



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:39 PM GMT

PDB ID : 1K5D
Title : Crystal structure of Ran-GPPNHP-RanBP1-RanGAPcomplex
Authors : Seewald, M.J.; Koerner, C.; Wittinghofer, A.; Vetter, I.R.
Deposited on : 2001-10-10
Resolution : 2.70 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>

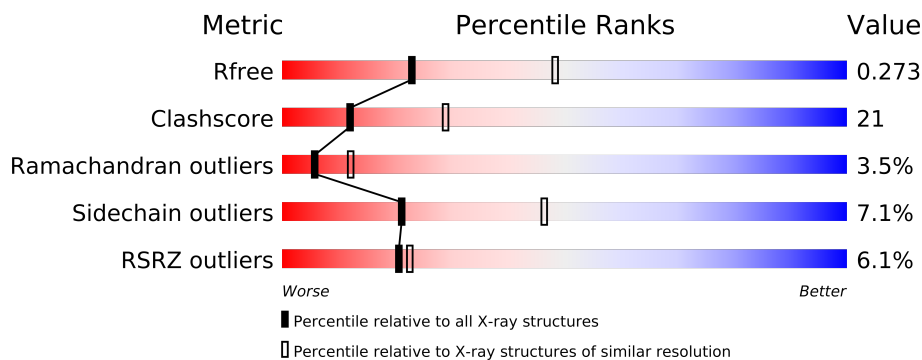
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.70 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	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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	216	
1	D	216	
1	G	216	
1	J	216	
2	B	201	
2	E	201	
2	H	201	
2	K	201	
3	C	386	
3	F	386	
3	I	386	
3	L	386	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22738 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 GTP-binding nuclear protein RAN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1652	1067	284	295	6			
1	D	206	Total	C	N	O	S	0	0	0
			1652	1067	284	295	6			
1	G	206	Total	C	N	O	S	0	0	0
			1652	1067	284	295	6			
1	J	206	Total	C	N	O	S	0	0	0
			1652	1067	284	295	6			

- Molecule 2 is a protein called Ran-specific GTPase-activating protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1216	769	214	226	7			
2	E	146	Total	C	N	O	S	0	0	0
			1216	769	214	226	7			
2	H	146	Total	C	N	O	S	0	0	0
			1216	769	214	226	7			
2	K	146	Total	C	N	O	S	0	0	0
			1216	769	214	226	7			

- Molecule 3 is a protein called Ran GTPase activating protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	344	Total	C	N	O	S	0	0	0
			2698	1699	469	522	8			
3	F	344	Total	C	N	O	S	0	0	0
			2698	1699	469	522	8			
3	I	344	Total	C	N	O	S	0	0	0
			2698	1699	469	522	8			
3	L	344	Total	C	N	O	S	0	0	0
			2698	1699	469	522	8			

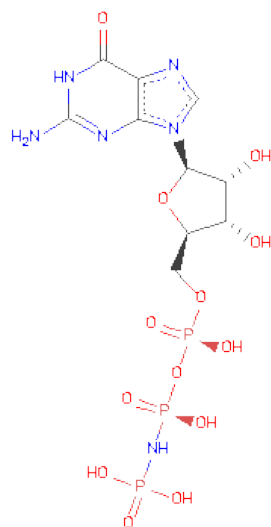
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	ALA	SER	SEE REMARK 999	UNP P41391
F	2	ALA	SER	SEE REMARK 999	UNP P41391
I	2	ALA	SER	SEE REMARK 999	UNP P41391
L	2	ALA	SER	SEE REMARK 999	UNP P41391

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Mg 1 1	0	0
4	J	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0

- Molecule 5 is PHOSPHOAMINOPHOSPHONICACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 32 10 6 13 3	0	0
5	D	1	Total C N O P 32 10 6 13 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	G	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
5	J	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 6 is water.

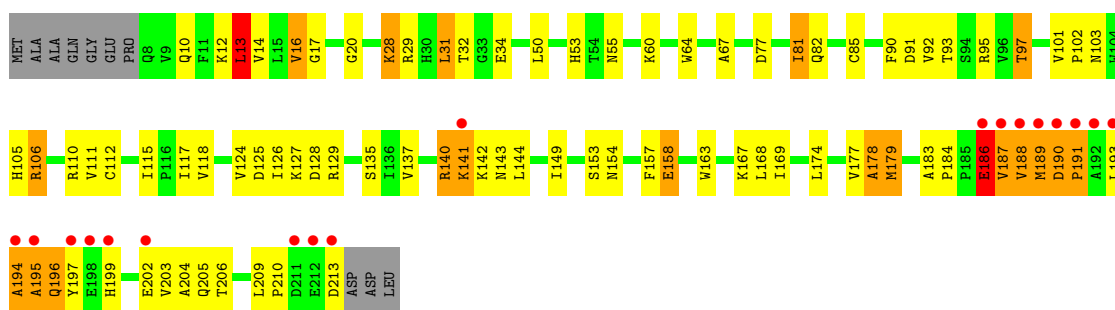
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	24	Total	O	0	0
			24	24		
6	B	3	Total	O	0	0
			3	3		
6	C	71	Total	O	0	0
			71	71		
6	D	29	Total	O	0	0
			29	29		
6	E	2	Total	O	0	0
			2	2		
6	F	47	Total	O	0	0
			47	47		
6	G	25	Total	O	0	0
			25	25		
6	H	5	Total	O	0	0
			5	5		
6	I	53	Total	O	0	0
			53	53		
6	J	31	Total	O	0	0
			31	31		
6	K	4	Total	O	0	0
			4	4		
6	L	48	Total	O	0	0
			48	48		

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.

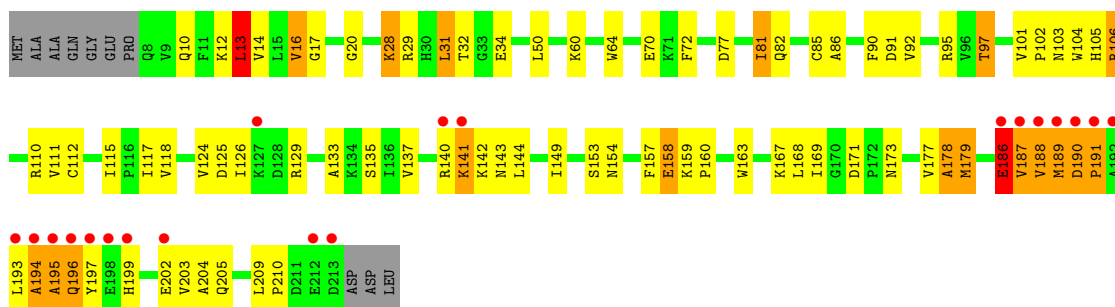
- Molecule 1: GTP-binding nuclear protein RAN

Chain A: 



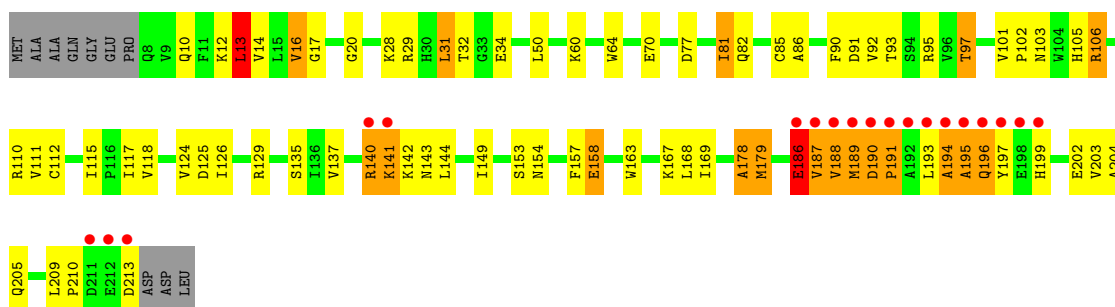
- Molecule 1: GTP-binding nuclear protein RAN

Chain D: 



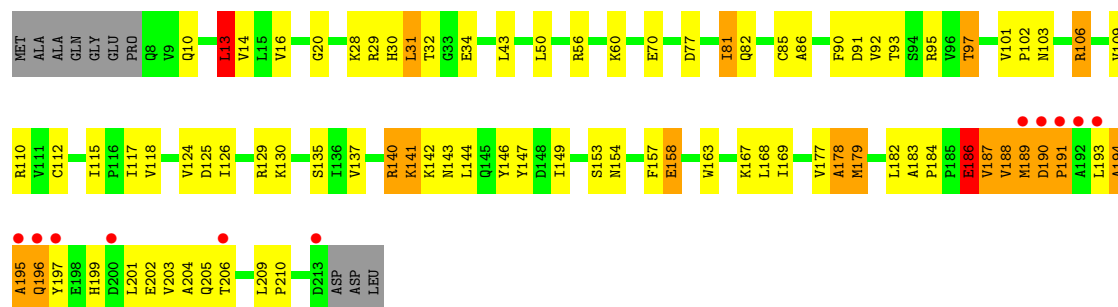
- Molecule 1: GTP-binding nuclear protein RAN

Chain G: 



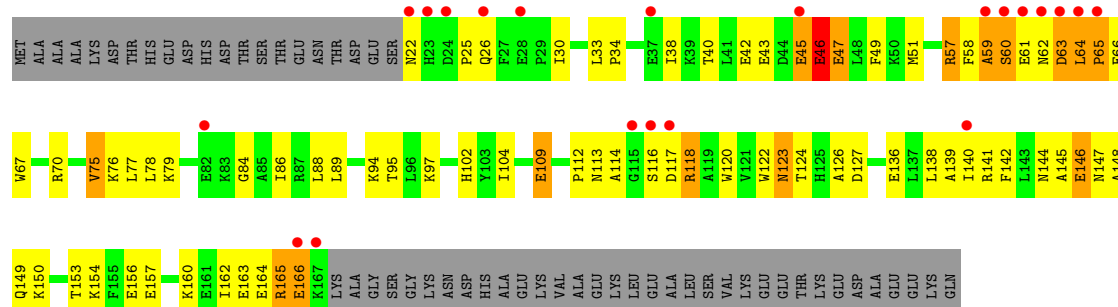
- Molecule 1: GTP-binding nuclear protein RAN

Chain J: 



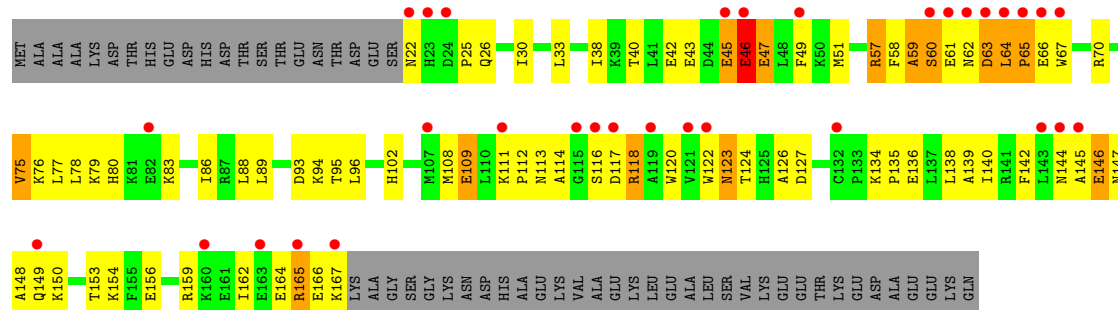
- Molecule 2: Ran-specific GTPase-activating protein

