



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:24 PM GMT

PDB ID : 3NNK
Title : Biochemical and Structural Characterization of a Ureidoglycine Aminotransferase in the Klebsiella pneumoniae Uric Acid Catabolic Pathway
Authors : French, J.B.; Ealick, S.E.
Deposited on : 2010-06-23
Resolution : 2.58 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

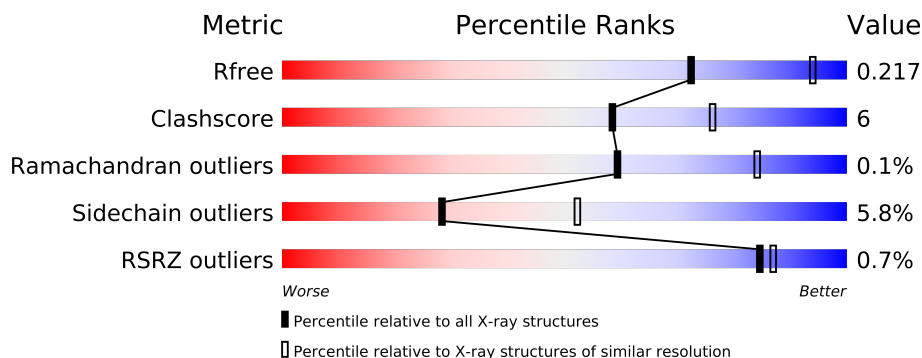
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.58 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}	66092	1891 (2.60-2.56)
Clashscore	79885	2358 (2.60-2.56)
Ramachandran outliers	78287	2316 (2.60-2.56)
Sidechain outliers	78261	2316 (2.60-2.56)
RSRZ outliers	66119	1891 (2.60-2.56)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	411	
1	B	411	
1	C	411	
1	D	411	
1	E	411	
1	F	411	
1	G	411	
1	H	411	
1	J	411	
1	K	411	
1	L	411	
1	M	411	
1	O	411	
1	P	411	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	R	411	
1	S	411	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 51634 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Ureidoglycine-glyoxylateaminotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	P	S	0	0	0
			3158	1987	558	586	1	26			
1	B	410	Total	C	N	O	P	S	0	0	0
			3175	1996	567	586	1	25			
1	C	410	Total	C	N	O	P	S	0	0	0
			3164	1988	565	585	1	25			
1	D	410	Total	C	N	O	P	S	0	0	0
			3180	1999	567	588	1	25			
1	E	410	Total	C	N	O	P	S	0	0	0
			3147	1981	557	583	1	25			
1	F	410	Total	C	N	O	P	S	0	0	0
			3171	1994	566	585	1	25			
1	G	410	Total	C	N	O	P	S	0	0	0
			3164	1988	565	585	1	25			
1	H	410	Total	C	N	O	P	S	0	0	0
			3183	2000	567	590	1	25			
1	J	410	Total	C	N	O	P	S	0	0	0
			3154	1984	558	586	1	25			
1	K	410	Total	C	N	O	P	S	0	0	0
			3175	1996	567	586	1	25			
1	L	409	Total	C	N	O	P	S	0	0	0
			3156	1982	564	584	1	25			
1	M	410	Total	C	N	O	P	S	0	0	0
			3183	2000	567	590	1	25			
1	O	410	Total	C	N	O	P	S	0	0	0
			3154	1984	558	586	1	25			
1	P	410	Total	C	N	O	P	S	0	0	0
			3175	1996	567	586	1	25			
1	R	410	Total	C	N	O	P	S	0	0	0
			3164	1988	565	585	1	25			
1	S	410	Total	C	N	O	P	S	0	0	0
			3179	1999	567	587	1	25			

- Molecule 2 is water.

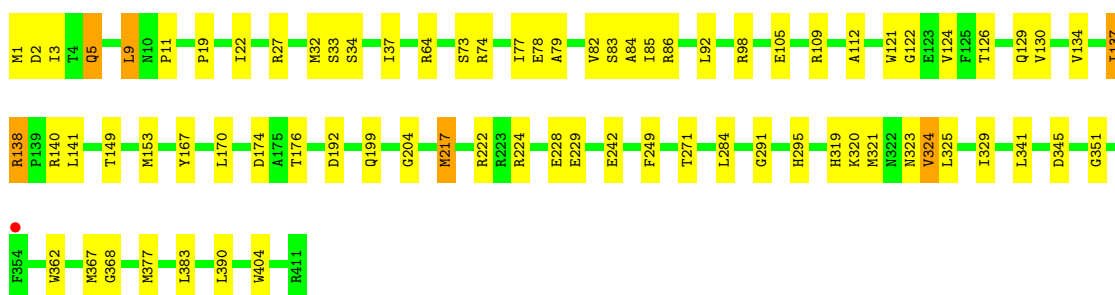
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	41	Total O 41 41	0	0
2	B	51	Total O 51 51	0	0
2	C	39	Total O 39 39	0	0
2	D	33	Total O 33 33	0	0
2	E	49	Total O 49 49	0	0
2	F	73	Total O 73 73	0	0
2	G	66	Total O 66 66	0	0
2	H	59	Total O 59 59	0	0
2	J	73	Total O 73 73	0	0
2	K	71	Total O 71 71	0	0
2	L	64	Total O 64 64	0	0
2	M	59	Total O 59 59	0	0
2	O	69	Total O 69 69	0	0
2	P	76	Total O 76 76	0	0
2	R	69	Total O 69 69	0	0
2	S	60	Total O 60 60	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.

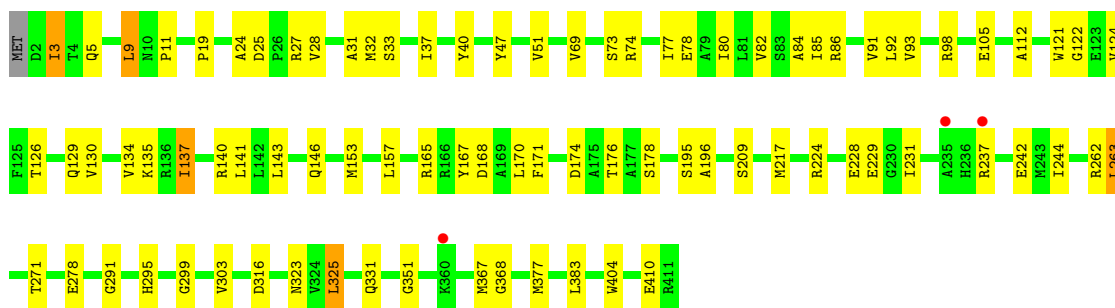
- Molecule 1: Ureidoglycine-glyoxylateaminotransferase

Chain A:



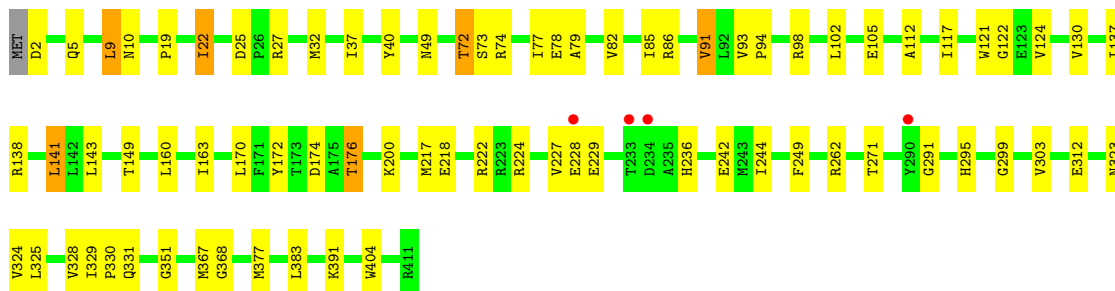
- Molecule 1: Ureidoglycine-glyoxylateaminotransferase

Chain B:



- Molecule 1: Ureidoglycine-glyoxylateaminotransferase

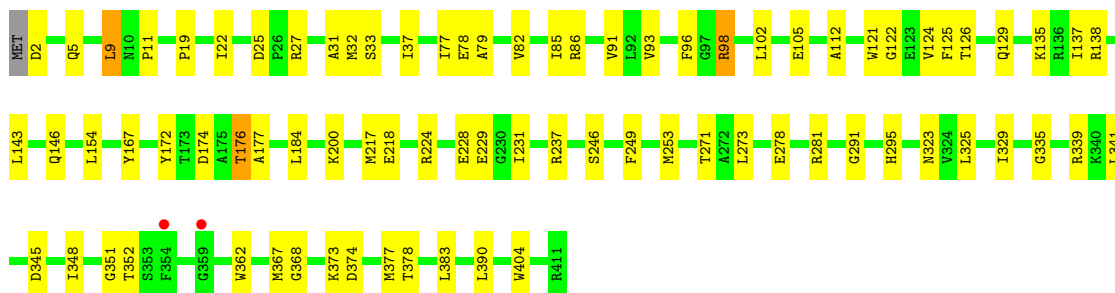
Chain C:



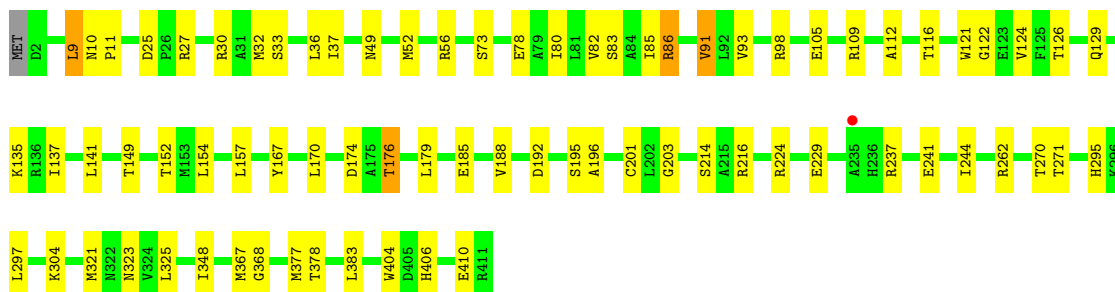
- Molecule 1: Ureidoglycine-glyoxylateaminotransferase

Chain D: 

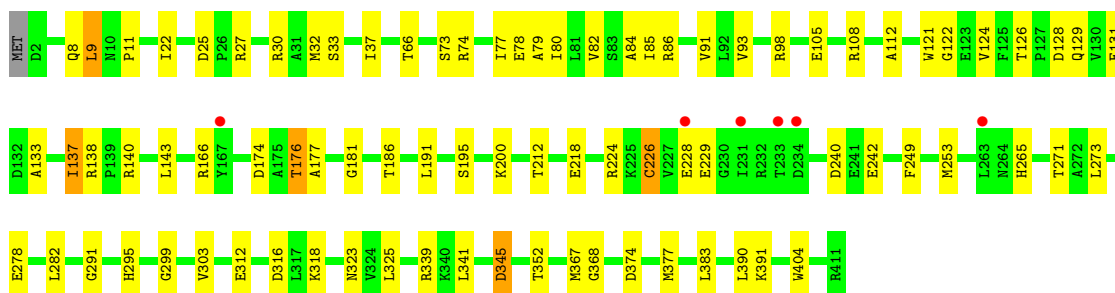
- Molecule 1: Ureidoglycine-glyoxylateaminotransferase

Chain E: 

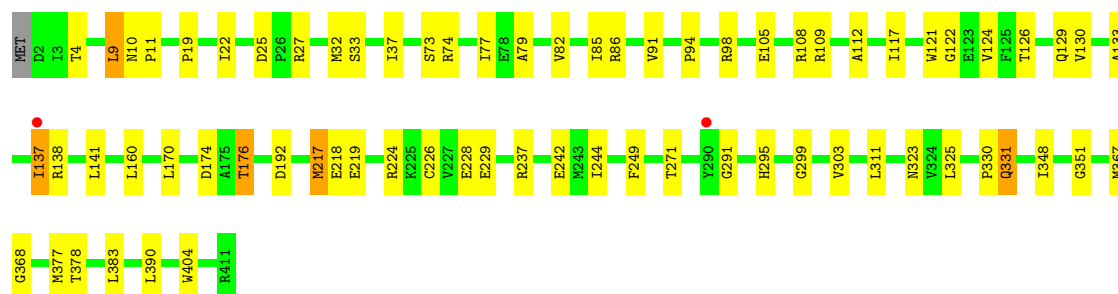
- Molecule 1: Ureidoglycine-glyoxylateaminotransferase

Chain F: 

- Molecule 1: Ureidoglycine-glyoxylateaminotransferase

Chain G: 

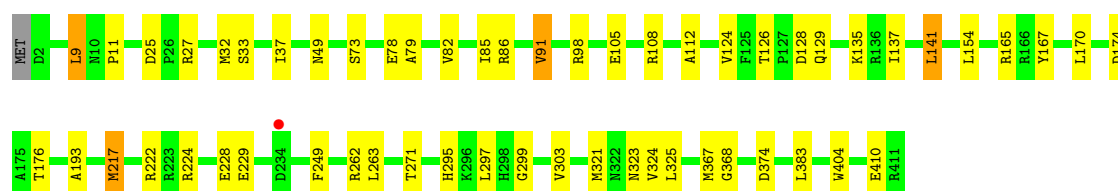
- Molecule 1: Ureidoglycine-glyoxylateaminotransferase

Chain H: 

