2.31	0.46
1:N:71:PHE:HB2	1:N:214:ILE:HB	1.98	0.46
1:H:47:CYS:HB3	1:H:101:LEU:HD13	1.97	0.46
3:M:136:ARG:HD2	1:N:236:LEU:HD21	1.98	0.45
2:I:80:TRP:HB3	2:I:85:VAL:HG22	1.96	0.45
2:L:164:TYR:O	2:L:171:PRO:HA	2.16	0.45
3:A:172:VAL:HB	3:A:248:THR:OG1	2.15	0.45
3:M:136:ARG:NH1	3:M:290:LYS:HG3	2.30	0.45
3:D:254:VAL:HG12	3:D:255:GLY:H	1.80	0.45
3:J:226:THR:CA	3:J:227:PHE:HD1	2.29	0.45
2:C:54:THR:N	2:C:245:PHE:O	2.49	0.45
2:I:12:ARG:HE	2:I:28:ALA:HA	1.81	0.45
1:N:60:THR:HA	1:N:61:ASN:HA	1.79	0.45
2:F:102:TYR:OH	2:F:104:SER:OG	2.26	0.45
2:C:17:THR:HG23	2:C:22:THR:OG1	2.16	0.45
2:L:80:TRP:HB3	2:L:85:VAL:CG2	2.47	0.45
3:G:81:ASP:O	3:G:85:SER:HB3	2.16	0.45
3:D:283:ARG:NH1	3:D:285:GLN:O	2.49	0.45
1:N:150:MET:O	1:N:154:HIS:ND1	2.49	0.45
3:M:134:GLN:O	3:M:138:LYS:HG3	2.16	0.45
1:H:122:THR:O	2:I:119:GLN:HB2	2.17	0.45
2:I:182:TRP:O	2:I:188:ASN:ND2	2.49	0.45
3:D:132:TYR:O	3:D:134:GLN:N	2.40	0.45
3:G:133:ALA:HB1	1:H:236:LEU:HB3	1.97	0.45
3:G:290:LYS:HZ1	1:H:236:LEU:HD11	1.82	0.45
3:D:234:LYS:NZ	3:D:236:LEU:HD12	2.31	0.45
1:H:146:ARG:HA	1:H:149:ALA:HB3	1.97	0.45
1:E:73:VAL:HA	1:E:198:TYR:OH	2.17	0.45
2:F:79:TYR:HA	2:F:215:LEU:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:99:HIS:HA	2:C:248:LEU:HA	1.99	0.45
1:N:122:THR:O	2:O:119:GLN:HB2	2.16	0.45
1:E:8:PRO:HG2	3:M:205:GLN:NE2	2.31	0.45
3:G:187:TRP:CD2	3:G:252:ARG:HD3	2.51	0.45
2:C:103:ARG:O	2:C:244:GLU:N	2.50	0.45
2:C:103:ARG:NH1	2:C:244:GLU:OE1	2.49	0.45
1:B:54:GLU:HB2	1:B:98:SER:HB3	1.98	0.45
2:L:80:TRP:HB3	2:L:85:VAL:HG21	1.98	0.45
2:O:31:ILE:HG13	2:O:32:ILE:H	1.80	0.45
3:M:195:VAL:HG21	3:M:206:VAL:HG21	1.98	0.45
1:H:163:SER:OG	2:I:186:ARG:HD3	2.17	0.45
3:J:77:GLU:HG3	1:K:227:GLN:HA	1.99	0.45
3:G:183:GLU:OE1	3:G:183:GLU:N	2.50	0.45
3:A:141:LEU:O	3:A:280:ARG:N	2.43	0.45
1:B:2:PHE:HA	1:B:3:PRO:HD3	1.78	0.45
2:F:152:GLN:HG2	2:F:210:CYS:SG	2.56	0.45
2:F:100:TYR:HE2	2:F:247:GLY:HA3	1.81	0.45
1:H:108:TYR:HA	1:H:228:LEU:O	2.17	0.45
3:J:308:THR:OG1	3:J:312:THR:HG21	2.17	0.45
3:G:202:PRO:HB3	1:H:11:ASN:HD22	1.82	0.45
1:E:22:ALA:HA	1:E:23:PRO:HD3	1.85	0.45
2:O:100:TYR:CZ	2:O:101:LEU:HD13	2.52	0.44
1:K:138:PRO:O	1:K:190:THR:OG1	2.25	0.44
2:C:115:SER:HB3	2:C:118:HIS:CE1	2.51	0.44
1:H:132:LEU:HD13	1:H:146:ARG:HG3	1.99	0.44
1:N:140:GLY:HA3	2:L:249:ARG:HD2	1.99	0.44
1:K:52:ILE:HB	2:L:173:SER:HA	1.99	0.44
1:B:201:ASN:OD1	1:B:202:TYR:N	2.47	0.44
3:G:150:GLU:OE2	3:G:270:ARG:NH2	2.42	0.44
2:I:250:GLN:CD	2:I:250:GLN:H	2.20	0.44
1:N:78:GLY:N	1:N:81:GLU:OE2	2.41	0.44
1:H:131:MET:HG3	1:H:159:PHE:CZ	2.52	0.44
3:G:217:TYR:OH	3:G:246:MET:SD	2.59	0.44
3:J:189:THR:C	3:J:191:THR:H	2.20	0.44
