



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:03 AM GMT

PDB ID : 3H06
Title : Crystal structure of the binding domain of the AMPA subunit GluR2 bound to the willardiine antagonist, UBP282
Authors : Ahmed, A.H.; Oswald, R.E.
Deposited on : 2009-04-08
Resolution : 2.80 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

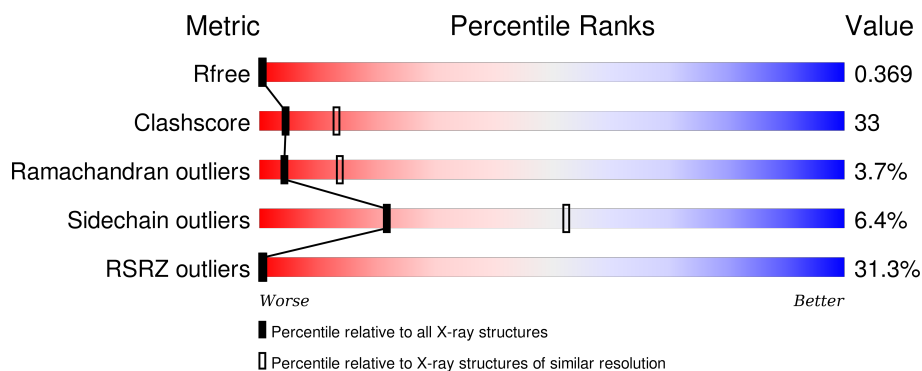
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	B	258	<div> <div>30%</div> <div>53%</div> <div>43%</div> <div>.</div> </div>
1	E	258	<div> <div>37%</div> <div>45%</div> <div>48%</div> <div>6%</div> </div>
1	G	258	<div> <div>25%</div> <div>57%</div> <div>38%</div> <div>5%</div> </div>
1	H	258	<div> <div>34%</div> <div>47%</div> <div>45%</div> <div>7%</div> </div>
1	J	258	<div> <div>30%</div> <div>51%</div> <div>43%</div> <div>5%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	L	258	
1	N	258	
1	P	258	

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
2	VBP	B	807	X	-	-	-
2	VBP	E	808	X	-	-	-
2	VBP	G	803	X	-	-	-
2	VBP	H	806	X	-	-	-
2	VBP	J	804	X	-	-	-
2	VBP	L	801	X	-	-	-
2	VBP	N	802	X	-	-	-
2	VBP	P	805	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16564 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 Glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	257	Total	C	N	O	S	0	0	0
			2010	1280	334	382	14			
1	B	257	Total	C	N	O	S	0	0	0
			2010	1280	334	382	14			
1	E	257	Total	C	N	O	S	0	0	0
			2010	1280	334	382	14			
1	H	257	Total	C	N	O	S	0	0	0
			2010	1280	334	382	14			
1	J	257	Total	C	N	O	S	0	0	0
			2010	1280	334	382	14			
1	L	257	Total	C	N	O	S	0	0	0
			2010	1280	334	382	14			
1	N	257	Total	C	N	O	S	0	0	0
			2010	1280	334	382	14			
1	P	257	Total	C	N	O	S	0	0	0
			2010	1280	334	382	14			

There are 16 discrepancies between the modelled and reference sequences:

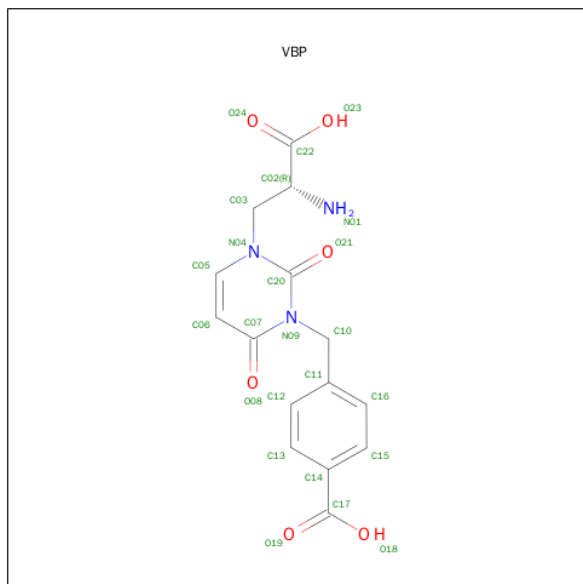
Chain	Residue	Modelled	Actual	Comment	Reference
G	118	GLY	-	LINKER	UNP P19491
G	119	THR	-	LINKER	UNP P19491
B	118	GLY	-	LINKER	UNP P19491
B	119	THR	-	LINKER	UNP P19491
E	118	GLY	-	LINKER	UNP P19491
E	119	THR	-	LINKER	UNP P19491
H	118	GLY	-	LINKER	UNP P19491
H	119	THR	-	LINKER	UNP P19491
J	118	GLY	-	LINKER	UNP P19491
J	119	THR	-	LINKER	UNP P19491
L	118	GLY	-	LINKER	UNP P19491
L	119	THR	-	LINKER	UNP P19491
N	118	GLY	-	LINKER	UNP P19491

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
N	119	THR	-	LINKER	UNP P19491
P	118	GLY	-	LINKER	UNP P19491
P	119	THR	-	LINKER	UNP P19491

- Molecule 2 is 4-({3-[(2R)-2-AMINO-2-CARBOXYETHYL]-2,6-DIOXO-3,6-DIHYDRO PYRIMIDIN-1(2H)-YL} METHYL) BENZOIC ACID (three-letter code: VBP) (formula: C₁₅H₁₅N₃O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	G	1	Total	C	N	O	0	0
			24	15	3	6		
2	B	1	Total	C	N	O	0	0
			24	15	3	6		
2	E	1	Total	C	N	O	0	0
			24	15	3	6		
2	H	1	Total	C	N	O	0	0
			24	15	3	6		
2	J	1	Total	C	N	O	0	0
			24	15	3	6		
2	L	1	Total	C	N	O	0	0
			24	15	3	6		
2	N	1	Total	C	N	O	0	0
			24	15	3	6		
2	P	1	Total	C	N	O	0	0
			24	15	3	6		

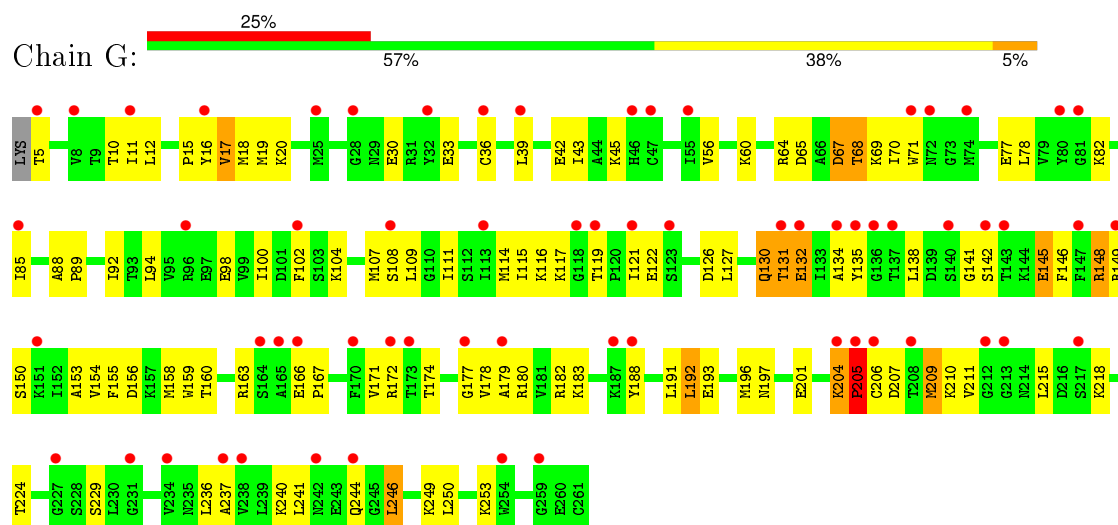
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	39	Total 39	O 39	0	0
3	B	42	Total 42	O 42	0	0
3	E	30	Total 30	O 30	0	0
3	H	30	Total 30	O 30	0	0
3	J	43	Total 43	O 43	0	0
3	L	34	Total 34	O 34	0	0
3	N	39	Total 39	O 39	0	0
3	P	35	Total 35	O 35	0	0

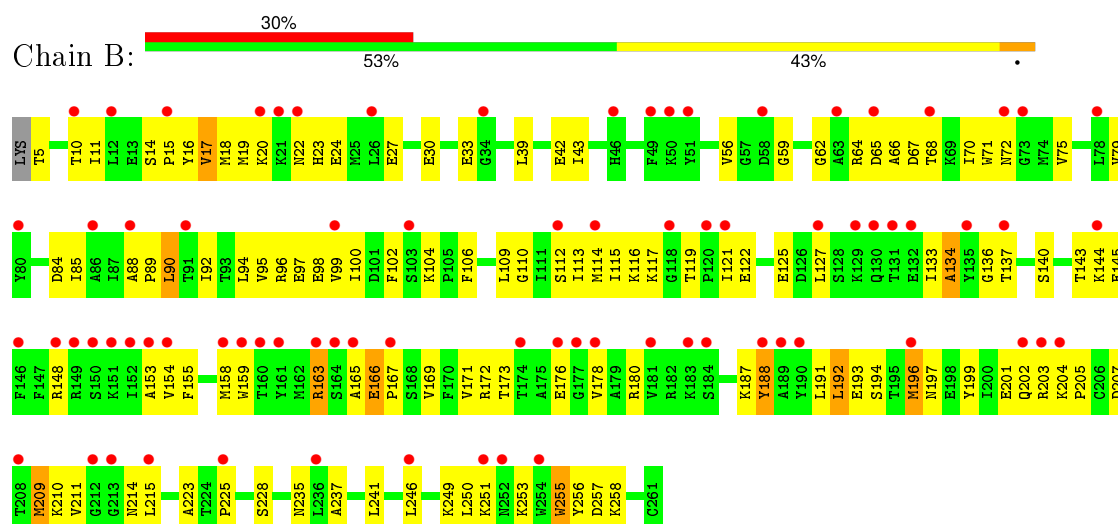
3 Residue-property plots

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: Glutamate receptor 2

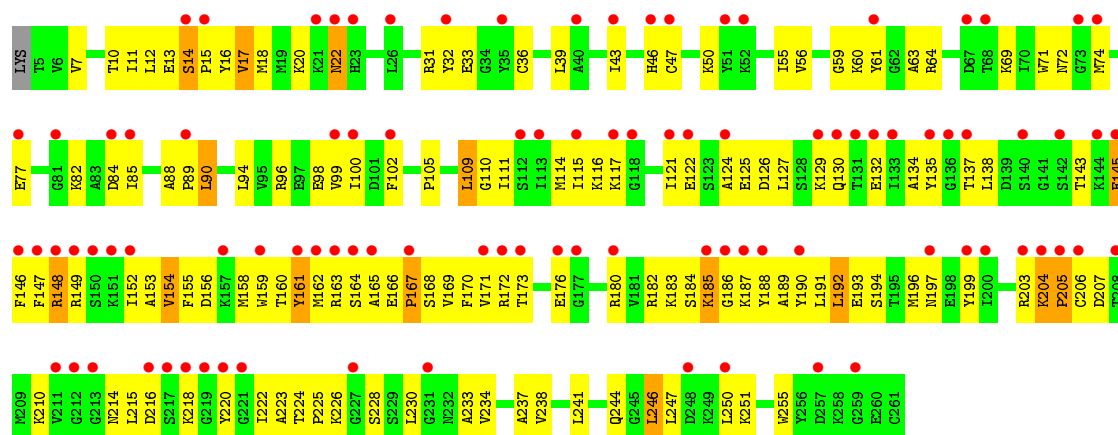


• Molecule 1: Glutamate receptor 2

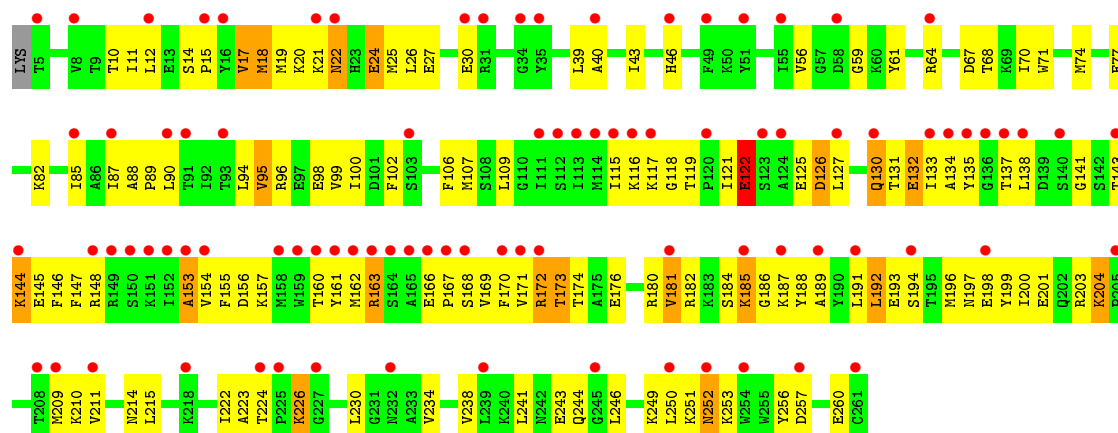


• Molecule 1: Glutamate receptor 2

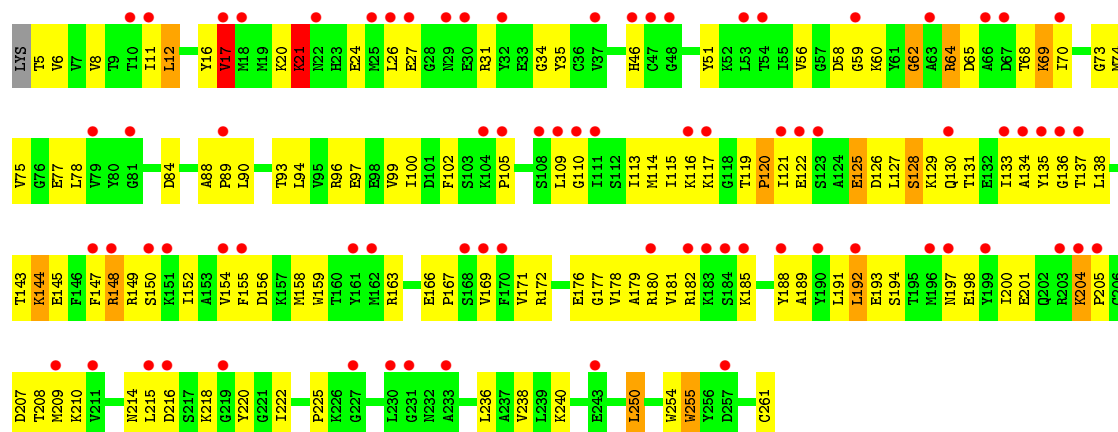




• Molecule 1: Glutamate receptor 2

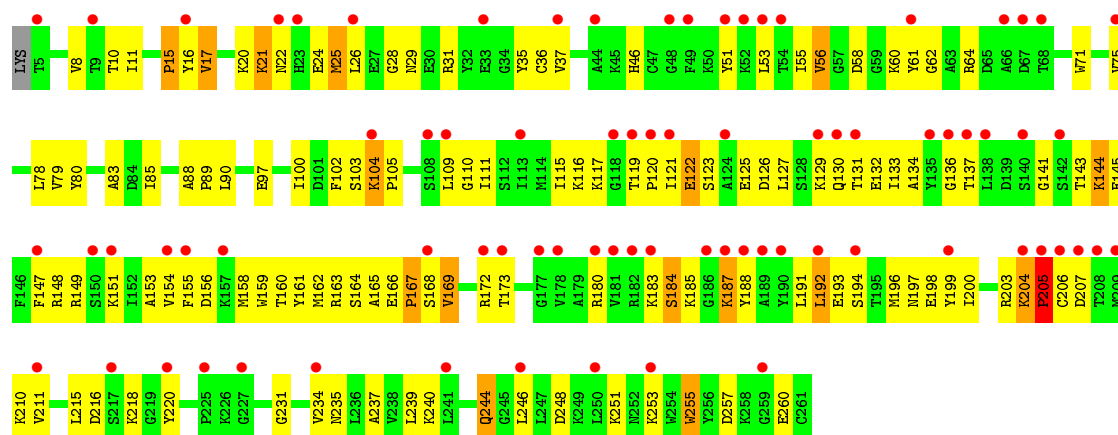


• Molecule 1: Glutamate receptor 2

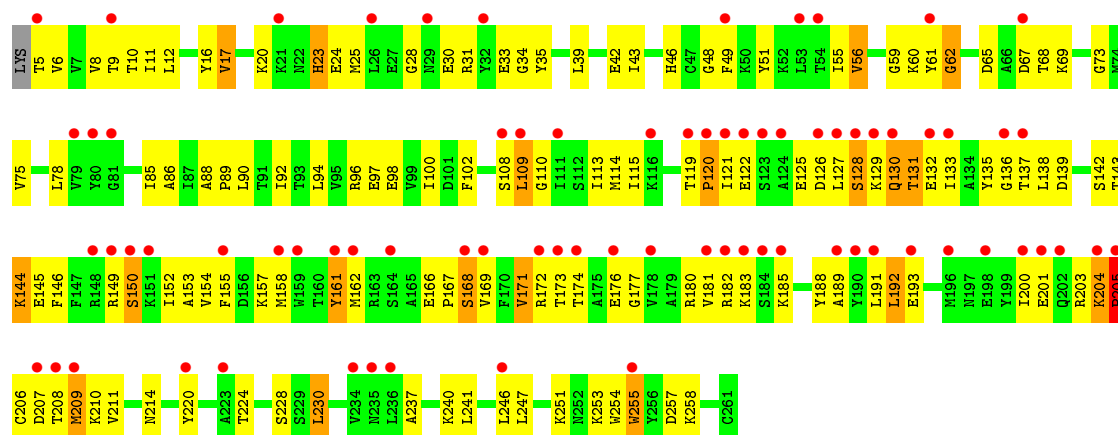


• Molecule 1: Glutamate receptor 2

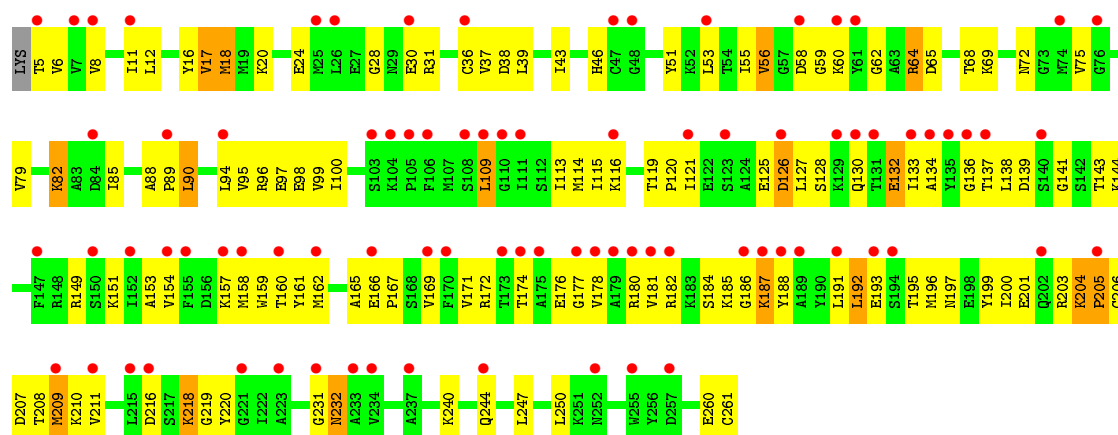




• Molecule 1: Glutamate receptor 2



• Molecule 1: Glutamate receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	91.01Å 90.92Å 92.51Å 85.61° 85.52° 72.40°	Depositor
Resolution (Å)	39.71 – 2.80 39.71 – 2.78	Depositor EDS
% Data completeness (in resolution range)	93.5 (39.71-2.80) 89.8 (39.71-2.78)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	64.73 (at 2.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.230 , 0.295 0.377 , 0.369	Depositor DCC
R_{free} test set	3242 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 16.5	EDS
Estimated twinning fraction	0.349 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.62$, $\langle L^2 \rangle = 0.49$	Xtriage
Outliers	0 of 64109 reflections	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	16564	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.87% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: VBP