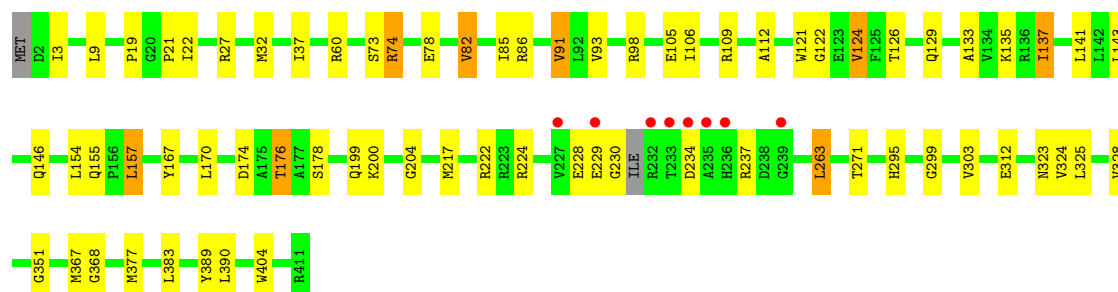
- Molecule 1: Ureidoglycine-glyoxylateaminotransferase

Chain J: 

- Molecule 1: Ureidoglycine-glyoxylateaminotransferase

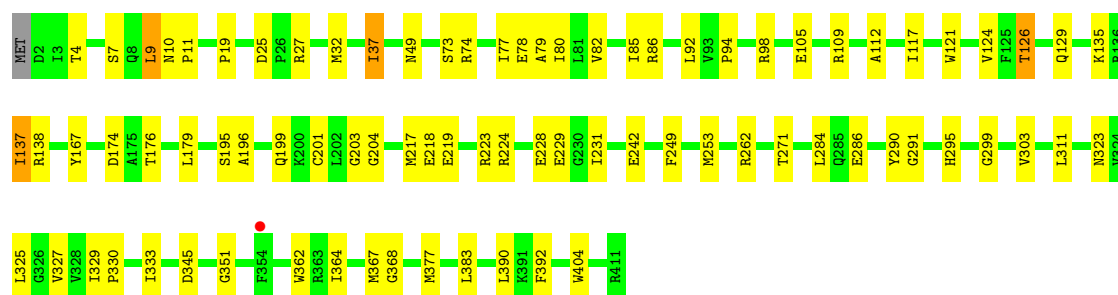
Chain K: 

- Molecule 1: Ureidoglycine-glyoxylateaminotransferase

Chain L: 

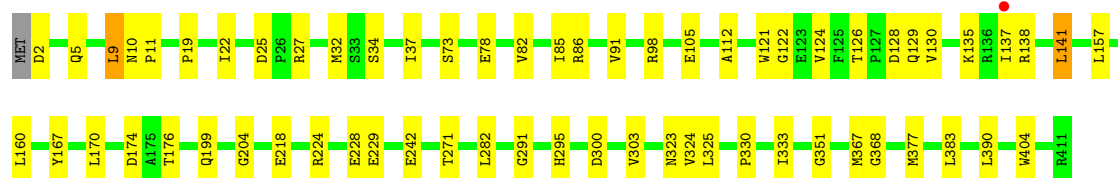
- Molecule 1: Ureidoglycine-glyoxylateaminotransferase

Chain M: 



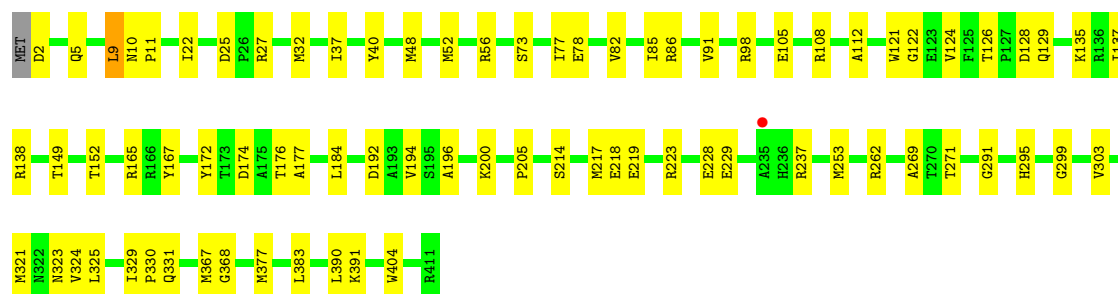
• Molecule 1: Ureidoglycine-glyoxylateaminotransferase

Chain O:



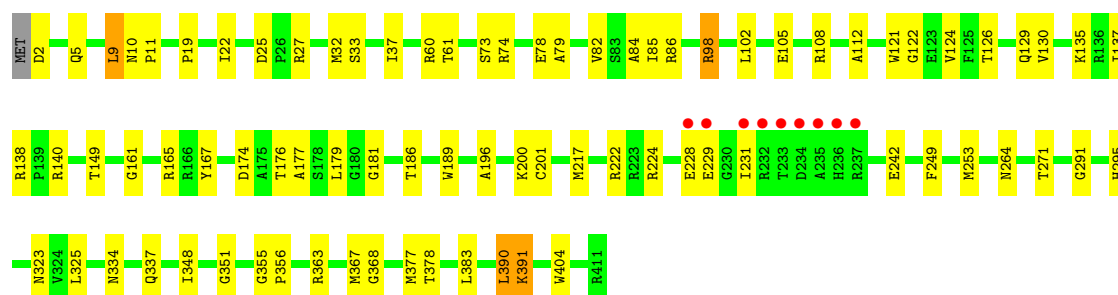
• Molecule 1: Ureidoglycine-glyoxylateaminotransferase

Chain P:



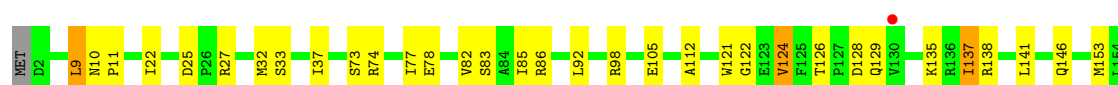
• Molecule 1: Ureidoglycine-glyoxylateaminotransferase

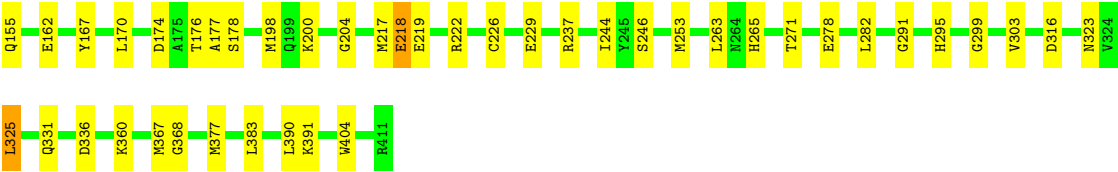
Chain R:



• Molecule 1: Ureidoglycine-glyoxylateaminotransferase

Chain S:





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	142.15Å 149.20Å 198.00Å 90.00° 90.28° 90.00°	Depositor
Resolution (Å)	50.00 – 2.58 49.85 – 2.58	Depositor EDS
% Data completeness (in resolution range)	93.8 (50.00-2.58) 93.9 (49.85-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.24 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.217 , 0.246 0.192 , 0.217	Depositor DCC
R_{free} test set	12155 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 7.8	EDS
Estimated twinning fraction	0.549 for H, K, L 0.451 for H, -K, -L 0.046 for -k,-h,-l 0.048 for k,h,-l 0.420 for h,-k,-l	Xtriage
Reported twinning fraction	0.549 for H, K, L 0.451 for H, -K, -L	Depositor
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	2 of 242432 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	51634	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	0/3198	0.52	0/4335
1	B	0.31	0/3215	0.51	0/4354
1	C	0.31	0/3204	0.52	1/4341 (0.0%)
1	D	0.32	0/3220	0.52	1/4360 (0.0%)
1	E	0.31	0/3187	0.51	0/4321
1	F	0.31	0/3211	0.52	0/4349
1	G	0.31	0/3204	0.51	0/4341
1	H	0.31	0/3223	0.51	0/4364
1	J	0.31	0/3194	0.52	0/4330
1	K	0.31	0/3215	0.52	2/4354 (0.0%)
1	L	0.31	0/3195	0.52	1/4327 (0.0%)
1	M	0.32	0/3223	0.51	0/4364
1	O	0.31	0/3194	0.52	1/4330 (0.0%)
1	P	0.31	0/3215	0.53	0/4354
1	R	0.31	0/3204	0.51	0/4341
1	S	0.32	0/3219	0.51	0/4358
All	All	0.31	0/51321	0.52	6/69523 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	141	LEU	CA-CB-CG	5.50	127.95	115.30
1	C	141	LEU	CA-CB-CG	5.26	127.40	115.30
1	D	141	LEU	CA-CB-CG	5.22	127.31	115.30
1	L	263	LEU	CA-CB-CG	5.14	127.13	115.30
1	O	141	LEU	CA-CB-CG	5.03	126.87	115.30
1	K	263	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3158	0	3092	45	0
1	B	3175	0	3129	51	0
1	C	3164	0	3103	46	0
1	D	3180	0	3135	52	0
1	E	3147	0	3078	41	0
1	F	3171	0	3123	47	0
1	G	3164	0	3103	52	0
1	H	3183	0	3137	45	0
1	J	3154	0	3086	42	0
1	K	3175	0	3129	35	0
1	L	3156	0	3091	40	0
1	M	3183	0	3137	47	0
1	O	3154	0	3086	36	0
1	P	3175	0	3129	45	0
1	R	3164	0	3103	45	0
1	S	3179	0	3135	46	0
2	A	41	0	0	0	0
2	B	51	0	0	3	0
2	C	39	0	0	1	0
2	D	33	0	0	0	0
2	E	49	0	0	0	0
2	F	73	0	0	2	0
2	G	66	0	0	2	0
2	H	59	0	0	0	0
2	J	73	0	0	0	0
2	K	71	0	0	0	0
2	L	64	0	0	0	0
2	M	59	0	0	0	0
2	O	69	0	0	0	0
2	P	76	0	0	3	0
2	R	69	0	0	0	0
2	S	60	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	51634	0	49796	626	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (626) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:72:THR:HG23	1:C:200:LLP:OP2	1.58	1.03
1:H:126:THR:H	1:H:129:GLN:HE21	1.14	0.96
1:K:174:ASP:OD1	1:K:176:THR:HG23	1.69	0.92
1:O:295:HIS:HE1	1:O:368:GLY:H	1.14	0.91
1:K:9:LEU:HD13	1:K:11:PRO:HD3	1.53	0.90
1:B:174:ASP:OD1	1:B:176:THR:HG23	1.72	0.89
1:K:126:THR:H	1:K:129:GLN:HE21	1.21	0.88
1:J:9:LEU:HD13	1:J:11:PRO:HD3	1.57	0.86
1:D:174:ASP:OD1	1:D:176:THR:HG23	1.77	0.85
1:G:295:HIS:HE1	1:G:368:GLY:H	1.25	0.83
1:O:126:THR:H	1:O:129:GLN:HE21	1.27	0.81
1:C:72:THR:CG2	1:C:200:LLP:OP2	2.29	0.81
1:R:390:LEU:O	1:R:391:LYS:HB2	1.80	0.80
1:M:25:ASP:OD1	1:M:27:ARG:HD3	1.80	0.80
1:S:78:GLU:O	1:S:82:VAL:HG23	1.81	0.79
1:J:174:ASP:OD1	1:J:176:THR:HG23	1.83	0.79
1:J:85:ILE:HG21	1:J:112:ALA:HB2	1.64	0.79
1:L:78:GLU:O	1:L:82:VAL:HG23	1.82	0.78
1:A:32:MET:SD	1:B:271:THR:HG21	2.23	0.78
1:E:85:ILE:HG21	1:E:112:ALA:HB2	1.66	0.78
1:J:229:GLU:H	1:K:105:GLU:HG3	1.50	0.77
1:S:174:ASP:OD1	1:S:176:THR:HG23	1.84	0.77
1:K:78:GLU:O	1:K:82:VAL:HG23	1.84	0.77
1:O:174:ASP:OD1	1:O:176:THR:HG23	1.85	0.77
1:C:295:HIS:HE1	1:C:368:GLY:H	1.29	0.76
1:F:295:HIS:HE1	1:F:368:GLY:H	1.30	0.76
1:J:295:HIS:HE1	1:J:368:GLY:H	1.32	0.75
1:J:32:MET:SD	1:K:271:THR:HG21	2.26	0.75
1:G:174:ASP:OD1	1:G:176:THR:HG23	1.88	0.73
1:M:295:HIS:HE1	1:M:368:GLY:H	1.34	0.73
1:F:297:LEU:HD13	1:F:410:GLU:HG2	1.69	0.73
1:G:9:LEU:HD13	1:G:11:PRO:HD3	1.70	0.73
1:G:78:GLU:O	1:G:82:VAL:HG23	1.89	0.73
1:O:330:PRO:HG2	1:O:333:ILE:HG13	1.69	0.73
1:J:105:GLU:HG3	1:K:229:GLU:H	1.52	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:323:ASN:HB2	1:B:367:MET:HG2	1.71	0.72
1:E:174:ASP:OD1	1:E:176:THR:HG22	1.89	0.72
1:F:85:ILE:HG21	1:F:112:ALA:HB2	1.71	0.72
1:A:73:SER:HB3	1:A:176:THR:HG21	1.72	0.72
1:A:85:ILE:HG21	1:A:112:ALA:HB2	1.69	0.72
1:H:9:LEU:HD13	1:H:11:PRO:HD3	1.70	0.72
1:P:295:HIS:HE1	1:P:368:GLY:H	1.34	0.72
1:B:25:ASP:OD1	1:B:27:ARG:HD3	1.90	0.71
1:F:126:THR:H	1:F:129:GLN:HE21	1.38	0.71
1:C:229:GLU:H	1:D:105:GLU:HG3	1.54	0.71
1:P:85:ILE:HG21	1:P:112:ALA:HB2	1.72	0.71
1:A:295:HIS:HE1	1:A:368:GLY:H	1.38	0.71
1:O:295:HIS:HE1	1:O:368:GLY:N	1.89	0.70
1:R:229:GLU:H	1:S:105:GLU:HG3	1.54	0.70
1:A:9:LEU:HD13	1:A:11:PRO:HD3	1.73	0.70
1:C:174:ASP:OD1	1:C:176:THR:HG23	1.92	0.70
1:R:32:MET:SD	1:S:271:THR:HG21	2.32	0.69
1:L:174:ASP:OD1	1:L:176:THR:HG23	1.93	0.69
1:K:295:HIS:HE1	1:K:368:GLY:H	1.40	0.69
1:B:126:THR:H	1:B:129:GLN:HE21	1.41	0.69
1:A:229:GLU:H	1:B:105:GLU:HG3	1.57	0.69
1:E:105:GLU:HG3	1:F:229:GLU:H	1.57	0.69
1:A:291:GLY:O	1:A:295:HIS:HD2	1.76	0.69
1:M:126:THR:H	1:M:129:GLN:HE21	1.39	0.69
1:D:82:VAL:HG12	1:D:244:ILE:HG23	1.73	0.68
1:K:323:ASN:HB2	1:K:367:MET:HG2	1.73	0.68
1:K:85:ILE:HG21	1:K:112:ALA:HB2	1.75	0.68
1:G:229:GLU:H	1:H:105:GLU:HG3	1.58	0.68
1:C:85:ILE:HG21	1:C:112:ALA:HB2	1.75	0.68
1:P:174:ASP:OD1	1:P:176:THR:HG23	1.94	0.68
1:B:295:HIS:HE1	1:B:368:GLY:H	1.42	0.67
1:H:295:HIS:HE1	1:H:368:GLY:H	1.43	0.67
1:R:126:THR:H	1:R:129:GLN:HE21	1.43	0.67
1:R:105:GLU:HG3	1:S:229:GLU:H	1.59	0.67
1:R:84:ALA:O	1:R:140:ARG:NH1	2.28	0.67
1:P:25:ASP:OD1	1:P:27:ARG:HD3	1.93	0.67
1:B:73:SER:HB3	1:B:176:THR:HG21	1.77	0.67
1:D:295:HIS:HE1	1:D:368:GLY:H	1.41	0.67
1:L:323:ASN:HB2	1:L:367:MET:HG2	1.77	0.66
1:R:174:ASP:OD1	1:R:176:THR:HG23	1.95	0.66
1:H:224:ARG:HD2	1:H:242:GLU:O	1.95	0.66
1:M:78:GLU:O	1:M:82:VAL:HG23	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:105:GLU:HG3	1:D:229:GLU:H	1.60	0.66
1:J:295:HIS:CE1	1:J:368:GLY:H	2.13	0.66
1:A:271:THR:HG21	1:B:32:MET:SD	2.36	0.66
1:K:141:LEU:HD13	1:K:170:LEU:HB2	1.78	0.66
1:E:9:LEU:HD13	1:E:11:PRO:HD3	1.78	0.66
1:K:126:THR:H	1:K:129:GLN:NE2	1.94	0.66
1:E:229:GLU:H	1:F:105:GLU:HG3	1.60	0.66
1:D:126:THR:H	1:D:129:GLN:HE21	1.44	0.65
1:B:3:ILE:HG13	1:B:3:ILE:O	1.94	0.65
1:G:291:GLY:O	1:G:295:HIS:HD2	1.79	0.65
1:M:291:GLY:O	1:M:295:HIS:HD2	1.78	0.65
1:R:271:THR:HG21	1:S:32:MET:SD	2.37	0.65
1:O:229:GLU:H	1:P:105:GLU:HG3	1.60	0.65
1:R:25:ASP:OD1	1:R:27:ARG:HD3	1.96	0.65
1:O:295:HIS:CE1	1:O:368:GLY:H	2.05	0.64
1:M:174:ASP:OD1	1:M:176:THR:HG23	1.97	0.64
1:D:85:ILE:HG21	1:D:112:ALA:HB2	1.79	0.64
1:R:85:ILE:HG21	1:R:112:ALA:HB2	1.79	0.64
1:S:73:SER:HB3	1:S:176:THR:HG21	1.78	0.64
1:O:228:GLU:HG2	1:P:105:GLU:HG3	1.79	0.64
1:D:177:ALA:HA	1:D:200:LLP:HG2	1.78	0.64
1:E:126:THR:H	1:E:129:GLN:HE21	1.45	0.64
1:S:126:THR:H	1:S:129:GLN:HE21	1.45	0.64
1:B:291:GLY:O	1:B:295:HIS:HD2	1.81	0.64
1:S:85:ILE:HG21	1:S:112:ALA:HB2	1.79	0.64
1:S:9:LEU:HD13	1:S:11:PRO:HD3	1.79	0.63
1:L:105:GLU:HG3	1:M:228:GLU:HG2	1.79	0.63
1:J:73:SER:HB3	1:J:176:THR:HG21	1.80	0.63
1:F:295:HIS:CE1	1:F:368:GLY:H	2.15	0.63
1:H:126:THR:H	1:H:129:GLN:NE2	1.94	0.63
1:J:271:THR:HG21	1:K:32:MET:SD	2.39	0.63
1:E:295:HIS:HE1	1:E:368:GLY:H	1.47	0.63
1:L:135:LYS:HE3	1:L:167:TYR:OH	1.98	0.62
1:O:323:ASN:HB2	1:O:367:MET:HG2	1.82	0.62
1:F:323:ASN:HB2	1:F:367:MET:HG2	1.80	0.62
1:P:135:LYS:HE3	1:P:167:TYR:OH	1.99	0.62
1:F:174:ASP:OD1	1:F:176:THR:HG23	1.98	0.62
1:R:231:ILE:HD13	1:R:264:ASN:O	2.00	0.62
1:G:32:MET:SD	1:H:271:THR:HG21	2.39	0.61
1:R:295:HIS:HE1	1:R:368:GLY:H	1.47	0.61
1:C:323:ASN:HB2	1:C:367:MET:HG2	1.81	0.61
1:A:33:SER:HB3	1:B:33:SER:HB3	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:73:SER:HB3	1:F:176:THR:HG21	1.83	0.61
1:A:284:LEU:HB2	1:B:3:ILE:HD13	1.82	0.61
1:P:73:SER:HB3	1:P:176:THR:HG21	1.81	0.61
1:B:85:ILE:HG21	1:B:112:ALA:HB2	1.82	0.61
1:C:2:ASP:O	1:C:5:GLN:HG2	2.01	0.61
1:A:295:HIS:CE1	1:A:368:GLY:H	2.19	0.61
1:M:295:HIS:CE1	1:M:368:GLY:H	2.16	0.61
1:M:333:ILE:HD11	1:M:392:PHE:HB2	1.82	0.61
1:G:105:GLU:HG3	1:H:229:GLU:H	1.66	0.60
1:H:85:ILE:HG21	1:H:112:ALA:HB2	1.83	0.60
1:M:176:THR:HG22	1:M:196:ALA:HA	1.82	0.60
1:L:295:HIS:HE1	1:L:368:GLY:H	1.47	0.60
1:K:25:ASP:OD1	1:K:27:ARG:HD3	2.01	0.60
1:M:323:ASN:HB2	1:M:367:MET:HG2	1.83	0.60
1:L:271:THR:HG21	1:M:32:MET:SD	2.41	0.60
1:S:295:HIS:CE1	1:S:368:GLY:H	2.19	0.60
1:D:141:LEU:HD13	1:D:170:LEU:HB2	1.84	0.60
1:A:105:GLU:HG3	1:B:229:GLU:H	1.65	0.60
1:F:304:LYS:HD2	1:F:406:HIS:HB2	1.84	0.60
1:G:224:ARG:HD2	1:G:242:GLU:O	2.02	0.59
1:E:373:LYS:HG2	2:G:921:HOH:O	2.01	0.59
1:G:295:HIS:HE1	1:G:368:GLY:N	1.98	0.59
1:L:85:ILE:HG21	1:L:112:ALA:HB2	1.84	0.59
1:L:229:GLU:H	1:M:105:GLU:HG3	1.66	0.59
1:M:85:ILE:HG21	1:M:112:ALA:HB2	1.84	0.59
1:O:25:ASP:OD1	1:O:27:ARG:HD3	2.02	0.59
1:S:295:HIS:HE1	1:S:368:GLY:H	1.50	0.59
1:L:74:ARG:HD2	1:L:200:LLP:OP2	2.01	0.59
1:L:73:SER:HB3	1:L:176:THR:HG21	1.83	0.59
1:L:228:GLU:HG2	1:L:230:GLY:H	1.67	0.59
1:P:149:THR:HG22	1:P:324:VAL:HG21	1.84	0.59
1:P:295:HIS:CE1	1:P:368:GLY:H	2.18	0.59
1:P:126:THR:H	1:P:129:GLN:HE21	1.50	0.59
1:J:84:ALA:O	1:J:140:ARG:NH1	2.36	0.59
1:C:295:HIS:CE1	1:C:368:GLY:H	2.17	0.59
1:J:152:THR:HA	1:J:321:MET:HE3	1.85	0.59
1:E:271:THR:HG21	1:F:32:MET:SD	2.42	0.59
1:R:177:ALA:HA	1:R:200:LLP:HG3	1.85	0.59
1:M:73:SER:HB3	1:M:176:THR:HG21	1.85	0.58
1:P:2:ASP:O	1:P:5:GLN:HG2	2.03	0.58
1:A:323:ASN:HB2	1:A:367:MET:HG2	1.85	0.58
1:O:32:MET:SD	1:P:271:THR:HG21	2.44	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:228:GLU:HG2	1:H:105:GLU:HG3	1.84	0.58
1:P:323:ASN:HB2	1:P:367:MET:HG2	1.85	0.58
1:R:323:ASN:HB2	1:R:367:MET:HG2	1.84	0.58
1:R:33:SER:HB3	1:S:33:SER:HB3	1.85	0.58
1:J:226:CYS:SG	1:K:108:ARG:NH1	2.75	0.58
1:K:154:LEU:HD23	1:K:321:MET:HG2	1.86	0.58
1:O:126:THR:H	1:O:129:GLN:NE2	2.00	0.58
1:B:295:HIS:HE1	1:B:368:GLY:N	2.02	0.58
1:P:27:ARG:HD2	1:S:10:ASN:ND2	2.19	0.58
1:E:32:MET:SD	1:F:271:THR:HG21	2.44	0.58
1:D:323:ASN:HB2	1:D:367:MET:HG2	1.84	0.58
1:G:85:ILE:HG21	1:G:112:ALA:HB2	1.84	0.57
1:D:78:GLU:O	1:D:82:VAL:HG23	2.04	0.57
1:F:25:ASP:OD1	1:F:27:ARG:HD3	2.04	0.57
1:H:330:PRO:O	1:H:331:GLN:CB	2.52	0.57
1:O:130:VAL:HG21	1:O:160:LEU:HG	1.85	0.57
1:P:330:PRO:O	1:P:331:GLN:HB2	2.04	0.57
1:C:271:THR:HG21	1:D:32:MET:SD	2.44	0.57
1:E:291:GLY:O	1:E:295:HIS:HD2	1.87	0.57
1:F:135:LYS:HE3	1:F:167:TYR:OH	2.04	0.57
1:O:78:GLU:O	1:O:82:VAL:HG23	2.03	0.57
1:O:105:GLU:HG3	1:P:228:GLU:HG2	1.86	0.57
1:E:135:LYS:HE3	1:E:167:TYR:OH	2.04	0.57
1:B:135:LYS:HE3	1:B:167:TYR:OH	2.04	0.57
1:P:126:THR:H	1:P:129:GLN:NE2	2.03	0.57
1:G:271:THR:HG21	1:H:32:MET:SD	2.45	0.57
1:D:25:ASP:OD1	1:D:27:ARG:HD3	2.04	0.57
1:E:79:ALA:HA	1:E:249:PHE:HB3	1.87	0.57
1:C:72:THR:HG21	1:D:266:HIS:HB2	1.87	0.56
1:B:40:TYR:HE1	1:B:262:ARG:HB3	1.70	0.56
1:L:32:MET:SD	1:M:271:THR:HG21	2.45	0.56
1:P:78:GLU:O	1:P:82:VAL:HG23	2.05	0.56
1:B:231:ILE:HD12	1:B:263:LEU:HD13	1.87	0.56
1:J:105:GLU:HG3	1:K:228:GLU:HG2	1.87	0.56
1:R:9:LEU:HD13	1:R:11:PRO:HD3	1.87	0.56
1:E:323:ASN:HB2	1:E:367:MET:HG2	1.87	0.56
1:M:311:LEU:CD2	1:M:330:PRO:HG3	2.35	0.56
1:B:93:VAL:HG22	1:B:143:LEU:HB2	1.87	0.56
1:M:49:ASN:HD21	1:M:262:ARG:HH22	1.53	0.56
1:C:25:ASP:OD1	1:C:27:ARG:HD3	2.06	0.56
1:A:174:ASP:OD1	1:A:176:THR:HG23	2.05	0.56
1:F:91:VAL:HG22	1:F:141:LEU:HB2	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:19:PRO:HD3	1:B:351:GLY:HA3	1.88	0.56
1:R:108:ARG:NH1	1:S:226:CYS:SG	2.79	0.56
1:G:105:GLU:HG3	1:H:228:GLU:HG2	1.88	0.56
1:O:105:GLU:HG3	1:P:229:GLU:H	1.71	0.55
1:G:25:ASP:OD1	1:G:27:ARG:HD3	2.06	0.55
1:G:33:SER:HB3	1:H:33:SER:HB3	1.86	0.55
1:K:126:THR:HG22	1:K:128:ASP:H	1.71	0.55
1:G:228:GLU:H	1:G:253:MET:HE3	1.71	0.55
1:D:299:GLY:O	1:D:303:VAL:HG23	2.06	0.55
1:H:25:ASP:OD1	1:H:27:ARG:HD3	2.06	0.55
1:O:141:LEU:HD13	1:O:170:LEU:HB2	1.87	0.55
1:K:295:HIS:CE1	1:K:368:GLY:H	2.21	0.55
1:H:82:VAL:HG12	1:H:244:ILE:HG23	1.88	0.55
1:B:27:ARG:HD2	1:D:10:ASN:ND2	2.22	0.55
1:P:299:GLY:O	1:P:303:VAL:HG23	2.07	0.55
1:L:199:GLN:HA	1:L:204:GLY:O	2.06	0.55
1:M:105:GLU:O	1:M:109:ARG:HG2	2.06	0.55
1:O:9:LEU:HD13	1:O:11:PRO:HD3	1.89	0.54
1:E:177:ALA:HA	1:E:200:LLP:HG3	1.90	0.54
1:O:271:THR:HG21	1:P:32:MET:SD	2.48	0.54
1:F:78:GLU:O	1:F:82:VAL:HG23	2.07	0.54
1:B:82:VAL:HG12	1:B:244:ILE:HG23	1.90	0.54
1:E:25:ASP:OD1	1:E:27:ARG:HD3	2.07	0.54
1:R:105:GLU:CG	1:S:229:GLU:H	2.19	0.54
1:K:49:ASN:HD21	1:K:262:ARG:HH22	1.55	0.54
1:R:390:LEU:O	1:R:391:LYS:CB	2.52	0.54
1:G:229:GLU:H	1:H:105:GLU:CG	2.21	0.54
1:H:141:LEU:HD13	1:H:170:LEU:HB2	1.90	0.54
1:S:299:GLY:O	1:S:303:VAL:HG23	2.08	0.53
1:E:341:LEU:O	1:E:345:ASP:HB2	2.08	0.53
1:J:33:SER:HB3	1:K:33:SER:HB3	1.90	0.53
1:S:323:ASN:HB2	1:S:367:MET:HG2	1.89	0.53
1:O:73:SER:HB3	1:O:176:THR:HG21	1.90	0.53
1:R:78:GLU:O	1:R:82:VAL:HG23	2.07	0.53
1:F:49:ASN:HD21	1:F:262:ARG:HH22	1.55	0.53
1:R:228:GLU:HG2	1:S:105:GLU:HG3	1.91	0.53
1:L:199:GLN:NE2	1:L:200:LLP:OP3	2.40	0.53
1:P:126:THR:HG22	1:P:128:ASP:H	1.72	0.53
1:H:82:VAL:HG12	1:H:244:ILE:CG2	2.39	0.53
1:J:149:THR:HA	1:J:321:MET:HE1	1.91	0.53
1:O:85:ILE:HG21	1:O:112:ALA:HB2	1.91	0.53
1:P:321:MET:SD	2:P:552:HOH:O	2.59	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:408:ARG:HB2	1:S:360:LYS:NZ	2.23	0.53
1:C:291:GLY:O	1:C:295:HIS:HD2	1.91	0.53
1:J:291:GLY:O	1:J:295:HIS:HD2	1.91	0.53
1:D:295:HIS:CE1	1:D:368:GLY:H	2.25	0.53
1:E:31:ALA:HB2	1:E:278:GLU:HG3	1.91	0.53
1:L:299:GLY:O	1:L:303:VAL:HG23	2.09	0.53
1:H:323:ASN:HB2	1:H:367:MET:HG2	1.91	0.53
1:G:177:ALA:HA	1:G:200:LLP:HG3	1.91	0.52
1:F:9:LEU:HD13	1:F:11:PRO:HD3	1.92	0.52
1:P:9:LEU:HD12	1:P:11:PRO:HD3	1.92	0.52
1:D:73:SER:HB3	1:D:176:THR:HG21	1.92	0.52
1:P:176:THR:HG22	1:P:196:ALA:C	2.30	0.52
1:B:84:ALA:O	1:B:140:ARG:NH1	2.43	0.52
1:F:83:SER:HA	1:F:244:ILE:HG12	1.91	0.52
1:R:295:HIS:HE1	1:R:368:GLY:N	2.08	0.52
1:J:405:ASP:O	1:S:360:LYS:HE3	2.10	0.52
1:M:79:ALA:HA	1:M:249:PHE:HB3	1.91	0.52
1:G:291:GLY:O	1:G:295:HIS:CD2	2.61	0.52
1:G:105:GLU:CG	1:H:229:GLU:H	2.22	0.52
1:J:105:GLU:CG	1:K:229:GLU:H	2.19	0.51
1:G:93:VAL:HG22	1:G:143:LEU:HB2	1.90	0.51
1:M:224:ARG:HD2	1:M:242:GLU:O	2.10	0.51
1:L:78:GLU:HG3	1:L:106:ILE:HG23	1.93	0.51
1:D:126:THR:HG22	1:D:128:ASP:H	1.74	0.51
1:C:94:PRO:HA	1:C:117:ILE:HG13	1.93	0.51
1:L:389:TYR:CZ	1:S:331:GLN:HB3	2.45	0.51
1:F:86:ARG:HH21	1:F:241:GLU:CD	2.13	0.51
1:C:9:LEU:HD23	1:D:277:ARG:HD3	1.92	0.51
1:S:153:MET:HE1	1:S:316:ASP:O	2.10	0.51
1:A:224:ARG:HD2	1:A:242:GLU:O	2.10	0.51
1:E:228:GLU:HG2	1:F:105:GLU:HG3	1.93	0.51
1:C:228:GLU:HG2	1:D:105:GLU:HG3	1.92	0.51
1:R:2:ASP:O	1:R:5:GLN:HG2	2.11	0.51
1:G:186:THR:HA	1:G:191:LEU:HD12	1.93	0.51
1:S:83:SER:HA	1:S:244:ILE:HG12	1.93	0.51
1:B:9:LEU:HD13	1:B:11:PRO:HD3	1.93	0.51
1:G:126:THR:H	1:G:129:GLN:NE2	2.07	0.51
1:B:24:ALA:HB1	2:B:833:HOH:O	2.10	0.51
1:K:135:LYS:HE3	1:K:167:TYR:OH	2.11	0.51
1:A:1:MET:HB3	1:A:2:ASP:HA	1.91	0.51
1:P:40:TYR:HE1	1:P:262:ARG:HB3	1.75	0.51
1:O:2:ASP:O	1:O:5:GLN:HG2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:27:ARG:HD2	1:H:10:ASN:ND2	2.26	0.51
1:B:80:ILE:HD12	1:B:195:SER:HB3	1.93	0.50
1:B:47:TYR:O	1:B:51:VAL:HG23	2.11	0.50
1:L:105:GLU:HG3	1:M:229:GLU:H	1.75	0.50
1:L:146:GLN:NE2	1:L:178:SER:OG	2.44	0.50
1:H:73:SER:HB3	1:H:176:THR:HG21	1.93	0.50
1:D:91:VAL:HG22	1:D:141:LEU:HB2	1.94	0.50
1:J:49:ASN:HD21	1:J:262:ARG:HH22	1.60	0.50
1:K:73:SER:HB3	1:K:176:THR:HG21	1.92	0.50
1:C:141:LEU:HD13	1:C:170:LEU:HB2	1.93	0.50
1:H:348:ILE:HD11	1:H:378:THR:HG22	1.93	0.50
1:E:281:ARG:HH22	1:G:8:GLN:NE2	2.10	0.50
1:C:40:TYR:HE1	1:C:262:ARG:HB3	1.76	0.50
1:J:228:GLU:HB3	1:J:253:MET:HE1	1.94	0.50
1:L:126:THR:H	1:L:129:GLN:HE21	1.60	0.50
1:G:82:VAL:O	1:G:224:ARG:NH2	2.45	0.50
1:L:133:ALA:O	1:L:137:ILE:HD13	2.12	0.50
1:G:126:THR:H	1:G:129:GLN:HE21	1.59	0.49
1:D:92:LEU:HB2	1:D:137:ILE:HD11	1.94	0.49
1:C:32:MET:SD	1:D:271:THR:HG21	2.52	0.49
1:K:27:ARG:HD2	1:M:10:ASN:ND2	2.27	0.49
1:F:141:LEU:HD13	1:F:170:LEU:HB2	1.95	0.49
1:G:323:ASN:HB2	1:G:367:MET:HG2	1.94	0.49
1:C:72:THR:HG23	1:C:200:LLP:P	2.49	0.49
1:R:229:GLU:H	1:S:105:GLU:CG	2.23	0.49
1:A:228:GLU:HG2	1:B:105:GLU:HG3	1.93	0.49
1:D:9:LEU:CD1	1:D:11:PRO:HD3	2.43	0.49
1:S:303:VAL:HG22	1:S:325:LEU:HG	1.94	0.49
1:B:176:THR:HG22	1:B:196:ALA:HA	1.93	0.49
1:L:389:TYR:CE1	1:S:331:GLN:HB3	2.47	0.49
1:H:174:ASP:OD1	1:H:176:THR:HG23	2.12	0.49
1:L:141:LEU:HD13	1:L:170:LEU:HB2	1.94	0.49
1:G:265:HIS:HB2	2:G:440:HOH:O	2.10	0.49
1:R:224:ARG:HD2	1:R:242:GLU:O	2.13	0.49
1:C:82:VAL:O	1:C:224:ARG:NH2	2.46	0.49
1:E:33:SER:HB3	1:F:33:SER:HB3	1.95	0.49
1:M:329:ILE:HG12	1:M:362:TRP:CE2	2.47	0.49
1:B:31:ALA:HB2	1:B:278:GLU:HG3	1.94	0.49
1:R:176:THR:HG22	1:R:196:ALA:HA	1.95	0.48
1:R:161:GLY:HA3	1:R:189:TRP:O	2.13	0.48
1:L:146:GLN:HG3	1:L:157:LEU:HD22	1.95	0.48
1:F:185:GLU:HB3	1:F:188:VAL:HB	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:19:PRO:HD3	1:J:351:GLY:HA3	1.94	0.48
1:A:126:THR:H	1:A:129:GLN:HE21	1.62	0.48
1:D:93:VAL:HG22	1:D:143:LEU:HB2	1.95	0.48
1:G:84:ALA:O	1:G:140:ARG:NH1	2.47	0.48
1:K:374:ASP:HA	1:M:345:ASP:O	2.13	0.48
1:D:121:TRP:HA	1:D:122:GLY:HA2	1.69	0.48
1:H:295:HIS:CE1	1:H:368:GLY:H	2.29	0.48
1:G:73:SER:HB3	1:G:176:THR:HG21	1.94	0.48
1:D:9:LEU:HD13	1:D:11:PRO:HD3	1.96	0.48
1:G:278:GLU:O	1:G:282:LEU:HG	2.13	0.48
1:J:78:GLU:O	1:J:82:VAL:HG23	2.14	0.48
1:F:85:ILE:O	1:F:224:ARG:NH2	2.47	0.48
1:L:3:ILE:HD13	1:M:284:LEU:HB2	1.94	0.48
1:F:152:THR:HA	1:F:321:MET:CE	2.43	0.48
1:R:181:GLY:HA2	1:R:295:HIS:CD2	2.49	0.48
1:F:152:THR:HA	1:F:321:MET:HE2	1.96	0.48
1:M:9:LEU:HD12	1:M:11:PRO:HD3	1.95	0.48
1:A:121:TRP:HA	1:A:122:GLY:HA2	1.71	0.48
1:F:52:MET:O	1:F:56:ARG:HG3	2.14	0.48
1:B:153:MET:HE1	1:B:316:ASP:HB3	1.95	0.48
1:G:79:ALA:HA	1:G:249:PHE:HB3	1.96	0.48
1:L:389:TYR:O	1:S:331:GLN:OE1	2.31	0.47
1:A:27:ARG:HD2	1:C:10:ASN:ND2	2.29	0.47
1:R:135:LYS:HE3	1:R:167:TYR:OH	2.14	0.47
1:H:19:PRO:HD3	1:H:351:GLY:HA3	1.96	0.47
1:E:78:GLU:O	1:E:82:VAL:HG23	2.14	0.47
1:J:331:GLN:HA	1:J:332:GLY:HA2	1.64	0.47
1:L:121:TRP:HA	1:L:122:GLY:HA2	1.71	0.47
1:H:94:PRO:HA	1:H:117:ILE:HG13	1.95	0.47
1:M:94:PRO:HA	1:M:117:ILE:HG13	1.96	0.47
1:C:74:ARG:HH21	1:C:102:LEU:HD13	1.79	0.47
1:J:229:GLU:H	1:K:105:GLU:CG	2.24	0.47
1:H:311:LEU:CD2	1:H:330:PRO:HG3	2.44	0.47
1:E:96:PHE:HB3	1:E:125:PHE:CE2	2.50	0.47
1:G:316:ASP:OD1	1:G:318:LYS:HE3	2.15	0.47
1:B:157:LEU:HG	1:B:171:PHE:HZ	1.80	0.47
1:F:192:ASP:HA	1:F:214:SER:HB3	1.96	0.47
1:L:93:VAL:HG22	1:L:143:LEU:HB2	1.95	0.47
1:A:1:MET:HB3	1:A:2:ASP:CA	2.45	0.47
1:A:79:ALA:HA	1:A:249:PHE:HB3	1.97	0.47
1:P:177:ALA:HA	1:P:200:LLP:HG3	1.97	0.47
1:S:177:ALA:HA	1:S:200:LLP:HG3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:78:GLU:O	1:A:82:VAL:HG23	2.15	0.47
1:P:205:PRO:HD2	2:P:903:HOH:O	2.14	0.47
1:B:299:GLY:O	1:B:303:VAL:HG23	2.14	0.47
1:P:192:ASP:HA	1:P:214:SER:HB3	1.96	0.47
1:C:79:ALA:HA	1:C:249:PHE:HB3	1.97	0.47
1:G:181:GLY:HA2	1:G:295:HIS:CD2	2.50	0.47
1:A:153:MET:HE1	1:A:319:HIS:HB2	1.95	0.47
1:C:227:VAL:HG21	1:C:236:HIS:CD2	2.49	0.47
1:L:295:HIS:CE1	1:L:368:GLY:H	2.32	0.47
1:G:66:THR:HG23	1:G:212:THR:HB	1.97	0.47
1:L:19:PRO:HD3	1:L:351:GLY:HA3	1.97	0.47
1:G:339:ARG:CZ	1:G:352:THR:HB	2.45	0.47
1:H:192:ASP:HB3	1:H:217:MET:HG2	1.97	0.47
1:C:49:ASN:HD21	1:C:262:ARG:HH22	1.63	0.47
1:H:299:GLY:O	1:H:303:VAL:HG23	2.16	0.47
1:D:254:VAL:O	1:D:258:TRP:HD1	1.98	0.46
1:O:105:GLU:CG	1:P:229:GLU:H	2.27	0.46
1:B:82:VAL:HG12	1:B:244:ILE:CG2	2.46	0.46
1:E:146:GLN:HE22	1:E:184:LEU:HD13	1.80	0.46
1:E:348:ILE:HD11	1:E:378:THR:HG22	1.96	0.46
1:C:105:GLU:HG3	1:D:228:GLU:HG2	1.96	0.46
1:B:224:ARG:HD2	1:B:242:GLU:O	2.16	0.46
1:J:80:ILE:HD12	1:J:195:SER:HB3	1.97	0.46
1:A:84:ALA:O	1:A:140:ARG:NH1	2.48	0.46
1:D:78:GLU:HG3	1:D:106:ILE:HG23	1.96	0.46
1:D:177:ALA:HB2	1:D:200:LLP:O3	2.16	0.46
1:D:82:VAL:O	1:D:224:ARG:NH2	2.49	0.46
1:B:28:VAL:HB	2:B:833:HOH:O	2.15	0.46
1:A:192:ASP:HB3	1:A:217:MET:HG2	1.97	0.46
1:S:121:TRP:HA	1:S:122:GLY:HA2	1.68	0.46
1:L:124:VAL:HG22	1:L:155:GLN:OE1	2.16	0.46
1:F:105:GLU:O	1:F:109:ARG:HG2	2.15	0.46
1:E:295:HIS:HE1	1:E:368:GLY:N	2.13	0.46
1:A:138:ARG:HH21	1:A:167:TYR:HB3	1.80	0.46
1:H:79:ALA:HA	1:H:249:PHE:HB3	1.98	0.46
1:J:121:TRP:HA	1:J:122:GLY:HA2	1.69	0.46
1:A:141:LEU:HD13	1:A:170:LEU:HB2	1.98	0.46
1:P:184:LEU:HD21	1:P:194:VAL:HG11	1.98	0.46
1:E:231:ILE:HD11	1:E:253:MET:HE3	1.97	0.46
1:G:74:ARG:HA	1:G:77:ILE:HD12	1.97	0.46
1:P:291:GLY:O	1:P:295:HIS:HD2	1.99	0.46
1:C:74:ARG:HA	1:C:77:ILE:HD12	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:329:ILE:HG12	1:A:362:TRP:CE2	2.50	0.46
1:G:121:TRP:HA	1:G:122:GLY:HA2	1.71	0.46
1:S:135:LYS:HE3	1:S:167:TYR:OH	2.16	0.46
1:H:91:VAL:HG22	1:H:141:LEU:HB2	1.97	0.45
1:A:199:GLN:HA	1:A:204:GLY:O	2.16	0.45
1:R:73:SER:HB3	1:R:176:THR:HG21	1.99	0.45
1:S:25:ASP:OD1	1:S:27:ARG:HD3	2.16	0.45
1:E:2:ASP:O	1:E:5:GLN:HG2	2.16	0.45
1:D:162:GLU:OE2	1:D:165:ARG:NH2	2.46	0.45
1:J:25:ASP:OD1	1:J:27:ARG:HD3	2.16	0.45
1:K:91:VAL:HG22	1:K:141:LEU:HB2	1.97	0.45
1:B:91:VAL:HG22	1:B:141:LEU:HB2	1.97	0.45
1:B:121:TRP:HA	1:B:122:GLY:HA2	1.72	0.45
1:P:295:HIS:HE1	1:P:368:GLY:N	2.08	0.45
1:K:299:GLY:O	1:K:303:VAL:HG23	2.16	0.45
1:G:299:GLY:O	1:G:303:VAL:HG23	2.16	0.45
1:M:219:GLU:O	1:M:223:ARG:HG3	2.16	0.45
1:P:329:ILE:HA	1:P:330:PRO:HD3	1.85	0.45
1:G:126:THR:HG22	1:G:128:ASP:H	1.81	0.45
1:L:3:ILE:HD13	1:M:284:LEU:CB	2.46	0.45
1:R:179:LEU:O	1:R:201:CYS:HB2	2.17	0.45
1:O:126:THR:HG22	1:O:128:ASP:H	1.82	0.45
1:J:224:ARG:HD2	1:J:242:GLU:O	2.17	0.45
1:R:98:ARG:NH1	1:R:102:LEU:HB2	2.31	0.45
1:M:231:ILE:HD11	1:M:253:MET:HE3	1.99	0.45
1:M:49:ASN:ND2	1:M:262:ARG:HH22	2.13	0.45
1:B:278:GLU:HG2	2:B:601:HOH:O	2.15	0.45
1:O:291:GLY:O	1:O:295:HIS:HD2	1.99	0.45
1:F:295:HIS:HE1	1:F:368:GLY:N	2.06	0.45
1:S:126:THR:HG22	1:S:128:ASP:H	1.82	0.45
1:A:105:GLU:O	1:A:109:ARG:HG2	2.17	0.45
1:D:152:THR:HA	1:D:321:MET:HE3	1.99	0.45
1:A:130:VAL:O	1:A:134:VAL:HG23	2.17	0.45
1:F:154:LEU:HD23	1:F:321:MET:HG2	1.99	0.45
1:C:93:VAL:HG22	1:C:143:LEU:HB2	1.99	0.45
1:D:84:ALA:O	1:D:140:ARG:NH1	2.49	0.45
1:F:216:ARG:HG3	2:F:488:HOH:O	2.16	0.45
1:M:92:LEU:HB2	1:M:137:ILE:HD11	1.99	0.45
1:D:40:TYR:HE1	1:D:262:ARG:HB3	1.82	0.45
1:M:74:ARG:HA	1:M:77:ILE:HD12	1.99	0.44
1:A:5:GLN:H	1:A:5:GLN:HG2	1.59	0.44
1:H:74:ARG:HA	1:H:77:ILE:HD12	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:80:ILE:HD12	1:D:195:SER:HB3	1.99	0.44
1:E:93:VAL:HG22	1:E:143:LEU:HB2	2.00	0.44
1:B:141:LEU:HD13	1:B:170:LEU:HB2	1.98	0.44
1:P:48:MET:O	1:P:52:MET:HG3	2.16	0.44
1:H:82:VAL:O	1:H:224:ARG:NH2	2.51	0.44
1:D:203:GLY:N	1:D:204:GLY:HA3	2.32	0.44
1:F:30:ARG:HD2	1:G:30:ARG:O	2.17	0.44
1:S:146:GLN:NE2	1:S:178:SER:OG	2.50	0.44
1:F:10:ASN:ND2	1:H:27:ARG:HD2	2.33	0.44
1:R:121:TRP:HA	1:R:122:GLY:HA2	1.72	0.44
1:A:73:SER:HB3	1:A:176:THR:CG2	2.44	0.44
1:H:330:PRO:O	1:H:331:GLN:HB3	2.17	0.44
1:S:124:VAL:HG22	1:S:155:GLN:OE1	2.18	0.44
1:G:108:ARG:NH1	1:H:226:CYS:SG	2.90	0.44
1:D:146:GLN:NE2	1:D:178:SER:OG	2.51	0.44
1:R:61:THR:HB	1:R:186:THR:HB	2.00	0.44
1:A:229:GLU:H	1:B:105:GLU:CG	2.26	0.44
1:H:291:GLY:O	1:H:295:HIS:HD2	2.01	0.44
1:D:291:GLY:O	1:D:295:HIS:HD2	2.00	0.44
1:B:92:LEU:HD22	1:B:137:ILE:CD1	2.48	0.44
1:R:291:GLY:O	1:R:295:HIS:HD2	2.01	0.44
1:F:348:ILE:HD11	1:F:378:THR:HG22	2.00	0.44
1:O:135:LYS:HE2	1:O:167:TYR:OH	2.18	0.44
1:C:299:GLY:O	1:C:303:VAL:HG23	2.18	0.44
1:R:19:PRO:HD3	1:R:351:GLY:HA3	1.98	0.44
1:C:312:GLU:HG3	1:C:328:VAL:HB	2.00	0.43
1:B:69:VAL:HB	1:B:209:SER:HB3	1.99	0.43
1:F:36:LEU:HD22	1:F:270:THR:HB	2.00	0.43
1:A:19:PRO:HD3	1:A:351:GLY:HA3	2.01	0.43
1:O:19:PRO:HD3	1:O:351:GLY:HA3	1.99	0.43
1:E:31:ALA:CB	1:E:278:GLU:HG3	2.49	0.43
1:G:74:ARG:HD2	1:G:200:LLP:OP2	2.19	0.43
1:L:121:TRP:N	1:L:121:TRP:CD1	2.86	0.43
1:F:93:VAL:HB	1:F:116:THR:HG22	2.01	0.43
1:M:19:PRO:HD3	1:M:351:GLY:HA3	1.99	0.43
1:C:91:VAL:HG22	1:C:141:LEU:HB2	2.00	0.43
1:C:160:LEU:HA	1:C:163:ILE:HD12	2.00	0.43
1:O:10:ASN:ND2	1:R:27:ARG:HD2	2.34	0.43
1:O:27:ARG:HD2	1:R:10:ASN:ND2	2.33	0.43
1:C:149:THR:HG22	1:C:324:VAL:HG21	2.00	0.43
1:D:231:ILE:HD11	1:D:253:MET:CE	2.49	0.43
1:E:329:ILE:HG12	1:E:362:TRP:CE2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:R:79:ALA:HA	1:R:249:PHE:HB3	2.01	0.43
1:M:80:ILE:HD12	1:M:195:SER:HB3	2.00	0.43
1:D:231:ILE:HD11	1:D:253:MET:HE3	2.00	0.43
1:K:85:ILE:O	1:K:224:ARG:NH2	2.52	0.43
1:S:253:MET:CE	1:S:265:HIS:HD2	2.32	0.43
1:J:92:LEU:HB2	1:J:137:ILE:HD11	2.01	0.43
1:J:146:GLN:NE2	1:J:184:LEU:HD13	2.34	0.43
1:M:299:GLY:O	1:M:303:VAL:HG23	2.19	0.43
1:E:345:ASP:O	1:G:374:ASP:HA	2.19	0.43
1:B:130:VAL:O	1:B:134:VAL:HG23	2.18	0.43
1:D:330:PRO:O	1:D:331:GLN:CB	2.67	0.43
1:D:161:GLY:HA3	1:D:189:TRP:O	2.18	0.43
1:O:27:ARG:NH2	1:O:282:LEU:HD22	2.33	0.43
1:E:329:ILE:HD13	1:E:335:GLY:HA3	2.01	0.43
1:H:295:HIS:HE1	1:H:368:GLY:N	2.14	0.42
1:S:141:LEU:HD13	1:S:170:LEU:HB2	2.00	0.42
1:P:219:GLU:O	1:P:223:ARG:HG3	2.19	0.42
1:R:149:THR:O	1:R:363:ARG:HD2	2.19	0.42
1:M:32:MET:HG2	1:M:271:THR:HG22	2.01	0.42
1:O:199:GLN:HA	1:O:204:GLY:O	2.19	0.42
1:B:146:GLN:NE2	1:B:178:SER:OG	2.52	0.42
1:J:179:LEU:O	1:J:201:CYS:HB2	2.19	0.42
1:A:341:LEU:O	1:A:345:ASP:HB2	2.18	0.42
1:F:121:TRP:HA	1:F:122:GLY:HA2	1.67	0.42
1:O:229:GLU:H	1:P:105:GLU:CG	2.27	0.42
1:P:52:MET:O	1:P:56:ARG:HG3	2.20	0.42
1:R:334:ASN:HB3	1:R:337:GLN:HB2	2.00	0.42
1:P:10:ASN:ND2	1:S:27:ARG:HD2	2.34	0.42
1:L:312:GLU:HB2	1:L:328:VAL:HB	2.01	0.42
1:S:74:ARG:HA	1:S:77:ILE:HD12	2.01	0.42
1:M:37:ILE:H	1:M:37:ILE:HD13	1.84	0.42
1:O:295:HIS:CE1	1:O:368:GLY:N	2.76	0.42
1:D:295:HIS:HE1	1:D:368:GLY:N	2.14	0.42
1:A:105:GLU:HG3	1:B:228:GLU:HG2	2.00	0.42
1:C:391:LYS:HB2	1:C:391:LYS:HE2	1.83	0.42
1:S:9:LEU:CD1	1:S:11:PRO:HD3	2.48	0.42
1:R:82:VAL:O	1:R:224:ARG:NH2	2.52	0.42
1:H:130:VAL:HG21	1:H:160:LEU:HG	2.02	0.42
1:M:135:LYS:HE3	1:M:167:TYR:OH	2.20	0.42
1:M:286:GLU:O	1:M:290:TYR:HD2	2.02	0.42
1:G:80:ILE:HD12	1:G:195:SER:HB3	2.00	0.42
1:E:19:PRO:HD3	1:E:351:GLY:HA3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:226:CYS:SG	1:H:108:ARG:NH1	2.92	0.42
1:D:105:GLU:O	1:D:109:ARG:HG2	2.20	0.42
1:F:80:ILE:HD12	1:F:195:SER:HB3	2.01	0.42
1:H:121:TRP:HA	1:H:122:GLY:HA2	1.69	0.42
1:J:73:SER:HB2	1:J:200:LLP:OP4	2.20	0.42
1:C:73:SER:HB3	1:C:176:THR:HG21	2.01	0.42
1:C:105:GLU:CG	1:D:229:GLU:H	2.29	0.42
1:E:96:PHE:HB3	1:E:125:PHE:HE2	1.85	0.42
1:K:193:ALA:HB2	1:K:217:MET:HG3	2.02	0.42
1:A:121:TRP:CD1	1:A:121:TRP:N	2.86	0.42
1:J:320:LYS:HE2	1:J:324:VAL:O	2.20	0.42
1:E:339:ARG:NE	1:E:352:THR:HB	2.35	0.42
1:M:126:THR:H	1:M:129:GLN:NE2	2.10	0.41
1:L:105:GLU:O	1:L:109:ARG:HG3	2.20	0.41
1:B:9:LEU:CD1	1:B:11:PRO:HD3	2.50	0.41
1:A:2:ASP:CG	1:A:3:ILE:H	2.23	0.41
1:B:303:VAL:HG22	1:B:325:LEU:HG	2.01	0.41
1:F:179:LEU:O	1:F:201:CYS:HB2	2.20	0.41
1:K:79:ALA:HA	1:K:249:PHE:HB3	2.02	0.41
1:R:253:MET:HB3	1:R:253:MET:HE2	1.87	0.41
1:A:83:SER:C	1:A:224:ARG:HH21	2.24	0.41
1:O:300:ASP:HA	1:O:303:VAL:HG12	2.02	0.41
1:O:121:TRP:HA	1:O:122:GLY:HA2	1.70	0.41
1:E:98:ARG:NH1	1:E:102:LEU:HB2	2.35	0.41
1:J:48:MET:O	1:J:52:MET:HG3	2.21	0.41
1:L:85:ILE:O	1:L:224:ARG:NH2	2.53	0.41
1:P:152:THR:HA	1:P:321:MET:CE	2.50	0.41
1:C:78:GLU:O	1:C:82:VAL:HG23	2.19	0.41
1:C:82:VAL:HG12	1:C:244:ILE:HG23	2.03	0.41
1:D:52:MET:O	1:D:56:ARG:HG3	2.20	0.41
1:C:121:TRP:HA	1:C:122:GLY:HA2	1.69	0.41
1:J:126:THR:H	1:J:129:GLN:NE2	2.19	0.41
1:J:91:VAL:HG22	1:J:141:LEU:HB2	2.02	0.41
1:F:203:GLY:HA2	2:F:586:HOH:O	2.19	0.41
1:C:224:ARG:HD2	1:C:242:GLU:O	2.21	0.41
1:F:149:THR:HA	1:F:321:MET:HE1	2.02	0.41
1:K:297:LEU:HD13	1:K:410:GLU:HG2	2.02	0.41
1:E:121:TRP:HA	1:E:122:GLY:HA2	1.68	0.41
1:C:19:PRO:HD3	1:C:351:GLY:HA3	2.02	0.41
1:F:295:HIS:CE1	1:F:368:GLY:N	2.85	0.41
1:P:218:GLU:HB3	2:P:523:HOH:O	2.21	0.41
1:S:198:MET:HB3	1:S:204:GLY:HA2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:S:218:GLU:HG3	1:S:219:GLU:N	2.34	0.41
1:M:121:TRP:CD1	1:M:121:TRP:N	2.87	0.41
1:D:86:ARG:HB2	1:D:86:ARG:HE	1.69	0.41
1:E:146:GLN:NE2	1:E:184:LEU:HD13	2.36	0.41
1:H:133:ALA:O	1:H:137:ILE:HD13	2.21	0.41
1:R:348:ILE:HD11	1:R:378:THR:HG22	2.02	0.41
1:P:228:GLU:H	1:P:253:MET:HE1	1.85	0.41
1:L:389:TYR:CE2	1:S:331:GLN:HG2	2.55	0.41
1:J:82:VAL:HG12	1:J:244:ILE:HG23	2.02	0.41
1:A:149:THR:HA	1:A:321:MET:HE1	2.03	0.41
1:A:320:LYS:HE2	1:A:324:VAL:O	2.21	0.41
1:G:341:LEU:O	1:G:345:ASP:HB2	2.21	0.41
1:A:74:ARG:HA	1:A:77:ILE:HD12	2.03	0.41
1:P:121:TRP:HA	1:P:122:GLY:HA2	1.70	0.41
1:E:77:ILE:HG12	1:E:172:TYR:OH	2.21	0.41
1:B:74:ARG:HA	1:B:77:ILE:HD12	2.03	0.41
1:C:77:ILE:HG12	1:C:172:TYR:OH	2.21	0.41
1:J:133:ALA:O	1:J:137:ILE:HD13	2.21	0.41
1:M:327:VAL:HG21	1:M:364:ILE:HD12	2.03	0.41
1:C:329:ILE:HA	1:C:330:PRO:HD3	1.93	0.41
1:G:295:HIS:CE1	1:G:368:GLY:H	2.17	0.40
1:M:176:THR:HG22	1:M:196:ALA:CA	2.49	0.40
1:G:131:GLU:OE2	1:G:166:ARG:NH2	2.53	0.40
1:J:228:GLU:HG2	1:K:105:GLU:HG3	2.03	0.40
1:E:374:ASP:HA	1:G:345:ASP:O	2.21	0.40
1:S:291:GLY:O	1:S:295:HIS:HD2	2.04	0.40
1:L:21:PRO:HB3	1:L:199:GLN:HB2	2.03	0.40
1:B:78:GLU:O	1:B:82:VAL:HG23	2.21	0.40
1:O:224:ARG:HD2	1:O:242:GLU:O	2.21	0.40
1:M:179:LEU:O	1:M:201:CYS:HB2	2.22	0.40
1:S:278:GLU:O	1:S:282:LEU:HG	2.22	0.40
1:P:77:ILE:HG12	1:P:172:TYR:OH	2.21	0.40
1:S:92:LEU:HB2	1:S:137:ILE:HD11	2.02	0.40
1:K:9:LEU:CD1	1:K:11:PRO:HD3	2.37	0.40
1:H:105:GLU:O	1:H:109:ARG:HG2	2.22	0.40
1:F:176:THR:HG22	1:F:196:ALA:HA	2.02	0.40
1:R:355:GLY:HA3	1:R:356:PRO:HD2	1.84	0.40
1:D:2:ASP:O	1:D:5:GLN:HG2	2.21	0.40
1:J:5:GLN:HE21	1:J:5:GLN:HB3	1.72	0.40
1:L:91:VAL:HG22	1:L:141:LEU:HB2	2.03	0.40
1:D:199:GLN:HA	1:D:204:GLY:O	2.22	0.40
1:M:199:GLN:HA	1:M:204:GLY:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:22:ILE:HD11	2:C:619:HOH:O	2.22	0.40
1:G:133:ALA:O	1:G:137:ILE:HD13	2.21	0.40
1:A:92:LEU:HB2	1:A:137:ILE:HD11	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	408/411 (99%)	388 (95%)	20 (5%)	0	100	100
1	B	407/411 (99%)	390 (96%)	17 (4%)	0	100	100
1	C	407/411 (99%)	384 (94%)	22 (5%)	1 (0%)	56	81
1	D	407/411 (99%)	392 (96%)	14 (3%)	1 (0%)	56	81
1	E	407/411 (99%)	391 (96%)	15 (4%)	1 (0%)	56	81
1	F	407/411 (99%)	390 (96%)	17 (4%)	0	100	100
1	G	407/411 (99%)	391 (96%)	15 (4%)	1 (0%)	56	81
1	H	407/411 (99%)	395 (97%)	11 (3%)	1 (0%)	56	81
1	J	407/411 (99%)	392 (96%)	15 (4%)	0	100	100
1	K	407/411 (99%)	395 (97%)	12 (3%)	0	100	100
1	L	404/411 (98%)	391 (97%)	13 (3%)	0	100	100
1	M	407/411 (99%)	392 (96%)	14 (3%)	1 (0%)	56	81
1	O	407/411 (99%)	393 (97%)	14 (3%)	0	100	100
1	P	407/411 (99%)	392 (96%)	14 (3%)	1 (0%)	56	81
1	R	407/411 (99%)	395 (97%)	11 (3%)	1 (0%)	56	81
1	S	407/411 (99%)	394 (97%)	12 (3%)	1 (0%)	56	81
All	All	6510/6576 (99%)	6265 (96%)	236 (4%)	9 (0%)	59	84