3:G:252:ARG:NH2	3:G:254:VAL:HB	2.32	0.44
3:J:77:GLU:OE1	1:B:28:PHE:HA	2.17	0.44
1:E:62:ALA:HA	1:E:65:LEU:HB2	1.99	0.44
2:L:101:LEU:HA	2:L:101:LEU:HD12	1.82	0.44
3:G:229:GLU:HB3	3:G:230:HIS:H	1.61	0.44
2:C:73:LYS:HG3	2:C:222:LEU:O	2.18	0.44
1:H:109:THR:HG22	1:H:230:LYS:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:THR:HA	2:C:184:ASN:HD21	1.81	0.44
3:A:224:TYR:HA	3:A:225:PRO:HD3	1.83	0.44
2:F:249:ARG:HD2	1:H:140:GLY:HA3	1.98	0.44
2:F:126:VAL:HG22	2:F:214:LEU:HD23	2.00	0.44
2:O:80:TRP:HB3	2:O:85:VAL:HG22	1.99	0.44
1:K:161:LEU:HD12	1:K:162:GLN:N	2.31	0.44
2:O:250:GLN:H	2:O:250:GLN:CD	2.20	0.44
1:H:74:SER:HA	1:H:211:THR:HA	2.00	0.44
1:B:74:SER:OG	1:B:76:GLN:O	2.35	0.44
3:M:275:ARG:HH21	1:N:39:GLU:CD	2.21	0.44
1:K:22:ALA:HA	1:K:23:PRO:HD3	1.79	0.44
1:E:238:THR:O	3:D:290:LYS:NZ	2.46	0.44
3:M:187:TRP:CD2	3:M:252:ARG:HD2	2.53	0.44
3:D:124:ASN:HB3	3:D:178:LYS:NZ	2.31	0.44
1:N:89:ASP:HA	1:N:90:PRO:HD3	1.86	0.44
3:A:78:THR:OG1	1:B:42:ASN:ND2	2.48	0.44
2:I:176:THR:HG22	2:I:180:HIS:CD2	2.53	0.44
2:F:239:ALA:HA	2:F:240:PRO:HD3	1.84	0.44
1:E:55:VAL:HB	1:E:71:PHE:CE1	2.50	0.44
1:K:48:GLN:HE22	1:K:222:LYS:HA	1.83	0.44
1:B:98:SER:HB2	2:C:173:SER:HB3	2.00	0.44
2:O:57:ASP:O	2:O:61:ASN:ND2	2.50	0.44
3:M:171:PHE:HB2	3:M:249:PHE:HE1	1.83	0.44
3:A:227:PHE:CG	3:A:228:GLY:N	2.86	0.44
1:N:146:ARG:HD2	1:N:199:GLN:OE1	2.17	0.44
3:M:132:TYR:OH	3:J:189:THR:O	2.23	0.43
1:K:140:GLY:HA3	2:C:249:ARG:HD3	2.00	0.43
3:M:200:SER:O	3:J:198:LYS:NZ	2.50	0.43
3:J:283:ARG:HD2	2:L:169:GLY:O	2.18	0.43
2:C:148:TYR:HD2	2:C:149:LYS:HD2	1.83	0.43
3:G:169:TYR:HB2	3:G:195:VAL:HB	1.98	0.43
2:C:21:SER:OG	2:C:63:PHE:HB2	2.18	0.43
2:C:23:ILE:HD11	2:C:63:PHE:CG	2.53	0.43
1:E:6:LEU:HD21	1:H:6:LEU:HD13	2.00	0.43
3:A:136:ARG:HG3	3:A:137:ARG:H	1.82	0.43
3:A:136:ARG:NH1	1:B:234:ASP:OD2	2.51	0.43
3:J:224:TYR:N	2:L:208:ASN:O	2.46	0.43
2:I:82:PHE:HE2	2:I:214:LEU:HB2	1.83	0.43
1:B:145:ASP:O	1:B:148:THR:OG1	2.32	0.43
2:F:71:TRP:CZ3	2:F:122:LEU:HD11	2.53	0.43
3:G:140:GLU:OE1	3:G:287:TYR:OH	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:TYR:HD2	2:C:221:PRO:HD2	1.83	0.43
2:O:115:SER:HB3	2:O:118:HIS:ND1	2.33	0.43
3:M:148:ASP:OD2	3:M:273:HIS:ND1	2.51	0.43
2:I:197:TYR:OH	2:I:204:ASP:OD2	2.18	0.43
1:E:60:THR:HA	1:E:61:ASN:HA	1.74	0.43
1:N:146:ARG:HB3	1:N:146:ARG:NH1	2.33	0.43
1:B:118:THR:N	1:B:217:LEU:O	2.46	0.43
2:I:175:LEU:HD21	2:I:215:LEU:HD11	2.00	0.43
3:J:306:SER:HB3	1:K:57:ASN:HB3	2.01	0.43
2:C:145:HIS:HA	2:C:146:PRO:HD3	1.85	0.43
3:A:288:LEU:HD23	3:A:288:LEU:HA	1.88	0.43
1:K:60:THR:HA	1:K:61:ASN:HA	1.74	0.43
1:B:109:THR:HG21	1:B:228:LEU:HD23	2.00	0.43
2:I:82:PHE:CE1	2:I:238:LEU:HD22	2.54	0.43