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	0.41	0/2046	0.64	0/2751
1	E	0.41	0/2046	0.63	0/2751
1	G	0.41	0/2046	0.65	0/2751
1	H	0.41	0/2046	0.61	0/2751
1	J	0.40	0/2046	0.62	0/2751
1	L	0.41	0/2046	0.62	0/2751
1	N	0.39	0/2046	0.62	0/2751
1	P	0.40	0/2046	0.64	0/2751
All	All	0.40	0/16368	0.63	0/22008

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2010	0	2037	133	0
1	E	2010	0	2037	140	0
1	G	2010	0	2037	116	0
1	H	2010	0	2037	139	0
1	J	2010	0	2037	134	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2010	0	2037	137	0
1	N	2010	0	2037	129	0
1	P	2010	0	2037	155	0
2	B	24	0	13	3	0
2	E	24	0	13	4	0
2	G	24	0	13	5	0
2	H	24	0	13	3	0
2	J	24	0	13	4	0
2	L	24	0	13	2	0
2	N	24	0	13	3	0
2	P	24	0	13	5	0
3	B	42	0	0	8	0
3	E	30	0	0	6	0
3	G	39	0	0	4	0
3	H	30	0	0	6	0
3	J	43	0	0	9	0
3	L	34	0	0	1	0
3	N	39	0	0	7	0
3	P	35	0	0	10	0
All	All	16564	0	16400	1065	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 33.