Chain B: 



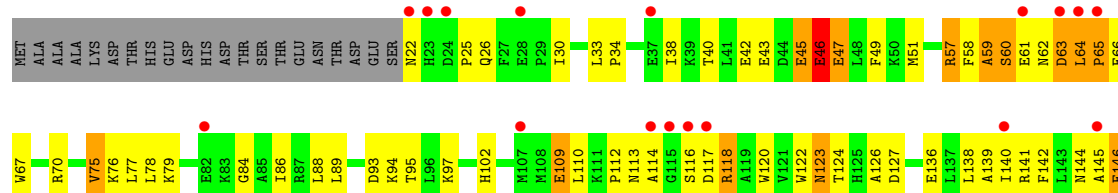
- Molecule 2: Ran-specific GTPase-activating protein

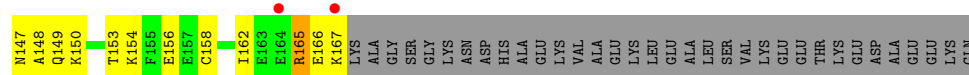
Chain E: 



- Molecule 2: Ran-specific GTPase-activating protein

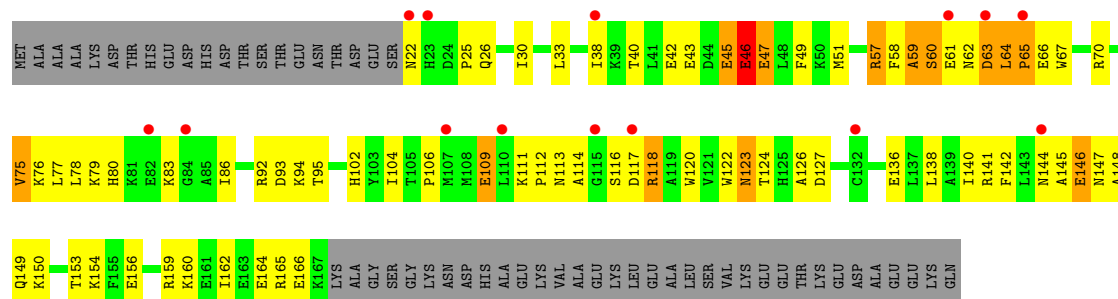
Chain H: 





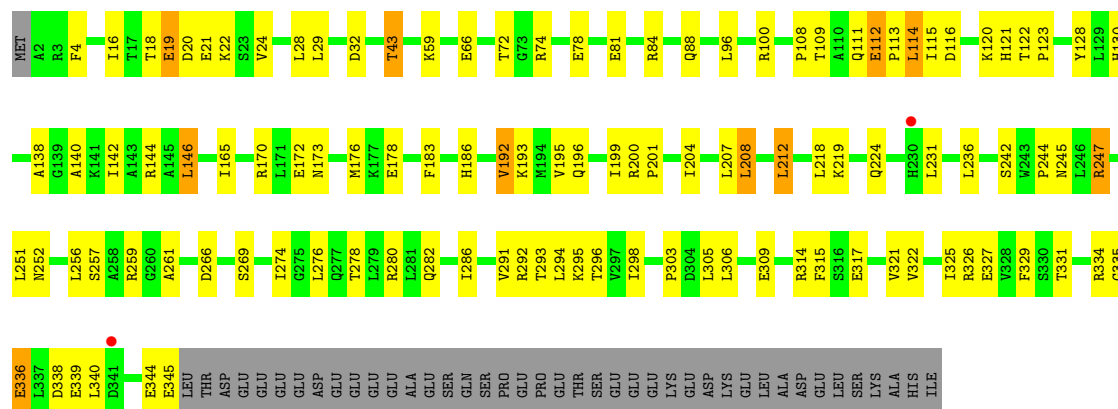
• Molecule 2: Ran-specific GTPase-activating protein

Chain K:



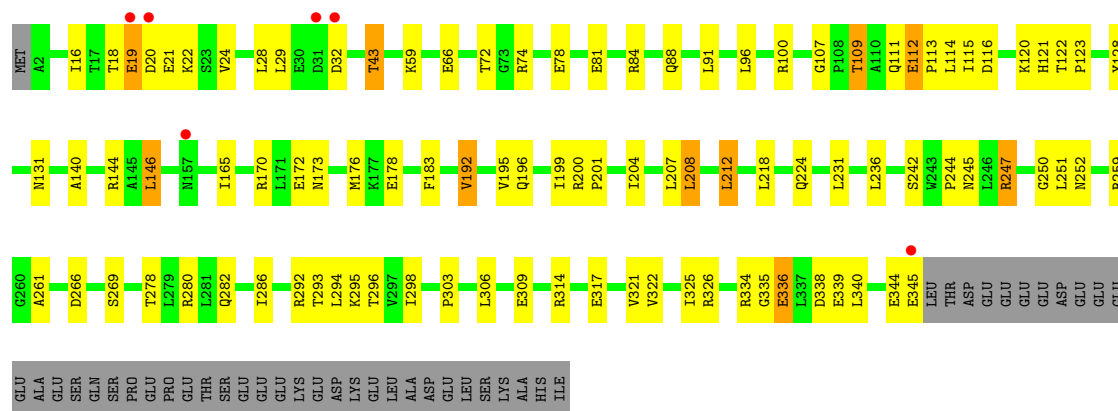
• Molecule 3: Ran GTPase activating protein 1

Chain C:



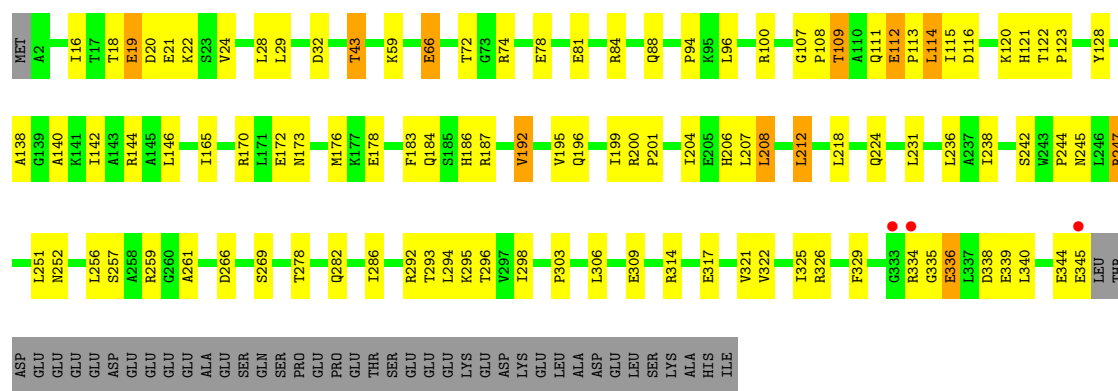
• Molecule 3: Ran GTPase activating protein 1

Chain F:



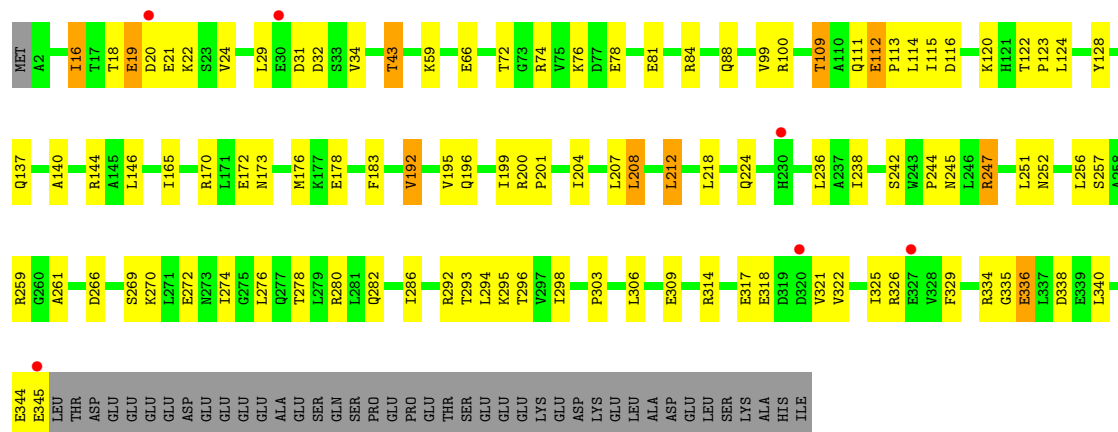
• Molecule 3: Ran GTPase activating protein 1

Chain I:



• Molecule 3: Ran GTPase activating protein 1

Chain L:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	101.55Å 103.11Å 120.18Å 71.59° 80.55° 67.78°	Depositor
Resolution (Å)	20.00 – 2.70 20.07 – 2.41	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.00-2.70) 96.4 (20.07-2.41)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.41Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.237 , 0.267 0.251 , 0.273	Depositor DCC
R_{free} test set	15265 reflections (10.61%)	DCC
Wilson B-factor (Å ²)	51.9	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 159097 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22738	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.36% 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: GNP, MG

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	0.41	0/1693	0.65	1/2296 (0.0%)
1	D	0.41	0/1693	0.64	1/2296 (0.0%)
1	G	0.42	0/1693	0.64	1/2296 (0.0%)
1	J	0.43	0/1693	0.65	1/2296 (0.0%)
2	B	0.36	0/1242	0.62	0/1666
2	E	0.34	0/1242	0.61	0/1666
2	H	0.36	0/1242	0.63	0/1666
2	K	0.36	0/1242	0.62	0/1666
3	C	0.41	0/2737	0.66	0/3697
3	F	0.39	0/2737	0.65	0/3697
3	I	0.39	0/2737	0.66	0/3697
3	L	0.39	0/2737	0.66	0/3697
All	All	0.39	0/22688	0.64	4/30636 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	13	LEU	CA-CB-CG	5.55	128.07	115.30
1	J	13	LEU	CA-CB-CG	5.54	128.03	115.30
1	A	13	LEU	CA-CB-CG	5.28	127.43	115.30
1	D	13	LEU	CA-CB-CG	5.26	127.41	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	1652	0	1659	76	0
1	D	1652	0	1659	77	0
1	G	1652	0	1659	71	0
1	J	1652	0	1659	89	0
2	B	1216	0	1208	80	0
2	E	1216	0	1208	85	0
2	H	1216	0	1208	79	0
2	K	1216	0	1208	88	0
3	C	2698	0	2733	103	0
3	F	2698	0	2733	85	0
3	I	2698	0	2733	98	0
3	L	2698	0	2733	93	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
5	A	32	0	13	2	0
5	D	32	0	13	3	0
5	G	32	0	13	3	0
5	J	32	0	13	6	0
6	A	24	0	0	4	0
6	B	3	0	0	0	0
6	C	71	0	0	17	0
6	D	29	0	0	5	0
6	E	2	0	0	0	0
6	F	47	0	0	7	0
6	G	25	0	0	4	0
6	H	5	0	0	0	0
6	I	53	0	0	8	0
6	J	31	0	0	6	0
6	K	4	0	0	1	0
6	L	48	0	0	5	0
All	All	22738	0	22452	964	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 21.