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	331	GLN
1	R	391	LYS
1	D	331	GLN
1	G	226	CYS
1	S	246	SER
1	C	331	GLN
1	P	269	ALA
1	E	246	SER
1	M	203	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	323/336 (96%)	304 (94%)	19 (6%)	28	51
1	B	327/336 (97%)	308 (94%)	19 (6%)	28	52
1	C	324/336 (96%)	305 (94%)	19 (6%)	28	51
1	D	328/336 (98%)	312 (95%)	16 (5%)	35	61
1	E	321/336 (96%)	300 (94%)	21 (6%)	24	45
1	F	326/336 (97%)	312 (96%)	14 (4%)	40	68
1	G	324/336 (96%)	303 (94%)	21 (6%)	24	45
1	H	329/336 (98%)	310 (94%)	19 (6%)	28	52
1	J	323/336 (96%)	305 (94%)	18 (6%)	30	54
1	K	327/336 (97%)	313 (96%)	14 (4%)	40	68
1	L	323/336 (96%)	297 (92%)	26 (8%)	17	32
1	M	329/336 (98%)	312 (95%)	17 (5%)	32	59
1	O	323/336 (96%)	305 (94%)	18 (6%)	30	54
1	P	327/336 (97%)	308 (94%)	19 (6%)	28	52
1	R	324/336 (96%)	305 (94%)	19 (6%)	28	51
1	S	328/336 (98%)	307 (94%)	21 (6%)	25	46
All	All	5206/5376 (97%)	4906 (94%)	300 (6%)	28	52