All (1065) 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)
1:E:204:LYS:HB3	1:E:205:PRO:HD2	1.12	1.11
1:L:204:LYS:HB3	1:L:205:PRO:HD2	1.09	1.09
1:P:204:LYS:HB3	1:P:205:PRO:HD2	1.31	1.09
1:H:173:THR:HG23	1:H:176:GLU:HB2	1.36	1.07
1:G:204:LYS:HB3	1:G:205:PRO:HD2	1.11	1.06
1:N:204:LYS:HB3	1:N:205:PRO:HD2	1.07	1.04
1:N:204:LYS:HB3	1:N:205:PRO:CD	1.91	1.01
1:J:21:LYS:HD3	1:J:21:LYS:H	1.28	0.99
1:B:95:VAL:HG11	1:E:69:LYS:HD3	1.42	0.99
1:L:104:LYS:H	1:L:104:LYS:NZ	1.61	0.97
1:L:104:LYS:HZ3	1:L:104:LYS:H	1.01	0.96
1:L:104:LYS:N	1:L:104:LYS:HZ3	1.62	0.96
1:G:117:LYS:HE2	1:G:209:MET:HE3	1.49	0.94
1:E:185:LYS:HB2	1:E:187:LYS:HE2	1.50	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:LYS:HB3	1:E:205:PRO:CD	1.99	0.92
1:L:204:LYS:HB3	1:L:205:PRO:CD	1.98	0.91
1:L:130:GLN:HE21	1:L:132:GLU:HB3	1.36	0.91
1:G:114:MET:HE1	1:G:178:VAL:HG13	1.52	0.90
1:H:116:LYS:HE2	1:N:25:MET:O	1.72	0.89
1:L:204:LYS:CB	1:L:205:PRO:HD2	2.01	0.89
1:J:21:LYS:CD	1:J:21:LYS:H	1.83	0.89
1:B:121:ILE:HD13	1:B:127:LEU:HD21	1.56	0.88
1:J:117:LYS:HA	1:J:209:MET:HE3	1.53	0.88
1:L:187:LYS:HE3	1:L:188:TYR:N	1.89	0.87
1:G:204:LYS:HB3	1:G:205:PRO:CD	2.01	0.87
1:N:150:SER:HA	3:N:285:HOH:O	1.75	0.86
1:E:204:LYS:CB	1:E:205:PRO:HD2	2.01	0.85
1:N:130:GLN:NE2	1:N:132:GLU:HB3	1.89	0.85
1:P:116:LYS:HE3	1:P:207:ASP:HB2	1.56	0.84
1:G:89:PRO:HB2	2:G:803:VBP:H05	1.56	0.83
1:E:172:ARG:HB3	1:E:176:GLU:OE1	1.78	0.83
1:P:204:LYS:CB	1:P:205:PRO:HD2	2.08	0.82
1:G:204:LYS:CB	1:G:205:PRO:HD2	2.03	0.82
1:B:39:LEU:O	1:B:43:ILE:HG12	1.78	0.82
1:H:64:ARG:NH1	1:H:71:TRP:HE1	1.78	0.81
1:J:204:LYS:HB3	1:J:205:PRO:HD3	1.63	0.81
1:B:122:GLU:HA	1:B:211:VAL:HG21	1.63	0.80
1:B:89:PRO:HB2	2:B:807:VBP:H05	1.63	0.80
1:E:99:VAL:HG23	1:E:100:ILE:HG23	1.63	0.80
1:G:130:GLN:OE1	1:G:132:GLU:HB3	1.82	0.79
1:P:204:LYS:HB3	1:P:205:PRO:CD	2.12	0.79
1:E:88:ALA:HB1	1:E:89:PRO:HD2	1.62	0.79
1:H:160:THR:HA	1:H:163:ARG:NH1	1.97	0.79
1:E:152:ILE:HG22	1:E:154:VAL:HG23	1.63	0.78
1:E:10:THR:HA	1:E:74:MET:HE1	1.64	0.78
1:N:130:GLN:HE21	1:N:132:GLU:HB3	1.48	0.78
1:B:159:TRP:O	1:B:163:ARG:HB2	1.83	0.78
1:J:182:ARG:HH12	1:J:205:PRO:HB2	1.48	0.77
1:J:89:PRO:HB2	2:J:804:VBP:H05	1.66	0.76
1:P:82:LYS:NZ	1:P:82:LYS:HA	2.00	0.76
1:L:100:ILE:HD12	1:L:100:ILE:O	1.86	0.76
1:P:94:LEU:O	1:P:98:GLU:HG3	1.85	0.76
1:H:153:ALA:HA	3:H:289:HOH:O	1.85	0.76
1:E:22:ASN:H	1:E:22:ASN:HD22	1.31	0.75
1:L:22:ASN:HB2	1:L:25:MET:HG3	1.66	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:166:GLU:HA	1:J:167:PRO:C	2.07	0.75
1:G:122:GLU:HA	1:G:211:VAL:HG21	1.65	0.75
1:N:128:SER:OG	1:N:154:VAL:HG13	1.86	0.75
1:H:64:ARG:HH11	1:H:71:TRP:HE1	1.35	0.75
1:G:122:GLU:HG2	1:G:126:ASP:OD2	1.87	0.74
1:N:56:VAL:HG13	1:N:59:GLY:HA2	1.69	0.74
1:H:15:PRO:HA	1:H:18:MET:HE3	1.70	0.74
1:H:130:GLN:HE21	1:H:132:GLU:N	1.85	0.74
1:P:232:ASN:HD22	1:P:232:ASN:N	1.82	0.74
1:P:58:ASP:O	1:P:60:LYS:HG3	1.88	0.73
1:E:39:LEU:O	1:E:43:ILE:HG12	1.89	0.73
1:H:56:VAL:HG13	1:H:59:GLY:HA2	1.70	0.73
1:B:114:MET:HE1	1:B:178:VAL:HG13	1.70	0.73
1:N:115:ILE:HD13	1:N:211:VAL:HG11	1.71	0.73
1:B:140:SER:HA	1:B:144:LYS:NZ	2.03	0.73
1:L:46:HIS:CD2	1:L:240:LYS:HD2	2.24	0.73
1:H:88:ALA:HB1	1:H:89:PRO:HD2	1.69	0.73
1:P:46:HIS:CD2	1:P:240:LYS:HD2	2.24	0.73
1:B:166:GLU:HA	1:B:167:PRO:C	2.08	0.72
1:L:154:VAL:O	1:L:158:MET:HG3	1.88	0.72
1:E:224:THR:HG23	3:E:268:HOH:O	1.89	0.72
1:N:204:LYS:CB	1:N:205:PRO:HD2	2.02	0.72
1:J:148:ARG:HG3	1:J:149:ARG:N	2.04	0.72
1:B:144:LYS:HE3	1:B:148:ARG:HH22	1.54	0.71
1:L:160:THR:HA	1:L:163:ARG:NH1	2.05	0.71
1:L:111:ILE:HD11	1:L:143:THR:HA	1.73	0.71
1:G:68:THR:OG1	1:G:70:ILE:HB	1.91	0.71
1:H:181:VAL:O	1:H:181:VAL:HG12	1.90	0.71
1:G:138:LEU:HD22	2:G:803:VBP:H15	1.73	0.71
1:G:159:TRP:O	1:G:163:ARG:HB2	1.90	0.71
1:E:216:ASP:OD1	1:E:218:LYS:HE3	1.91	0.71
1:H:135:TYR:HB3	1:H:189:ALA:HB3	1.72	0.71
1:L:156:ASP:O	1:L:160:THR:HG23	1.90	0.71
1:L:21:LYS:H	1:L:21:LYS:HD3	1.56	0.70
1:B:241:LEU:HD22	1:B:246:LEU:CD2	2.21	0.70
1:E:20:LYS:HG2	1:E:31:ARG:O	1.91	0.70
1:B:241:LEU:HD22	1:B:246:LEU:HD23	1.74	0.70
1:N:154:VAL:O	1:N:158:MET:HG3	1.91	0.70
1:B:20:LYS:HG2	1:B:33:GLU:CD	2.12	0.70
1:G:145:GLU:HA	1:G:148:ARG:HG2	1.73	0.70
1:H:141:GLY:O	1:H:145:GLU:HG2	1.92	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:192:LEU:H	1:L:192:LEU:HD12	1.57	0.70
1:P:134:ALA:N	1:P:187:LYS:O	2.25	0.70
1:L:166:GLU:HA	1:L:167:PRO:C	2.12	0.70
1:N:162:MET:HE1	1:N:191:LEU:HD12	1.73	0.70
1:E:230:LEU:O	1:E:234:VAL:HG23	1.91	0.70
1:E:50:LYS:HE2	1:E:50:LYS:HA	1.73	0.70
1:J:261:CYS:HB3	3:J:300:HOH:O	1.92	0.70
1:N:135:TYR:HB3	1:N:189:ALA:HB3	1.74	0.69
1:L:184:SER:O	1:L:187:LYS:HE2	1.92	0.69
1:H:10:THR:HA	1:H:74:MET:HE1	1.74	0.69
1:P:121:ILE:HG22	1:P:126:ASP:HB3	1.73	0.69
1:E:193:GLU:HG3	3:E:279:HOH:O	1.92	0.69
1:L:187:LYS:NZ	1:L:188:TYR:HB3	2.08	0.69
1:N:137:THR:HG22	1:N:191:LEU:HB2	1.75	0.69
1:H:39:LEU:O	1:H:43:ILE:HG12	1.93	0.69
1:B:251:LYS:HE3	3:B:293:HOH:O	1.93	0.69
1:B:204:LYS:HB2	3:B:300:HOH:O	1.92	0.69
1:B:210:LYS:HD2	3:B:298:HOH:O	1.93	0.69
1:L:104:LYS:CE	1:L:104:LYS:H	2.04	0.68
1:P:64:ARG:HD3	1:P:69:LYS:HA	1.76	0.68
1:J:134:ALA:O	1:J:188:TYR:HA	1.94	0.68
1:L:130:GLN:NE2	1:L:133:ILE:HG13	2.07	0.68
1:E:172:ARG:HG2	1:E:173:THR:HG23	1.76	0.68
1:G:130:GLN:HA	1:G:130:GLN:HE21	1.58	0.68
1:H:230:LEU:O	1:H:234:VAL:HG23	1.94	0.68
1:L:125:GLU:OE2	1:L:154:VAL:HG21	1.93	0.67
1:N:89:PRO:HB2	2:N:802:VBP:H05	1.76	0.67
1:P:16:TYR:CD1	1:P:89:PRO:HG3	2.28	0.67
1:J:185:LYS:N	1:J:185:LYS:HD2	2.09	0.67
1:J:46:HIS:CD2	1:J:240:LYS:HD2	2.29	0.67
1:E:205:PRO:O	1:E:207:ASP:N	2.26	0.67
1:G:16:TYR:CD1	1:G:89:PRO:HG3	2.29	0.67
1:J:129:LYS:O	1:J:131:THR:N	2.28	0.67
1:G:193:GLU:HG3	3:G:264:HOH:O	1.94	0.66
1:E:203:ARG:O	1:E:204:LYS:O	2.13	0.66
1:E:156:ASP:O	1:E:160:THR:HG23	1.96	0.66
1:L:115:ILE:HG21	1:L:121:ILE:CD1	2.26	0.66
1:J:69:LYS:NZ	1:J:69:LYS:HB2	2.10	0.66
1:H:117:LYS:HA	1:H:209:MET:HE2	1.78	0.66
1:P:114:MET:HE1	1:P:178:VAL:HA	1.77	0.66
1:B:145:GLU:HG2	1:B:148:ARG:HH21	1.61	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:121:ILE:HG23	1:H:133:ILE:HD12	1.77	0.66
1:J:149:ARG:HG2	3:J:265:HOH:O	1.95	0.66
1:P:169:VAL:HA	1:P:180:ARG:HH12	1.61	0.66
1:P:193:GLU:H	2:P:805:VBP:H13	1.61	0.66
1:J:152:ILE:HB	1:J:155:PHE:HD2	1.60	0.66
1:E:14:SER:O	1:E:18:MET:SD	2.54	0.65
1:G:166:GLU:HA	1:G:167:PRO:C	2.17	0.65
1:G:180:ARG:HD2	1:G:188:TYR:CZ	2.31	0.65
1:L:203:ARG:O	1:L:204:LYS:O	2.15	0.65
1:N:152:ILE:HG22	3:N:280:HOH:O	1.95	0.65
1:L:244:GLN:HB3	1:L:246:LEU:HD13	1.79	0.65
1:N:110:GLY:HA3	1:N:214:ASN:HB3	1.78	0.65
1:J:35:TYR:CE1	1:J:250:LEU:HB3	2.30	0.65
1:N:121:ILE:HD13	1:N:127:LEU:CD2	2.27	0.65
1:B:251:LYS:O	1:B:255:TRP:HB2	1.97	0.65
1:B:95:VAL:HG11	1:E:69:LYS:CD	2.25	0.65
1:L:164:SER:O	1:L:165:ALA:HB3	1.97	0.65
1:J:64:ARG:HD3	1:J:69:LYS:HA	1.78	0.65
1:H:11:ILE:HG13	3:H:268:HOH:O	1.97	0.65
1:J:6:VAL:O	1:J:51:TYR:HA	1.97	0.65
1:B:154:VAL:O	1:B:158:MET:HG3	1.97	0.65
1:L:89:PRO:HB2	2:L:801:VBP:H05	1.79	0.65
1:H:197:ASN:ND2	1:H:210:LYS:HG3	2.12	0.64
1:E:154:VAL:O	1:E:158:MET:HG3	1.97	0.64
1:H:130:GLN:HG2	1:H:131:THR:N	2.11	0.64
1:J:148:ARG:HA	1:J:159:TRP:CD1	2.31	0.64
1:H:144:LYS:HE3	1:H:148:ARG:NH2	2.13	0.64
1:G:205:PRO:O	1:G:207:ASP:N	2.30	0.64
1:G:193:GLU:OE1	1:G:218:LYS:NZ	2.29	0.64
1:B:172:ARG:HB3	1:B:172:ARG:NH1	2.12	0.64
1:J:178:VAL:HG12	1:J:182:ARG:HE	1.61	0.64
1:P:138:LEU:HD11	1:P:172:ARG:O	1.97	0.64
1:G:193:GLU:HG2	2:G:803:VBP:H13	1.80	0.64
1:N:20:LYS:HG2	1:N:31:ARG:O	1.97	0.64
1:H:224:THR:HG23	3:H:287:HOH:O	1.98	0.64
1:N:158:MET:O	1:N:162:MET:HG3	1.98	0.64
1:L:10:THR:OG1	1:L:17:VAL:HG11	1.97	0.64
1:P:116:LYS:HG3	1:P:207:ASP:O	1.98	0.63
1:H:166:GLU:HA	1:H:167:PRO:C	2.18	0.63
1:J:90:LEU:O	1:J:220:TYR:HA	1.99	0.63
1:B:92:ILE:HG23	1:B:102:PHE:CD2	2.32	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:177:GLY:O	1:J:181:VAL:HG23	1.97	0.63
1:E:64:ARG:NH1	1:E:71:TRP:HE1	1.96	0.63
1:B:16:TYR:CD1	1:B:89:PRO:HG3	2.34	0.63
1:G:197:ASN:ND2	1:G:210:LYS:HG3	2.14	0.63
1:P:115:ILE:HB	1:P:119:THR:HB	1.81	0.63
1:N:157:LYS:HE3	1:N:161:TYR:CE1	2.34	0.63
1:B:19:MET:HG3	3:J:289:HOH:O	1.98	0.63
1:N:180:ARG:O	1:N:188:TYR:HD2	1.82	0.63
1:H:134:ALA:HB3	1:H:187:LYS:O	1.99	0.63
1:L:103:SER:HB2	1:L:104:LYS:HZ1	1.64	0.62
1:G:183:LYS:H	1:G:183:LYS:HD2	1.64	0.62
1:E:166:GLU:HA	1:E:167:PRO:C	2.20	0.62
1:P:199:TYR:HE1	1:P:203:ARG:NH1	1.96	0.62
1:N:16:TYR:CD1	1:N:89:PRO:HG3	2.34	0.62
1:H:163:ARG:HH11	1:H:163:ARG:CB	2.12	0.62
1:L:8:VAL:HG22	1:L:85:ILE:CG2	2.29	0.62
1:L:104:LYS:HE3	1:L:239:LEU:HG	1.81	0.62
1:L:192:LEU:HD13	1:L:197:ASN:HB2	1.82	0.62
1:H:180:ARG:HG2	1:H:188:TYR:CD2	2.34	0.62
1:N:144:LYS:HB3	1:N:144:LYS:NZ	2.15	0.62
1:L:137:THR:HG22	1:L:191:LEU:HB2	1.82	0.62
1:B:191:LEU:N	1:B:191:LEU:HD12	2.15	0.62
1:B:42:GLU:HG3	1:B:246:LEU:HD21	1.81	0.62
1:P:201:GLU:HG3	1:P:209:MET:HA	1.82	0.62
1:L:16:TYR:CD1	1:L:89:PRO:HG3	2.34	0.62
1:B:100:ILE:HD12	1:B:223:ALA:HB1	1.80	0.62
1:E:100:ILE:HD13	1:E:223:ALA:HB1	1.82	0.62
1:H:117:LYS:HG3	1:H:209:MET:HE2	1.82	0.62
1:J:110:GLY:HA3	1:J:214:ASN:HB3	1.82	0.62
1:N:251:LYS:HD2	1:N:255:TRP:CE3	2.34	0.62
1:E:138:LEU:HD22	2:E:808:VBP:H15	1.81	0.62
1:N:152:ILE:HB	1:N:155:PHE:CD2	2.35	0.62
1:L:172:ARG:HG2	1:L:173:THR:HG23	1.81	0.62
1:L:58:ASP:O	1:L:60:LYS:HG3	2.00	0.62
1:J:20:LYS:HB2	1:J:31:ARG:O	1.99	0.62
1:P:171:VAL:HB	1:P:176:GLU:HB3	1.81	0.62
1:L:24:GLU:H	1:L:24:GLU:CD	2.04	0.62
1:L:104:LYS:HD2	1:L:239:LEU:HD21	1.81	0.61
1:H:137:THR:HG22	1:H:191:LEU:HB2	1.80	0.61
1:E:204:LYS:O	1:E:205:PRO:C	2.39	0.61
1:G:159:TRP:HE1	1:G:163:ARG:NH1	1.97	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:157:LYS:HE2	1:H:161:TYR:CE1	2.35	0.61
1:E:183:LYS:HB2	1:E:183:LYS:NZ	2.15	0.61
1:B:144:LYS:HE3	1:B:148:ARG:HH12	1.65	0.61
1:E:125:GLU:N	1:E:125:GLU:OE1	2.25	0.61
1:E:169:VAL:HA	1:E:180:ARG:HH12	1.65	0.61
1:H:172:ARG:HB3	1:H:176:GLU:OE1	2.00	0.61
1:N:130:GLN:HG3	1:N:133:ILE:H	1.64	0.61
1:B:92:ILE:HA	1:B:102:PHE:CE2	2.35	0.61
1:G:240:LYS:O	1:G:244:GLN:HG3	1.99	0.61
1:P:232:ASN:N	1:P:232:ASN:ND2	2.48	0.61
1:J:148:ARG:HB2	1:J:148:ARG:HH11	1.66	0.61
1:P:79:VAL:HG22	1:P:99:VAL:HG12	1.82	0.61
1:G:172:ARG:NH1	1:G:172:ARG:HB3	2.16	0.61
1:J:222:ILE:HD13	1:J:238:VAL:HG21	1.83	0.61
1:H:10:THR:HA	1:H:74:MET:CE	2.30	0.60
1:J:121:ILE:HG13	1:J:126:ASP:HB3	1.83	0.60
1:H:147:PHE:CE2	1:H:191:LEU:HD13	2.37	0.60
1:N:166:GLU:HA	1:N:167:PRO:C	2.22	0.60
1:E:155:PHE:CE1	1:E:215:LEU:HD13	2.37	0.60
1:B:144:LYS:NZ	3:B:273:HOH:O	2.32	0.60
1:P:125:GLU:OE1	1:P:154:VAL:HG11	2.02	0.60
1:P:154:VAL:O	1:P:158:MET:HG3	2.02	0.60
1:J:152:ILE:HB	1:J:155:PHE:CD2	2.36	0.60
1:B:11:ILE:O	1:B:17:VAL:HG13	2.02	0.60
1:P:203:ARG:O	1:P:204:LYS:O	2.19	0.59
1:H:130:GLN:NE2	1:H:132:GLU:N	2.49	0.59
1:N:130:GLN:HE21	1:N:133:ILE:H	1.50	0.59
1:J:114:MET:HE1	1:J:178:VAL:HA	1.84	0.59
1:L:192:LEU:N	1:L:192:LEU:HD12	2.15	0.59
1:H:134:ALA:O	1:H:188:TYR:HA	2.03	0.59
1:B:42:GLU:CG	1:B:246:LEU:HD21	2.33	0.59
1:P:172:ARG:HB2	1:P:172:ARG:NH1	2.18	0.59
1:H:26:LEU:HD22	1:H:30:GLU:OE2	2.03	0.59
1:L:78:LEU:HD23	1:L:83:ALA:HB3	1.84	0.59
1:E:11:ILE:O	1:E:17:VAL:CG1	2.50	0.59
1:H:133:ILE:HG23	1:H:186:GLY:O	2.02	0.59
1:E:147:PHE:CE2	1:E:191:LEU:HD13	2.37	0.59
1:G:109:LEU:HD12	1:G:193:GLU:HB3	1.83	0.59
1:B:62:GLY:HA3	1:B:75:VAL:HG23	1.84	0.59
1:L:199:TYR:O	1:L:203:ARG:HG2	2.02	0.59
1:L:163:ARG:HG3	1:L:164:SER:N	2.17	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:21:LYS:HG2	1:L:22:ASN:H	1.67	0.59
1:H:99:VAL:HG23	1:H:100:ILE:HG23	1.84	0.59
1:L:183:LYS:O	1:L:184:SER:HB3	2.02	0.59
1:J:121:ILE:HD13	1:J:133:ILE:HD12	1.85	0.59
1:L:20:LYS:HD2	1:L:26:LEU:HD12	1.85	0.59
1:J:125:GLU:HA	1:J:128:SER:OG	2.03	0.59
1:J:194:SER:O	1:J:198:GLU:HG3	2.01	0.59
1:E:10:THR:HA	1:E:74:MET:CE	2.31	0.59
1:L:121:ILE:HG22	1:L:126:ASP:HB3	1.85	0.59
1:N:253:LYS:HE2	1:N:258:LYS:NZ	2.18	0.59
1:E:121:ILE:HD13	1:E:127:LEU:HD21	1.85	0.59
1:P:11:ILE:O	1:P:17:VAL:HG13	2.02	0.59
1:B:115:ILE:CG2	1:B:121:ILE:HD11	2.33	0.59
1:B:144:LYS:HE3	1:B:148:ARG:NH2	2.17	0.59
1:P:46:HIS:HD2	1:P:240:LYS:HD2	1.67	0.59
1:G:171:VAL:HG11	1:G:177:GLY:HA2	1.83	0.59
1:L:155:PHE:CE1	1:L:215:LEU:HD13	2.37	0.59
1:J:117:LYS:HG2	1:J:209:MET:CE	2.33	0.58
1:N:136:GLY:HA3	1:N:169:VAL:O	2.02	0.58
1:P:53:LEU:HD11	3:P:292:HOH:O	2.02	0.58
1:B:137:THR:HG22	1:B:191:LEU:HB2	1.85	0.58
1:G:100:ILE:HD12	1:G:100:ILE:C	2.23	0.58
1:P:203:ARG:HD3	1:P:260:GLU:HG2	1.85	0.58
1:H:163:ARG:HB2	1:H:163:ARG:HH11	1.67	0.58
1:H:130:GLN:NE2	1:H:133:ILE:N	2.51	0.58
1:B:20:LYS:HD3	1:B:33:GLU:HB3	1.85	0.58
1:P:37:VAL:HG13	3:P:292:HOH:O	2.02	0.58
1:P:56:VAL:HG13	1:P:59:GLY:HA2	1.85	0.58
1:B:134:ALA:O	1:B:188:TYR:HA	2.03	0.58
1:L:197:ASN:HD21	1:L:210:LYS:HA	1.69	0.58
1:N:152:ILE:HB	1:N:155:PHE:HD2	1.69	0.58
1:L:172:ARG:HB2	1:L:172:ARG:HH11	1.66	0.58
1:B:225:PRO:HD2	1:B:228:SER:HB2	1.84	0.58
1:H:77:GLU:HG2	1:H:82:LYS:HB2	1.84	0.58
1:G:130:GLN:HG3	1:G:131:THR:N	2.18	0.58
1:G:172:ARG:CZ	1:G:172:ARG:HB3	2.31	0.58
1:G:154:VAL:O	1:G:158:MET:HG3	2.04	0.58
1:E:134:ALA:HA	1:E:161:TYR:OH	2.04	0.58
1:L:104:LYS:HB3	1:L:105:PRO:HD2	1.84	0.58
1:E:152:ILE:O	1:E:156:ASP:N	2.34	0.58
1:L:21:LYS:H	1:L:21:LYS:CD	2.17	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:141:GLY:O	1:L:145:GLU:HG2	2.03	0.58
1:G:109:LEU:HD23	1:G:109:LEU:N	2.19	0.58
1:N:46:HIS:CD2	1:N:240:LYS:HD2	2.38	0.58
1:B:196:MET:HA	1:B:196:MET:CE	2.34	0.58
1:E:22:ASN:H	1:E:22:ASN:ND2	2.02	0.58
1:P:121:ILE:CG2	1:P:126:ASP:HB3	2.34	0.58
1:E:56:VAL:HG13	1:E:59:GLY:HA2	1.86	0.58
1:P:166:GLU:HA	1:P:167:PRO:C	2.23	0.58
1:G:119:THR:HG22	1:G:121:ILE:HG12	1.85	0.57
1:P:180:ARG:HD2	1:P:188:TYR:CD2	2.38	0.57
1:E:31:ARG:HH21	1:E:32:TYR:HE2	1.51	0.57
1:L:29:ASN:HB2	3:L:282:HOH:O	2.05	0.57
1:J:216:ASP:OD2	1:J:218:LYS:HE2	2.05	0.57
1:J:135:TYR:HB3	1:J:189:ALA:HB3	1.87	0.57
1:G:160:THR:O	1:G:163:ARG:HB3	2.04	0.57
1:N:20:LYS:HG3	1:N:30:GLU:O	2.04	0.57
1:L:11:ILE:O	1:L:17:VAL:HG13	2.04	0.57
1:E:153:ALA:HA	1:E:156:ASP:HB3	1.87	0.57
1:P:125:GLU:HA	1:P:128:SER:OG	2.04	0.57
1:P:193:GLU:OE1	1:P:218:LYS:HE2	2.04	0.57
1:L:121:ILE:HG22	1:L:126:ASP:O	2.05	0.57
1:H:162:MET:HA	1:H:169:VAL:HG21	1.86	0.57
1:B:192:LEU:H	1:B:192:LEU:HD12	1.69	0.57
1:N:204:LYS:O	1:N:205:PRO:C	2.42	0.57
1:H:160:THR:HA	1:H:163:ARG:HH11	1.67	0.57
1:N:180:ARG:HG2	1:N:188:TYR:CD2	2.40	0.57
1:E:125:GLU:O	1:E:129:LYS:HG2	2.04	0.57
1:E:192:LEU:HD13	1:E:197:ASN:HB2	1.85	0.57
1:P:210:LYS:HE3	3:P:290:HOH:O	2.04	0.57
1:N:172:ARG:HG2	1:N:173:THR:HG23	1.86	0.57
1:E:20:LYS:HD3	1:E:33:GLU:HB3	1.87	0.57
1:J:90:LEU:HD22	1:J:96:ARG:NH1	2.19	0.57
1:N:130:GLN:O	1:N:130:GLN:HG3	2.05	0.56
1:J:182:ARG:HH12	1:J:205:PRO:CB	2.16	0.56
1:E:152:ILE:CG2	1:E:154:VAL:HG23	2.34	0.56
1:L:16:TYR:CG	1:L:89:PRO:HG3	2.39	0.56
1:G:246:LEU:O	1:G:250:LEU:HG	2.05	0.56
1:J:182:ARG:HG2	1:J:207:ASP:OD2	2.05	0.56
1:H:130:GLN:HG2	1:H:131:THR:H	1.69	0.56
1:P:119:THR:HG22	1:P:121:ILE:HG12	1.87	0.56
1:J:8:VAL:HG23	1:J:51:TYR:HB2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:243:GLU:O	1:L:149:ARG:HD2	2.05	0.56
1:H:203:ARG:O	1:H:260:GLU:HB2	2.05	0.56
1:L:21:LYS:HD3	1:L:21:LYS:N	2.20	0.56
1:P:121:ILE:HD12	1:P:127:LEU:CD2	2.35	0.56
1:G:179:ALA:O	1:G:183:LYS:HD3	2.06	0.56
1:G:92:ILE:HG23	1:G:102:PHE:CD2	2.40	0.56
1:P:157:LYS:HD3	1:P:157:LYS:O	2.05	0.56
1:P:182:ARG:HH21	1:P:200:ILE:CG2	2.18	0.56
1:B:155:PHE:CE1	1:B:215:LEU:HD13	2.40	0.56
1:N:139:ASP:HB2	1:N:171:VAL:O	2.06	0.56
1:P:28:GLY:HA2	1:P:31:ARG:HH21	1.69	0.56
1:P:141:GLY:HA3	3:P:262:HOH:O	2.06	0.56
1:J:58:ASP:OD1	1:J:73:GLY:HA2	2.05	0.56
1:P:151:LYS:HE2	1:P:151:LYS:HA	1.88	0.56
1:L:155:PHE:HE1	1:L:215:LEU:HD13	1.68	0.56
1:L:166:GLU:CA	1:L:167:PRO:C	2.73	0.56
1:P:109:LEU:CD2	1:P:219:GLY:HA2	2.36	0.56
1:J:138:LEU:HD22	2:J:804:VBP:H15	1.87	0.56
1:N:144:LYS:HE2	1:N:144:LYS:C	2.27	0.56
1:B:20:LYS:HE2	1:B:30:GLU:O	2.06	0.55
1:B:115:ILE:C	1:B:115:ILE:HD12	2.27	0.55
1:G:156:ASP:O	1:G:160:THR:HG23	2.05	0.55
1:H:196:MET:HE2	2:H:806:VBP:H10	1.87	0.55
1:P:82:LYS:HZ2	1:P:82:LYS:HA	1.71	0.55
1:G:148:ARG:HG3	1:G:149:ARG:HG3	1.88	0.55
1:J:155:PHE:HE1	1:J:215:LEU:HD22	1.70	0.55
1:H:148:ARG:NH2	3:H:269:HOH:O	2.32	0.55
1:J:192:LEU:HD12	1:J:192:LEU:N	2.20	0.55
1:G:183:LYS:N	1:G:183:LYS:HD2	2.21	0.55
1:N:24:GLU:H	1:N:24:GLU:CD	2.10	0.55
1:B:193:GLU:H	2:B:807:VBP:H13	1.71	0.55
1:G:122:GLU:O	1:G:211:VAL:HG22	2.06	0.55
1:B:16:TYR:CG	1:B:89:PRO:HG3	2.42	0.55
1:B:140:SER:HA	1:B:144:LYS:CE	2.36	0.55
1:L:172:ARG:NH1	1:L:172:ARG:HB2	2.22	0.55
1:L:100:ILE:HD11	1:L:102:PHE:CE2	2.42	0.55
1:L:166:GLU:HB2	1:L:168:SER:N	2.22	0.55
1:P:125:GLU:C	1:P:127:LEU:H	2.09	0.55
1:H:19:MET:HG3	3:P:281:HOH:O	2.05	0.55
1:P:121:ILE:HD12	1:P:127:LEU:HD23	1.88	0.55
1:P:192:LEU:HD12	1:P:192:LEU:N	2.20	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:147:PHE:CZ	1:L:191:LEU:HD13	2.41	0.55
1:B:136:GLY:O	1:B:191:LEU:HD13	2.06	0.55
1:H:138:LEU:HD22	2:H:806:VBP:H15	1.88	0.55
1:N:247:LEU:HB2	3:N:276:HOH:O	2.07	0.55
1:P:195:THR:HG21	1:P:220:TYR:HE2	1.71	0.55
1:J:136:GLY:HA3	1:J:169:VAL:O	2.06	0.55
1:L:205:PRO:O	1:L:207:ASP:N	2.40	0.55
1:B:122:GLU:HA	1:B:211:VAL:CG2	2.35	0.55
1:P:208:THR:O	1:P:209:MET:HB2	2.06	0.55
1:B:192:LEU:HD13	1:B:197:ASN:HB2	1.89	0.55
1:H:115:ILE:O	1:H:115:ILE:HD12	2.07	0.55
1:H:201:GLU:HG3	1:H:209:MET:HA	1.89	0.55
1:H:193:GLU:H	2:H:806:VBP:H13	1.72	0.55
1:B:95:VAL:HB	1:E:64:ARG:HH21	1.71	0.54
1:N:115:ILE:CD1	1:N:211:VAL:HG11	2.36	0.54
1:N:16:TYR:HA	1:N:35:TYR:HB3	1.89	0.54
1:G:180:ARG:HD2	1:G:188:TYR:CE2	2.41	0.54
1:L:121:ILE:HD12	1:L:121:ILE:O	2.08	0.54
1:G:39:LEU:O	1:G:43:ILE:HG12	2.07	0.54
1:E:226:LYS:HE3	3:P:285:HOH:O	2.08	0.54
1:P:182:ARG:NH1	1:P:205:PRO:HB2	2.23	0.54
1:L:194:SER:O	1:L:198:GLU:HG3	2.08	0.54
1:G:148:ARG:HB2	1:G:148:ARG:NH1	2.22	0.54
1:N:185:LYS:N	1:N:185:LYS:HD2	2.23	0.54
1:P:192:LEU:HD13	1:P:197:ASN:HB2	1.89	0.54
1:H:109:LEU:HD23	1:H:109:LEU:N	2.23	0.54
1:B:180:ARG:HG2	1:B:188:TYR:CD2	2.42	0.54
1:P:115:ILE:HB	1:P:119:THR:CB	2.38	0.54
1:N:88:ALA:HB1	1:N:89:PRO:CD	2.38	0.54
1:N:203:ARG:O	1:N:204:LYS:O	2.26	0.54
1:N:205:PRO:O	1:N:207:ASP:N	2.33	0.54
1:N:208:THR:O	1:N:209:MET:HB3	2.07	0.54
1:H:27:GLU:HG2	3:H:285:HOH:O	2.07	0.54
1:B:159:TRP:NE1	1:B:163:ARG:NH1	2.56	0.54
1:L:115:ILE:HG21	1:L:121:ILE:HD13	1.89	0.54
1:N:8:VAL:HG22	1:N:85:ILE:CG2	2.38	0.54
1:H:64:ARG:NH1	1:H:71:TRP:NE1	2.49	0.53
1:J:20:LYS:HG2	1:J:26:LEU:CD1	2.37	0.53
1:P:82:LYS:HZ3	1:P:82:LYS:HA	1.72	0.53
1:L:97:GLU:OE2	1:L:102:PHE:HB2	2.08	0.53
1:H:156:ASP:HB3	3:H:289:HOH:O	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:GLU:H	1:B:166:GLU:CD	2.11	0.53
1:N:121:ILE:HD13	1:N:127:LEU:HD21	1.91	0.53
1:G:18:MET:N	1:G:33:GLU:O	2.32	0.53
1:L:187:LYS:HZ2	1:L:188:TYR:HB3	1.72	0.53
1:G:159:TRP:HE1	1:G:163:ARG:HH11	1.57	0.53
1:N:119:THR:HG23	1:N:133:ILE:HD13	1.90	0.53
1:P:125:GLU:C	1:P:127:LEU:N	2.62	0.53
1:J:65:ASP:O	1:J:69:LYS:HA	2.09	0.53
1:P:62:GLY:HA3	1:P:75:VAL:HG23	1.91	0.53
1:G:92:ILE:HG12	1:G:102:PHE:CG	2.44	0.53
1:B:90:LEU:HD22	1:B:96:ARG:NH1	2.23	0.53
1:E:100:ILE:HD11	1:E:102:PHE:CE2	2.44	0.53
1:H:192:LEU:HD13	1:H:197:ASN:HB2	1.91	0.53
1:N:20:LYS:O	1:N:23:HIS:HB3	2.07	0.53
1:H:118:GLY:HA2	1:N:30:GLU:CG	2.39	0.53
1:G:94:LEU:HD12	1:J:236:LEU:HD22	1.91	0.53
1:N:237:ALA:O	1:N:241:LEU:HG	2.09	0.53
1:G:197:ASN:HD22	1:G:210:LYS:HG3	1.73	0.52
1:E:246:LEU:O	1:E:250:LEU:HG	2.09	0.52
1:J:21:LYS:HD3	1:J:21:LYS:N	2.10	0.52
1:E:64:ARG:NH1	1:E:71:TRP:NE1	2.57	0.52
1:P:89:PRO:HB2	2:P:805:VBP:H05	1.91	0.52
1:B:62:GLY:HA2	1:B:72:ASN:O	2.09	0.52
1:E:127:LEU:HB3	1:E:135:TYR:CE2	2.44	0.52
1:H:17:VAL:C	1:H:18:MET:HG3	2.28	0.52
1:L:36:CYS:SG	1:L:88:ALA:HA	2.49	0.52
1:B:20:LYS:CE	1:B:30:GLU:O	2.57	0.52
1:N:125:GLU:HA	1:N:125:GLU:OE1	2.09	0.52
1:L:134:ALA:O	1:L:188:TYR:HA	2.10	0.52
1:J:148:ARG:HG3	1:J:149:ARG:H	1.74	0.52
1:N:20:LYS:HD3	1:N:33:GLU:HB3	1.90	0.52
1:J:115:ILE:HD13	1:J:121:ILE:O	2.10	0.52
1:H:115:ILE:C	1:H:115:ILE:HD12	2.30	0.52
1:P:199:TYR:CE1	1:P:203:ARG:NH1	2.77	0.52
1:P:232:ASN:HA	3:P:289:HOH:O	2.09	0.52
1:L:46:HIS:HD2	1:L:240:LYS:HD2	1.75	0.52
1:P:180:ARG:O	1:P:180:ARG:HG2	2.10	0.52
1:H:144:LYS:HE3	1:H:148:ARG:HH21	1.73	0.52
1:G:20:LYS:NZ	1:G:30:GLU:HG2	2.25	0.52
1:B:110:GLY:HA3	1:B:214:ASN:HB3	1.91	0.52
1:G:114:MET:HE2	1:G:178:VAL:HA	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:122:GLU:HG3	1:J:126:ASP:OD2	2.10	0.52
1:P:6:VAL:O	1:P:51:TYR:HA	2.09	0.52
1:P:109:LEU:HD23	1:P:219:GLY:HA2	1.91	0.52
1:G:201:GLU:HG2	1:G:201:GLU:O	2.09	0.52
1:H:173:THR:O	1:H:176:GLU:HB3	2.10	0.52
1:P:193:GLU:HG2	2:P:805:VBP:H13	1.92	0.52
1:J:68:THR:HB	1:J:70:ILE:HG12	1.91	0.52
1:B:112:SER:OG	1:B:194:SER:HA	2.10	0.52
1:H:252:ASN:ND2	1:H:256:TYR:HB2	2.25	0.51
1:H:24:GLU:HG2	1:H:25:MET:N	2.25	0.51
1:N:200:ILE:HG22	1:N:208:THR:OG1	2.09	0.51
1:P:134:ALA:O	1:P:188:TYR:HA	2.11	0.51
1:J:154:VAL:O	1:J:158:MET:HG3	2.11	0.51
1:H:21:LYS:O	1:H:22:ASN:HB3	2.10	0.51
1:P:113:ILE:HG12	1:P:191:LEU:HD21	1.92	0.51
1:E:11:ILE:HG12	1:E:12:LEU:N	2.25	0.51
1:L:134:ALA:N	1:L:187:LYS:O	2.41	0.51
1:N:16:TYR:CG	1:N:89:PRO:HG3	2.45	0.51
1:G:191:LEU:HD12	1:G:191:LEU:N	2.25	0.51
1:B:140:SER:HA	1:B:144:LYS:HZ3	1.73	0.51
1:B:114:MET:HE2	1:B:178:VAL:HA	1.91	0.51
1:N:171:VAL:HG22	1:N:176:GLU:HB3	1.93	0.51
1:H:109:LEU:HB2	1:H:194:SER:OG	2.10	0.51
1:N:121:ILE:HD13	1:N:127:LEU:HD23	1.92	0.51
1:E:22:ASN:N	1:E:22:ASN:ND2	2.59	0.51
1:E:130:GLN:OE1	1:E:132:GLU:N	2.44	0.51
1:H:234:VAL:O	1:H:238:VAL:HG23	2.11	0.51
1:P:196:MET:HE2	2:P:805:VBP:H10	1.93	0.51
1:J:117:LYS:HE3	3:J:279:HOH:O	2.11	0.51
1:L:111:ILE:CD1	1:L:143:THR:HA	2.40	0.51
1:B:19:MET:HB3	1:B:23:HIS:CD2	2.46	0.51
1:E:135:TYR:HB3	1:E:189:ALA:HB3	1.93	0.51
1:E:225:PRO:HD2	1:E:228:SER:HB2	1.93	0.51
1:J:56:VAL:HG13	1:J:59:GLY:HA2	1.92	0.51
1:J:210:LYS:HE2	3:J:267:HOH:O	2.10	0.50
1:B:89:PRO:HB2	2:B:807:VBP:C05	2.38	0.50
1:N:142:SER:HA	1:N:145:GLU:HB2	1.93	0.50
1:L:79:VAL:HG12	1:L:80:TYR:CD1	2.45	0.50
1:P:24:GLU:H	1:P:24:GLU:CD	2.14	0.50
1:E:153:ALA:O	1:E:154:VAL:C	2.49	0.50
1:B:159:TRP:HE1	1:B:163:ARG:NH1	2.08	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:166:GLU:HA	1:J:167:PRO:O	2.12	0.50
1:H:130:GLN:HE21	1:H:131:THR:C	2.13	0.50
1:J:180:ARG:HG2	1:J:188:TYR:CD2	2.46	0.50
1:J:46:HIS:NE2	1:J:240:LYS:HD2	2.26	0.50
1:B:95:VAL:HG13	3:B:270:HOH:O	2.11	0.50
1:J:114:MET:CE	1:J:178:VAL:HA	2.42	0.50
1:B:144:LYS:HE3	1:B:148:ARG:NH1	2.25	0.50
1:P:209:MET:HG2	1:P:210:LYS:O	2.11	0.50
1:P:39:LEU:O	1:P:43:ILE:HG12	2.12	0.50
1:B:92:ILE:HA	1:B:102:PHE:CZ	2.47	0.50
1:E:125:GLU:H	1:E:125:GLU:CD	2.13	0.50
1:E:11:ILE:O	1:E:17:VAL:HG11	2.10	0.50
1:E:64:ARG:HH12	1:E:71:TRP:HE1	1.59	0.50
1:L:180:ARG:HG2	1:L:188:TYR:CD2	2.46	0.50
1:N:129:LYS:O	1:N:131:THR:N	2.44	0.50
1:G:127:LEU:HD22	1:G:135:TYR:CD2	2.47	0.50
1:E:18:MET:HG2	1:E:33:GLU:O	2.11	0.50
1:E:161:TYR:CD1	1:E:161:TYR:C	2.85	0.50
1:G:42:GLU:OE2	1:G:246:LEU:HD22	2.12	0.50
1:E:90:LEU:HD23	1:E:96:ARG:NH1	2.27	0.50
1:L:204:LYS:O	1:L:205:PRO:C	2.50	0.50
1:G:88:ALA:HB1	1:G:89:PRO:CD	2.42	0.50
1:E:218:LYS:HD3	3:E:280:HOH:O	2.12	0.50
1:L:123:SER:HB3	1:L:126:ASP:OD1	2.12	0.50
1:H:117:LYS:HG3	1:H:209:MET:CE	2.42	0.50
1:H:144:LYS:HD2	1:H:144:LYS:O	2.11	0.50
1:H:253:LYS:O	1:H:257:ASP:HB2	2.12	0.50
1:L:110:GLY:HA3	1:L:216:ASP:O	2.11	0.50
1:J:88:ALA:HB1	1:J:89:PRO:CD	2.42	0.50