All (964) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:165:ILE:HA	6:C:445:HOH:O	1.52	1.09
5:J:4250:GNP:PG	6:J:4252:HOH:O	2.14	1.03
1:A:91:ASP:H	1:A:97:THR:HG21	1.22	1.01
1:G:91:ASP:H	1:G:97:THR:HG21	1.21	1.00
1:J:91:ASP:H	1:J:97:THR:HG21	1.23	0.99
1:D:91:ASP:H	1:D:97:THR:HG21	1.24	0.98
2:H:86:ILE:HB	2:H:162:ILE:HD11	1.49	0.94
2:E:86:ILE:HB	2:E:162:ILE:HD11	1.46	0.93
2:E:42:GLU:O	2:E:45:GLU:HB3	1.69	0.93
2:B:42:GLU:O	2:B:45:GLU:HB3	1.70	0.91
2:H:42:GLU:O	2:H:45:GLU:HB3	1.68	0.91
2:K:42:GLU:O	2:K:45:GLU:HB3	1.71	0.91
1:J:158:GLU:HG2	2:K:94:LYS:HB3	1.52	0.90
1:D:158:GLU:HG2	2:E:94:LYS:HB3	1.55	0.88
1:J:206:THR:O	2:K:114:ALA:HB2	1.74	0.88
1:A:90:PHE:HB2	1:A:97:THR:HG23	1.57	0.86
2:B:86:ILE:HB	2:B:162:ILE:HD11	1.58	0.85
1:A:158:GLU:HG2	2:B:94:LYS:HB3	1.59	0.84
5:J:4250:GNP:O2G	6:J:4252:HOH:O	1.93	0.83
1:J:209:LEU:HD23	2:K:113:ASN:ND2	1.93	0.83
3:C:317:GLU:HG2	3:C:340:LEU:HB2	1.61	0.83
1:J:90:PHE:HB2	1:J:97:THR:HG23	1.62	0.81
1:G:90:PHE:HB2	1:G:97:THR:HG23	1.61	0.80
3:C:176:MET:HE3	3:C:207:LEU:HB2	1.63	0.80
1:G:91:ASP:H	1:G:97:THR:CG2	1.95	0.80
3:I:317:GLU:HG2	3:I:340:LEU:HB2	1.62	0.80
3:I:176:MET:HE3	3:I:207:LEU:HB2	1.63	0.80
1:D:90:PHE:HB2	1:D:97:THR:HG23	1.62	0.79
3:F:317:GLU:HG2	3:F:340:LEU:HB2	1.64	0.79
2:H:124:THR:HG22	2:H:126:ALA:H	1.47	0.79
3:L:176:MET:HE3	3:L:207:LEU:HB2	1.64	0.79
1:J:205:GLN:O	2:K:114:ALA:N	2.15	0.78
3:C:173:ASN:HD21	3:C:200:ARG:H	1.31	0.78
1:D:143:ASN:ND2	2:E:25:PRO:HB3	1.99	0.78
2:B:124:THR:HG22	2:B:126:ALA:H	1.49	0.78
1:J:205:GLN:HB2	2:K:112:PRO:O	1.84	0.77
1:G:158:GLU:HG2	2:H:94:LYS:HB3	1.64	0.77
2:K:124:THR:HG22	2:K:126:ALA:H	1.49	0.77
3:L:317:GLU:HG2	3:L:340:LEU:HB2	1.65	0.77
1:G:91:ASP:N	1:G:97:THR:HG21	1.98	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:91:ASP:N	1:J:97:THR:HG21	1.99	0.76
3:C:173:ASN:ND2	3:C:200:ARG:H	1.83	0.76
6:G:3266:HOH:O	3:I:72:THR:HG21	1.84	0.76
3:I:72:THR:HG23	6:I:431:HOH:O	1.84	0.76
1:J:91:ASP:H	1:J:97:THR:CG2	1.98	0.76
1:A:91:ASP:N	1:A:97:THR:HG21	2.00	0.76
3:F:173:ASN:HD21	3:F:200:ARG:H	1.33	0.76
1:J:143:ASN:HA	2:K:22:ASN:ND2	1.99	0.75
3:F:173:ASN:ND2	3:F:200:ARG:H	1.84	0.75
2:E:124:THR:HG22	2:E:126:ALA:H	1.51	0.75
3:F:176:MET:HE3	3:F:207:LEU:HB2	1.67	0.75
1:A:91:ASP:H	1:A:97:THR:CG2	2.00	0.75
1:D:91:ASP:H	1:D:97:THR:CG2	1.99	0.75
1:A:186:GLU:CD	1:A:187:VAL:H	1.90	0.74
3:L:259:ARG:HB3	3:L:259:ARG:NH1	2.02	0.74
1:J:186:GLU:CD	1:J:187:VAL:H	1.91	0.74
3:C:193:LYS:HB2	6:C:445:HOH:O	1.85	0.74
3:I:173:ASN:ND2	3:I:200:ARG:H	1.85	0.74
3:F:259:ARG:HB3	3:F:259:ARG:NH1	2.02	0.74
3:I:259:ARG:NH1	3:I:259:ARG:HB3	2.02	0.74
1:D:91:ASP:N	1:D:97:THR:HG21	2.00	0.74
3:C:259:ARG:HB3	3:C:259:ARG:NH1	2.02	0.74
1:G:20:GLY:H	5:G:3250:GNP:HNB3	1.34	0.73
1:G:186:GLU:CD	1:G:187:VAL:H	1.90	0.73
3:L:173:ASN:ND2	3:L:200:ARG:H	1.87	0.73
3:C:176:MET:CE	3:C:207:LEU:HB2	2.19	0.73
1:D:186:GLU:CD	1:D:187:VAL:H	1.92	0.73
3:I:173:ASN:HD21	3:I:200:ARG:H	1.36	0.72
1:A:20:GLY:H	5:A:1250:GNP:HNB3	1.38	0.71
2:E:46:GLU:HB2	2:E:79:LYS:O	1.91	0.71
3:L:43:THR:HG22	3:L:74:ARG:HE	1.56	0.71
1:D:70:GLU:HA	6:F:406:HOH:O	1.90	0.70
1:J:143:ASN:ND2	2:K:25:PRO:HB3	2.06	0.70
1:A:209:LEU:HD23	2:B:113:ASN:ND2	2.06	0.70
1:D:20:GLY:H	5:D:2250:GNP:HNB3	1.40	0.70
3:F:112:GLU:HB2	6:F:425:HOH:O	1.92	0.70
2:H:46:GLU:HB2	2:H:79:LYS:O	1.92	0.70
1:J:29:ARG:HD3	1:J:154:ASN:OD1	1.92	0.70
3:I:43:THR:HG22	3:I:74:ARG:HE	1.57	0.70
2:K:46:GLU:HB2	2:K:79:LYS:O	1.92	0.70
2:K:59:ALA:O	2:K:60:SER:HB2	1.93	0.69
2:H:146:GLU:O	2:H:150:LYS:HG3	1.93	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:146:GLU:O	2:E:150:LYS:HG3	1.91	0.69
2:H:59:ALA:O	2:H:60:SER:HB2	1.92	0.69
1:J:20:GLY:H	5:J:4250:GNP:HNB3	1.41	0.69
2:B:146:GLU:O	2:B:150:LYS:HG3	1.93	0.69
3:L:32:ASP:HA	3:L:59:LYS:HE2	1.74	0.69
2:E:59:ALA:O	2:E:60:SER:HB2	1.92	0.68
3:F:20:ASP:O	3:F:22:LYS:N	2.26	0.68
1:J:189:MET:O	1:J:190:ASP:HB2	1.91	0.68
2:B:46:GLU:HB2	2:B:79:LYS:O	1.94	0.68
1:A:189:MET:O	1:A:190:ASP:HB2	1.91	0.68
1:D:189:MET:O	1:D:190:ASP:HB2	1.92	0.68
5:D:2250:GNP:PG	6:D:2252:HOH:O	2.51	0.68
2:E:75:VAL:HG21	2:E:140:ILE:HD11	1.76	0.68
3:L:173:ASN:HD21	3:L:200:ARG:H	1.42	0.68
3:F:170:ARG:NH1	6:F:426:HOH:O	2.22	0.68
1:G:143:ASN:ND2	2:H:25:PRO:HB3	2.08	0.68
1:G:189:MET:O	1:G:190:ASP:HB2	1.92	0.68
3:I:176:MET:CE	3:I:207:LEU:HB2	2.23	0.68
2:K:146:GLU:O	2:K:150:LYS:HG3	1.94	0.68
2:B:59:ALA:O	2:B:60:SER:HB2	1.93	0.67
1:D:29:ARG:HD3	1:D:154:ASN:OD1	1.94	0.67
3:F:43:THR:HG22	3:F:74:ARG:HE	1.59	0.67
2:K:75:VAL:HG21	2:K:140:ILE:HD11	1.75	0.67
2:B:75:VAL:HG21	2:B:140:ILE:HD11	1.77	0.67
1:G:29:ARG:HD3	1:G:154:ASN:OD1	1.94	0.67
3:F:204:ILE:HG23	3:F:208:LEU:CD2	2.25	0.67
3:F:32:ASP:HA	3:F:59:LYS:HE2	1.77	0.67
1:G:169:ILE:HD12	2:H:33:LEU:HD12	1.75	0.67
3:L:204:ILE:HG23	3:L:208:LEU:CD2	2.25	0.67
3:L:176:MET:CE	3:L:207:LEU:HB2	2.25	0.66
3:C:20:ASP:O	3:C:22:LYS:N	2.28	0.66
1:D:32:THR:HG22	1:D:34:GLU:H	1.59	0.66
3:L:20:ASP:O	3:L:22:LYS:N	2.28	0.66
2:B:117:ASP:OD2	2:B:145:ALA:HB2	1.95	0.66
3:I:192:VAL:HG12	3:I:218:LEU:HD11	1.76	0.66
1:G:32:THR:HG22	1:G:34:GLU:H	1.61	0.66
2:B:123:ASN:HD22	2:B:124:THR:H	1.44	0.66
2:E:62:ASN:O	2:E:64:LEU:HD22	1.96	0.66
3:C:327:GLU:HG3	1:J:109:VAL:HG21	1.76	0.66
2:K:59:ALA:HB2	2:K:65:PRO:HA	1.78	0.66
2:E:59:ALA:HB2	2:E:65:PRO:HA	1.78	0.66
2:E:123:ASN:HD22	2:E:124:THR:H	1.44	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:192:VAL:HG12	3:F:218:LEU:HD11	1.76	0.65
3:L:192:VAL:HG12	3:L:218:LEU:HD11	1.78	0.65
1:A:13:LEU:HB2	1:A:85:CYS:SG	2.36	0.65
2:K:117:ASP:OD2	2:K:145:ALA:HB2	1.96	0.65