3:M:289:PHE:HB2	3:M:292:ASN:OD1	2.18	0.43
3:M:128:ASP:N	3:M:128:ASP:OD1	2.52	0.43
2:I:101:LEU:HA	2:I:101:LEU:HD12	1.78	0.43
1:H:212:ALA:HA	2:I:119:GLN:HE22	1.84	0.43
3:D:232:GLN:HG2	3:D:234:LYS:O	2.18	0.43
1:N:22:ALA:HA	1:N:23:PRO:HD3	1.82	0.43
3:M:307:ARG:H	1:N:57:ASN:HB3	1.84	0.43
3:M:77:GLU:N	3:M:77:GLU:OE1	2.41	0.43
2:O:249:ARG:HG3	2:O:250:GLN:N	2.34	0.43
1:H:146:ARG:HD2	1:H:199:GLN:OE1	2.18	0.43
1:E:132:LEU:HD21	1:E:134:ALA:HB2	2.01	0.43
3:J:281:PRO:HG2	2:L:170:ILE:CG2	2.49	0.43
3:A:254:VAL:HG23	3:A:255:GLY:O	2.18	0.43
1:K:146:ARG:HB3	1:K:146:ARG:NH1	2.33	0.43
1:B:73:VAL:HA	1:B:198:TYR:OH	2.19	0.43
2:F:23:ILE:HD11	2:F:63:PHE:CD1	2.53	0.43
3:D:260:LYS:HE3	3:G:159:THR:HG21	2.01	0.43
1:K:122:THR:O	2:L:119:GLN:HB2	2.19	0.43
3:G:128:ASP:OD1	3:G:128:ASP:N	2.51	0.43
1:N:158:ASP:OD1	1:N:161:LEU:HG	2.19	0.43
1:N:143:PRO:HD3	2:L:250:GLN:HE21	1.83	0.43
1:H:134:ALA:HA	1:H:154:HIS:HA	2.01	0.43
3:G:172:VAL:HA	3:G:173:PRO:HD2	1.76	0.43
3:A:292:ASN:CG	3:A:294:ASN:HD22	2.18	0.43
3:J:213:PRO:HG3	1:N:110:GLN:NE2	2.34	0.42
3:A:290:LYS:HA	3:A:290:LYS:HD3	1.67	0.42
2:O:101:LEU:HD12	2:O:101:LEU:HA	1.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:130:THR:OG1	3:D:131:GLY:N	2.52	0.42
1:K:82:LEU:HD23	1:K:197:TRP:CE2	2.53	0.42
3:A:232:GLN:C	3:A:234:LYS:H	2.23	0.42
2:I:133:GLY:N	2:I:167:ASP:O	2.47	0.42
3:A:292:ASN:OD1	3:A:294:ASN:ND2	2.26	0.42
1:E:29:HIS:HA	1:E:30:PRO:HD3	1.86	0.42
3:A:183:GLU:OE1	3:A:183:GLU:N	2.51	0.42
3:A:136:ARG:HH12	1:B:235:ILE:C	2.22	0.42
1:E:24:ILE:CG2	3:D:193:PRO:HG2	2.48	0.42
3:A:132:TYR:OH	3:A:134:GLN:NE2	2.45	0.42
2:O:199:ASN:HB3	2:O:201:LEU:O	2.20	0.42
2:L:17:THR:HB	2:L:22:THR:HG23	2.01	0.42
1:E:39:GLU:CD	3:D:275:ARG:HH21	2.22	0.42
3:G:261:TYR:HA	3:G:262:PRO:HD3	1.83	0.42
3:M:210:PHE:CZ	3:M:212:SER:HB3	2.53	0.42
3:M:132:TYR:O	3:M:134:GLN:N	2.48	0.42
3:A:136:ARG:NH1	1:B:235:ILE:O	2.49	0.42
3:G:136:ARG:CZ	3:G:287:TYR:HE2	2.32	0.42
1:H:48:GLN:NE2	1:H:222:LYS:HA	2.28	0.42
3:G:307:ARG:NH1	3:G:310:ILE:HA	2.34	0.42
3:A:205:GLN:NE2	1:K:8:PRO:HG2	2.34	0.42
2:F:94:GLN:C	2:F:96:ALA:H	2.21	0.42
3:G:215:SER:OG	1:H:34:ILE:HG12	2.19	0.42
1:K:67:GLU:HG2	1:K:70:ARG:NH2	2.34	0.42
1:B:60:THR:HA	1:B:61:ASN:HA	1.70	0.42
3:G:278:ILE:HD13	2:I:128:PRO:HB2	2.01	0.42
1:H:123:GLY:O	2:I:186:ARG:HB2	2.19	0.42
3:G:236:LEU:HD12	2:I:145:HIS:CE1	2.55	0.42
2:F:30:ASN:ND2	2:F:181:GLN:OE1	2.53	0.42
2:I:93:GLY:O	2:I:97:GLN:HG2	2.19	0.42
1:B:35:HIS:C	1:B:35:HIS:CD2	2.92	0.42
3:A:281:PRO:HG2	2:C:170:ILE:CG2	2.49	0.42
3:J:172:VAL:HA	3:J:173:PRO:HD2	1.85	0.42
3:M:198:LYS:HD2	3:M:200:SER:OG	2.20	0.42
2:F:146:PRO:HA	2:F:147:PRO:HD3	1.74	0.42