1:E:32:TYR:HE2	3:E:287:HOH:O	1.94	0.50
1:H:143:THR:O	1:H:146:PHE:HB3	2.12	0.50
1:E:196:MET:HG2	2:E:808:VBP:O08	2.12	0.49
1:H:130:GLN:OE1	1:H:133:ILE:HB	2.11	0.49
1:H:197:ASN:HD22	1:H:210:LYS:HG3	1.77	0.49
1:N:5:THR:O	1:N:5:THR:HG22	2.12	0.49
1:L:103:SER:HB2	1:L:104:LYS:NZ	2.27	0.49
1:J:117:LYS:HG2	1:J:209:MET:HE3	1.93	0.49
1:L:192:LEU:CD1	1:L:197:ASN:HB2	2.41	0.49
1:P:121:ILE:HG21	1:P:126:ASP:O	2.12	0.49
1:N:12:LEU:HD23	1:N:17:VAL:O	2.12	0.49
1:H:157:LYS:HE2	1:H:161:TYR:HE1	1.74	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:94:LEU:O	1:E:98:GLU:HG3	2.11	0.49
1:P:210:LYS:HB3	1:P:210:LYS:NZ	2.28	0.49
1:L:88:ALA:HB1	1:L:89:PRO:CD	2.43	0.49
1:P:172:ARG:HB2	1:P:172:ARG:HH11	1.78	0.49
1:L:216:ASP:OD2	1:L:218:LYS:HE3	2.12	0.49
1:L:28:GLY:HA2	1:L:31:ARG:HH21	1.77	0.49
1:B:148:ARG:HG3	1:B:159:TRP:CZ2	2.47	0.49
1:L:160:THR:O	1:L:163:ARG:HG2	2.13	0.49
1:J:222:ILE:N	1:J:222:ILE:HD12	2.28	0.49
1:B:117:LYS:HD3	1:B:209:MET:HE3	1.93	0.49
1:H:135:TYR:CB	1:H:189:ALA:HB3	2.42	0.49
1:P:115:ILE:HG12	1:P:211:VAL:HG11	1.94	0.49
1:J:185:LYS:N	1:J:185:LYS:CD	2.74	0.49
1:N:65:ASP:O	1:N:69:LYS:HA	2.12	0.49
1:N:6:VAL:O	1:N:51:TYR:HA	2.13	0.49
1:J:204:LYS:HB3	1:J:205:PRO:CD	2.38	0.49
1:J:159:TRP:O	1:J:163:ARG:HB2	2.13	0.49
1:B:75:VAL:O	1:B:79:VAL:HG23	2.13	0.49
1:E:182:ARG:HG2	1:E:207:ASP:OD2	2.13	0.49
1:H:121:ILE:HD13	1:H:127:LEU:HG	1.94	0.49
1:P:158:MET:O	1:P:162:MET:HG3	2.13	0.49
1:N:253:LYS:O	1:N:257:ASP:HB2	2.13	0.49
1:E:197:ASN:HD22	1:E:210:LYS:HG3	1.77	0.49
1:N:94:LEU:O	1:N:98:GLU:HG3	2.13	0.49
1:B:171:VAL:HB	1:B:176:GLU:HG2	1.94	0.49
1:N:108:SER:C	1:N:109:LEU:HD23	2.33	0.49
1:H:122:GLU:OE1	1:H:126:ASP:OD2	2.31	0.49
1:J:148:ARG:HB2	1:J:148:ARG:NH1	2.26	0.49
1:H:99:VAL:O	1:H:226:LYS:HD3	2.13	0.49
1:E:244:GLN:HA	1:P:149:ARG:CD	2.43	0.49
1:E:105:PRO:HA	1:E:220:TYR:O	2.13	0.49
1:B:95:VAL:CB	1:E:64:ARG:HH21	2.25	0.48
1:N:143:THR:HG21	3:N:266:HOH:O	2.13	0.48
1:B:122:GLU:O	1:B:211:VAL:HG22	2.13	0.48
1:B:241:LEU:HD22	1:B:246:LEU:HD22	1.95	0.48
1:P:114:MET:CE	1:P:208:THR:HG21	2.43	0.48
1:E:159:TRP:O	1:E:163:ARG:HB2	2.13	0.48
1:L:100:ILE:HD12	1:L:100:ILE:C	2.33	0.48
1:P:125:GLU:O	1:P:127:LEU:N	2.46	0.48
1:E:148:ARG:CG	1:E:148:ARG:O	2.61	0.48
1:G:11:ILE:HG13	3:G:290:HOH:O	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:GLU:HG2	1:E:82:LYS:HB2	1.95	0.48
1:P:97:GLU:O	1:P:97:GLU:HG3	2.13	0.48
1:G:36:CYS:SG	1:G:88:ALA:HA	2.53	0.48
1:H:144:LYS:CE	1:H:148:ARG:NH2	2.76	0.48
1:E:137:THR:HG22	1:E:191:LEU:HB2	1.95	0.48
1:P:143:THR:HB	3:P:262:HOH:O	2.13	0.48
1:J:27:GLU:HA	1:J:27:GLU:OE1	2.14	0.48
1:N:182:ARG:NH1	1:N:208:THR:HG23	2.29	0.48
1:B:88:ALA:HB1	1:B:89:PRO:CD	2.43	0.48
1:H:163:ARG:NH1	1:H:163:ARG:HB2	2.27	0.48
1:P:177:GLY:O	1:P:181:VAL:HG23	2.13	0.48
1:N:193:GLU:H	2:N:802:VBP:H13	1.79	0.48
1:J:200:ILE:HG22	1:J:208:THR:OG1	2.14	0.48
1:H:249:LYS:HD3	1:L:151:LYS:HB3	1.95	0.48
1:P:203:ARG:HA	1:P:260:GLU:CG	2.43	0.48
1:H:162:MET:HB3	1:H:170:PHE:CZ	2.49	0.48
1:E:159:TRP:CE3	1:E:159:TRP:HA	2.49	0.48
1:N:60:LYS:HB2	1:N:73:GLY:CA	2.44	0.48
1:B:250:LEU:O	1:B:253:LYS:HB3	2.14	0.48
1:L:160:THR:HG22	1:L:163:ARG:HH12	1.78	0.48
1:H:100:ILE:HD11	1:H:102:PHE:CE2	2.49	0.48
1:G:237:ALA:O	1:G:241:LEU:HG	2.14	0.48
1:J:182:ARG:NH1	1:J:207:ASP:OD1	2.46	0.48
1:B:237:ALA:O	1:B:241:LEU:HG	2.14	0.48
1:H:147:PHE:CZ	1:H:191:LEU:HD13	2.49	0.48
1:B:199:TYR:O	1:B:203:ARG:HG2	2.14	0.48
1:G:115:ILE:HD12	1:G:119:THR:HB	1.95	0.48
1:P:65:ASP:HB3	1:P:68:THR:OG1	2.14	0.48
1:G:180:ARG:HD2	1:G:188:TYR:CE1	2.49	0.48
1:J:192:LEU:HD12	1:J:192:LEU:H	1.78	0.48
1:P:182:ARG:HH12	1:P:205:PRO:HB2	1.79	0.48
1:J:197:ASN:ND2	1:J:210:LYS:HG3	2.29	0.48
1:L:15:PRO:HD3	1:L:199:TYR:CD1	2.49	0.47
1:J:138:LEU:O	1:J:144:LYS:HB2	2.14	0.47
1:L:164:SER:O	1:L:165:ALA:CB	2.60	0.47
1:H:181:VAL:CG1	1:H:181:VAL:O	2.62	0.47
1:E:234:VAL:O	1:E:237:ALA:HB3	2.14	0.47
1:H:196:MET:O	1:H:200:ILE:HG12	2.13	0.47
1:P:247:LEU:HB2	3:P:273:HOH:O	2.13	0.47
1:E:247:LEU:HB2	3:E:286:HOH:O	2.14	0.47
1:B:68:THR:OG1	1:B:70:ILE:HB	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:MET:CE	1:B:178:VAL:HA	2.44	0.47
1:P:133:ILE:HG23	1:P:187:LYS:C	2.34	0.47
1:P:113:ILE:HG12	1:P:191:LEU:CD2	2.44	0.47
1:L:147:PHE:CE2	1:L:191:LEU:HD13	2.49	0.47
1:E:127:LEU:HD22	1:E:135:TYR:CD2	2.49	0.47
1:L:166:GLU:HA	1:L:167:PRO:O	2.13	0.47
1:H:192:LEU:CD1	1:H:197:ASN:HB2	2.45	0.47
1:N:144:LYS:HD3	3:N:262:HOH:O	2.15	0.47
1:H:249:LYS:HD3	1:L:151:LYS:CB	2.43	0.47
1:B:62:GLY:HA3	1:B:75:VAL:CG2	2.43	0.47
1:H:115:ILE:HD13	1:H:119:THR:HB	1.95	0.47
1:P:203:ARG:HA	1:P:260:GLU:HG3	1.96	0.47
1:G:182:ARG:NH1	1:G:205:PRO:HB2	2.29	0.47
1:N:130:GLN:NE2	1:N:133:ILE:HG13	2.28	0.47
1:J:145:GLU:OE1	1:J:148:ARG:HD2	2.14	0.47
1:P:192:LEU:HD12	1:P:192:LEU:H	1.80	0.47
1:J:16:TYR:HA	1:J:35:TYR:HB3	1.95	0.47
1:L:251:LYS:O	1:L:255:TRP:HB2	2.14	0.47
1:E:13:GLU:HB3	1:E:16:TYR:HD2	1.79	0.47
1:P:204:LYS:O	1:P:205:PRO:C	2.49	0.47
1:P:205:PRO:O	1:P:207:ASP:N	2.48	0.47
1:B:11:ILE:O	1:B:17:VAL:CG1	2.62	0.47
1:E:7:VAL:HB	1:E:84:ASP:OD2	2.14	0.47
1:B:97:GLU:HG3	1:B:97:GLU:O	2.13	0.47
1:G:77:GLU:HG2	1:G:82:LYS:HB2	1.97	0.47
1:G:117:LYS:HE2	1:G:209:MET:CE	2.34	0.47
1:G:114:MET:CE	1:G:178:VAL:HA	2.44	0.47
1:J:114:MET:HE3	1:J:178:VAL:HG13	1.96	0.47
1:G:130:GLN:HA	1:G:130:GLN:NE2	2.25	0.47
1:E:88:ALA:HB1	1:E:89:PRO:CD	2.39	0.47
1:P:240:LYS:O	1:P:244:GLN:HG3	2.14	0.47
1:J:105:PRO:HA	1:J:220:TYR:O	2.15	0.47
1:E:11:ILE:HG21	1:E:61:TYR:CE1	2.49	0.47
1:J:171:VAL:HB	1:J:176:GLU:HB3	1.96	0.47
1:J:5:THR:O	1:J:5:THR:HG23	2.15	0.47
1:N:130:GLN:HG2	1:N:133:ILE:HB	1.96	0.47
1:B:42:GLU:CD	1:B:246:LEU:HD21	2.35	0.47
1:P:65:ASP:O	1:P:69:LYS:N	2.47	0.47
1:P:65:ASP:O	1:P:69:LYS:HA	2.15	0.47
1:L:115:ILE:HG21	1:L:121:ILE:HD11	1.95	0.47
1:L:193:GLU:H	2:L:801:VBP:H13	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:113:ILE:HG22	1:J:115:ILE:HG23	1.97	0.47
1:E:147:PHE:CZ	1:E:191:LEU:HD13	2.49	0.47
1:N:11:ILE:O	1:N:17:VAL:HG13	2.15	0.47
1:P:130:GLN:HE21	1:P:132:GLU:HB3	1.80	0.47
1:J:137:THR:HG22	1:J:191:LEU:HB2	1.96	0.47
1:E:63:ALA:N	1:E:72:ASN:OD1	2.43	0.47
1:P:100:ILE:HD12	1:P:100:ILE:O	2.15	0.47
1:P:203:ARG:HA	1:P:203:ARG:HD3	1.70	0.47
1:B:172:ARG:CB	1:B:172:ARG:NH1	2.78	0.47
1:J:62:GLY:HA3	1:J:75:VAL:HG23	1.97	0.47
1:J:99:VAL:HG23	1:J:100:ILE:HG23	1.96	0.47
1:G:182:ARG:HH12	1:G:205:PRO:HB2	1.80	0.46
1:N:182:ARG:NH1	1:N:207:ASP:OD1	2.48	0.46
1:G:115:ILE:HG22	1:G:121:ILE:HD11	1.98	0.46
1:N:113:ILE:HG22	1:N:115:ILE:HG23	1.96	0.46
1:P:75:VAL:O	1:P:79:VAL:HG23	2.14	0.46
1:P:180:ARG:O	1:P:184:SER:HB3	2.15	0.46
1:J:185:LYS:HD2	1:J:185:LYS:H	1.77	0.46
1:B:172:ARG:CB	1:B:172:ARG:HH11	2.28	0.46
1:E:22:ASN:N	1:E:22:ASN:HD22	1.96	0.46
1:B:155:PHE:CZ	1:B:215:LEU:HD22	2.50	0.46
1:E:241:LEU:HD22	1:E:246:LEU:HD22	1.98	0.46
1:N:51:TYR:N	1:N:51:TYR:CD2	2.83	0.46
1:P:130:GLN:HE21	1:P:130:GLN:HB3	1.57	0.46
1:B:133:ILE:HG23	1:B:187:LYS:HA	1.97	0.46
1:N:42:GLU:HG3	1:N:246:LEU:CD2	2.45	0.46
1:J:97:GLU:HA	1:J:97:GLU:OE2	2.16	0.46
1:N:61:TYR:CE1	2:N:802:VBP:H03A	2.50	0.46
1:G:68:THR:C	1:G:70:ILE:H	2.17	0.46
1:N:180:ARG:HG2	1:N:180:ARG:O	2.16	0.46
1:B:115:ILE:O	1:B:115:ILE:HD12	2.16	0.46
1:J:182:ARG:NH1	1:J:205:PRO:CB	2.78	0.46
1:P:96:ARG:C	1:P:98:GLU:H	2.19	0.46
1:G:148:ARG:HB2	1:G:148:ARG:HH11	1.80	0.46
1:G:192:LEU:HD13	1:G:197:ASN:HB2	1.98	0.46
1:E:169:VAL:CA	1:E:180:ARG:HH12	2.29	0.46
1:E:148:ARG:HA	1:E:159:TRP:CD1	2.51	0.46
1:J:147:PHE:CE2	1:J:191:LEU:HD13	2.51	0.46
1:P:184:SER:O	1:P:186:GLY:N	2.48	0.46
1:P:36:CYS:SG	1:P:88:ALA:HA	2.56	0.46
1:H:118:GLY:HA2	1:N:30:GLU:HG3	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:64:ARG:HG3	1:J:64:ARG:NH1	2.30	0.46
1:P:138:LEU:HD12	1:P:139:ASP:H	1.81	0.46
1:N:144:LYS:HB3	1:N:144:LYS:HZ3	1.80	0.46
1:L:144:LYS:NZ	1:L:148:ARG:NH2	2.64	0.46
1:G:67:ASP:O	1:G:69:LYS:HD3	2.16	0.46
1:L:136:GLY:HA3	1:L:169:VAL:O	2.16	0.46
1:N:92:ILE:HG12	1:N:102:PHE:CD1	2.51	0.46
1:H:14:SER:CB	1:H:18:MET:HE3	2.46	0.46
1:N:60:LYS:HB2	1:N:73:GLY:HA2	1.97	0.46
1:P:100:ILE:C	1:P:100:ILE:HD12	2.36	0.46
1:G:111:ILE:HD12	1:G:146:PHE:CD2	2.51	0.46
1:N:137:THR:HB	3:N:266:HOH:O	2.16	0.45
1:H:121:ILE:HD12	1:H:122:GLU:N	2.31	0.45
1:P:137:THR:HG22	1:P:191:LEU:HB2	1.97	0.45
1:P:62:GLY:HA3	1:P:75:VAL:CG2	2.46	0.45
1:B:211:VAL:O	1:B:211:VAL:HG13	2.16	0.45
1:H:11:ILE:O	1:H:17:VAL:HG13	2.15	0.45
1:L:121:ILE:HA	1:L:126:ASP:HB3	1.98	0.45
1:E:111:ILE:O	1:E:214:ASN:HA	2.16	0.45
1:G:5:THR:N	3:G:262:HOH:O	2.49	0.45
1:J:21:LYS:CE	1:J:21:LYS:H	2.26	0.45
1:P:180:ARG:O	1:P:184:SER:CB	2.64	0.45
1:N:180:ARG:O	1:N:188:TYR:CD2	2.66	0.45
1:L:172:ARG:CB	1:L:172:ARG:NH1	2.80	0.45
1:N:171:VAL:CG2	1:N:176:GLU:HB3	2.46	0.45
1:B:173:THR:O	1:B:176:GLU:HB3	2.16	0.45
1:B:125:GLU:N	1:B:125:GLU:OE1	2.39	0.45
1:H:155:PHE:CE1	1:H:215:LEU:HD13	2.51	0.45
1:P:197:ASN:ND2	1:P:210:LYS:HA	2.31	0.45
1:B:99:VAL:HG23	1:B:100:ILE:HG23	1.98	0.45
1:P:8:VAL:HG22	1:P:85:ILE:CG2	2.47	0.45
1:L:90:LEU:O	1:L:220:TYR:HA	2.15	0.45
1:B:106:PHE:C	1:B:106:PHE:CD1	2.90	0.45
1:G:229:SER:HB2	3:G:282:HOH:O	2.17	0.45
1:L:205:PRO:O	1:L:207:ASP:OD1	2.34	0.45
1:N:207:ASP:OD1	1:N:208:THR:HG23	2.17	0.45
1:H:121:ILE:CG2	1:H:133:ILE:HD12	2.46	0.45
1:J:222:ILE:HD13	1:J:238:VAL:CG2	2.46	0.45
1:E:11:ILE:O	1:E:17:VAL:HG13	2.15	0.45
1:B:196:MET:HA	1:B:196:MET:HE3	1.98	0.45
1:N:172:ARG:HB3	1:N:176:GLU:OE1	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:PRO:HG2	1:B:207:ASP:OD1	2.16	0.45
1:E:171:VAL:HB	1:E:176:GLU:HB2	1.99	0.45
1:J:182:ARG:NH1	1:J:205:PRO:HB2	2.24	0.45
1:P:64:ARG:HG3	1:P:64:ARG:HH11	1.82	0.45
1:J:51:TYR:CD2	1:J:51:TYR:N	2.84	0.45
1:E:147:PHE:C	1:E:149:ARG:H	2.20	0.45
1:P:121:ILE:CB	1:P:126:ASP:HB3	2.47	0.45
1:B:155:PHE:HE1	1:B:215:LEU:HD13	1.82	0.45
1:N:109:LEU:HD23	1:N:109:LEU:N	2.31	0.45
1:N:10:THR:O	1:N:55:ILE:HA	2.17	0.45
1:J:84:ASP:O	1:J:225:PRO:HD3	2.17	0.45
1:L:64:ARG:HB2	1:L:71:TRP:CE2	2.51	0.45
1:J:117:LYS:HG2	1:J:209:MET:HE2	1.98	0.45
1:G:159:TRP:O	1:G:163:ARG:CB	2.63	0.45
1:P:64:ARG:HG3	1:P:64:ARG:NH1	2.30	0.45
1:L:16:TYR:HA	1:L:35:TYR:HB3	1.99	0.45
1:H:115:ILE:HB	1:H:119:THR:HB	1.98	0.45
1:L:187:LYS:HZ2	1:L:188:TYR:CB	2.29	0.45
1:B:159:TRP:HE1	1:B:163:ARG:HH12	1.64	0.45
1:J:100:ILE:C	1:J:100:ILE:HD12	2.37	0.45
1:G:19:MET:HG3	3:N:272:HOH:O	2.17	0.45
1:E:251:LYS:HD3	1:E:255:TRP:CE3	2.52	0.45
1:L:116:LYS:HE3	1:L:207:ASP:HB2	1.98	0.44
1:B:42:GLU:OE2	1:B:246:LEU:HD21	2.18	0.44
1:P:161:TYR:CD2	1:P:162:MET:N	2.86	0.44
1:H:180:ARG:C	1:H:182:ARG:H	2.20	0.44
1:E:124:ALA:O	1:E:127:LEU:N	2.50	0.44
1:P:195:THR:HG21	1:P:220:TYR:CE2	2.50	0.44
1:B:201:GLU:OE1	1:B:209:MET:HB2	2.16	0.44
1:L:122:GLU:HA	1:L:211:VAL:HG21	2.00	0.44
1:E:109:LEU:HD12	1:E:193:GLU:OE1	2.18	0.44
1:N:28:GLY:O	1:N:31:ARG:HG3	2.17	0.44
1:J:121:ILE:CD1	1:J:133:ILE:HD12	2.47	0.44
1:E:114:MET:CE	1:E:192:LEU:HD21	2.47	0.44
1:E:197:ASN:ND2	1:E:210:LYS:HA	2.32	0.44
1:G:20:LYS:HZ2	1:G:30:GLU:HG2	1.81	0.44
1:J:11:ILE:HD11	1:J:59:GLY:O	2.17	0.44
1:N:201:GLU:OE1	1:N:210:LYS:N	2.48	0.44
1:J:150:SER:HA	3:J:276:HOH:O	2.17	0.44
1:J:34:GLY:HA2	1:J:254:TRP:CZ3	2.52	0.44
1:G:85:ILE:HG13	1:G:224:THR:HG22	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:65:ASP:O	1:N:69:LYS:N	2.50	0.44
1:N:129:LYS:O	1:N:130:GLN:C	2.54	0.44
1:E:14:SER:HA	3:E:278:HOH:O	2.17	0.44
1:J:137:THR:HB	1:J:143:THR:HG22	1.98	0.44
1:J:24:GLU:H	1:J:24:GLU:CD	2.20	0.44
1:J:178:VAL:CG1	1:J:182:ARG:HE	2.28	0.44
1:P:169:VAL:HA	1:P:180:ARG:NH1	2.31	0.44
1:P:113:ILE:HD13	1:P:127:LEU:CD1	2.47	0.44
1:J:115:ILE:CD1	1:J:121:ILE:O	2.64	0.44
1:H:96:ARG:O	1:H:100:ILE:HG13	2.17	0.44
1:B:155:PHE:CZ	1:B:215:LEU:HB3	2.53	0.44
1:E:241:LEU:CD2	1:E:246:LEU:HD22	2.48	0.44
1:H:106:PHE:CD1	1:H:106:PHE:C	2.91	0.44
1:J:179:ALA:HA	1:J:182:ARG:HD2	1.99	0.44
1:E:234:VAL:O	1:E:238:VAL:HG23	2.17	0.44
1:J:121:ILE:HG12	1:J:127:LEU:HD23	1.98	0.44
1:B:104:LYS:HG2	1:B:235:ASN:OD1	2.18	0.44
1:H:68:THR:O	1:H:70:ILE:HG13	2.18	0.44
1:P:204:LYS:CB	1:P:205:PRO:CD	2.87	0.44
1:L:161:TYR:HD2	1:L:162:MET:HG3	1.83	0.44
1:J:69:LYS:HB2	1:J:69:LYS:HZ3	1.80	0.44
1:J:73:GLY:O	1:J:77:GLU:HG2	2.17	0.44
1:P:109:LEU:N	1:P:109:LEU:HD23	2.32	0.44
1:P:130:GLN:NE2	1:P:132:GLU:HB3	2.32	0.44
1:H:122:GLU:HB3	1:H:211:VAL:HG21	1.99	0.44
1:J:152:ILE:N	1:J:152:ILE:HD12	2.32	0.44
1:E:197:ASN:ND2	1:E:210:LYS:HG3	2.33	0.44
1:J:74:MET:O	1:J:77:GLU:HB2	2.18	0.44
1:N:183:LYS:O	1:N:185:LYS:HD2	2.18	0.44
1:P:38:ASP:HB3	1:P:250:LEU:HD11	1.99	0.44
1:E:162:MET:HB3	1:E:170:PHE:CZ	2.53	0.44
1:P:136:GLY:HA2	1:P:162:MET:SD	2.58	0.44
1:H:20:LYS:CE	1:H:30:GLU:O	2.66	0.44
1:L:196:MET:HE2	1:L:200:ILE:HG12	1.99	0.44
1:H:107:MET:HE1	1:H:251:LYS:HG2	2.00	0.44
1:E:185:LYS:HB3	1:E:186:GLY:H	1.68	0.43
1:E:193:GLU:H	2:E:808:VBP:H13	1.82	0.43
1:G:179:ALA:O	1:G:183:LYS:CD	2.66	0.43
1:B:165:ALA:HB2	3:B:290:HOH:O	2.17	0.43
1:N:9:THR:O	1:N:86:ALA:HA	2.18	0.43
1:P:260:GLU:O	1:P:261:CYS:SG	2.76	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:60:LYS:HD3	1:P:72:ASN:ND2	2.33	0.43
1:G:68:THR:C	1:G:70:ILE:N	2.72	0.43
1:B:136:GLY:HA3	1:B:169:VAL:O	2.18	0.43
1:G:155:PHE:CZ	1:G:215:LEU:HD22	2.52	0.43
1:N:114:MET:CE	1:N:192:LEU:HD21	2.48	0.43
1:B:115:ILE:HG22	1:B:121:ILE:HD11	2.00	0.43
1:P:137:THR:HB	1:P:143:THR:HG22	2.00	0.43
1:H:201:GLU:CG	1:H:209:MET:HA	2.48	0.43
1:E:12:LEU:HD13	1:E:55:ILE:CD1	2.48	0.43
1:G:11:ILE:HG12	1:G:12:LEU:N	2.33	0.43
1:J:143:THR:HB	3:J:288:HOH:O	2.19	0.43
1:H:94:LEU:O	1:H:98:GLU:HG3	2.17	0.43
1:B:56:VAL:HG13	1:B:59:GLY:HA2	2.01	0.43
1:B:14:SER:HB2	3:B:279:HOH:O	2.17	0.43
1:L:125:GLU:C	1:L:127:LEU:N	2.70	0.43
1:G:121:ILE:HD13	1:G:127:LEU:HD21	1.99	0.43
1:H:153:ALA:O	1:H:154:VAL:C	2.57	0.43
1:H:121:ILE:HG23	1:H:133:ILE:CD1	2.46	0.43
1:J:113:ILE:N	3:J:287:HOH:O	2.48	0.43
1:B:67:ASP:OD2	1:B:68:THR:HG23	2.18	0.43
1:G:193:GLU:CD	1:G:218:LYS:HZ2	2.18	0.43
1:G:16:TYR:CG	1:G:89:PRO:HG3	2.53	0.43
1:H:11:ILE:HG12	1:H:12:LEU:N	2.33	0.43
1:L:159:TRP:HA	1:L:159:TRP:CE3	2.54	0.43
1:H:100:ILE:HD13	1:H:223:ALA:HB1	1.99	0.43
1:E:47:CYS:SG	1:E:233:ALA:HB1	2.58	0.43
1:J:119:THR:HA	1:J:120:PRO:HD3	1.84	0.43
1:L:184:SER:HB2	1:L:187:LYS:NZ	2.33	0.43
1:N:143:THR:O	1:N:146:PHE:HB3	2.18	0.43
1:B:143:THR:HG21	1:B:191:LEU:O	2.19	0.43
1:J:20:LYS:HB2	1:J:31:ARG:C	2.39	0.43
1:E:183:LYS:HB2	1:E:183:LYS:HZ2	1.83	0.43
1:N:253:LYS:HE2	1:N:258:LYS:HZ3	1.84	0.43
1:E:115:ILE:CG2	1:E:121:ILE:HD11	2.49	0.43
1:G:11:ILE:CG1	1:G:12:LEU:N	2.82	0.43
1:B:94:LEU:O	1:B:98:GLU:HG3	2.17	0.43
1:E:116:LYS:NZ	1:E:185:LYS:HA	2.32	0.43
1:E:159:TRP:HA	1:E:159:TRP:HE3	1.82	0.43
1:G:236:LEU:HD22	1:J:94:LEU:CD1	2.49	0.43
1:N:130:GLN:HE21	1:N:132:GLU:CB	2.25	0.43
1:P:193:GLU:HG2	2:P:805:VBP:C13	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:144:LYS:NZ	1:H:148:ARG:NH2	2.67	0.43
1:H:20:LYS:HZ2	1:H:30:GLU:HG2	1.84	0.43
1:J:5:THR:N	3:J:291:HOH:O	2.51	0.43
1:N:130:GLN:HE21	1:N:133:ILE:N	2.16	0.43
1:G:122:GLU:HA	1:G:211:VAL:CG2	2.41	0.43
1:P:197:ASN:HD21	1:P:210:LYS:HA	1.84	0.43
1:B:10:THR:OG1	1:B:11:ILE:N	2.48	0.43
1:L:37:VAL:HG13	1:L:53:LEU:HD11	2.00	0.43
1:G:64:ARG:HG3	1:G:71:TRP:CE2	2.54	0.43
1:B:84:ASP:O	1:B:85:ILE:HB	2.18	0.43
1:H:172:ARG:HG2	1:H:173:THR:N	2.34	0.42
1:B:92:ILE:HG12	1:B:102:PHE:CG	2.54	0.42
1:E:180:ARG:HD3	1:E:188:TYR:CE2	2.54	0.42
1:E:115:ILE:HG22	1:E:121:ILE:HD11	2.00	0.42
1:E:161:TYR:O	1:E:165:ALA:HB2	2.18	0.42
1:H:250:LEU:O	1:H:253:LYS:HB3	2.19	0.42
1:N:65:ASP:HB3	1:N:68:THR:OG1	2.18	0.42
1:N:100:ILE:HD12	1:N:100:ILE:C	2.40	0.42
1:L:55:ILE:O	1:L:56:VAL:C	2.58	0.42
1:H:40:ALA:HA	1:H:87:ILE:HD13	2.01	0.42
1:P:12:LEU:HD22	1:P:18:MET:HA	2.00	0.42
1:H:184:SER:O	1:H:186:GLY:N	2.53	0.42
1:H:118:GLY:HA2	1:N:30:GLU:HG2	2.01	0.42
1:B:171:VAL:HB	1:B:176:GLU:CG	2.48	0.42
1:P:250:LEU:HA	1:P:250:LEU:HD23	1.78	0.42
1:J:116:LYS:HG3	1:J:207:ASP:O	2.19	0.42
1:P:96:ARG:C	1:P:98:GLU:N	2.73	0.42
1:P:181:VAL:HG22	1:P:188:TYR:O	2.18	0.42
1:P:16:TYR:CE1	1:P:89:PRO:HG3	2.54	0.42
1:J:16:TYR:CE1	1:J:255:TRP:HH2	2.37	0.42
1:J:12:LEU:HD12	1:J:17:VAL:O	2.20	0.42
1:L:21:LYS:HG2	1:L:22:ASN:N	2.33	0.42
1:P:88:ALA:HB1	1:P:89:PRO:CD	2.49	0.42
1:P:114:MET:HE2	1:P:208:THR:HG21	2.01	0.42
1:J:60:LYS:HB2	1:J:73:GLY:CA	2.50	0.42
1:E:145:GLU:O	1:E:146:PHE:C	2.58	0.42
1:G:130:GLN:HG3	1:G:131:THR:H	1.84	0.42
1:L:11:ILE:HG21	1:L:61:TYR:CE1	2.54	0.42
1:B:203:ARG:NH1	1:B:258:LYS:O	2.52	0.42
1:E:100:ILE:HD13	1:E:223:ALA:CB	2.50	0.42
1:H:11:ILE:HG21	1:H:61:TYR:CE1	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:122:GLU:HA	1:N:211:VAL:CG2	2.49	0.42
1:P:125:GLU:OE2	1:P:125:GLU:N	2.52	0.42
1:P:216:ASP:OD2	1:P:218:LYS:HD2	2.20	0.42
1:J:68:THR:CB	1:J:70:ILE:HG12	2.49	0.42
1:H:100:ILE:HD12	1:H:100:ILE:C	2.39	0.42
1:P:159:TRP:O	1:P:160:THR:C	2.57	0.42
1:E:172:ARG:N	1:E:176:GLU:OE2	2.42	0.42
1:E:210:LYS:HB3	1:E:210:LYS:NZ	2.34	0.42
1:B:24:GLU:N	1:B:24:GLU:OE1	2.43	0.42
1:L:8:VAL:HG13	1:L:85:ILE:HG23	2.02	0.42
1:B:116:LYS:O	1:B:117:LYS:C	2.58	0.42
1:G:196:MET:CE	1:G:196:MET:HA	2.50	0.42
1:H:11:ILE:O	1:H:17:VAL:CG1	2.68	0.42
1:P:16:TYR:CG	1:P:89:PRO:HG3	2.55	0.42
1:L:119:THR:HA	1:L:120:PRO:HD3	1.86	0.42
1:J:64:ARG:HH11	1:J:64:ARG:HG3	1.83	0.42
1:P:79:VAL:HG22	1:P:99:VAL:CG1	2.50	0.42
1:E:192:LEU:CD1	1:E:197:ASN:HB2	2.48	0.42
1:L:144:LYS:NZ	1:L:148:ARG:HH21	2.18	0.42
1:G:104:LYS:NZ	1:J:102:PHE:O	2.36	0.42
1:N:90:LEU:O	1:N:220:TYR:HA	2.19	0.42
1:H:116:LYS:HG3	1:H:185:LYS:O	2.18	0.42
1:B:119:THR:HG22	1:B:121:ILE:H	1.85	0.42
1:J:193:GLU:H	2:J:804:VBP:H13	1.84	0.42
1:H:201:GLU:HG2	1:H:201:GLU:O	2.20	0.42
1:H:20:LYS:C	1:H:22:ASN:H	2.22	0.42
1:G:246:LEU:O	1:G:249:LYS:HB3	2.19	0.42
1:G:94:LEU:O	1:G:98:GLU:HG3	2.19	0.42
1:E:110:GLY:O	1:E:194:SER:N	2.38	0.42
1:H:171:VAL:HB	1:H:176:GLU:OE2	2.20	0.41
1:E:116:LYS:O	1:E:117:LYS:C	2.58	0.41
1:H:88:ALA:O	1:H:90:LEU:N	2.52	0.41
1:B:246:LEU:O	1:B:249:LYS:HB3	2.21	0.41
1:L:234:VAL:O	1:L:237:ALA:HB3	2.20	0.41
1:G:10:THR:O	1:G:56:VAL:HG12	2.20	0.41
1:H:46:HIS:CE1	1:H:241:LEU:HD21	2.54	0.41
1:G:116:LYS:O	1:G:117:LYS:C	2.58	0.41
1:N:119:THR:HA	1:N:120:PRO:HD3	1.82	0.41
1:N:127:LEU:O	1:N:128:SER:C	2.58	0.41
1:E:20:LYS:HB3	1:E:22:ASN:ND2	2.35	0.41
1:H:121:ILE:C	1:H:122:GLU:HG3	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:134:ALA:O	1:G:188:TYR:HA	2.20	0.41
1:J:93:THR:OG1	1:J:96:ARG:HD2	2.20	0.41
1:B:19:MET:HA	1:B:19:MET:HE3	2.02	0.41
1:N:167:PRO:O	1:N:168:SER:C	2.58	0.41
1:G:11:ILE:O	1:G:17:VAL:HG13	2.21	0.41
1:H:214:ASN:N	1:H:214:ASN:HD22	2.17	0.41
1:G:141:GLY:O	1:G:142:SER:C	2.58	0.41
1:L:21:LYS:N	1:L:21:LYS:CD	2.82	0.41
1:B:166:GLU:N	1:B:166:GLU:CD	2.73	0.41
1:B:92:ILE:HG12	1:B:102:PHE:CD1	2.56	0.41
1:E:190:TYR:CD2	1:E:192:LEU:HG	2.55	0.41
1:N:97:GLU:O	1:N:97:GLU:HG3	2.19	0.41
1:G:193:GLU:H	2:G:803:VBP:H13	1.84	0.41
1:G:121:ILE:CD1	1:G:127:LEU:HD21	2.50	0.41
1:G:127:LEU:O	1:G:130:GLN:HB3	2.21	0.41
1:N:122:GLU:HA	1:N:211:VAL:HG21	2.02	0.41
1:P:137:THR:HB	1:P:143:THR:CG2	2.50	0.41
1:L:121:ILE:HG22	1:L:126:ASP:C	2.41	0.41
1:B:113:ILE:C	1:B:197:ASN:HD21	2.23	0.41
1:B:15:PRO:HB3	1:B:199:TYR:CE1	2.55	0.41
1:N:62:GLY:HA3	1:N:75:VAL:CG2	2.51	0.41
1:P:20:LYS:NZ	1:P:30:GLU:O	2.45	0.41
1:L:204:LYS:HG2	1:L:260:GLU:OE1	2.21	0.41
1:H:15:PRO:HA	1:H:18:MET:CE	2.43	0.41
1:B:109:LEU:HB2	1:B:194:SER:OG	2.20	0.41
1:E:60:LYS:HD2	1:E:72:ASN:ND2	2.36	0.41
1:E:143:THR:O	1:E:146:PHE:HB3	2.20	0.41
1:H:125:GLU:OE1	1:H:125:GLU:N	2.38	0.41
1:N:138:LEU:HA	1:N:138:LEU:HD12	1.95	0.41
1:B:95:VAL:HG12	1:E:69:LYS:HB3	2.03	0.41
1:G:209:MET:HB3	1:G:209:MET:HE3	1.93	0.41
1:G:119:THR:CG2	1:G:121:ILE:HG12	2.50	0.41
1:G:65:ASP:HB3	1:G:68:THR:HG23	2.03	0.41
1:H:169:VAL:HA	1:H:180:ARG:HH22	1.85	0.41
1:P:171:VAL:HB	1:P:176:GLU:CB	2.46	0.41
1:P:55:ILE:O	1:P:56:VAL:C	2.59	0.41
1:G:15:PRO:HA	1:G:18:MET:SD	2.60	0.41
1:E:148:ARG:HG3	1:E:148:ARG:O	2.21	0.41
1:B:65:ASP:HB3	1:B:68:THR:OG1	2.20	0.41
1:H:85:ILE:HD11	1:H:222:ILE:HG21	2.02	0.41
1:B:95:VAL:CG1	1:E:69:LYS:HB3	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:136:GLY:HA2	1:N:162:MET:HE2	2.03	0.41
1:L:62:GLY:HA3	1:L:75:VAL:HG23	2.03	0.41
1:N:177:GLY:O	1:N:181:VAL:HG23	2.21	0.41
1:J:109:LEU:HD23	1:J:109:LEU:N	2.35	0.41
1:G:205:PRO:O	1:G:207:ASP:OD1	2.39	0.41
1:G:204:LYS:O	1:G:205:PRO:C	2.56	0.41
1:J:21:LYS:CD	1:J:21:LYS:N	2.63	0.41
1:L:130:GLN:NE2	1:L:132:GLU:HB3	2.19	0.41
1:L:187:LYS:C	1:L:187:LYS:HE3	2.39	0.41
1:G:130:GLN:CG	1:G:131:THR:N	2.83	0.41
1:H:211:VAL:HG13	1:H:211:VAL:O	2.20	0.41
1:H:88:ALA:HB1	1:H:89:PRO:CD	2.45	0.41
1:L:161:TYR:O	1:L:164:SER:O	2.38	0.41
1:P:115:ILE:HD12	1:P:119:THR:HB	2.03	0.41
1:J:155:PHE:O	1:J:158:MET:HB2	2.21	0.41
1:E:192:LEU:N	1:E:192:LEU:HD12	2.36	0.41
1:E:148:ARG:HB2	1:E:159:TRP:CE2	2.55	0.41
1:E:16:TYR:HB3	1:E:36:CYS:SG	2.61	0.41
1:N:96:ARG:O	1:N:100:ILE:HG13	2.20	0.41
1:B:256:TYR:O	1:B:257:ASP:C	2.59	0.41
1:E:199:TYR:CE1	1:E:203:ARG:NE	2.89	0.41
1:N:204:LYS:CB	1:N:205:PRO:CD	2.77	0.41
1:J:201:GLU:HG3	1:J:209:MET:HA	2.02	0.41
1:L:159:TRP:O	1:L:160:THR:C	2.60	0.41
1:G:148:ARG:HB3	1:G:159:TRP:CZ2	2.55	0.41
1:J:68:THR:O	1:J:69:LYS:HB3	2.20	0.41
1:E:110:GLY:HA3	1:E:214:ASN:HB3	2.03	0.41
1:P:144:LYS:HZ2	1:P:159:TRP:HH2	1.69	0.41
1:N:34:GLY:HA2	1:N:254:TRP:CZ3	2.56	0.41
1:L:131:THR:O	1:L:132:GLU:C	2.59	0.40
1:P:119:THR:HG22	1:P:121:ILE:CG1	2.51	0.40
1:L:119:THR:HG22	1:L:121:ILE:HG13	2.03	0.40
1:P:192:LEU:CD1	1:P:197:ASN:HB2	2.50	0.40
1:P:201:GLU:CG	1:P:209:MET:HA	2.50	0.40
1:L:8:VAL:HG23	1:L:51:TYR:HB2	2.02	0.40
1:E:164:SER:O	1:E:165:ALA:HB2	2.21	0.40
1:G:250:LEU:O	1:G:253:LYS:HB3	2.22	0.40
1:H:203:ARG:HB3	1:H:204:LYS:H	1.65	0.40
1:P:90:LEU:O	1:P:220:TYR:HA	2.21	0.40
1:L:79:VAL:HG12	1:L:80:TYR:CE1	2.56	0.40
1:E:85:ILE:HD11	1:E:222:ILE:CG2	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:198:GLU:O	1:H:199:TYR:C	2.59	0.40
1:J:89:PRO:HB2	2:J:804:VBP:C05	2.44	0.40
1:P:180:ARG:HD2	1:P:188:TYR:CE2	2.55	0.40
1:B:67:ASP:N	1:B:67:ASP:OD2	2.53	0.40
1:J:201:GLU:OE1	1:J:210:LYS:N	2.48	0.40
1:P:133:ILE:HG23	1:P:187:LYS:O	2.21	0.40
1:B:201:GLU:HG2	1:B:202:GLN:NE2	2.36	0.40
1:G:146:PHE:O	1:G:150:SER:HB2	2.22	0.40
1:B:5:THR:N	3:B:262:HOH:O	2.54	0.40
1:L:253:LYS:HA	1:L:257:ASP:HB2	2.02	0.40
1:J:204:LYS:O	1:J:205:PRO:C	2.60	0.40
1:L:166:GLU:HB2	1:L:167:PRO:CA	2.52	0.40
1:J:20:LYS:HG2	1:J:26:LEU:HD12	2.04	0.40
1:H:244:GLN:O	1:L:149:ARG:HG2	2.20	0.40
1:N:11:ILE:O	1:N:17:VAL:CG1	2.69	0.40
1:N:228:SER:OG	1:N:230:LEU:HD12	2.21	0.40
1:B:64:ARG:HG3	1:B:71:TRP:CZ2	2.56	0.40
1:N:127:LEU:O	1:N:129:LYS:N	2.55	0.40
1:N:136:GLY:HA2	1:N:162:MET:CE	2.51	0.40
1:G:193:GLU:HG2	2:G:803:VBP:C13	2.51	0.40
1:E:89:PRO:HB2	2:E:808:VBP:H05	2.04	0.40
1:H:130:GLN:HE22	1:H:133:ILE:N	2.17	0.40
1:N:39:LEU:O	1:N:43:ILE:HG12	2.20	0.40
1:G:107:MET:HG2	1:G:108:SER:N	2.36	0.40
1:N:49:PHE:CD1	1:N:49:PHE:C	2.95	0.40
1:P:5:THR:N	3:P:283:HOH:O	2.54	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	255/258 (99%)	227 (89%)	23 (9%)	5 (2%)	9	30
1	E	255/258 (99%)	222 (87%)	20 (8%)	13 (5%)	2	8
1	G	255/258 (99%)	223 (88%)	27 (11%)	5 (2%)	9	30
1	H	255/258 (99%)	211 (83%)	35 (14%)	9 (4%)	4	15
1	J	255/258 (99%)	228 (89%)	19 (8%)	8 (3%)	5	17
1	L	255/258 (99%)	212 (83%)	32 (12%)	11 (4%)	3	10
1	N	255/258 (99%)	220 (86%)	23 (9%)	12 (5%)	3	9
1	P	255/258 (99%)	206 (81%)	37 (14%)	12 (5%)	3	9
All	All	2040/2064 (99%)	1749 (86%)	216 (11%)	75 (4%)	4	14