3:I:204:ILE:HG23	3:I:208:LEU:CD2	2.26	0.65
3:C:176:MET:HE1	3:C:207:LEU:HD22	1.77	0.65
2:E:122:TRP:HZ3	2:E:140:ILE:HG22	1.62	0.65
1:J:32:THR:HG22	1:J:34:GLU:H	1.61	0.65
3:C:43:THR:HG22	3:C:74:ARG:HE	1.61	0.65
3:I:32:ASP:HA	3:I:59:LYS:HE2	1.78	0.65
1:D:143:ASN:HA	2:E:22:ASN:ND2	2.11	0.65
2:B:123:ASN:ND2	2:B:124:THR:H	1.95	0.65
2:H:46:GLU:HG3	2:H:79:LYS:HB3	1.77	0.65
2:E:123:ASN:ND2	2:E:124:THR:H	1.95	0.65
1:A:92:VAL:HG13	1:A:129:ARG:HG3	1.79	0.65
2:K:62:ASN:O	2:K:64:LEU:HD22	1.97	0.65
2:B:49:PHE:HB3	2:B:77:LEU:HD12	1.79	0.65
2:H:123:ASN:ND2	2:H:124:THR:H	1.95	0.65
2:K:46:GLU:HG3	2:K:79:LYS:HB3	1.79	0.65
1:A:143:ASN:ND2	2:B:25:PRO:HB3	2.12	0.65
3:F:200:ARG:HB3	3:F:201:PRO:CD	2.27	0.65
2:B:62:ASN:O	2:B:64:LEU:HD22	1.97	0.65
1:A:29:ARG:HD3	1:A:154:ASN:OD1	1.96	0.65
2:H:75:VAL:HG21	2:H:140:ILE:HD11	1.78	0.65
1:A:53:HIS:ND1	6:A:1269:HOH:O	2.28	0.65
2:H:123:ASN:HD22	2:H:124:THR:H	1.45	0.64
3:I:20:ASP:O	3:I:22:LYS:N	2.31	0.64
3:C:200:ARG:HB3	3:C:201:PRO:CD	2.28	0.64
3:I:187:ARG:NH1	3:L:272:GLU:HG3	2.11	0.64
2:E:117:ASP:OD2	2:E:145:ALA:HB2	1.96	0.64
3:F:176:MET:CE	3:F:207:LEU:HB2	2.27	0.64
1:J:193:LEU:HD12	1:J:193:LEU:H	1.62	0.64
2:H:117:ASP:OD2	2:H:145:ALA:HB2	1.97	0.64
2:H:59:ALA:HB2	2:H:65:PRO:HA	1.80	0.64
2:B:59:ALA:HB2	2:B:65:PRO:HA	1.79	0.64
3:C:112:GLU:HB2	6:C:388:HOH:O	1.98	0.64
3:F:252:ASN:ND2	3:F:282:GLN:H	1.95	0.64
2:B:46:GLU:HG3	2:B:79:LYS:HB3	1.80	0.63
2:B:122:TRP:HZ3	2:B:140:ILE:HG22	1.62	0.63
3:C:204:ILE:HG23	3:C:208:LEU:CD2	2.28	0.63
3:C:192:VAL:HG12	3:C:218:LEU:HD11	1.80	0.63
2:H:167:LYS:N	2:H:167:LYS:HD2	2.13	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:176:MET:HE1	3:I:207:LEU:HD22	1.78	0.63
3:L:112:GLU:HB2	6:L:423:HOH:O	1.98	0.63
3:C:32:ASP:HA	3:C:59:LYS:HE2	1.79	0.63
6:D:2277:HOH:O	3:F:109:THR:CG2	2.47	0.63
1:A:169:ILE:HD12	2:B:33:LEU:HD12	1.81	0.63
3:L:200:ARG:HB3	3:L:201:PRO:CD	2.28	0.63
1:D:92:VAL:HG13	1:D:129:ARG:HG3	1.81	0.63
1:A:127:LYS:HB3	6:A:1262:HOH:O	1.98	0.63
1:G:13:LEU:HB2	1:G:85:CYS:SG	2.39	0.63
1:A:193:LEU:H	1:A:193:LEU:HD12	1.64	0.63
1:G:126:ILE:HD11	5:G:3250:GNP:N2	2.14	0.62
1:A:92:VAL:CG1	1:A:129:ARG:HG3	2.29	0.62
2:K:104:ILE:O	2:K:162:ILE:HD13	1.99	0.62
2:K:123:ASN:HD22	2:K:124:THR:H	1.47	0.62
2:E:49:PHE:HB3	2:E:77:LEU:HD12	1.79	0.62
2:E:46:GLU:HG3	2:E:79:LYS:HB3	1.80	0.62
1:G:153:SER:O	1:G:154:ASN:HB2	1.99	0.62
2:E:47:GLU:HA	2:E:78:LEU:HD23	1.82	0.62
1:A:153:SER:O	1:A:154:ASN:HB2	1.98	0.62
3:L:176:MET:HE1	3:L:207:LEU:HD22	1.80	0.62
3:F:200:ARG:HB3	3:F:201:PRO:HD2	1.81	0.62
2:K:136:GLU:HG2	2:K:138:LEU:HD21	1.80	0.62
2:B:47:GLU:HA	2:B:78:LEU:HD23	1.81	0.62
2:K:47:GLU:HA	2:K:78:LEU:HD23	1.80	0.62
1:A:32:THR:HG22	1:A:34:GLU:H	1.65	0.62
1:D:143:ASN:HD21	2:E:25:PRO:HB3	1.64	0.62
2:H:62:ASN:O	2:H:64:LEU:HD22	1.99	0.62
1:D:189:MET:HB2	1:D:193:LEU:HD22	1.82	0.62
1:J:153:SER:O	1:J:154:ASN:HB2	2.00	0.61
3:C:200:ARG:HB3	3:C:201:PRO:HD2	1.82	0.61
1:D:209:LEU:HD23	2:E:113:ASN:ND2	2.15	0.61
1:G:117:ILE:HB	1:G:144:LEU:HD22	1.83	0.61
3:C:193:LYS:N	6:C:445:HOH:O	2.27	0.61
1:J:77:ASP:OD2	1:J:110:ARG:NH2	2.34	0.61
2:B:136:GLU:HG2	2:B:138:LEU:HD21	1.81	0.61
1:J:169:ILE:HD12	2:K:33:LEU:HD12	1.83	0.61
3:I:112:GLU:HB2	6:I:425:HOH:O	2.00	0.61
3:F:111:GLN:O	3:F:115:ILE:HG13	2.01	0.61
2:H:136:GLU:HG2	2:H:138:LEU:HD21	1.82	0.61
2:E:144:ASN:HB2	2:E:146:GLU:HG3	1.83	0.61
2:K:92:ARG:HD2	6:K:202:HOH:O	2.00	0.61
3:F:176:MET:HE1	3:F:207:LEU:HD22	1.83	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:126:ILE:HD11	5:D:2250:GNP:N2	2.15	0.61
1:G:193:LEU:H	1:G:193:LEU:HD12	1.64	0.61
2:H:47:GLU:HA	2:H:78:LEU:HD23	1.82	0.61
2:E:136:GLU:HG2	2:E:138:LEU:HD21	1.83	0.61
1:G:92:VAL:HG13	1:G:129:ARG:HG3	1.82	0.61
1:D:92:VAL:CG1	1:D:129:ARG:HG3	2.30	0.61
3:L:335:GLY:O	3:L:336:GLU:HB2	1.99	0.61
2:K:122:TRP:HZ3	2:K:140:ILE:HG22	1.65	0.60
1:J:143:ASN:HA	2:K:22:ASN:HD22	1.64	0.60
2:K:144:ASN:HB2	2:K:146:GLU:HG3	1.83	0.60
3:I:200:ARG:HB3	3:I:201:PRO:CD	2.31	0.60
2:B:144:ASN:HB2	2:B:146:GLU:HG3	1.83	0.60
2:K:49:PHE:HB3	2:K:77:LEU:HD12	1.83	0.60
1:D:117:ILE:HB	1:D:144:LEU:HD22	1.82	0.60
2:H:144:ASN:HB2	2:H:146:GLU:HG3	1.84	0.60
2:H:49:PHE:HB3	2:H:77:LEU:HD12	1.83	0.60
3:I:184:GLN:HE22	3:L:270:LYS:NZ	2.00	0.60
1:A:117:ILE:HB	1:A:144:LEU:HD22	1.84	0.60
2:B:43:GLU:C	2:B:45:GLU:H	2.03	0.60
3:I:116:ASP:OD2	3:I:120:LYS:HE2	2.02	0.60
1:D:13:LEU:HD12	1:D:13:LEU:C	2.22	0.60
2:E:167:LYS:N	2:E:167:LYS:HD2	2.16	0.60
3:I:200:ARG:HB3	3:I:201:PRO:HD2	1.83	0.60
1:D:193:LEU:H	1:D:193:LEU:HD12	1.66	0.60
2:H:122:TRP:HZ3	2:H:140:ILE:HG22	1.66	0.59
1:G:101:VAL:HB	1:G:102:PRO:HD3	1.84	0.59
3:I:252:ASN:ND2	3:I:282:GLN:H	2.00	0.59
1:J:101:VAL:HB	1:J:102:PRO:HD3	1.84	0.59
2:K:123:ASN:ND2	2:K:124:THR:H	1.99	0.59
1:A:168:LEU:HD22	2:B:30:ILE:HD12	1.84	0.59
3:L:200:ARG:HB3	3:L:201:PRO:HD2	1.85	0.59
1:D:153:SER:O	1:D:154:ASN:HB2	2.01	0.59
3:L:252:ASN:ND2	3:L:282:GLN:H	2.01	0.59
2:E:43:GLU:C	2:E:45:GLU:H	2.05	0.59
1:A:189:MET:HB2	1:A:193:LEU:HD22	1.83	0.59
2:B:109:GLU:CD	2:B:109:GLU:H	2.06	0.59
2:K:109:GLU:CD	2:K:109:GLU:H	2.06	0.59
3:C:140:ALA:O	3:C:144:ARG:HG3	2.03	0.59
2:H:43:GLU:C	2:H:45:GLU:H	2.04	0.59
1:G:168:LEU:HD22	2:H:30:ILE:HD12	1.85	0.59
1:J:92:VAL:HG13	1:J:129:ARG:HG3	1.84	0.59
2:H:62:ASN:O	2:H:63:ASP:HB2	2.02	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:140:ALA:O	3:I:144:ARG:HG3	2.03	0.58
3:F:116:ASP:OD2	3:F:120:LYS:HE2	2.03	0.58
1:D:169:ILE:HD12	2:E:33:LEU:HD12	1.85	0.58
2:E:109:GLU:H	2:E:109:GLU:CD	2.06	0.58
1:J:189:MET:HB2	1:J:193:LEU:HD22	1.84	0.58
3:C:192:VAL:CG1	3:C:218:LEU:HD11	2.33	0.58