2:O:21:SER:OG	2:O:63:PHE:HB2	2.20	0.42
3:M:157:THR:OG1	3:M:161:GLU:N	2.53	0.42
2:I:81:LYS:O	2:I:84:ASP:HB3	2.20	0.42
1:B:75:ALA:HA	1:B:202:TYR:HB3	2.01	0.42
3:A:284:ASN:HD21	2:C:165:VAL:HG12	1.85	0.42
1:E:146:ARG:HB3	1:E:146:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:125:TRP:CZ3	3:M:127:ILE:HA	2.55	0.42
3:A:283:ARG:HD2	2:C:169:GLY:O	2.20	0.42
2:L:239:ALA:HA	2:L:240:PRO:HD3	1.87	0.42
2:L:17:THR:HA	2:L:22:THR:HA	2.00	0.42
3:D:288:LEU:HD23	3:D:288:LEU:HA	1.84	0.42
2:I:164:TYR:O	2:I:171:PRO:HA	2.20	0.42
3:A:145:MET:O	3:A:217:TYR:N	2.51	0.42
2:O:23:ILE:HD11	2:O:63:PHE:CD1	2.55	0.42
3:J:281:PRO:HG2	2:L:170:ILE:HG21	2.02	0.42
3:M:212:SER:HA	3:M:213:PRO:HD3	1.94	0.42
3:A:147:PHE:HB3	3:A:274:VAL:HG12	2.02	0.42
3:D:172:VAL:HB	3:D:248:THR:OG1	2.19	0.42
1:H:93:SER:HA	1:H:94:GLY:HA3	1.53	0.42
1:E:54:GLU:OE2	2:F:164:TYR:OH	2.16	0.42
3:M:281:PRO:HG2	2:O:170:ILE:CG2	2.50	0.42
2:F:70:LEU:HD13	2:F:231:VAL:HG11	2.01	0.42
2:F:185:LEU:HD12	2:F:185:LEU:H	1.85	0.42
3:M:130:THR:OG1	3:M:131:GLY:N	2.53	0.42
3:M:282:MET:HG3	1:N:100:LEU:HD11	2.01	0.42
3:G:277:TRP:NE1	1:H:39:GLU:HB2	2.34	0.42
2:C:110:VAL:O	2:C:191:ALA:N	2.50	0.42
1:E:228:LEU:HD21	3:M:173:PRO:HB2	2.02	0.42
3:A:232:GLN:O	3:A:233:GLU:HB3	2.19	0.42
1:K:158:ASP:OD1	1:K:161:LEU:HG	2.20	0.42
2:I:84:ASP:OD2	2:I:154:GLY:N	2.48	0.42
2:O:107:CYS:HB2	2:O:241:MET:SD	2.60	0.42
2:I:119:GLN:O	2:I:222:LEU:HA	2.20	0.41
1:K:221:GLN:HG3	1:K:222:LYS:H	1.85	0.41
3:D:90:VAL:HG12	3:D:125:TRP:HZ2	1.85	0.41
1:H:140:GLY:HA2	1:H:141:PRO:HD3	1.89	0.41
2:F:71:TRP:HB3	2:F:232:ILE:O	2.20	0.41
1:H:114:SER:OG	1:H:170:PRO:O	2.29	0.41
1:K:145:ASP:O	1:K:148:THR:OG1	2.30	0.41
2:L:152:GLN:HG2	2:L:210:CYS:SG	2.60	0.41
1:B:67:GLU:HG2	1:B:70:ARG:CZ	2.50	0.41
3:D:173:PRO:HB2	1:H:228:LEU:HD21	2.01	0.41
1:E:16:THR:HG21	3:M:193:PRO:HG3	2.01	0.41
2:F:23:ILE:HG22	2:F:24:THR:H	1.84	0.41
1:H:130:LYS:O	1:H:199:GLN:HB3	2.20	0.41
2:I:111:GLN:O	2:I:235:THR:N	2.52	0.41
1:E:42:ASN:ND2	3:D:78:THR:OG1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:124:SER:O	2:L:186:ARG:NH2	2.53	0.41
2:C:162:HIS:HA	2:C:163:PRO:HD2	1.95	0.41
2:C:18:ILE:O	2:C:20:ASN:N	2.53	0.41
1:H:122:THR:HA	2:I:184:ASN:ND2	2.29	0.41
3:J:136:ARG:NE	3:J:287:TYR:CE2	2.88	0.41
2:O:164:TYR:O	2:O:171:PRO:HA	2.20	0.41
2:I:81:LYS:HD2	2:I:151:THR:O	2.20	0.41
2:O:239:ALA:HA	2:O:240:PRO:HD3	1.92	0.41
2:O:152:GLN:HG2	2:O:210:CYS:SG	2.61	0.41
3:D:84:PHE:HE1	3:D:138:LYS:HG2	1.85	0.41
3:M:285:GLN:HA	3:M:301:LYS:HE3	2.02	0.41
3:J:189:THR:O	3:J:191:THR:N	2.52	0.41
2:I:188:ASN:C	2:I:188:ASN:OD1	2.58	0.41
3:M:192:ASN:OD1	3:M:192:ASN:N	2.52	0.41
1:B:122:THR:OG1	1:B:213:TYR:O	2.22	0.41