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	205	PRO
1	G	206	CYS
1	B	163	ARG
1	E	14	SER
1	E	185	LYS
1	E	204	LYS
1	E	205	PRO
1	E	206	CYS
1	H	22	ASN
1	H	122	GLU
1	H	153	ALA
1	J	130	GLN
1	J	204	LYS
1	L	184	SER
1	L	204	LYS
1	L	205	PRO
1	L	206	CYS
1	N	130	GLN
1	N	204	LYS
1	N	205	PRO
1	N	206	CYS
1	P	153	ALA
1	P	165	ALA
1	P	204	LYS
1	P	205	PRO
1	G	204	LYS
1	B	66	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	148	ARG
1	E	184	SER
1	J	120	PRO
1	J	128	SER
1	L	153	ALA
1	N	153	ALA
1	N	168	SER
1	P	206	CYS
1	G	153	ALA
1	B	153	ALA
1	E	15	PRO
1	H	172	ARG
1	H	185	LYS
1	J	21	LYS
1	N	128	SER
1	P	132	GLU
1	B	134	ALA
1	E	46	HIS
1	E	122	GLU
1	E	168	SER
1	H	132	GLU
1	H	168	SER
1	L	117	LYS
1	L	167	PRO
1	L	185	LYS
1	P	120	PRO
1	P	185	LYS
1	P	209	MET
1	G	131	THR
1	L	122	GLU
1	L	231	GLY
1	N	209	MET
1	P	126	ASP
1	B	188	TYR
1	J	172	ARG
1	L	56	VAL
1	N	120	PRO
1	H	181	VAL
1	J	17	VAL
1	J	62	GLY
1	P	56	VAL
1	E	154	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	231	GLY
1	N	48	GLY
1	N	56	VAL
1	N	62	GLY
1	H	95	VAL
1	E	167	PRO