3:F:335:GLY:O	3:F:336:GLU:HB2	2.02	0.58
3:I:192:VAL:CG1	3:I:218:LEU:HD11	2.33	0.58
1:G:92:VAL:CG1	1:G:129:ARG:HG3	2.33	0.58
3:I:111:GLN:O	3:I:115:ILE:HG13	2.03	0.58
1:G:189:MET:HB2	1:G:193:LEU:HD22	1.85	0.58
3:C:331:THR:HG21	1:J:142:LYS:HA	1.85	0.58
1:A:101:VAL:HB	1:A:102:PRO:HD3	1.84	0.58
1:A:126:ILE:HD11	5:A:1250:GNP:N2	2.18	0.58
2:E:75:VAL:HG21	2:E:140:ILE:CD1	2.33	0.58
3:C:219:LYS:NZ	6:C:436:HOH:O	2.35	0.58
3:L:116:ASP:OD2	3:L:120:LYS:HE2	2.03	0.58
2:K:59:ALA:HB2	2:K:66:GLU:H	1.69	0.58
2:E:62:ASN:O	2:E:63:ASP:HB2	2.04	0.58
1:A:190:ASP:H	1:A:193:LEU:HD13	1.69	0.58
3:L:18:THR:HG22	3:L:21:GLU:OE1	2.04	0.58
1:J:70:GLU:HA	6:L:411:HOH:O	2.03	0.58
2:K:62:ASN:HB3	2:K:64:LEU:HD22	1.86	0.58
2:B:62:ASN:O	2:B:63:ASP:HB2	2.03	0.58
1:J:56:ARG:NH1	2:K:33:LEU:O	2.36	0.58
2:H:109:GLU:H	2:H:109:GLU:CD	2.06	0.58
1:D:77:ASP:OD2	1:D:110:ARG:NH2	2.36	0.58
2:B:75:VAL:HG21	2:B:140:ILE:CD1	2.34	0.57
3:I:344:GLU:HG2	3:I:345:GLU:N	2.19	0.57
1:D:190:ASP:H	1:D:193:LEU:HD13	1.68	0.57
3:C:112:GLU:CB	3:C:113:PRO:HD3	2.35	0.57
1:G:70:GLU:HA	6:I:391:HOH:O	2.04	0.57
1:J:92:VAL:CG1	1:J:129:ARG:HG3	2.34	0.57
3:F:192:VAL:CG1	3:F:218:LEU:HD11	2.34	0.57
3:L:112:GLU:CB	3:L:113:PRO:HD3	2.34	0.57
5:J:4250:GNP:O3G	6:J:4252:HOH:O	2.16	0.57
1:J:190:ASP:H	1:J:193:LEU:HD13	1.69	0.57
3:C:344:GLU:HG2	3:C:345:GLU:N	2.20	0.57
2:K:43:GLU:C	2:K:45:GLU:H	2.05	0.57
2:K:62:ASN:O	2:K:63:ASP:HB2	2.04	0.57
1:G:143:ASN:HA	2:H:22:ASN:ND2	2.20	0.57
3:C:335:GLY:O	3:C:336:GLU:HB2	2.05	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:31:LEU:HB3	1:A:50:LEU:CD2	2.35	0.57
3:L:344:GLU:HG2	3:L:345:GLU:N	2.19	0.57
3:L:192:VAL:CG1	3:L:218:LEU:HD11	2.35	0.57
2:K:86:ILE:HB	2:K:162:ILE:HD11	1.86	0.57
2:H:63:ASP:C	2:H:64:LEU:HD13	2.26	0.57
2:E:122:TRP:CZ3	2:E:140:ILE:HG22	2.40	0.57
2:B:62:ASN:HB3	2:B:64:LEU:HD22	1.87	0.57
3:F:112:GLU:CB	3:F:113:PRO:HD3	2.35	0.56
1:G:77:ASP:OD2	1:G:110:ARG:NH2	2.38	0.56
1:G:190:ASP:H	1:G:193:LEU:HD13	1.70	0.56
3:I:18:THR:HG22	3:I:21:GLU:CG	2.35	0.56
2:E:51:MET:HE3	2:E:147:ASN:HB3	1.87	0.56
2:K:75:VAL:HG21	2:K:140:ILE:CD1	2.36	0.56
1:J:117:ILE:HB	1:J:144:LEU:HD22	1.87	0.56
3:C:18:THR:HG22	3:C:21:GLU:CG	2.35	0.56
1:A:77:ASP:OD2	1:A:110:ARG:NH2	2.38	0.56
3:I:335:GLY:O	3:I:336:GLU:HB2	2.04	0.56
3:L:140:ALA:O	3:L:144:ARG:HG3	2.05	0.56
3:F:306:LEU:HD21	3:F:334:ARG:HD2	1.87	0.56
2:E:86:ILE:CB	2:E:162:ILE:HD11	2.28	0.56
3:L:137:GLN:HB2	6:L:414:HOH:O	2.06	0.56
1:G:31:LEU:HB3	1:G:50:LEU:CD2	2.36	0.56
3:C:165:ILE:HD13	6:C:445:HOH:O	2.05	0.55
1:J:168:LEU:HD22	2:K:30:ILE:HD12	1.87	0.55
3:F:140:ALA:O	3:F:144:ARG:HG3	2.06	0.55
2:H:62:ASN:HB3	2:H:64:LEU:HD22	1.86	0.55
2:B:63:ASP:C	2:B:64:LEU:HD13	2.27	0.55
3:I:199:ILE:CG2	3:I:204:ILE:HD12	2.36	0.55
2:E:153:THR:HG23	2:E:154:LYS:N	2.22	0.55
1:J:126:ILE:HD11	5:J:4250:GNP:N2	2.20	0.55
3:F:334:ARG:HG2	3:F:334:ARG:HH11	1.71	0.55
2:H:144:ASN:CB	2:H:146:GLU:HG3	2.37	0.55
3:L:18:THR:HG22	3:L:21:GLU:CG	2.37	0.55
3:I:112:GLU:CB	3:I:113:PRO:HD3	2.35	0.55
1:D:101:VAL:HB	1:D:102:PRO:HD3	1.88	0.55
3:C:116:ASP:OD2	3:C:120:LYS:HE2	2.07	0.55
3:F:344:GLU:HG2	3:F:345:GLU:N	2.20	0.55
2:H:153:THR:HG23	2:H:154:LYS:N	2.22	0.55
3:C:252:ASN:ND2	3:C:282:GLN:H	2.05	0.55
2:E:59:ALA:HB2	2:E:66:GLU:H	1.72	0.55
2:B:59:ALA:HB2	2:B:66:GLU:H	1.72	0.55
2:B:122:TRP:CZ3	2:B:140:ILE:HG22	2.40	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:18:THR:HG22	3:F:21:GLU:CG	2.37	0.54
3:C:199:ILE:CG2	3:C:204:ILE:HD12	2.38	0.54
1:J:31:LEU:HB3	1:J:50:LEU:CD2	2.37	0.54
3:C:334:ARG:HG2	3:C:334:ARG:HH11	1.72	0.54
3:C:245:ASN:O	3:C:247:ARG:HD2	2.06	0.54
3:F:176:MET:CE	3:F:207:LEU:HD22	2.38	0.54
2:B:153:THR:HG23	2:B:154:LYS:N	2.23	0.54
2:E:112:PRO:HG3	2:E:120:TRP:HZ3	1.73	0.54
3:L:245:ASN:O	3:L:247:ARG:HD2	2.08	0.54
1:J:178:ALA:HB3	2:K:38:ILE:HD11	1.90	0.54
3:F:112:GLU:HA	3:F:112:GLU:OE1	2.07	0.54
1:A:13:LEU:C	1:A:13:LEU:HD12	2.28	0.54
1:J:13:LEU:HB2	1:J:85:CYS:SG	2.48	0.54
1:A:141:LYS:HE3	1:A:142:LYS:HD2	1.90	0.54
2:B:49:PHE:CB	2:B:77:LEU:HD12	2.38	0.54
2:B:58:PHE:HB2	2:B:67:TRP:CZ3	2.43	0.54
2:B:144:ASN:CB	2:B:146:GLU:HG3	2.38	0.54
3:L:199:ILE:CG2	3:L:204:ILE:HD12	2.38	0.54
1:D:141:LYS:HE3	1:D:142:LYS:HD2	1.90	0.54
1:D:168:LEU:HD22	2:E:30:ILE:HD12	1.89	0.54
3:C:183:PHE:HE1	3:C:207:LEU:HD11	1.72	0.54
2:E:62:ASN:HB3	2:E:64:LEU:HD22	1.89	0.54
3:I:334:ARG:HH11	3:I:334:ARG:HG2	1.73	0.54
1:G:141:LYS:HE3	1:G:142:LYS:HD2	1.90	0.54
3:I:259:ARG:HH11	3:I:259:ARG:HB3	1.72	0.54
3:F:261:ALA:CB	3:F:286:ILE:HG12	2.38	0.54
3:F:306:LEU:HD23	3:F:334:ARG:HH11	1.74	0.53
3:C:111:GLN:O	3:C:115:ILE:HG13	2.07	0.53
2:K:153:THR:HG23	2:K:154:LYS:N	2.22	0.53
1:J:95:ARG:HB2	1:J:95:ARG:NH1	2.23	0.53
2:E:144:ASN:CB	2:E:146:GLU:HG3	2.38	0.53
2:E:49:PHE:CB	2:E:77:LEU:HD12	2.38	0.53
3:F:199:ILE:CG2	3:F:204:ILE:HD12	2.38	0.53
1:D:13:LEU:HB2	1:D:85:CYS:SG	2.47	0.53
2:H:59:ALA:HB2	2:H:66:GLU:H	1.73	0.53
2:B:51:MET:HE3	2:B:147:ASN:HB3	1.89	0.53
2:K:144:ASN:CB	2:K:146:GLU:HG3	2.39	0.53
6:A:1256:HOH:O	3:C:108:PRO:HD3	2.08	0.53
2:B:104:ILE:O	2:B:162:ILE:HD13	2.09	0.53
3:C:18:THR:CG2	3:C:21:GLU:HG3	2.39	0.53
3:I:245:ASN:O	3:I:247:ARG:HD2	2.09	0.53
3:F:43:THR:CG2	3:F:72:THR:O	2.57	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:43:THR:HG21	3:C:72:THR:O	2.09	0.53
3:L:112:GLU:OE1	3:L:112:GLU:HA	2.08	0.53
2:B:123:ASN:ND2	2:B:124:THR:N	2.57	0.53
2:B:57:ARG:HG3	2:B:70:ARG:HD3	1.91	0.53
3:I:306:LEU:HD21	3:I:334:ARG:HD2	1.90	0.53
3:I:94:PRO:O	6:I:417:HOH:O	2.19	0.53
3:F:18:THR:HG22	3:F:21:GLU:OE1	2.08	0.53
1:G:190:ASP:N	1:G:191:PRO:CD	2.72	0.53