All (300) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	9	LEU
1	A	22	ILE
1	A	34	SER
1	A	37	ILE
1	A	64	ARG
1	A	86	ARG
1	A	98	ARG
1	A	124	VAL
1	A	137	ILE
1	A	138	ARG
1	A	217	MET
1	A	222	ARG
1	A	324	VAL
1	A	325	LEU
1	A	377	MET
1	A	383	LEU
1	A	390	LEU
1	A	404	TRP
1	B	3	ILE
1	B	5	GLN
1	B	9	LEU
1	B	37	ILE
1	B	86	ARG
1	B	98	ARG
1	B	124	VAL
1	B	137	ILE
1	B	165	ARG
1	B	168	ASP
1	B	217	MET
1	B	237	ARG
1	B	263	LEU
1	B	325	LEU
1	B	331	GLN
1	B	377	MET
1	B	383	LEU
1	B	404	TRP
1	B	410	GLU
1	C	9	LEU
1	C	22	ILE
1	C	37	ILE
1	C	72	THR
1	C	86	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	91	VAL
1	C	98	ARG
1	C	124	VAL
1	C	130	VAL
1	C	137	ILE
1	C	138	ARG
1	C	176	THR
1	C	217	MET
1	C	218	GLU
1	C	222	ARG
1	C	325	LEU
1	C	377	MET
1	C	383	LEU
1	C	404	TRP
1	D	9	LEU
1	D	37	ILE
1	D	86	ARG
1	D	98	ARG
1	D	124	VAL
1	D	137	ILE
1	D	138	ARG
1	D	176	THR
1	D	217	MET
1	D	218	GLU
1	D	237	ARG
1	D	263	LEU
1	D	325	LEU
1	D	377	MET
1	D	383	LEU
1	D	404	TRP
1	E	9	LEU
1	E	22	ILE
1	E	37	ILE
1	E	86	ARG
1	E	91	VAL
1	E	98	ARG
1	E	124	VAL
1	E	137	ILE
1	E	138	ARG
1	E	154	LEU
1	E	176	THR
1	E	217	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	218	GLU
1	E	224	ARG
1	E	237	ARG
1	E	273	LEU
1	E	325	LEU
1	E	377	MET
1	E	383	LEU
1	E	390	LEU
1	E	404	TRP
1	F	9	LEU
1	F	37	ILE
1	F	86	ARG
1	F	91	VAL
1	F	98	ARG
1	F	124	VAL
1	F	137	ILE
1	F	157	LEU
1	F	176	THR
1	F	237	ARG
1	F	325	LEU
1	F	377	MET
1	F	383	LEU
1	F	404	TRP
1	G	9	LEU
1	G	22	ILE
1	G	37	ILE
1	G	86	ARG
1	G	91	VAL
1	G	98	ARG
1	G	124	VAL
1	G	137	ILE
1	G	138	ARG
1	G	176	THR
1	G	218	GLU
1	G	240	ASP
1	G	273	LEU
1	G	312	GLU
1	G	325	LEU
1	G	345	ASP
1	G	377	MET
1	G	383	LEU
1	G	390	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	391	LYS
1	G	404	TRP
1	H	4	THR
1	H	9	LEU
1	H	22	ILE
1	H	37	ILE
1	H	86	ARG
1	H	98	ARG
1	H	124	VAL
1	H	137	ILE
1	H	138	ARG
1	H	176	THR
1	H	217	MET
1	H	218	GLU
1	H	219	GLU
1	H	237	ARG
1	H	325	LEU
1	H	377	MET
1	H	383	LEU
1	H	390	LEU
1	H	404	TRP
1	J	5	GLN
1	J	9	LEU
1	J	22	ILE
1	J	37	ILE
1	J	86	ARG
1	J	98	ARG
1	J	124	VAL
1	J	137	ILE
1	J	138	ARG
1	J	162	GLU
1	J	217	MET
1	J	218	GLU
1	J	222	ARG
1	J	324	VAL
1	J	325	LEU
1	J	377	MET
1	J	383	LEU
1	J	404	TRP
1	K	9	LEU
1	K	37	ILE
1	K	86	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	91	VAL
1	K	98	ARG
1	K	124	VAL
1	K	137	ILE
1	K	165	ARG
1	K	217	MET
1	K	222	ARG
1	K	324	VAL
1	K	325	LEU
1	K	383	LEU
1	K	404	TRP
1	L	9	LEU
1	L	22	ILE
1	L	27	ARG
1	L	37	ILE
1	L	60	ARG
1	L	74	ARG
1	L	82	VAL
1	L	86	ARG
1	L	91	VAL
1	L	98	ARG
1	L	124	VAL
1	L	137	ILE
1	L	154	LEU
1	L	157	LEU
1	L	176	THR
1	L	217	MET
1	L	222	ARG
1	L	234	ASP
1	L	237	ARG
1	L	263	LEU
1	L	324	VAL
1	L	325	LEU
1	L	377	MET
1	L	383	LEU
1	L	390	LEU
1	L	404	TRP
1	M	4	THR
1	M	7	SER
1	M	9	LEU
1	M	37	ILE
1	M	86	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	98	ARG
1	M	124	VAL
1	M	126	THR
1	M	137	ILE
1	M	138	ARG
1	M	217	MET
1	M	218	GLU
1	M	325	LEU
1	M	377	MET
1	M	383	LEU
1	M	390	LEU
1	M	404	TRP
1	O	9	LEU
1	O	22	ILE
1	O	34	SER
1	O	37	ILE
1	O	86	ARG
1	O	91	VAL
1	O	98	ARG
1	O	124	VAL
1	O	137	ILE
1	O	138	ARG
1	O	157	LEU
1	O	218	GLU
1	O	324	VAL
1	O	325	LEU
1	O	377	MET
1	O	383	LEU
1	O	390	LEU
1	O	404	TRP
1	P	9	LEU
1	P	22	ILE
1	P	37	ILE
1	P	86	ARG
1	P	91	VAL
1	P	98	ARG
1	P	108	ARG
1	P	124	VAL
1	P	137	ILE
1	P	138	ARG
1	P	165	ARG
1	P	217	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	237	ARG
1	P	325	LEU
1	P	377	MET
1	P	383	LEU
1	P	390	LEU
1	P	391	LYS
1	P	404	TRP
1	R	9	LEU
1	R	22	ILE
1	R	37	ILE
1	R	60	ARG
1	R	74	ARG
1	R	86	ARG
1	R	98	ARG
1	R	124	VAL
1	R	130	VAL
1	R	137	ILE
1	R	138	ARG
1	R	165	ARG
1	R	217	MET
1	R	222	ARG
1	R	325	LEU
1	R	377	MET
1	R	383	LEU
1	R	390	LEU
1	R	404	TRP
1	S	9	LEU
1	S	22	ILE
1	S	37	ILE
1	S	86	ARG
1	S	98	ARG
1	S	124	VAL
1	S	137	ILE
1	S	138	ARG
1	S	162	GLU
1	S	217	MET
1	S	218	GLU
1	S	222	ARG
1	S	237	ARG
1	S	263	LEU
1	S	325	LEU
1	S	336	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S	377	MET
1	S	383	LEU
1	S	390	LEU
1	S	391	LYS
1	S	404	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (131) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	49	ASN
1	A	129	GLN
1	A	146	GLN
1	A	295	HIS
1	A	406	HIS
1	B	10	ASN
1	B	49	ASN
1	B	129	GLN
1	B	146	GLN
1	B	285	GLN
1	B	295	HIS
1	B	331	GLN
1	C	8	GLN
1	C	10	ASN
1	C	39	GLN
1	C	49	ASN
1	C	129	GLN
1	C	146	GLN
1	C	295	HIS
1	C	406	HIS
1	D	5	GLN
1	D	10	ASN
1	D	39	GLN
1	D	49	ASN
1	D	129	GLN
1	D	146	GLN
1	D	295	HIS
1	D	406	HIS
1	E	5	GLN
1	E	10	ASN
1	E	49	ASN
1	E	101	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	129	GLN
1	E	146	GLN
1	E	295	HIS
1	E	406	HIS
1	F	10	ASN
1	F	49	ASN
1	F	129	GLN
1	F	146	GLN
1	F	295	HIS
1	F	388	ASN
1	G	5	GLN
1	G	8	GLN
1	G	10	ASN
1	G	39	GLN
1	G	46	HIS
1	G	49	ASN
1	G	129	GLN
1	G	146	GLN
1	G	295	HIS
1	G	406	HIS
1	H	5	GLN
1	H	10	ASN
1	H	39	GLN
1	H	49	ASN
1	H	129	GLN
1	H	146	GLN
1	H	295	HIS
1	H	406	HIS
1	J	5	GLN
1	J	10	ASN
1	J	39	GLN
1	J	49	ASN
1	J	129	GLN
1	J	146	GLN
1	J	295	HIS
1	J	401	GLN
1	J	406	HIS
1	K	5	GLN
1	K	8	GLN
1	K	10	ASN
1	K	39	GLN
1	K	49	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	129	GLN
1	K	146	GLN
1	K	295	HIS
1	K	331	GLN
1	K	406	HIS
1	L	5	GLN
1	L	10	ASN
1	L	39	GLN
1	L	49	ASN
1	L	129	GLN
1	L	146	GLN
1	L	295	HIS
1	L	319	HIS
1	L	388	ASN
1	M	5	GLN
1	M	10	ASN
1	M	39	GLN
1	M	49	ASN
1	M	129	GLN
1	M	146	GLN
1	M	295	HIS
1	M	388	ASN
1	M	406	HIS
1	O	5	GLN
1	O	10	ASN
1	O	39	GLN
1	O	49	ASN
1	O	129	GLN
1	O	146	GLN
1	O	295	HIS
1	O	388	ASN
1	O	406	HIS
1	P	5	GLN
1	P	10	ASN
1	P	39	GLN
1	P	49	ASN
1	P	129	GLN
1	P	146	GLN
1	P	295	HIS
1	P	406	HIS
1	R	5	GLN
1	R	10	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	R	39	GLN
1	R	49	ASN
1	R	129	GLN
1	R	146	GLN
1	R	295	HIS
1	S	5	GLN
1	S	10	ASN
1	S	39	GLN
1	S	49	ASN
1	S	129	GLN
1	S	146	GLN
1	S	295	HIS
1	S	331	GLN
1	S	406	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