2:I:23:ILE:HG22	2:I:24:THR:H	1.85	0.41
3:G:189:THR:HG23	3:G:192:ASN:OD1	2.19	0.41
1:E:124:SER:OG	1:E:125:PHE:N	2.53	0.41
2:C:106:PHE:N	2:C:195:VAL:O	2.46	0.41
3:G:77:GLU:OE1	1:H:227:GLN:HA	2.21	0.41
2:I:104:SER:OG	2:I:105:GLY:N	2.52	0.41
1:B:122:THR:O	2:C:119:GLN:HB2	2.21	0.41
3:G:128:ASP:HB2	3:G:130:THR:HG22	2.02	0.41
3:M:144:TYR:OH	2:O:129:GLU:OE2	2.37	0.41
3:G:277:TRP:HB3	3:G:278:ILE:H	1.63	0.41
3:A:306:SER:HB3	1:B:57:ASN:HB3	2.02	0.41
3:M:281:PRO:HB3	2:O:174:GLN:HB2	2.02	0.41
1:H:145:ASP:O	1:H:148:THR:OG1	2.39	0.41
1:B:22:ALA:HA	1:B:23:PRO:HD3	1.74	0.41
3:A:84:PHE:O	3:A:86:ARG:N	2.49	0.41
2:C:82:PHE:CE1	2:C:238:LEU:HD22	2.54	0.41
3:A:172:VAL:HA	3:A:173:PRO:HD2	1.82	0.41
2:L:86:LEU:HD11	2:L:238:LEU:HD11	2.02	0.41
1:N:7:LYS:HE2	1:N:7:LYS:HB3	1.82	0.41
3:A:137:ARG:NH2	1:B:103:GLN:OE1	2.54	0.41
1:E:21:SER:OG	3:D:205:GLN:OE1	2.39	0.41
3:G:275:ARG:HH21	1:H:39:GLU:CD	2.22	0.41
1:N:120:MET:HE1	2:O:182:TRP:CD2	2.55	0.41
3:M:172:VAL:HA	3:M:173:PRO:HD2	1.86	0.41
1:N:146:ARG:HA	1:N:149:ALA:HB3	2.02	0.41
3:J:143:THR:HB	3:J:278:ILE:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:189:THR:HG23	3:D:192:ASN:OD1	2.20	0.41
3:M:150:GLU:HA	3:M:207:SER:HA	2.02	0.41
1:N:54:GLU:HG3	1:N:98:SER:HB3	2.03	0.41
3:D:171:PHE:HD2	3:D:249:PHE:CE1	2.39	0.41
2:F:68:THR:HG22	2:F:235:THR:HA	2.02	0.41
1:N:36:ILE:HA	1:N:37:PRO:HD3	1.95	0.41
1:E:133:ILE:HG22	1:E:167:LEU:HD22	2.02	0.41
3:M:165:GLN:OE1	3:M:166:LEU:N	2.46	0.41
2:F:23:ILE:HD11	2:F:63:PHE:CG	2.55	0.41
1:N:14:LEU:HD23	1:N:17:ASP:HB3	2.03	0.41
2:C:23:ILE:HD11	2:C:63:PHE:CD1	2.55	0.41
2:I:44:ASP:OD1	2:I:44:ASP:N	2.53	0.41
3:A:249:PHE:HD1	3:A:249:PHE:HA	1.77	0.41
3:A:297:GLY:H	2:C:135:VAL:HG13	1.86	0.40
2:F:174:GLN:HB2	3:D:281:PRO:HB3	2.02	0.40
2:C:100:TYR:CD1	2:C:101:LEU:HD13	2.55	0.40
3:A:86:ARG:HH21	3:A:138:LYS:NZ	2.20	0.40
3:D:187:TRP:CG	3:D:252:ARG:HD2	2.56	0.40
1:H:100:LEU:HA	1:H:100:LEU:HD12	1.95	0.40
1:N:142:LEU:HA	1:N:143:PRO:HD2	1.94	0.40
1:E:52:ILE:HB	2:F:173:SER:HA	2.03	0.40
2:O:94:GLN:C	2:O:96:ALA:H	2.25	0.40
2:I:14:ALA:HB2	2:I:26:GLN:NE2	2.37	0.40
2:I:188:ASN:OD1	2:I:189:ASN:N	2.54	0.40
3:M:173:PRO:HD2	3:M:192:ASN:HB3	2.04	0.40
2:I:109:HIS:N	2:I:237:THR:O	2.53	0.40
2:L:23:ILE:HG22	2:L:24:THR:H	1.86	0.40
1:B:114:SER:HB2	1:B:221:GLN:CB	2.50	0.40
1:B:14:LEU:HG	1:B:16:THR:H	1.87	0.40
2:L:103:ARG:HD2	2:L:202:PRO:O	2.21	0.40
2:C:103:ARG:HG3	2:C:197:TYR:CG	2.56	0.40
1:H:130:LYS:HG2	1:H:158:ASP:HA	2.03	0.40
2:L:81:LYS:O	2:L:85:VAL:HG23	2.21	0.40
3:G:133:ALA:HA	1:H:236:LEU:HD13	2.03	0.40
2:I:103:ARG:HG3	2:I:197:TYR:CG	2.56	0.40
2:L:249:ARG:HG3	2:L:250:GLN:O	2.22	0.40
3:M:285:GLN:NE2	2:O:165:VAL:HG11	2.37	0.40