2:H:123:ASN:ND2	2:H:124:THR:N	2.57	0.52
3:L:259:ARG:HB3	3:L:259:ARG:HH11	1.74	0.52
2:K:63:ASP:C	2:K:64:LEU:HD13	2.29	0.52
1:G:13:LEU:C	1:G:13:LEU:HD12	2.30	0.52
3:L:111:GLN:O	3:L:115:ILE:HG13	2.10	0.52
2:B:164:GLU:O	2:B:165:ARG:C	2.47	0.52
1:G:209:LEU:HD23	2:H:113:ASN:ND2	2.24	0.52
3:F:245:ASN:O	3:F:247:ARG:HD2	2.08	0.52
3:I:176:MET:CE	3:I:207:LEU:HD22	2.40	0.52
3:I:266:ASP:O	3:I:269:SER:HB3	2.10	0.52
1:G:143:ASN:HD21	2:H:25:PRO:HB3	1.73	0.52
1:J:13:LEU:HD12	1:J:13:LEU:C	2.30	0.52
3:F:292:ARG:HG2	3:F:321:VAL:HG11	1.92	0.52
3:L:306:LEU:HD21	3:L:334:ARG:HD2	1.91	0.52
3:L:334:ARG:HG2	3:L:334:ARG:HH11	1.74	0.52
3:F:43:THR:HG21	3:F:72:THR:O	2.10	0.52
1:J:190:ASP:N	1:J:191:PRO:CD	2.72	0.52
2:B:112:PRO:HG3	2:B:120:TRP:HZ3	1.74	0.52
3:C:112:GLU:HA	3:C:112:GLU:OE1	2.09	0.52
2:K:106:PRO:O	2:K:159:ARG:NE	2.43	0.52
1:J:163:TRP:CZ2	1:J:167:LYS:HE3	2.44	0.52
1:J:209:LEU:HD23	2:K:113:ASN:HD21	1.73	0.52
3:L:176:MET:CE	3:L:207:LEU:HD22	2.40	0.52
2:E:63:ASP:C	2:E:64:LEU:HD13	2.30	0.52
1:G:188:VAL:C	1:G:189:MET:HG2	2.30	0.52
1:D:31:LEU:HB3	1:D:50:LEU:CD2	2.39	0.52
3:I:43:THR:HG21	3:I:72:THR:O	2.10	0.52
2:E:123:ASN:ND2	2:E:124:THR:N	2.57	0.52
2:H:64:LEU:HD13	2:H:64:LEU:N	2.24	0.52
3:L:204:ILE:HG23	3:L:208:LEU:HD23	1.91	0.52
1:D:103:ASN:OD1	1:D:106:ARG:NH2	2.43	0.52
3:L:43:THR:CG2	3:L:72:THR:O	2.58	0.52
2:K:58:PHE:HB2	2:K:67:TRP:CZ3	2.44	0.52
2:K:51:MET:HE3	2:K:147:ASN:HB3	1.92	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:120:LYS:HD3	3:L:318:GLU:HB3	1.92	0.52
3:C:173:ASN:HD21	3:C:200:ARG:N	2.06	0.51
1:J:140:ARG:O	2:K:22:ASN:OD1	2.28	0.51
2:E:58:PHE:HB2	2:E:67:TRP:CZ3	2.45	0.51
1:A:190:ASP:N	1:A:191:PRO:CD	2.73	0.51
1:D:190:ASP:N	1:D:191:PRO:CD	2.72	0.51
1:J:141:LYS:HE3	1:J:142:LYS:HD2	1.91	0.51
3:F:178:GLU:HB2	6:F:413:HOH:O	2.10	0.51
3:C:259:ARG:HH11	3:C:259:ARG:HB3	1.72	0.51
3:L:43:THR:HG21	3:L:72:THR:O	2.10	0.51
2:B:64:LEU:N	2:B:64:LEU:HD13	2.26	0.51
3:C:306:LEU:HD23	3:C:334:ARG:HH11	1.75	0.51
3:L:306:LEU:HD23	3:L:334:ARG:HH11	1.75	0.51
1:D:199:HIS:O	1:D:203:VAL:HG23	2.10	0.51
2:K:112:PRO:HG3	2:K:120:TRP:HZ3	1.76	0.51
3:I:43:THR:CG2	3:I:72:THR:O	2.58	0.51
3:C:306:LEU:HD21	3:C:334:ARG:HD2	1.93	0.51
1:G:209:LEU:HD13	2:H:67:TRP:CG	2.44	0.51
3:F:131:ASN:ND2	6:F:414:HOH:O	2.43	0.51
1:G:188:VAL:O	1:G:189:MET:O	2.27	0.51
2:H:75:VAL:HG21	2:H:140:ILE:CD1	2.39	0.51
2:H:112:PRO:HG3	2:H:120:TRP:HZ3	1.76	0.51
3:L:292:ARG:HG2	3:L:321:VAL:HG11	1.92	0.51
3:I:112:GLU:OE1	3:I:112:GLU:HA	2.10	0.51
3:I:306:LEU:HD23	3:I:334:ARG:HH11	1.74	0.51
1:G:190:ASP:OD2	1:G:194:ALA:HB2	2.10	0.51
3:F:204:ILE:HG23	3:F:208:LEU:HD23	1.92	0.51
3:C:204:ILE:HG23	3:C:208:LEU:HD23	1.92	0.51
3:L:242:SER:O	3:L:244:PRO:HD3	2.11	0.51
1:J:143:ASN:CA	2:K:22:ASN:ND2	2.72	0.51
1:J:188:VAL:O	1:J:189:MET:O	2.29	0.51
3:C:43:THR:CG2	3:C:72:THR:O	2.58	0.51
2:K:136:GLU:CG	2:K:138:LEU:HD21	2.41	0.51
1:D:163:TRP:CZ2	1:D:167:LYS:HE3	2.45	0.51
3:I:18:THR:HG22	3:I:21:GLU:OE1	2.10	0.51
3:I:20:ASP:O	3:I:21:GLU:HB2	2.11	0.51
3:C:18:THR:HG22	3:C:21:GLU:OE1	2.11	0.51
3:F:245:ASN:ND2	6:F:391:HOH:O	2.40	0.51
3:C:236:LEU:HD21	3:C:251:LEU:HD11	1.93	0.51
2:H:51:MET:HE3	2:H:147:ASN:HB3	1.93	0.50
1:D:190:ASP:OD2	1:D:194:ALA:HB2	2.11	0.50
2:K:122:TRP:CZ3	2:K:140:ILE:HG22	2.45	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:261:ALA:CB	3:I:286:ILE:HG12	2.41	0.50
6:G:3275:HOH:O	3:I:109:THR:CG2	2.59	0.50
1:J:190:ASP:OD2	1:J:194:ALA:HB2	2.10	0.50
3:F:259:ARG:HB3	3:F:259:ARG:HH11	1.73	0.50
3:C:294:LEU:O	3:C:298:ILE:HG13	2.11	0.50
3:C:176:MET:CE	3:C:207:LEU:HD22	2.40	0.50
1:A:188:VAL:C	1:A:189:MET:HG2	2.32	0.50
3:C:72:THR:HG23	6:C:389:HOH:O	2.12	0.50
5:J:4250:GNP:O1G	6:J:4252:HOH:O	2.17	0.50
2:B:78:LEU:O	2:B:86:ILE:HA	2.11	0.50
1:G:163:TRP:CZ2	1:G:167:LYS:HE3	2.47	0.50
1:A:12:LYS:HE3	1:A:64:TRP:CE2	2.46	0.50
3:C:130:HIS:HE1	6:C:435:HOH:O	1.94	0.50
1:G:199:HIS:O	1:G:203:VAL:HG23	2.11	0.50
2:K:123:ASN:ND2	2:K:124:THR:N	2.59	0.50
1:A:209:LEU:HD23	2:B:113:ASN:HD21	1.76	0.50
3:L:20:ASP:O	3:L:21:GLU:HB2	2.12	0.50
1:D:95:ARG:NH1	1:D:95:ARG:HB2	2.26	0.50
1:J:199:HIS:O	1:J:203:VAL:HG23	2.11	0.50
2:H:78:LEU:O	2:H:86:ILE:HA	2.11	0.50
1:J:188:VAL:C	1:J:189:MET:HG2	2.33	0.50
1:D:188:VAL:O	1:D:189:MET:O	2.29	0.50
3:C:100:ARG:HA	3:C:128:TYR:HB2	1.94	0.50
3:C:317:GLU:HB2	6:C:441:HOH:O	2.10	0.50
2:H:49:PHE:CB	2:H:77:LEU:HD12	2.41	0.50
1:J:32:THR:HG21	1:J:34:GLU:OE1	2.12	0.50
2:H:122:TRP:CZ3	2:H:140:ILE:HG22	2.45	0.49
2:H:57:ARG:HG3	2:H:70:ARG:HD3	1.93	0.49
1:A:199:HIS:O	1:A:203:VAL:HG23	2.12	0.49
3:C:19:GLU:C	3:C:20:ASP:O	2.50	0.49
1:A:143:ASN:HD21	2:B:25:PRO:HB3	1.75	0.49
3:I:295:LYS:HG3	3:I:325:ILE:HG13	1.94	0.49
3:C:326:ARG:NH2	6:C:442:HOH:O	2.45	0.49
3:L:294:LEU:O	3:L:298:ILE:HG13	2.12	0.49
3:F:195:VAL:HG22	3:F:224:GLN:HB3	1.95	0.49
2:H:38:ILE:HG13	2:H:38:ILE:O	2.12	0.49
1:D:188:VAL:C	1:D:189:MET:HG2	2.33	0.49
1:D:193:LEU:O	1:D:196:GLN:NE2	2.45	0.49
1:G:124:VAL:HG22	1:G:149:ILE:O	2.12	0.49
3:I:183:PHE:HE1	3:I:207:LEU:HD11	1.77	0.49
3:L:18:THR:CG2	3:L:21:GLU:HG3	2.42	0.49
2:H:136:GLU:CG	2:H:138:LEU:HD21	2.42	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:195:VAL:HG22	3:C:224:GLN:HB3	1.95	0.49
3:L:309:GLU:HA	3:L:338:ASP:OD1	2.11	0.49
3:I:292:ARG:HG2	3:I:321:VAL:HG11	1.94	0.49
3:C:128:TYR:CE2	3:C:165:ILE:HG13	2.47	0.49
2:E:78:LEU:O	2:E:86:ILE:HA	2.12	0.49
1:J:143:ASN:HD21	2:K:25:PRO:HB3	1.76	0.49
3:F:20:ASP:O	3:F:21:GLU:HB2	2.12	0.49
1:A:190:ASP:OD2	1:A:194:ALA:HB2	2.12	0.49
3:I:18:THR:CG2	3:I:21:GLU:HG3	2.41	0.49
2:K:57:ARG:HG3	2:K:70:ARG:HD3	1.94	0.49