16 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	LLP	A	200	1	24,24,25	4.11	2 (8%)	30,32,34	1.54	6 (20%)
1	LLP	B	200	1	24,24,25	4.06	2 (8%)	30,32,34	1.81	6 (20%)
1	LLP	C	200	1	24,24,25	4.10	3 (12%)	30,32,34	1.68	7 (23%)
1	LLP	D	200	1	24,24,25	4.13	3 (12%)	30,32,34	1.75	5 (16%)
1	LLP	E	200	1	24,24,25	4.05	3 (12%)	30,32,34	1.77	6 (20%)
1	LLP	F	200	1	24,24,25	4.06	2 (8%)	30,32,34	1.55	5 (16%)
1	LLP	G	200	1	24,24,25	4.10	2 (8%)	30,32,34	1.71	6 (20%)
1	LLP	H	200	1	24,24,25	4.10	3 (12%)	30,32,34	1.82	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	LLP	J	200	1	24,24,25	4.13	2 (8%)	30,32,34	1.62	5 (16%)
1	LLP	K	200	1	24,24,25	4.06	2 (8%)	30,32,34	1.64	7 (23%)
1	LLP	L	200	1	24,24,25	4.05	3 (12%)	30,32,34	1.62	6 (20%)
1	LLP	M	200	1	24,24,25	4.07	3 (12%)	30,32,34	1.75	6 (20%)
1	LLP	O	200	1	24,24,25	4.15	3 (12%)	30,32,34	1.79	6 (20%)
1	LLP	P	200	1	24,24,25	4.08	2 (8%)	30,32,34	1.64	5 (16%)
1	LLP	R	200	1	24,24,25	4.11	3 (12%)	30,32,34	1.55	6 (20%)
1	LLP	S	200	1	24,24,25	4.12	3 (12%)	30,32,34	1.62	6 (20%)