1:K:49:VAL:HG11	2:L:177:VAL:HA	2.03	0.40
2:O:33:VAL:HG21	2:O:181:GLN:HG2	2.04	0.40
2:F:81:LYS:HD3	3:D:222:ASP:OD2	2.22	0.40

There are no symmetry-related clashes.

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	B	219/242 (90%)	193 (88%)	23 (10%)	3 (1%)	14	59
1	E	219/242 (90%)	192 (88%)	25 (11%)	2 (1%)	21	68
1	H	219/242 (90%)	191 (87%)	26 (12%)	2 (1%)	21	68
1	K	219/242 (90%)	193 (88%)	24 (11%)	2 (1%)	21	68
1	N	219/242 (90%)	194 (89%)	22 (10%)	3 (1%)	14	59
2	C	232/323 (72%)	195 (84%)	30 (13%)	7 (3%)	5	46
2	F	232/323 (72%)	200 (86%)	29 (12%)	3 (1%)	15	61
2	I	232/323 (72%)	201 (87%)	26 (11%)	5 (2%)	8	52
2	L	232/323 (72%)	203 (88%)	24 (10%)	5 (2%)	8	52
2	O	232/323 (72%)	201 (87%)	26 (11%)	5 (2%)	8	52
3	A	217/313 (69%)	192 (88%)	20 (9%)	5 (2%)	8	51
3	D	217/313 (69%)	193 (89%)	20 (9%)	4 (2%)	11	55
3	G	217/313 (69%)	192 (88%)	20 (9%)	5 (2%)	8	51
3	J	217/313 (69%)	189 (87%)	22 (10%)	6 (3%)	6	47
3	M	217/313 (69%)	188 (87%)	24 (11%)	5 (2%)	8	51
All	All	3340/4390 (76%)	2917 (87%)	361 (11%)	62 (2%)	10	54

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	205	PRO
2	F	211	ASN
3	D	130	THR
3	M	130	THR
3	J	234	LYS
3	J	235	ASP
1	N	205	PRO
1	B	205	PRO

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Mol	Chain	Res	Type
1	H	205	PRO
1	K	205	PRO
2	O	211	ASN
2	C	13	VAL
2	C	26	GLN
2	C	211	ASN
2	I	211	ASN
2	L	211	ASN
2	F	19	GLY
3	A	130	THR
3	A	231	LYS
3	A	232	GLN
3	G	130	THR
3	G	231	LYS
3	G	232	GLN
3	J	130	THR
1	H	94	GLY
2	O	31	ILE
2	C	19	GLY
2	I	19	GLY
2	I	31	ILE
2	L	19	GLY
3	M	231	LYS
3	G	235	ASP
2	C	12	ARG
2	C	14	ALA
2	I	140	GLY
2	I	229	THR
3	M	132	TYR
3	M	233	GLU
3	G	132	TYR
1	N	11	ASN
1	N	94	GLY
1	B	94	GLY
1	K	94	GLY
2	O	95	ASN
2	L	229	THR
1	E	94	GLY
3	D	222	ASP
3	A	132	TYR
3	J	132	TYR
3	J	229	GLU

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Mol	Chain	Res	Type
1	B	11	ASN
2	O	229	THR
2	C	229	THR
2	L	61	ASN
2	L	95	ASN
2	F	229	THR
3	D	132	TYR
3	A	222	ASP
3	D	131	GLY
2	O	19	GLY
3	M	131	GLY
3	J	131	GLY

5.3.2 Protein sidechains (i)

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	B	187/202 (93%)	183 (98%)	4 (2%)	61	86
1	E	187/202 (93%)	185 (99%)	2 (1%)	80	92
1	H	187/202 (93%)	183 (98%)	4 (2%)	61	86
1	K	187/202 (93%)	184 (98%)	3 (2%)	70	89
1	N	187/202 (93%)	185 (99%)	2 (1%)	80	92
2	C	200/272 (74%)	195 (98%)	5 (2%)	55	83
2	F	200/272 (74%)	198 (99%)	2 (1%)	82	92
2	I	200/272 (74%)	193 (96%)	7 (4%)	43	78
2	L	200/272 (74%)	197 (98%)	3 (2%)	72	90
2	O	200/272 (74%)	193 (96%)	7 (4%)	43	78
3	A	190/265 (72%)	183 (96%)	7 (4%)	41	76
3	D	190/265 (72%)	186 (98%)	4 (2%)	61	86
3	G	190/265 (72%)	181 (95%)	9 (5%)	32	72