2:K:64:LEU:N	2:K:64:LEU:HD13	2.28	0.49
3:C:242:SER:O	3:C:244:PRO:HD3	2.12	0.49
2:K:61:GLU:O	2:K:61:GLU:HG3	2.12	0.49
3:C:20:ASP:O	3:C:21:GLU:HB2	2.13	0.49
2:B:136:GLU:CG	2:B:138:LEU:HD21	2.41	0.49
2:H:61:GLU:HG3	2:H:61:GLU:O	2.13	0.49
2:B:61:GLU:HG3	2:B:61:GLU:O	2.13	0.49
1:G:95:ARG:HB2	1:G:95:ARG:NH1	2.28	0.49
2:E:64:LEU:HD13	2:E:64:LEU:N	2.28	0.49
1:A:188:VAL:O	1:A:189:MET:O	2.29	0.49
1:G:188:VAL:O	1:G:189:MET:HG2	2.13	0.49
2:K:49:PHE:CB	2:K:77:LEU:HD12	2.42	0.49
3:I:326:ARG:NH2	6:I:430:HOH:O	2.40	0.49
1:G:10:GLN:HE21	1:G:60:LYS:HD2	1.78	0.49
1:G:193:LEU:O	1:G:196:GLN:NE2	2.46	0.49
1:D:32:THR:HG21	1:D:34:GLU:OE1	2.12	0.49
2:H:58:PHE:HB2	2:H:67:TRP:CZ3	2.47	0.49
1:G:213:ASP:OD2	2:H:141:ARG:NH1	2.38	0.49
3:F:183:PHE:HE1	3:F:207:LEU:HD11	1.76	0.49
2:B:109:GLU:OE1	2:B:109:GLU:N	2.44	0.49
2:B:38:ILE:O	2:B:38:ILE:HG13	2.13	0.49
1:A:143:ASN:HA	2:B:22:ASN:ND2	2.28	0.48
1:D:13:LEU:HD12	1:D:14:VAL:N	2.28	0.48
3:F:18:THR:CG2	3:F:21:GLU:HG3	2.42	0.48
3:I:204:ILE:HG23	3:I:208:LEU:HD23	1.95	0.48
2:K:78:LEU:O	2:K:86:ILE:HA	2.13	0.48
2:B:109:GLU:CD	2:B:109:GLU:N	2.66	0.48
1:A:202:GLU:C	1:A:204:ALA:H	2.15	0.48
1:D:125:ASP:OD2	1:D:126:ILE:HD12	2.14	0.48
1:A:32:THR:HG21	1:A:34:GLU:OE1	2.13	0.48
2:H:58:PHE:HD2	2:H:67:TRP:CE2	2.32	0.48
1:G:202:GLU:C	1:G:204:ALA:H	2.16	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:125:ASP:OD2	1:A:126:ILE:HD12	2.13	0.48
3:I:199:ILE:HG22	3:I:204:ILE:HD12	1.96	0.48
1:G:81:ILE:HD13	1:G:82:GLN:HG3	1.95	0.48
2:E:61:GLU:O	2:E:61:GLU:HG3	2.13	0.48
3:L:236:LEU:HD21	3:L:251:LEU:HD11	1.95	0.48
1:D:189:MET:CB	1:D:193:LEU:HD22	2.43	0.48
1:G:32:THR:HG21	1:G:34:GLU:OE1	2.13	0.48
3:I:295:LYS:HG3	3:I:325:ILE:CG1	2.43	0.48
1:J:201:LEU:HG	2:K:111:LYS:HD3	1.94	0.48
3:F:173:ASN:HD21	3:F:200:ARG:N	2.08	0.48
2:K:109:GLU:N	2:K:109:GLU:OE1	2.47	0.48
3:C:292:ARG:HG2	3:C:321:VAL:HG11	1.95	0.48
1:D:10:GLN:HE21	1:D:60:LYS:HD2	1.79	0.48
3:L:183:PHE:HE1	3:L:207:LEU:HD11	1.79	0.48
3:I:259:ARG:CB	3:I:259:ARG:HH11	2.27	0.48
2:K:58:PHE:HD2	2:K:67:TRP:CE2	2.31	0.48
2:K:49:PHE:HZ	2:K:51:MET:CE	2.26	0.48
3:C:314:ARG:NH1	3:C:344:GLU:OE1	2.47	0.48
2:B:58:PHE:HD2	2:B:67:TRP:CE2	2.31	0.48
3:I:303:PRO:O	3:I:334:ARG:NH2	2.47	0.48
3:L:128:TYR:CE2	3:L:165:ILE:HG13	2.49	0.48
3:F:242:SER:O	3:F:244:PRO:HD3	2.14	0.48
3:F:236:LEU:HD21	3:F:251:LEU:HD11	1.96	0.48
3:C:259:ARG:CB	3:C:259:ARG:HH11	2.27	0.47
3:I:19:GLU:C	3:I:20:ASP:O	2.48	0.47
2:H:109:GLU:OE1	2:H:109:GLU:N	2.45	0.47
2:E:108:MET:O	2:E:159:ARG:HG3	2.14	0.47
1:A:189:MET:CB	1:A:193:LEU:HD22	2.44	0.47
1:D:178:ALA:O	1:D:179:MET:HB2	2.14	0.47
1:D:202:GLU:C	1:D:204:ALA:H	2.16	0.47
3:I:242:SER:O	3:I:244:PRO:HD3	2.14	0.47
2:B:40:THR:HB	2:B:43:GLU:OE2	2.14	0.47
1:J:13:LEU:HD12	1:J:14:VAL:N	2.29	0.47
3:I:122:THR:N	3:I:123:PRO:CD	2.77	0.47
1:A:193:LEU:O	1:A:196:GLN:NE2	2.46	0.47
3:L:18:THR:HG22	3:L:21:GLU:CD	2.34	0.47
3:I:322:VAL:HG12	3:I:326:ARG:NH1	2.29	0.47
3:L:261:ALA:CB	3:L:286:ILE:HG12	2.44	0.47
3:L:266:ASP:O	3:L:269:SER:HB3	2.14	0.47
2:E:109:GLU:N	2:E:109:GLU:CD	2.67	0.47
3:C:309:GLU:HA	3:C:338:ASP:OD1	2.13	0.47
1:J:10:GLN:HE21	1:J:60:LYS:HD2	1.80	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:100:ARG:HA	3:I:128:TYR:HB2	1.96	0.47
2:K:40:THR:HB	2:K:43:GLU:OE2	2.14	0.47
3:L:259:ARG:CB	3:L:259:ARG:HH11	2.27	0.47
3:F:19:GLU:C	3:F:20:ASP:O	2.52	0.47
3:F:303:PRO:O	3:F:334:ARG:NH2	2.48	0.47
1:J:178:ALA:O	1:J:179:MET:HB2	2.15	0.47
1:A:163:TRP:CZ2	1:A:167:LYS:HE3	2.49	0.47
1:A:95:ARG:HB2	1:A:95:ARG:NH1	2.30	0.47
3:F:259:ARG:CB	3:F:259:ARG:HH11	2.27	0.47
2:E:49:PHE:HZ	2:E:51:MET:CE	2.28	0.47
1:J:189:MET:CB	1:J:193:LEU:HD22	2.45	0.47
1:J:193:LEU:O	1:J:196:GLN:NE2	2.47	0.47
1:D:189:MET:O	1:D:190:ASP:CB	2.63	0.47
1:A:13:LEU:HD12	1:A:14:VAL:N	2.30	0.47
2:E:136:GLU:CG	2:E:138:LEU:HD21	2.44	0.47
3:C:322:VAL:HG12	3:C:326:ARG:NH1	2.30	0.47
1:A:16:VAL:HG13	1:A:17:GLY:N	2.30	0.47
1:D:81:ILE:HD13	1:D:82:GLN:HG3	1.96	0.47
3:F:122:THR:N	3:F:123:PRO:CD	2.78	0.47
3:F:100:ARG:HA	3:F:128:TYR:HB2	1.96	0.47
3:F:295:LYS:HG3	3:F:325:ILE:CG1	2.45	0.47
2:E:58:PHE:HD2	2:E:67:TRP:CE2	2.32	0.47
3:C:28:LEU:O	3:C:59:LYS:NZ	2.48	0.47
2:K:160:LYS:O	2:K:164:GLU:HG3	2.15	0.47
1:J:81:ILE:HD13	1:J:82:GLN:N	2.30	0.47
2:E:57:ARG:HG3	2:E:70:ARG:HD3	1.97	0.47
3:L:100:ARG:HA	3:L:128:TYR:HB2	1.97	0.47
2:E:95:THR:O	2:E:96:LEU:HB2	2.14	0.47
3:C:295:LYS:HG3	3:C:325:ILE:CG1	2.45	0.47
2:E:86:ILE:HB	2:E:162:ILE:CD1	2.32	0.47
3:L:176:MET:CE	3:L:207:LEU:HD13	2.45	0.47
1:A:188:VAL:O	1:A:189:MET:HG2	2.14	0.47
3:C:144:ARG:HG2	3:C:178:GLU:CG	2.45	0.47
3:I:144:ARG:HG2	3:I:178:GLU:CG	2.45	0.47
1:J:177:VAL:HG23	2:K:38:ILE:CD1	2.45	0.47
3:C:122:THR:N	3:C:123:PRO:CD	2.78	0.47
1:J:195:ALA:O	1:J:197:TYR:N	2.48	0.47
2:H:158:CYS:O	2:H:162:ILE:HG13	2.15	0.46
2:H:49:PHE:HZ	2:H:51:MET:CE	2.28	0.46
1:G:81:ILE:HD13	1:G:82:GLN:N	2.30	0.46
1:J:202:GLU:C	1:J:204:ALA:H	2.18	0.46
3:L:19:GLU:C	3:L:20:ASP:O	2.52	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:242:SER:C	3:I:244:PRO:HD3	2.35	0.46
3:F:295:LYS:HG3	3:F:325:ILE:HG13	1.97	0.46
3:C:261:ALA:CB	3:C:286:ILE:HG12	2.45	0.46
3:C:266:ASP:O	3:C:269:SER:HB3	2.15	0.46
1:A:10:GLN:HE21	1:A:60:LYS:HD2	1.81	0.46
1:D:188:VAL:O	1:D:189:MET:HG2	2.15	0.46
1:J:177:VAL:HG23	2:K:38:ILE:HD13	1.98	0.46
1:D:205:GLN:HE22	2:E:111:LYS:HE2	1.79	0.46
1:A:186:GLU:O	1:A:187:VAL:HB	2.16	0.46
3:F:144:ARG:HG2	3:F:178:GLU:CG	2.45	0.46
6:G:3275:HOH:O	3:I:107:GLY:HA3	2.14	0.46
3:I:195:VAL:HG22	3:I:224:GLN:HB3	1.97	0.46
2:H:84:GLY:H	2:H:165:ARG:HH21	1.63	0.46