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	B	216/217 (100%)	206 (95%)	10 (5%)	33	67
1	E	216/217 (100%)	207 (96%)	9 (4%)	36	71
1	G	216/217 (100%)	201 (93%)	15 (7%)	19	48
1	H	216/217 (100%)	199 (92%)	17 (8%)	15	40
1	J	216/217 (100%)	203 (94%)	13 (6%)	24	56
1	L	216/217 (100%)	200 (93%)	16 (7%)	17	43
1	N	216/217 (100%)	198 (92%)	18 (8%)	14	38
1	P	216/217 (100%)	204 (94%)	12 (6%)	26	59
All	All	1728/1736 (100%)	1618 (94%)	110 (6%)	22	52

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	17	VAL
1	G	45	LYS
1	G	60	LYS
1	G	67	ASP
1	G	68	THR
1	G	78	LEU
1	G	130	GLN
1	G	132	GLU
1	G	145	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	148	ARG
1	G	174	THR
1	G	192	LEU
1	G	205	PRO
1	G	209	MET
1	G	246	LEU
1	B	17	VAL
1	B	18	MET
1	B	22	ASN
1	B	27	GLU
1	B	90	LEU
1	B	166	GLU
1	B	192	LEU
1	B	196	MET
1	B	209	MET
1	B	255	TRP
1	E	17	VAL
1	E	22	ASN
1	E	90	LEU
1	E	109	LEU
1	E	126	ASP
1	E	145	GLU
1	E	161	TYR
1	E	192	LEU
1	E	246	LEU
1	H	17	VAL
1	H	18	MET
1	H	24	GLU
1	H	67	ASP
1	H	95	VAL
1	H	122	GLU
1	H	126	ASP
1	H	130	GLN
1	H	144	LYS
1	H	163	ARG
1	H	173	THR
1	H	174	THR
1	H	192	LEU
1	H	204	LYS
1	H	226	LYS
1	H	246	LEU
1	H	252	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	12	LEU
1	J	17	VAL
1	J	21	LYS
1	J	64	ARG
1	J	69	LYS
1	J	78	LEU
1	J	125	GLU
1	J	144	LYS
1	J	148	ARG
1	J	156	ASP
1	J	192	LEU
1	J	250	LEU
1	J	255	TRP
1	L	15	PRO
1	L	17	VAL
1	L	21	LYS
1	L	25	MET
1	L	104	LYS
1	L	109	LEU
1	L	129	LYS
1	L	144	LYS
1	L	169	VAL
1	L	187	LYS
1	L	192	LEU
1	L	205	PRO
1	L	235	ASN
1	L	244	GLN
1	L	248	ASP
1	L	255	TRP
1	N	17	VAL
1	N	23	HIS
1	N	67	ASP
1	N	78	LEU
1	N	109	LEU
1	N	126	ASP
1	N	131	THR
1	N	144	LYS
1	N	149	ARG
1	N	150	SER
1	N	161	TYR
1	N	171	VAL
1	N	174	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	192	LEU
1	N	205	PRO
1	N	224	THR
1	N	230	LEU
1	N	255	TRP
1	P	17	VAL
1	P	18	MET
1	P	64	ARG
1	P	82	LYS
1	P	90	LEU
1	P	95	VAL
1	P	109	LEU
1	P	174	THR
1	P	187	LYS
1	P	192	LEU
1	P	218	LYS
1	P	232	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	46	HIS
1	B	46	HIS
1	B	130	GLN
1	B	244	GLN
1	E	22	ASN
1	E	46	HIS
1	E	197	ASN
1	E	244	GLN
1	H	130	GLN
1	H	197	ASN
1	H	214	ASN
1	H	244	GLN
1	H	252	ASN
1	J	130	GLN
1	J	244	GLN
1	L	46	HIS
1	L	130	GLN
1	L	197	ASN
1	L	252	ASN
1	N	46	HIS
1	N	130	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	197	ASN
1	N	244	GLN
1	P	46	HIS
1	P	130	GLN
1	P	197	ASN
1	P	232	ASN