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
1	LLP	A	200	1	-	0/15/17/19	0/1/1/1
1	LLP	B	200	1	-	0/15/17/19	0/1/1/1
1	LLP	C	200	1	-	0/15/17/19	0/1/1/1
1	LLP	D	200	1	-	0/15/17/19	0/1/1/1
1	LLP	E	200	1	-	0/15/17/19	0/1/1/1
1	LLP	F	200	1	-	0/15/17/19	0/1/1/1
1	LLP	G	200	1	-	0/15/17/19	0/1/1/1
1	LLP	H	200	1	-	0/15/17/19	0/1/1/1
1	LLP	J	200	1	-	0/15/17/19	0/1/1/1
1	LLP	K	200	1	-	0/15/17/19	0/1/1/1
1	LLP	L	200	1	-	0/15/17/19	0/1/1/1
1	LLP	M	200	1	-	0/15/17/19	0/1/1/1
1	LLP	O	200	1	-	0/15/17/19	0/1/1/1
1	LLP	P	200	1	-	0/15/17/19	0/1/1/1
1	LLP	R	200	1	-	0/15/17/19	0/1/1/1
1	LLP	S	200	1	-	0/15/17/19	0/1/1/1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	200	LLP	O-C	19.84	1.25	1.11
1	J	200	LLP	O-C	19.72	1.25	1.11
1	D	200	LLP	O-C	19.71	1.25	1.11
1	S	200	LLP	O-C	19.66	1.25	1.11
1	G	200	LLP	O-C	19.61	1.24	1.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	200	LLP	O-C	19.61	1.24	1.11
1	A	200	LLP	O-C	19.60	1.24	1.11
1	R	200	LLP	O-C	19.57	1.24	1.11
1	C	200	LLP	O-C	19.48	1.24	1.11
1	P	200	LLP	O-C	19.46	1.24	1.11
1	F	200	LLP	O-C	19.42	1.24	1.11
1	B	200	LLP	O-C	19.39	1.24	1.11
1	K	200	LLP	O-C	19.34	1.24	1.11
1	E	200	LLP	O-C	19.33	1.24	1.11
1	M	200	LLP	O-C	19.31	1.24	1.11
1	L	200	LLP	O-C	19.29	1.24	1.11
1	M	200	LLP	CA-C	2.98	1.53	1.48
1	C	200	LLP	CA-C	2.84	1.53	1.48
1	K	200	LLP	CA-C	2.78	1.53	1.48
1	R	200	LLP	CA-C	2.72	1.53	1.48
1	S	200	LLP	CA-C	2.71	1.53	1.48
1	L	200	LLP	CA-C	2.70	1.53	1.48
1	A	200	LLP	CA-C	2.68	1.53	1.48
1	F	200	LLP	CA-C	2.61	1.53	1.48
1	G	200	LLP	CA-C	2.58	1.53	1.48
1	P	200	LLP	CA-C	2.58	1.53	1.48
1	D	200	LLP	CA-C	2.54	1.53	1.48
1	J	200	LLP	CA-C	2.54	1.53	1.48
1	B	200	LLP	CA-C	2.50	1.52	1.48
1	E	200	LLP	CA-C	2.47	1.52	1.48
1	M	200	LLP	CB-CA	2.44	1.55	1.53
1	O	200	LLP	CA-C	2.40	1.52	1.48
1	H	200	LLP	CA-C	2.39	1.52	1.48
1	S	200	LLP	CB-CA	2.18	1.55	1.53
1	C	200	LLP	CB-CA	2.11	1.55	1.53
1	E	200	LLP	CB-CA	2.07	1.55	1.53
1	R	200	LLP	CB-CA	2.07	1.55	1.53
1	O	200	LLP	CB-CA	2.05	1.55	1.53
1	D	200	LLP	CB-CA	2.04	1.55	1.53
1	L	200	LLP	CB-CA	2.02	1.55	1.53
1	H	200	LLP	CB-CA	2.00	1.55	1.53