3	J	190/265 (72%)	185 (97%)	5 (3%)	54	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	M	190/265 (72%)	186 (98%)	4 (2%)	61 86
All	All	2885/3695 (78%)	2817 (98%)	68 (2%)	57 84

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	70	ARG
1	E	161	LEU
2	F	35	TYR
2	F	248	LEU
3	D	77	GLU
3	D	245	MET
3	D	249	PHE
3	D	310	ILE
3	M	201	ASP
3	M	227	PHE
3	M	249	PHE
3	M	290	LYS
3	A	130	THR
3	A	163	VAL
3	A	206	VAL
3	A	229	GLU
3	A	249	PHE
3	A	253	THR
3	A	258	LYS
3	G	81	ASP
3	G	122	TYR
3	G	130	THR
3	G	227	PHE
3	G	229	GLU
3	G	253	THR
3	G	283	ARG
3	G	308	THR
3	G	310	ILE
3	J	146	ARG
3	J	192	ASN
3	J	249	PHE
3	J	253	THR
3	J	310	ILE
1	N	79	LYS
1	N	161	LEU
1	B	10	THR

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Mol	Chain	Res	Type
1	B	33	CYS
1	B	35	HIS
1	B	79	LYS
1	H	60	THR
1	H	70	ARG
1	H	79	LYS
1	H	97	GLN
1	K	79	LYS
1	K	161	LEU
1	K	235	ILE
2	O	35	TYR
2	O	76	LYS
2	O	95	ASN
2	O	100	TYR
2	O	101	LEU
2	O	142	GLU
2	O	248	LEU
2	C	23	ILE
2	C	31	ILE
2	C	35	TYR
2	C	62	ARG
2	C	101	LEU
2	I	13	VAL
2	I	20	ASN
2	I	23	ILE
2	I	35	TYR
2	I	101	LEU
2	I	104	SER
2	I	180	HIS
2	L	23	ILE
2	L	35	TYR
2	L	181	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	227	GLN
2	F	26	GLN
2	F	199	ASN
3	D	134	GLN
3	D	243	ASN
3	M	205	GLN

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Mol	Chain	Res	Type
3	A	244	ASN
3	J	205	GLN
1	N	237	GLN
2	C	30	ASN
2	C	209	HIS
2	C	211	ASN
2	I	30	ASN
2	I	181	GLN
2	L	97	GLN
2	L	181	GLN
2	L	209	HIS

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	B	223/242 (92%)	-0.11	7 (3%)	52	36	80, 97, 139, 197	0
1	E	223/242 (92%)	-0.14	4 (1%)	71	56	80, 95, 135, 176	0
1	H	223/242 (92%)	-0.15	2 (0%)	85	74	80, 96, 135, 179	0
1	K	223/242 (92%)	-0.11	2 (0%)	85	74	80, 97, 140, 188	0
1	N	223/242 (92%)	-0.21	4 (1%)	71	56	80, 97, 134, 201	0
2	C	236/323 (73%)	0.19	18 (7%)	17	10	78, 105, 203, 251	0
2	F	236/323 (73%)	0.30	20 (8%)	13	9	78, 103, 198, 239	0
2	I	236/323 (73%)	0.24	18 (7%)	17	10	78, 105, 205, 239	0
2	L	236/323 (73%)	0.25	19 (8%)	15	9	78, 107, 203, 235	0
2	O	236/323 (73%)	0.20	13 (5%)	29	19	78, 105, 205, 234	0
3	A	221/313 (70%)	-0.02	9 (4%)	41	27	75, 95, 166, 239	0
3	D	221/313 (70%)	0.05	11 (4%)	32	21	75, 93, 164, 211	0
3	G	221/313 (70%)	-0.10	10 (4%)	37	24	75, 95, 167, 237	0
3	J	221/313 (70%)	0.06	12 (5%)	29	19	75, 95, 170, 255	0
3	M	221/313 (70%)	-0.00	7 (3%)	51	35	75, 95, 159, 219	0
All	All	3400/4390 (77%)	0.03	156 (4%)	36	24	75, 97, 184, 255	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	233	GLU	9.8
2	F	141	THR	8.2
2	F	143	ASP	7.4
3	J	235	ASP	7.0
2	C	139	THR	6.2
2	I	141	THR	6.2
2	F	142	GLU	6.1