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 ⓘ

8 ligands are modelled in this entry.

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	$\# Z > 2$
2	VBP	B	807	-	15,25,25	6.21	11 (73%)	16,35,35	1.41	1 (6%)
2	VBP	E	808	-	15,25,25	6.28	11 (73%)	16,35,35	1.55	1 (6%)
2	VBP	G	803	-	15,25,25	6.36	11 (73%)	16,35,35	1.51	1 (6%)
2	VBP	H	806	-	15,25,25	6.05	11 (73%)	16,35,35	1.69	3 (18%)
2	VBP	J	804	-	15,25,25	6.19	12 (80%)	16,35,35	1.45	1 (6%)
2	VBP	L	801	-	15,25,25	6.28	12 (80%)	16,35,35	1.41	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	VBP	N	802	-	15,25,25	6.15	12 (80%)	16,35,35	1.33	1 (6%)
2	VBP	P	805	-	15,25,25	6.51	11 (73%)	16,35,35	1.22	1 (6%)

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
2	VBP	B	807	-	1/1/3/3	0/8/16/16	0/2/2/2
2	VBP	E	808	-	1/1/3/3	0/8/16/16	0/2/2/2
2	VBP	G	803	-	1/1/3/3	0/8/16/16	0/2/2/2
2	VBP	H	806	-	1/1/3/3	0/8/16/16	0/2/2/2
2	VBP	J	804	-	1/1/3/3	0/8/16/16	0/2/2/2
2	VBP	L	801	-	1/1/3/3	0/8/16/16	0/2/2/2
2	VBP	N	802	-	1/1/3/3	0/8/16/16	0/2/2/2
2	VBP	P	805	-	1/1/3/3	0/8/16/16	0/2/2/2

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	806	VBP	C03-N04	-5.91	1.42	1.48
2	N	802	VBP	C03-N04	-5.80	1.42	1.48
2	G	803	VBP	C03-N04	-5.44	1.42	1.48
2	B	807	VBP	C03-N04	-5.19	1.42	1.48
2	E	808	VBP	C03-N04	-5.09	1.43	1.48
2	J	804	VBP	C03-N04	-4.72	1.43	1.48
2	L	801	VBP	C03-N04	-4.62	1.43	1.48
2	P	805	VBP	C03-N04	-4.48	1.43	1.48
2	L	801	VBP	C10-N09	-2.36	1.44	1.48
2	N	802	VBP	C10-N09	-2.29	1.44	1.48
2	J	804	VBP	C10-N09	-2.17	1.44	1.48
2	N	802	VBP	C05-C06	5.31	1.49	1.38
2	J	804	VBP	C05-C06	5.40	1.49	1.38
2	H	806	VBP	C05-C06	5.44	1.49	1.38
2	P	805	VBP	C05-C06	5.45	1.49	1.38
2	G	803	VBP	C05-C06	5.45	1.50	1.38
2	B	807	VBP	C05-C06	5.59	1.50	1.38
2	L	801	VBP	C05-C06	5.67	1.50	1.38
2	E	808	VBP	C05-C06	5.68	1.50	1.38
2	H	806	VBP	O08-C07	6.29	1.39	1.24
2	B	807	VBP	O08-C07	6.30	1.39	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	802	VBP	O08-C07	6.39	1.39	1.24
2	N	802	VBP	C12-C11	6.47	1.52	1.38
2	H	806	VBP	C12-C11	6.48	1.52	1.38
2	J	804	VBP	C13-C14	6.53	1.53	1.39
2	H	806	VBP	C13-C14	6.54	1.53	1.39
2	G	803	VBP	C13-C14	6.58	1.53	1.39
2	N	802	VBP	C13-C14	6.58	1.53	1.39
2	B	807	VBP	C12-C11	6.66	1.53	1.38
2	P	805	VBP	C13-C14	6.66	1.53	1.39
2	G	803	VBP	O08-C07	6.67	1.40	1.24
2	J	804	VBP	C12-C11	6.68	1.53	1.38
2	J	804	VBP	O08-C07	6.71	1.40	1.24
2	L	801	VBP	C12-C11	6.74	1.53	1.38
2	L	801	VBP	C13-C14	6.75	1.53	1.39
2	P	805	VBP	O08-C07	6.75	1.40	1.24
2	E	808	VBP	C05-N04	6.76	1.48	1.36
2	B	807	VBP	C13-C14	6.76	1.53	1.39
2	E	808	VBP	O08-C07	6.78	1.40	1.24
2	P	805	VBP	C12-C11	6.83	1.53	1.38
2	L	801	VBP	C16-C11	6.85	1.53	1.38
2	N	802	VBP	C15-C14	6.96	1.54	1.39
2	H	806	VBP	C07-N09	6.97	1.48	1.38
2	E	808	VBP	C12-C11	6.98	1.53	1.38
2	L	801	VBP	O08-C07	6.98	1.41	1.24
2	J	804	VBP	C16-C11	7.00	1.53	1.38
2	G	803	VBP	C12-C11	7.00	1.53	1.38
2	E	808	VBP	C13-C14	7.03	1.54	1.39
2	N	802	VBP	C16-C11	7.07	1.53	1.38
2	H	806	VBP	C05-N04	7.11	1.48	1.36
2	L	801	VBP	C15-C14	7.13	1.54	1.39
2	B	807	VBP	C16-C11	7.17	1.54	1.38
2	H	806	VBP	C16-C11	7.22	1.54	1.38
2	G	803	VBP	C16-C11	7.24	1.54	1.38
2	B	807	VBP	C05-N04	7.27	1.49	1.36
2	J	804	VBP	C15-C14	7.37	1.55	1.39
2	B	807	VBP	C15-C14	7.40	1.55	1.39
2	H	806	VBP	C15-C14	7.44	1.55	1.39
2	P	805	VBP	C16-C11	7.45	1.54	1.38
2	G	803	VBP	C15-C14	7.48	1.55	1.39
2	L	801	VBP	C05-N04	7.50	1.49	1.36
2	E	808	VBP	C16-C11	7.50	1.54	1.38
2	J	804	VBP	C05-N04	7.54	1.49	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	803	VBP	C05-N04	7.67	1.49	1.36
2	N	802	VBP	C07-N09	7.69	1.49	1.38
2	E	808	VBP	C15-C14	7.70	1.55	1.39
2	P	805	VBP	C15-C14	7.76	1.56	1.39
2	P	805	VBP	C05-N04	7.81	1.49	1.36
2	N	802	VBP	C05-N04	7.86	1.50	1.36
2	J	804	VBP	C07-N09	7.95	1.50	1.38
2	E	808	VBP	C07-N09	7.97	1.50	1.38
2	B	807	VBP	C07-N09	8.25	1.50	1.38
2	G	803	VBP	C07-N09	8.29	1.50	1.38
2	N	802	VBP	C12-C13	8.47	1.54	1.38
2	H	806	VBP	C12-C13	8.48	1.54	1.38
2	L	801	VBP	C07-N09	8.48	1.50	1.38
2	E	808	VBP	C12-C13	8.70	1.54	1.38
2	B	807	VBP	C12-C13	8.75	1.54	1.38
2	J	804	VBP	C12-C13	8.76	1.54	1.38
2	H	806	VBP	C16-C15	8.84	1.54	1.38
2	L	801	VBP	C16-C15	9.03	1.55	1.38
2	B	807	VBP	C16-C15	9.08	1.55	1.38
2	G	803	VBP	C16-C15	9.11	1.55	1.38
2	N	802	VBP	C16-C15	9.14	1.55	1.38
2	L	801	VBP	C12-C13	9.18	1.55	1.38
2	P	805	VBP	C07-N09	9.18	1.51	1.38
2	P	805	VBP	C12-C13	9.23	1.55	1.38
2	J	804	VBP	C16-C15	9.25	1.55	1.38
2	E	808	VBP	C16-C15	9.28	1.55	1.38
2	G	803	VBP	C12-C13	9.32	1.55	1.38
2	P	805	VBP	C16-C15	10.02	1.56	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	806	VBP	C15-C16-C11	-2.02	118.28	121.04
2	H	806	VBP	C16-C11-C12	2.16	121.59	118.13
2	P	805	VBP	C10-N09-C20	3.87	122.63	118.05
2	N	802	VBP	C10-N09-C20	4.08	122.88	118.05
2	J	804	VBP	C10-N09-C20	4.48	123.35	118.05
2	L	801	VBP	C10-N09-C20	4.68	123.59	118.05
2	B	807	VBP	C10-N09-C20	4.71	123.63	118.05
2	E	808	VBP	C10-N09-C20	4.91	123.87	118.05
2	G	803	VBP	C10-N09-C20	5.07	124.05	118.05
2	H	806	VBP	C10-N09-C20	5.45	124.50	118.05

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	H	806	VBP	C02
2	E	808	VBP	C02
2	N	802	VBP	C02
2	B	807	VBP	C02
2	P	805	VBP	C02
2	J	804	VBP	C02
2	G	803	VBP	C02
2	L	801	VBP	C02

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	807	VBP	3	0
2	E	808	VBP	4	0
2	G	803	VBP	5	0
2	H	806	VBP	3	0
2	J	804	VBP	4	0
2	L	801	VBP	2	0
2	N	802	VBP	3	0
2	P	805	VBP	5	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	B	257/258 (99%)	1.56	78 (30%) 1 0	12, 32, 65, 76	0
1	E	257/258 (99%)	1.79	96 (37%) 0 0	17, 37, 70, 91	0
1	G	257/258 (99%)	1.50	64 (24%) 1 0	14, 34, 61, 71	0
1	H	257/258 (99%)	1.71	89 (34%) 0 0	13, 36, 72, 89	0
1	J	257/258 (99%)	1.64	78 (30%) 1 0	18, 35, 60, 68	0
1	L	257/258 (99%)	1.66	78 (30%) 1 0	18, 36, 64, 74	0
1	N	257/258 (99%)	1.65	76 (29%) 1 0	16, 35, 65, 74	0
1	P	257/258 (99%)	1.80	84 (32%) 1 0	17, 36, 63, 73	0
All	All	2056/2064 (99%)	1.66	643 (31%) 1 0	12, 35, 65, 91	0