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	200	LLP	C-CA-N	-5.39	108.45	113.83
1	B	200	LLP	OP4-C5'-C5	5.23	119.90	109.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	200	LLP	C-CA-N	-5.20	108.64	113.83
1	K	200	LLP	OP4-C5'-C5	5.10	119.62	109.26
1	B	200	LLP	C-CA-N	-5.06	108.77	113.83
1	D	200	LLP	C-CA-N	-5.04	108.79	113.83
1	E	200	LLP	OP4-C5'-C5	5.01	119.44	109.26
1	M	200	LLP	OP4-C5'-C5	4.83	119.07	109.26
1	P	200	LLP	OP4-C5'-C5	4.78	118.98	109.26
1	H	200	LLP	OP4-C5'-C5	4.58	118.58	109.26
1	S	200	LLP	OP4-C5'-C5	4.57	118.54	109.26
1	O	200	LLP	OP4-C5'-C5	4.46	118.32	109.26
1	G	200	LLP	OP4-C5'-C5	4.44	118.29	109.26
1	J	200	LLP	C-CA-N	-4.39	109.44	113.83
1	E	200	LLP	C-CA-N	-4.36	109.47	113.83
1	D	200	LLP	OP4-C5'-C5	4.32	118.05	109.26
1	C	200	LLP	OP4-C5'-C5	4.23	117.85	109.26
1	M	200	LLP	C-CA-N	-4.19	109.64	113.83
1	R	200	LLP	OP4-C5'-C5	4.06	117.52	109.26
1	G	200	LLP	C4-C4'-NZ	3.94	118.86	111.52
1	A	200	LLP	C4-C4'-NZ	3.91	118.80	111.52
1	L	200	LLP	OP4-C5'-C5	3.86	117.10	109.26
1	F	200	LLP	OP4-C5'-C5	3.75	116.89	109.26
1	C	200	LLP	C6-C5-C4	3.60	120.83	118.10
1	L	200	LLP	C4-C4'-NZ	3.58	118.18	111.52
1	F	200	LLP	C4-C4'-NZ	3.58	118.18	111.52
1	C	200	LLP	C4-C4'-NZ	3.51	118.06	111.52
1	S	200	LLP	C4-C4'-NZ	3.48	118.00	111.52
1	H	200	LLP	C4-C4'-NZ	3.46	117.96	111.52
1	D	200	LLP	C4-C4'-NZ	3.46	117.96	111.52
1	L	200	LLP	C-CA-N	-3.41	110.42	113.83
1	J	200	LLP	OP4-C5'-C5	3.41	116.20	109.26
1	G	200	LLP	C-CA-N	-3.36	110.47	113.83
1	P	200	LLP	C4-C4'-NZ	3.36	117.78	111.52
1	A	200	LLP	C6-C5-C4	3.34	120.64	118.10
1	E	200	LLP	C4-C4'-NZ	3.25	117.58	111.52
1	J	200	LLP	C6-C5-C4	3.21	120.54	118.10
1	P	200	LLP	C6-C5-C4	3.17	120.51	118.10
1	A	200	LLP	OP4-C5'-C5	3.16	115.69	109.26
1	R	200	LLP	C4-C4'-NZ	3.15	117.39	111.52
1	H	200	LLP	C6-C5-C4	3.15	120.49	118.10
1	M	200	LLP	C6-C5-C4	3.15	120.49	118.10
1	G	200	LLP	C6-C5-C4	3.13	120.48	118.10
1	J	200	LLP	C4-C4'-NZ	3.13	117.34	111.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	200	LLP	C6-C5-C4	3.11	120.46	118.10
1	F	200	LLP	C6-C5-C4	3.09	120.45	118.10
1	B	200	LLP	C6-C5-C4	3.05	120.42	118.10
1	R	200	LLP	C6-C5-C4	3.02	120.40	118.10
1	O	200	LLP	C6-C5-C4	2.99	120.37	118.10
1	K	200	LLP	C4-C4'-NZ	2.98	117.06	111.52
1	E	200	LLP	C6-C5-C4	2.97	120.35	118.10
1	O	200	LLP	C4-C4'-NZ	2.93	116.97	111.52
1	S	200	LLP	C6-C5-C4	2.89	120.29	118.10
1	D	200	LLP	C6-C5-C4	2.85	120.26	118.10
1	M	200	LLP	C4-C4'-NZ	2.81	116.75	111.52
1	K	200	LLP	C6-C5-C4	2.74	120.18	118.10
1	F	200	LLP	C-CA-N	-2.71	111.12	113.83
1	S	200	LLP	C-CA-N	-2.67	111.17	113.83
1	K	200	LLP	C-CA-N	-2.66	111.18	113.83
1	A	200	LLP	C4'-C4-C5	2.64	122.12	119.70
1	P	200	LLP	C-CA-N	-2.60	111.24	113.83
1	C	200	LLP	C4'-C4-C5	2.57	122.06	119.70
1	L	200	LLP	C4'-C4-C5	2.54	122.03	119.70
1	R	200	LLP	C-CA-N	-2.49	111.34	113.83
1	M	200	LLP	C5-C6-N1	-2.49	119.37	123.86
1	B	200	LLP	C5-C6-N1	-2.46	119.42	123.86
1	P	200	LLP	C5-C6-N1	-2.42	119.50	123.86
1	C	200	LLP	C-CA-N	-2.40	111.43	113.83
1	E	200	LLP	C5-C6-N1	-2.40	119.54	123.86
1	H	200	LLP	C5-C6-N1	-2.39	119.55	123.86
1	C	200	LLP	C5-C6-N1	-2.38	119.57	123.86
1	G	200	LLP	C4'-C4-C5	2.37	121.88	119.70
1	M	200	LLP	CD-CE-NZ	2.34	118.31	112.09
1	O	200	LLP	C5-C6-N1	-2.34	119.64	123.86
1	K	200	LLP	C5-C6-N1	-2.32	119.68	123.86
1	B	200	LLP	C4'-C4-C5	2.28	121.79	119.70
1	J	200	LLP	C5-C6-N1	-2.28	119.75	123.86
1	S	200	LLP	C5-C6-N1	-2.27	119.77	123.86
1	R	200	LLP	C5-C6-N1	-2.26	119.79	123.86
1	G	200	LLP	C5-C6-N1	-2.24	119.82	123.86
1	F	200	LLP	C5-C6-N1	-2.22	119.85	123.86
1	L	200	LLP	C5-C6-N1	-2.21	119.88	123.86
1	D	200	LLP	C5-C6-N1	-2.16	119.97	123.86
1	A	200	LLP	C5-C6-N1	-2.10	120.06	123.86
1	S	200	LLP	CD-CE-NZ	2.10	117.67	112.09
1	O	200	LLP	CD-CE-NZ	2.10	117.66	112.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	200	LLP	OP3-P-OP4	2.07	112.37	106.65
1	B	200	LLP	O3-C3-C2	2.06	121.27	117.61
1	K	200	LLP	CD-CE-NZ	2.06	117.56	112.09
1	R	200	LLP	C4'-C4-C5	2.05	121.59	119.70
1	K	200	LLP	C4'-C4-C5	2.04	121.57	119.70
1	A	200	LLP	C-CA-N	-2.02	111.81	113.83
1	E	200	LLP	O3-C3-C2	2.00	121.16	117.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	411/411 (100%)	0.01	1 (0%) 93 95	26, 36, 45, 53	0
1	B	410/411 (99%)	-0.03	3 (0%) 84 87	27, 33, 43, 57	0
1	C	410/411 (99%)	0.00	4 (0%) 79 81	26, 34, 47, 57	0
1	D	410/411 (99%)	-0.08	2 (0%) 88 90	26, 33, 42, 46	0
1	E	410/411 (99%)	-0.00	2 (0%) 88 90	25, 35, 44, 48	0
1	F	410/411 (99%)	-0.06	1 (0%) 93 95	26, 32, 43, 56	0
1	G	410/411 (99%)	0.02	6 (1%) 70 71	26, 34, 45, 58	0
1	H	410/411 (99%)	-0.05	2 (0%) 88 90	25, 32, 41, 47	0
1	J	410/411 (99%)	-0.09	2 (0%) 88 90	25, 31, 41, 46	0
1	K	410/411 (99%)	0.01	1 (0%) 93 95	25, 31, 44, 55	0
1	L	409/411 (99%)	0.05	8 (1%) 62 61	25, 32, 43, 61	0
1	M	410/411 (99%)	-0.05	1 (0%) 93 95	25, 33, 42, 46	0
1	O	410/411 (99%)	-0.04	1 (0%) 93 95	24, 31, 41, 46	0
1	P	410/411 (99%)	-0.05	1 (0%) 93 95	25, 32, 44, 55	0
1	R	410/411 (99%)	0.05	9 (2%) 59 57	27, 32, 43, 61	0
1	S	410/411 (99%)	-0.05	1 (0%) 93 95	27, 33, 43, 46	0
All	All	6560/6576 (99%)	-0.02	45 (0%) 84 87	24, 33, 44, 61	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	234	ASP	5.3
1	R	236	HIS	4.8
1	L	234	ASP	4.6
1	L	235	ALA	4.5
1	R	233	THR	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	R	237	ARG	3.7
1	L	233	THR	3.6
1	G	231	ILE	3.6
1	R	232	ARG	3.6
1	L	232	ARG	3.2
1	B	237	ARG	3.1
1	J	354	PHE	2.9
1	R	228	GLU	2.9
1	L	229	GLU	2.7
1	C	233	THR	2.7
1	L	236	HIS	2.7
1	S	130	VAL	2.7
1	E	354	PHE	2.6
1	C	228	GLU	2.6
1	A	354	PHE	2.6
1	O	137	ILE	2.6
1	G	234	ASP	2.4
1	R	229	GLU	2.4
1	C	234	ASP	2.4
1	H	290	TYR	2.4
1	L	227	VAL	2.3
1	J	290	TYR	2.3
1	G	263	LEU	2.3
1	B	235	ALA	2.3
1	M	354	PHE	2.3
1	E	359	GLY	2.3
1	K	234	ASP	2.2
1	B	360	LYS	2.2
1	D	137	ILE	2.2
1	P	235	ALA	2.2
1	G	228	GLU	2.2
1	H	137	ILE	2.2
1	C	290	TYR	2.2
1	R	231	ILE	2.1
1	G	233	THR	2.1
1	D	354	PHE	2.1
1	R	235	ALA	2.1
1	G	167	TYR	2.0
1	L	239	GLY	2.0
1	F	235	ALA	2.0

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

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	LLP	J	200	24/25	0.16	0.82	28,30,30,30	0
1	LLP	L	200	24/25	0.16	0.79	28,29,30,30	0
1	LLP	E	200	24/25	0.15	0.78	31,32,33,33	0
1	LLP	M	200	24/25	0.15	0.44	30,33,34,35	0
1	LLP	H	200	24/25	0.16	0.34	28,31,32,33	0
1	LLP	O	200	24/25	0.15	0.24	28,30,31,31	0
1	LLP	C	200	24/25	0.15	0.24	32,33,33,34	0
1	LLP	A	200	24/25	0.15	0.24	32,33,35,35	0
1	LLP	K	200	24/25	0.15	0.15	29,31,31,32	0
1	LLP	P	200	24/25	0.15	-0.07	30,32,32,32	0
1	LLP	R	200	24/25	0.14	-0.12	29,31,31,32	0
1	LLP	G	200	24/25	0.13	-0.30	30,31,31,31	0
1	LLP	S	200	24/25	0.13	-0.35	31,32,33,33	0
1	LLP	B	200	24/25	0.13	-0.38	29,30,32,32	0
1	LLP	D	200	24/25	0.13	-0.62	29,30,30,31	0
1	LLP	F	200	24/25	0.12	-0.63	28,30,30,31	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.