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Mol	Chain	Res	Type	RSRZ
2	C	140	GLY	5.7
2	C	141	THR	5.6
3	J	232	GLN	5.4
2	L	142	GLU	5.4
3	J	234	LYS	5.3
2	O	29	ALA	5.2
2	I	143	ASP	5.2
2	F	140	GLY	5.2
3	J	228	GLY	5.1
2	O	250	GLN	5.1
1	K	238	THR	5.0
2	L	14	ALA	4.9
1	B	174	ASN	4.9
2	I	252	VAL	4.8
3	G	233	GLU	4.8
2	O	14	ALA	4.7
2	F	144	SER	4.7
2	C	142	GLU	4.6
2	F	11	ASP	4.5
3	G	234	LYS	4.4
3	G	232	GLN	4.4
2	L	137	GLY	4.4
1	B	238	THR	4.4
3	M	235	ASP	4.3
2	C	251	ALA	4.3
2	O	139	THR	4.3
2	F	251	ALA	4.1
2	L	143	ASP	4.1
2	I	11	ASP	4.1
2	C	252	VAL	4.1
2	L	250	GLN	4.1
2	O	251	ALA	4.0
2	O	143	ASP	4.0
2	I	251	ALA	3.9
2	I	142	GLU	3.9
3	G	73	HIS	3.9
2	L	140	GLY	3.8
3	A	232	GLN	3.8
3	D	233	GLU	3.8
1	H	238	THR	3.7
2	F	250	GLN	3.7
2	I	140	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
2	O	27	GLU	3.6
2	L	138	GLY	3.6
3	A	228	GLY	3.6
2	I	14	ALA	3.6
3	J	226	THR	3.6
2	O	28	ALA	3.6
2	L	15	GLN	3.6
1	N	238	THR	3.6
3	G	226	THR	3.5
3	M	234	LYS	3.5
3	G	230	HIS	3.5
2	L	141	THR	3.5
3	M	233	GLU	3.5
2	F	139	THR	3.5
2	C	28	ALA	3.4
3	D	120	ASN	3.4
3	A	233	GLU	3.4
3	M	230	HIS	3.4
2	L	139	THR	3.3
3	G	231	LYS	3.3
2	L	144	SER	3.3
3	A	119	PRO	3.2
2	L	11	ASP	3.2
3	D	232	GLN	3.2
3	G	235	ASP	3.2
3	D	235	ASP	3.1
1	N	174	ASN	3.1
2	C	14	ALA	3.1
3	A	229	GLU	3.1
1	B	237	GLN	3.0
2	O	138	GLY	3.0
2	C	138	GLY	3.0
2	L	136	ALA	3.0
2	F	14	ALA	3.0
2	O	141	THR	3.0
2	F	136	ALA	3.0
2	O	140	GLY	3.0
2	I	246	ALA	2.9
2	I	247	GLY	2.8
2	F	45	SER	2.8
1	K	174	ASN	2.8
2	O	142	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	135	VAL	2.8
2	C	143	ASP	2.8
2	F	137	GLY	2.8
2	C	225	ASP	2.7
2	C	57	ASP	2.7
2	L	45	SER	2.7
2	F	42	CYS	2.7
3	M	227	PHE	2.7
2	I	26	GLN	2.7
1	B	236	LEU	2.6
1	E	1	GLY	2.6
2	C	226	GLN	2.6
2	I	15	GLN	2.6
2	L	28	ALA	2.6
3	J	313	LEU	2.6
2	I	59	SER	2.6
1	B	41	ARG	2.5
2	C	136	ALA	2.5
3	D	236	LEU	2.5
3	J	124	ASN	2.5
2	I	139	THR	2.5
3	M	228	GLY	2.5
2	C	29	ALA	2.5
2	F	44	ASP	2.5
3	G	225	PRO	2.5
3	D	228	GLY	2.5
2	L	47	ALA	2.5
2	F	57	ASP	2.5
3	M	229	GLU	2.5
2	F	55	ARG	2.4
3	D	313	LEU	2.4
3	D	234	LYS	2.4
1	E	2	PHE	2.4
2	L	135	VAL	2.4
2	O	11	ASP	2.4
3	D	308	THR	2.4
2	I	45	SER	2.3
2	F	47	ALA	2.3
1	E	174	ASN	2.3
2	F	46	ASP	2.3
3	A	120	ASN	2.3
3	G	236	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	I	55	ARG	2.3
1	B	2	PHE	2.3
2	L	30	ASN	2.2
3	A	236	LEU	2.2
3	J	231	LYS	2.2
3	D	237	GLU	2.2
3	A	231	LYS	2.2
1	N	233	SER	2.2
2	C	137	GLY	2.2
3	J	122	TYR	2.2
2	I	29	ALA	2.2
3	A	230	HIS	2.2
2	L	29	ALA	2.2
2	F	32	ILE	2.1
1	H	61	ASN	2.1
2	I	24	THR	2.1
3	J	236	LEU	2.1
1	E	85	VAL	2.1
1	B	235	ILE	2.1
3	D	180	ASP	2.1
1	N	41	ARG	2.0
2	C	27	GLU	2.0
3	J	230	HIS	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.