All (643) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	121	ILE	11.0
1	H	164	SER	10.0
1	E	147	PHE	9.5
1	E	219	GLY	8.7
1	J	109	LEU	8.5
1	P	121	ILE	8.4
1	N	183	LYS	8.1
1	E	151	LYS	7.8
1	J	147	PHE	7.7
1	G	164	SER	7.7
1	L	108	SER	7.5
1	P	223	ALA	7.5
1	J	47	CYS	7.4
1	E	122	GLU	6.8
1	L	190	TYR	6.7
1	P	188	TYR	6.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	164	SER	6.5
1	N	136	GLY	6.4
1	B	161	TYR	6.4
1	N	161	TYR	6.4
1	H	135	TYR	6.4
1	L	49	PHE	6.4
1	H	153	ALA	6.2
1	H	154	VAL	6.2
1	E	167	PRO	6.2
1	B	151	LYS	6.1
1	E	205	PRO	6.1
1	L	246	LEU	6.0
1	N	124	ALA	6.0
1	N	121	ILE	5.9
1	E	204	LYS	5.8
1	N	159	TRP	5.8
1	P	11	ILE	5.7
1	J	135	TYR	5.7
1	H	167	PRO	5.6
1	H	148	ARG	5.6
1	G	118	GLY	5.5
1	N	80	TYR	5.5
1	L	205	PRO	5.5
1	G	136	GLY	5.5
1	L	150	SER	5.5
1	P	108	SER	5.5
1	N	209	MET	5.5
1	H	5	THR	5.5
1	E	213	GLY	5.5
1	L	207	ASP	5.4
1	H	144	LYS	5.4
1	L	5	THR	5.4
1	E	190	TYR	5.4
1	H	150	SER	5.3
1	N	148	ARG	5.3
1	H	114	MET	5.2
1	J	121	ILE	5.2
1	H	161	TYR	5.2
1	H	149	ARG	5.1
1	E	188	TYR	5.1
1	E	212	GLY	5.1
1	J	188	TYR	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	212	GLY	5.0
1	G	205	PRO	5.0
1	N	162	MET	4.9
1	L	157	LYS	4.9
1	P	136	GLY	4.9
1	P	126	ASP	4.9
1	B	114	MET	4.9
1	L	204	LYS	4.8
1	J	79	VAL	4.8
1	G	151	LYS	4.8
1	B	130	GLN	4.7
1	J	48	GLY	4.7
1	L	137	THR	4.7
1	G	16	TYR	4.7
1	E	26	LEU	4.7
1	J	134	ALA	4.7
1	H	151	LYS	4.7
1	P	182	ARG	4.7
1	J	123	SER	4.6
1	P	134	ALA	4.6
1	G	80	TYR	4.6
1	G	212	GLY	4.6
1	E	164	SER	4.6
1	H	127	LEU	4.6
1	L	48	GLY	4.6
1	G	165	ALA	4.5
1	J	151	LYS	4.5
1	P	110	GLY	4.5
1	B	150	SER	4.5
1	H	159	TRP	4.5
1	N	155	PHE	4.5
1	B	153	ALA	4.5
1	P	7	VAL	4.4
1	N	185	LYS	4.4
1	B	51	TYR	4.4
1	L	211	VAL	4.4
1	N	130	GLN	4.4
1	P	174	THR	4.4
1	H	257	ASP	4.4
1	N	223	ALA	4.4
1	L	129	LYS	4.4
1	B	176	GLU	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	127	LEU	4.3
1	N	149	ARG	4.3
1	J	211	VAL	4.3
1	G	227	GLY	4.3
1	B	144	LYS	4.2
1	B	154	VAL	4.2
1	P	169	VAL	4.2
1	P	109	LEU	4.2
1	E	199	TYR	4.2
1	B	78	LEU	4.1
1	J	130	GLN	4.1
1	H	261	CYS	4.1
1	E	142	SER	4.1
1	P	155	PHE	4.1
1	J	209	MET	4.1
1	P	180	ARG	4.1
1	B	129	LYS	4.1
1	H	112	SER	4.1
1	P	170	PHE	4.1
1	N	109	LEU	4.0
1	E	248	ASP	4.0
1	N	26	LEU	4.0
1	E	81	GLY	4.0
1	L	136	GLY	4.0
1	P	137	THR	4.0
1	P	233	ALA	4.0
1	H	250	LEU	4.0
1	N	172	ARG	4.0
1	J	154	VAL	4.0
1	L	120	PRO	4.0
1	P	189	ALA	4.0
1	N	182	ARG	4.0
1	G	213	GLY	4.0
1	E	162	MET	4.0
1	N	126	ASP	3.9
1	P	187	LYS	3.9
1	N	168	SER	3.9
1	E	171	VAL	3.9
1	H	168	SER	3.9
1	J	197	ASN	3.9
1	H	120	PRO	3.9
1	H	152	ILE	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	110	GLY	3.9
1	B	137	THR	3.9
1	G	142	SER	3.8
1	N	158	MET	3.8
1	J	11	ILE	3.8
1	P	30	GLU	3.8
1	J	204	LYS	3.8
1	L	208	THR	3.8
1	N	137	THR	3.8
1	B	152	ILE	3.8
1	B	159	TRP	3.8
1	J	137	THR	3.8
1	E	159	TRP	3.8
1	L	109	LEU	3.8
1	N	54	THR	3.8
1	E	21	LYS	3.8
1	H	137	THR	3.8
1	B	50	LYS	3.7
1	B	49	PHE	3.7
1	P	150	SER	3.7
1	P	193	GLU	3.7
1	G	46	HIS	3.7
1	L	75	VAL	3.7
1	P	135	TYR	3.7
1	B	181	VAL	3.7
1	P	105	PRO	3.7
1	E	144	LYS	3.7
1	P	173	THR	3.7
1	H	58	ASP	3.7
1	J	81	GLY	3.7
1	L	189	ALA	3.7
1	G	113	ILE	3.6
1	L	181	VAL	3.6
1	L	194	SER	3.6
1	P	215	LEU	3.6
1	L	147	PHE	3.6
1	L	177	GLY	3.6
1	B	196	MET	3.6
1	N	176	GLU	3.6
1	B	213	GLY	3.6
1	E	118	GLY	3.6
1	G	188	TYR	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	N	196	MET	3.6
1	N	204	LYS	3.6
1	N	123	SER	3.6
1	N	53	LEU	3.5
1	B	149	ARG	3.5
1	N	5	THR	3.5
1	J	219	GLY	3.5
1	E	211	VAL	3.5
1	P	5	THR	3.5
1	L	178	VAL	3.5
1	B	203	ARG	3.5
1	E	163	ARG	3.5
1	B	26	LEU	3.5
1	J	185	LYS	3.5
1	P	131	THR	3.5
1	H	162	MET	3.4
1	J	105	PRO	3.4
1	P	202	GLN	3.4
1	N	234	VAL	3.4
1	G	134	ALA	3.4
1	E	257	ASP	3.4
1	H	252	ASN	3.4
1	J	66	ALA	3.4
1	G	173	THR	3.4
1	J	215	LEU	3.4
1	B	99	VAL	3.4
1	E	51	TYR	3.4
1	H	51	TYR	3.4
1	J	122	GLU	3.4
1	P	178	VAL	3.4
1	N	246	LEU	3.3
1	P	36	CYS	3.3
1	J	257	ASP	3.3
1	L	26	LEU	3.3
1	E	136	GLY	3.3
1	G	96	ARG	3.3
1	J	230	LEU	3.3
1	G	147	PHE	3.3
1	P	94	LEU	3.3
1	N	174	THR	3.3
1	J	216	ASP	3.3
1	P	181	VAL	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	P	48	GLY	3.3
1	L	188	TYR	3.3
1	E	23	HIS	3.3
1	G	231	GLY	3.3
1	E	14	SER	3.3
1	H	158	MET	3.2
1	J	111	ILE	3.2
1	H	227	GLY	3.2
1	L	142	SER	3.2
1	P	140	SER	3.2
1	N	127	LEU	3.2
1	J	26	LEU	3.2
1	P	53	LEU	3.2
1	L	130	GLN	3.2
1	E	131	THR	3.2
1	N	208	THR	3.2
1	E	121	ILE	3.2
1	H	172	ARG	3.2
1	G	81	GLY	3.2
1	B	177	GLY	3.2
1	L	209	MET	3.2
1	J	148	ARG	3.1
1	G	11	ILE	3.1
1	E	150	SER	3.1
1	B	158	MET	3.1
1	B	204	LYS	3.1
1	N	122	GLU	3.1
1	E	99	VAL	3.1
1	E	102	PHE	3.1
1	E	146	PHE	3.1
1	L	119	THR	3.1
1	P	123	SER	3.1
1	P	186	GLY	3.1
1	G	25	MET	3.1
1	G	32	TYR	3.1
1	H	30	GLU	3.1
1	E	208	THR	3.0
1	P	106	PHE	3.0
1	E	40	ALA	3.0
1	J	199	TYR	3.0
1	B	184	SER	3.0
1	B	120	PRO	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	27	GLU	3.0
1	H	181	VAL	3.0
1	E	129	LYS	3.0
1	H	254	TRP	3.0
1	L	22	ASN	3.0
1	E	32	TYR	3.0
1	E	130	GLN	3.0
1	P	191	LEU	3.0
1	J	22	ASN	3.0
1	E	67	ASP	3.0
1	E	84	ASP	3.0
1	H	163	ARG	3.0
1	E	186	GLY	3.0
1	J	53	LEU	3.0
1	G	254	TRP	3.0
1	N	129	LYS	3.0
1	N	220	TYR	3.0
1	N	150	SER	3.0
1	B	63	ALA	3.0
1	L	183	LYS	3.0
1	B	135	TYR	3.0
1	G	137	THR	2.9
1	G	74	MET	2.9
1	H	8	VAL	2.9
1	J	89	PRO	2.9
1	P	60	LYS	2.9
1	E	85	ILE	2.9
1	J	59	GLY	2.9
1	J	108	SER	2.9
1	P	237	ALA	2.9
1	G	47	CYS	2.9
1	E	117	LYS	2.9
1	E	68	THR	2.9
1	E	250	LEU	2.9
1	J	190	TYR	2.9
1	L	118	GLY	2.9
1	G	28	GLY	2.9
1	G	108	SER	2.9
1	B	160	THR	2.9
1	B	118	GLY	2.9
1	P	216	ASP	2.9
1	H	171	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	154	VAL	2.9
1	H	189	ALA	2.9
1	P	234	VAL	2.8
1	E	43	ILE	2.8
1	H	111	ILE	2.8
1	H	194	SER	2.8
1	E	52	LYS	2.8
1	L	187	LYS	2.8
1	N	116	LYS	2.8
1	P	25	MET	2.8
1	H	166	GLU	2.8
1	L	113	ILE	2.8
1	H	117	LYS	2.8
1	E	133	ILE	2.8
1	E	148	ARG	2.8
1	G	135	TYR	2.8
1	B	46	HIS	2.8
1	N	178	VAL	2.8
1	N	190	TYR	2.8
1	B	15	PRO	2.8
1	H	113	ILE	2.8
1	H	138	LEU	2.8
1	N	132	GLU	2.8
1	B	86	ALA	2.8
1	P	47	CYS	2.8
1	N	119	THR	2.8
1	G	217	SER	2.8
1	L	37	VAL	2.8
1	L	217	SER	2.8
1	N	79	VAL	2.8
1	B	246	LEU	2.8
1	E	22	ASN	2.8
1	J	30	GLU	2.8
1	P	257	ASP	2.8
1	E	149	ARG	2.8
1	J	37	VAL	2.8
1	P	154	VAL	2.8
1	J	32	TYR	2.7
1	J	17	VAL	2.7
1	E	140	SER	2.7
1	E	115	ILE	2.7
1	G	72	ASN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	237	ALA	2.7
1	H	134	ALA	2.7
1	L	61	TYR	2.7
1	N	61	TYR	2.7
1	B	132	GLU	2.7
1	N	200	ILE	2.7
1	G	119	THR	2.7
1	E	145	GLU	2.7
1	E	221	GLY	2.7
1	E	227	GLY	2.7
1	H	239	LEU	2.7
1	N	49	PHE	2.7
1	J	67	ASP	2.7
1	B	121	ILE	2.7
1	L	206	CYS	2.7
1	N	108	SER	2.7
1	H	22	ASN	2.7
1	B	22	ASN	2.7
1	B	21	LYS	2.6
1	H	116	LYS	2.6
1	L	131	THR	2.6
1	J	180	ARG	2.6
1	E	185	LYS	2.6
1	L	259	GLY	2.6
1	G	242	ASN	2.6
1	B	236	LEU	2.6
1	G	149	ARG	2.6
1	J	18	MET	2.6
1	J	196	MET	2.6
1	L	173	THR	2.6
1	P	103	SER	2.6
1	P	252	ASN	2.6
1	B	146	PHE	2.6
1	B	254	TRP	2.6
1	L	220	TYR	2.6
1	G	206	CYS	2.6
1	E	231	GLY	2.6
1	J	136	GLY	2.6
1	P	74	MET	2.6
1	B	215	LEU	2.6
1	B	88	ALA	2.6
1	B	167	PRO	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	184	SER	2.6
1	N	198	GLU	2.6
1	H	124	ALA	2.6
1	H	130	GLN	2.6
1	P	179	ALA	2.6
1	J	203	ARG	2.5
1	E	113	ILE	2.5
1	B	165	ALA	2.5
1	P	244	GLN	2.5
1	N	67	ASP	2.5
1	G	170	PHE	2.5
1	G	143	THR	2.5
1	H	87	ILE	2.5
1	B	251	LYS	2.5
1	E	132	GLU	2.5
1	L	53	LEU	2.5
1	N	133	ILE	2.5
1	B	148	ARG	2.5
1	N	189	ALA	2.5
1	H	123	SER	2.5
1	G	204	LYS	2.5
1	N	236	LEU	2.5
1	E	46	HIS	2.5
1	P	162	MET	2.5
1	E	152	ILE	2.5
1	P	111	ILE	2.5
1	E	137	THR	2.5
1	J	162	MET	2.5
1	N	151	LYS	2.5
1	H	115	ILE	2.5
1	N	202	GLN	2.5
1	P	175	ALA	2.5
1	N	169	VAL	2.5
1	G	187	LYS	2.5
1	L	227	GLY	2.5
1	E	61	TYR	2.5
1	H	64	ARG	2.5
1	B	131	THR	2.5
1	P	130	GLN	2.5
1	J	117	LYS	2.5
1	J	170	PHE	2.5
1	E	89	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	179	ALA	2.4
1	B	73	GLY	2.4
1	G	131	THR	2.4
1	H	160	THR	2.4
1	J	150	SER	2.4
1	E	161	TYR	2.4
1	H	35	TYR	2.4
1	J	29	ASN	2.4
1	H	209	MET	2.4
1	P	209	MET	2.4
1	L	104	LYS	2.4
1	N	191	LEU	2.4
1	G	172	ARG	2.4
1	G	102	PHE	2.4
1	E	73	GLY	2.4
1	B	65	ASP	2.4
1	G	132	GLU	2.4
1	G	71	TRP	2.4
1	E	197	ASN	2.4
1	H	16	TYR	2.4
1	H	91	THR	2.4
1	E	157	LYS	2.4
1	N	181	VAL	2.4
1	N	201	GLU	2.4
1	B	12	LEU	2.4
1	L	192	LEU	2.4
1	L	66	ALA	2.4
1	B	91	THR	2.4
1	E	77	GLU	2.4
1	E	177	GLY	2.4
1	P	194	SER	2.4
1	J	54	THR	2.4
1	P	211	VAL	2.4
1	J	25	MET	2.4
1	H	55	ILE	2.4
1	L	168	SER	2.4
1	B	188	TYR	2.4
1	H	31	ARG	2.4
1	H	143	THR	2.4
1	J	70	ILE	2.4
1	B	163	ARG	2.4
1	B	34	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	200	ILE	2.3
1	E	259	GLY	2.3
1	P	221	GLY	2.3
1	P	116	LYS	2.3
1	P	129	LYS	2.3
1	G	36	CYS	2.3
1	H	21	LYS	2.3
1	J	155	PHE	2.3
1	G	123	SER	2.3
1	L	234	VAL	2.3
1	N	29	ASN	2.3
1	J	243	GLU	2.3
1	E	74	MET	2.3
1	E	206	CYS	2.3
1	H	170	PHE	2.3
1	G	39	LEU	2.3
1	G	121	ILE	2.3
1	L	225	PRO	2.3
1	N	205	PRO	2.3
1	P	58	ASP	2.3
1	L	51	TYR	2.3
1	L	54	THR	2.3
1	P	205	PRO	2.3
1	H	187	LYS	2.3
1	L	253	LYS	2.3
1	N	9	THR	2.3
1	H	198	GLU	2.3
1	E	15	PRO	2.3
1	G	259	GLY	2.3
1	L	172	ARG	2.3
1	G	140	SER	2.3
1	P	152	ILE	2.3
1	H	93	THR	2.3
1	B	225	PRO	2.3
1	H	136	GLY	2.3
1	E	176	GLU	2.2
1	B	174	THR	2.2
1	E	173	THR	2.2
1	B	202	GLN	2.2
1	N	255	TRP	2.2
1	B	252	ASN	2.2
1	B	183	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	N	128	SER	2.2
1	G	8	VAL	2.2
1	G	244	GLN	2.2
1	L	250	LEU	2.2
1	E	165	ALA	2.2
1	H	205	PRO	2.2
1	L	180	ARG	2.2
1	L	155	PHE	2.2
1	P	61	TYR	2.2
1	P	76	GLY	2.2
1	G	208	THR	2.2
1	B	10	THR	2.2
1	L	68	THR	2.2
1	N	207	ASP	2.2
1	H	218	LYS	2.2
1	E	217	SER	2.2
1	J	116	LYS	2.2
1	L	44	ALA	2.2
1	G	5	THR	2.2
1	J	10	THR	2.2
1	L	182	ARG	2.2
1	N	32	TYR	2.2
1	P	231	GLY	2.2
1	B	58	ASP	2.2
1	B	208	THR	2.2
1	J	133	ILE	2.2
1	P	133	ILE	2.2
1	G	166	GLU	2.2
1	J	46	HIS	2.2
1	L	135	TYR	2.2
1	P	158	MET	2.2
1	L	241	LEU	2.2
1	L	67	ASP	2.2
1	N	21	LYS	2.2
1	H	46	HIS	2.2
1	B	72	ASN	2.2
1	J	233	ALA	2.2
1	B	20	LYS	2.2
1	P	104	LYS	2.2
1	P	147	PHE	2.2
1	H	208	THR	2.2
1	L	9	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	124	ALA	2.2
1	P	84	ASP	2.1
1	G	177	GLY	2.1
1	E	47	CYS	2.1
1	J	182	ARG	2.1
1	G	234	VAL	2.1
1	E	220	TYR	2.1
1	N	164	SER	2.1
1	H	34	GLY	2.1
1	H	85	ILE	2.1
1	J	231	GLY	2.1
1	P	8	VAL	2.1
1	B	189	ALA	2.1
1	P	166	GLU	2.1
1	P	255	TRP	2.1
1	E	187	LYS	2.1
1	H	12	LEU	2.1
1	E	124	ALA	2.1
1	H	40	ALA	2.1
1	H	165	ALA	2.1
1	L	23	HIS	2.1
1	H	245	GLY	2.1
1	J	183	LYS	2.1
1	H	15	PRO	2.1
1	N	120	PRO	2.1
1	L	33	GLU	2.1
1	H	224	THR	2.1
1	E	135	TYR	2.1
1	E	218	LYS	2.1
1	H	211	VAL	2.1
1	N	193	GLU	2.1
1	L	151	LYS	2.1
1	B	190	TYR	2.1
1	L	199	TYR	2.1
1	B	103	SER	2.1
1	E	100	ILE	2.1
1	E	203	ARG	2.1
1	H	103	SER	2.1
1	J	168	SER	2.1
1	N	111	ILE	2.1
1	J	104	LYS	2.1
1	B	68	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	P	177	GLY	2.1
1	J	161	TYR	2.1
1	H	140	SER	2.1
1	N	184	SER	2.1
1	H	191	LEU	2.1
1	J	63	ALA	2.1
1	L	186	GLY	2.1
1	G	55	ILE	2.1
1	N	173	THR	2.1
1	H	185	LYS	2.1
1	N	235	ASN	2.1
1	H	225	PRO	2.1
1	J	169	VAL	2.1
1	L	52	LYS	2.0
1	L	16	TYR	2.0
1	H	232	ASN	2.0
1	E	112	SER	2.0
1	E	172	ARG	2.0
1	J	192	LEU	2.0
1	L	140	SER	2.0
1	H	49	PHE	2.0
1	G	85	ILE	2.0
1	E	180	ARG	2.0
1	G	238	VAL	2.0
1	B	112	SER	2.0
1	E	216	ASP	2.0
1	B	80	TYR	2.0
1	E	35	TYR	2.0
1	B	178	VAL	2.0
1	H	90	LEU	2.0
1	J	227	GLY	2.0
1	N	81	GLY	2.0
1	J	205	PRO	2.0
1	P	89	PRO	2.0
1	H	133	ILE	2.0
1	P	157	LYS	2.0
1	L	138	LEU	2.0
1	P	26	LEU	2.0
1	P	160	THR	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(Å ²)	Q<0.9
2	VBP	B	807	24/24	0.75	0.31	0.33	22,26,35,38	0
2	VBP	J	804	24/24	0.74	0.33	0.33	27,30,34,38	0
2	VBP	G	803	24/24	0.82	0.33	0.13	18,28,38,43	0
2	VBP	P	805	24/24	0.79	0.33	0.08	18,27,38,40	0
2	VBP	N	802	24/24	0.76	0.32	-0.09	21,25,38,38	0
2	VBP	E	808	24/24	0.77	0.30	-0.39	25,30,38,42	0
2	VBP	L	801	24/24	0.82	0.28	-0.58	22,25,31,38	0
2	VBP	H	806	24/24	0.78	0.28	-0.80	25,30,35,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.