3:I:236:LEU:HD21	3:I:251:LEU:HD11	1.97	0.46
3:L:195:VAL:HG22	3:L:224:GLN:HB3	1.97	0.46
2:E:118:ARG:HA	2:E:148:ALA:HB2	1.97	0.46
2:H:59:ALA:O	2:H:60:SER:CB	2.62	0.46
3:F:322:VAL:HG12	3:F:326:ARG:NH1	2.30	0.46
2:K:59:ALA:O	2:K:60:SER:CB	2.63	0.46
1:J:188:VAL:O	1:J:189:MET:HG2	2.14	0.46
3:I:314:ARG:NH1	3:I:344:GLU:OE1	2.49	0.46
3:C:183:PHE:CE1	3:C:207:LEU:HD11	2.50	0.46
3:F:314:ARG:NH1	3:F:344:GLU:OE1	2.49	0.46
3:L:122:THR:N	3:L:123:PRO:CD	2.79	0.46
2:H:123:ASN:HD22	2:H:124:THR:N	2.13	0.46
1:G:186:GLU:O	1:G:187:VAL:HB	2.16	0.46
2:H:144:ASN:HD22	2:H:147:ASN:HD21	1.64	0.46
2:B:63:ASP:C	2:B:65:PRO:HD3	2.36	0.46
1:G:31:LEU:HB3	1:G:50:LEU:HD21	1.98	0.46
3:L:322:VAL:HG12	3:L:326:ARG:NH1	2.31	0.46
2:H:49:PHE:O	2:H:76:LYS:HA	2.16	0.46
2:E:63:ASP:C	2:E:65:PRO:HD3	2.36	0.46
2:E:109:GLU:N	2:E:109:GLU:OE1	2.46	0.46
1:D:124:VAL:HG22	1:D:149:ILE:O	2.16	0.46
1:G:135:SER:O	1:G:137:VAL:HG23	2.16	0.46
3:C:4:PHE:HA	6:C:398:HOH:O	2.15	0.46
2:H:88:LEU:HD23	2:H:89:LEU:N	2.31	0.46
3:C:186:HIS:HD2	6:C:456:HOH:O	1.99	0.45
2:H:63:ASP:C	2:H:65:PRO:HD3	2.37	0.45
2:B:49:PHE:HZ	2:B:51:MET:CE	2.29	0.45
3:F:199:ILE:HG22	3:F:204:ILE:HD12	1.98	0.45
1:J:112:CYS:HB3	1:J:115:ILE:HD13	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:18:THR:HG22	3:F:21:GLU:CD	2.37	0.45
2:B:59:ALA:O	2:B:60:SER:CB	2.63	0.45
3:C:18:THR:HG22	3:C:21:GLU:CD	2.37	0.45
1:G:112:CYS:HB3	1:G:115:ILE:HD13	1.98	0.45
1:J:169:ILE:HD12	2:K:33:LEU:CD1	2.45	0.45
1:D:81:ILE:HD13	1:D:82:GLN:N	2.32	0.45
2:B:157:GLU:HA	2:B:160:LYS:HE2	1.97	0.45
1:J:183:ALA:HA	1:J:184:PRO:HD3	1.83	0.45
1:G:178:ALA:O	1:G:179:MET:HB2	2.16	0.45
1:A:128:ASP:HB2	6:C:430:HOH:O	2.17	0.45
3:C:256:LEU:O	3:C:257:SER:CB	2.65	0.45
1:D:16:VAL:HG13	1:D:17:GLY:N	2.32	0.45
1:A:112:CYS:HB3	1:A:115:ILE:HD13	1.97	0.45
1:D:186:GLU:O	1:D:187:VAL:HB	2.17	0.45
2:K:63:ASP:C	2:K:65:PRO:HD3	2.37	0.45
1:G:115:ILE:O	1:G:117:ILE:HG13	2.16	0.45
1:D:112:CYS:HB3	1:D:115:ILE:HD13	1.98	0.45
1:D:205:GLN:NE2	2:E:111:LYS:HE2	2.31	0.45
1:J:209:LEU:HB3	2:K:141:ARG:NH2	2.31	0.45
1:J:135:SER:O	1:J:137:VAL:HG23	2.16	0.45
3:I:28:LEU:O	3:I:59:LYS:NZ	2.50	0.45
3:I:18:THR:HG22	3:I:21:GLU:CD	2.37	0.45
1:G:105:HIS:CD2	1:G:144:LEU:HD21	2.52	0.45
1:A:31:LEU:HB3	1:A:50:LEU:HD21	1.98	0.45
6:J:4278:HOH:O	3:L:109:THR:CG2	2.65	0.45
1:D:12:LYS:HE3	1:D:64:TRP:CE2	2.51	0.45
1:A:135:SER:O	1:A:137:VAL:HG23	2.16	0.45
1:J:93:THR:O	1:J:130:LYS:HD2	2.17	0.45
3:I:187:ARG:NH2	3:L:270:LYS:O	2.39	0.45
2:H:109:GLU:CD	2:H:109:GLU:N	2.66	0.45
1:A:93:THR:HG21	1:A:126:ILE:HG21	1.99	0.45
1:J:103:ASN:OD1	1:J:106:ARG:NH2	2.50	0.45
3:L:256:LEU:O	3:L:257:SER:CB	2.65	0.45
3:L:303:PRO:O	3:L:334:ARG:NH2	2.50	0.45
1:A:195:ALA:O	1:A:197:TYR:N	2.50	0.45
2:K:118:ARG:HA	2:K:148:ALA:HB2	1.97	0.45
3:L:18:THR:O	3:L:20:ASP:O	2.35	0.44
6:D:2277:HOH:O	3:F:107:GLY:HA3	2.17	0.44
3:C:303:PRO:O	3:C:334:ARG:NH2	2.50	0.44
2:K:38:ILE:O	2:K:38:ILE:HG13	2.16	0.44
1:A:103:ASN:OD1	1:A:106:ARG:NH2	2.48	0.44
1:A:81:ILE:HD13	1:A:82:GLN:N	2.32	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:209:LEU:HD13	2:E:67:TRP:CG	2.51	0.44
1:G:189:MET:CB	1:G:193:LEU:HD22	2.47	0.44
2:E:149:GLN:O	2:E:153:THR:HG22	2.17	0.44
3:L:170:ARG:NH1	6:L:405:HOH:O	2.50	0.44
3:I:108:PRO:HD3	6:I:435:HOH:O	2.16	0.44
3:F:72:THR:HG22	6:F:406:HOH:O	2.16	0.44
1:D:105:HIS:CD2	1:D:144:LEU:HD21	2.53	0.44
2:E:40:THR:HB	2:E:43:GLU:OE2	2.17	0.44
3:I:21:GLU:O	3:I:24:VAL:HB	2.18	0.44
3:L:314:ARG:NH1	3:L:344:GLU:OE1	2.50	0.44
1:A:178:ALA:O	1:A:179:MET:HB2	2.17	0.44
3:L:295:LYS:HG3	3:L:325:ILE:HG13	2.00	0.44
3:L:295:LYS:HG3	3:L:325:ILE:CG1	2.47	0.44
1:J:186:GLU:O	1:J:187:VAL:HB	2.17	0.44
3:I:173:ASN:HD21	3:I:200:ARG:N	2.10	0.44
3:C:21:GLU:O	3:C:24:VAL:HB	2.17	0.44
1:D:115:ILE:O	1:D:117:ILE:HG13	2.18	0.44
1:A:202:GLU:C	1:A:204:ALA:N	2.70	0.44
1:J:81:ILE:HD13	1:J:82:GLN:HG3	1.99	0.44
2:B:118:ARG:HA	2:B:148:ALA:HB2	1.98	0.44
3:L:84:ARG:O	3:L:88:GLN:HB2	2.17	0.44
1:G:13:LEU:HD12	1:G:14:VAL:N	2.33	0.44
2:H:149:GLN:O	2:H:153:THR:HG22	2.17	0.44
1:D:202:GLU:C	1:D:204:ALA:N	2.71	0.44
3:F:128:TYR:CE2	3:F:165:ILE:HG13	2.52	0.44
3:I:96:LEU:O	3:I:121:HIS:HE1	2.01	0.44
1:D:133:ALA:N	6:D:2269:HOH:O	2.37	0.44
1:D:135:SER:O	1:D:137:VAL:HG23	2.17	0.44
1:G:103:ASN:OD1	1:G:106:ARG:NH2	2.50	0.44
1:G:125:ASP:OD2	1:G:126:ILE:HD12	2.17	0.44
1:J:124:VAL:HG22	1:J:149:ILE:O	2.18	0.44
3:F:250:GLY:HA2	3:F:280:ARG:HB2	2.00	0.44
1:J:125:ASP:OD2	1:J:126:ILE:HD12	2.18	0.44
2:H:70:ARG:HD2	2:H:70:ARG:HA	1.83	0.44
1:A:105:HIS:CD2	1:A:144:LEU:HD21	2.53	0.44
2:B:149:GLN:O	2:B:153:THR:HG22	2.18	0.44
2:E:93:ASP:O	2:E:95:THR:N	2.43	0.44
2:K:59:ALA:CB	2:K:65:PRO:HA	2.47	0.43
2:B:49:PHE:O	2:B:76:LYS:HA	2.17	0.43
2:K:49:PHE:O	2:K:76:LYS:HA	2.18	0.43
1:J:31:LEU:HB3	1:J:50:LEU:HD21	1.99	0.43
1:D:159:LYS:HB2	1:D:160:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:294:LEU:O	3:I:298:ILE:HG13	2.18	0.43
1:A:213:ASP:OD2	2:B:141:ARG:NH1	2.44	0.43
1:G:16:VAL:HG13	1:G:17:GLY:N	2.33	0.43
3:I:186:HIS:HD2	6:I:411:HOH:O	2.02	0.43
2:K:123:ASN:HD22	2:K:124:THR:N	2.14	0.43
1:A:206:THR:O	2:B:114:ALA:HB2	2.17	0.43
3:C:199:ILE:HG22	3:C:204:ILE:HD12	1.98	0.43
1:J:178:ALA:O	1:J:179:MET:CB	2.66	0.43
1:G:202:GLU:C	1:G:204:ALA:N	2.71	0.43
1:J:30:HIS:HD2	6:J:4260:HOH:O	2.00	0.43
1:D:195:ALA:O	1:D:197:TYR:N	2.51	0.43
2:H:51:MET:HE3	2:H:142:PHE:CD1	2.54	0.43
2:H:102:HIS:CE1	2:H:122:TRP:HE1	2.36	0.43
3:C:252:ASN:ND2	3:C:280:ARG:HB3	2.33	0.43
3:F:309:GLU:HA	3:F:338:ASP:OD1	2.18	0.43
2:E:49:PHE:O	2:E:76:LYS:HA	2.18	0.43
3:F:28:LEU:O	3:F:59:LYS:NZ	2.52	0.43
2:E:57:ARG:HD3	2:E:136:GLU:OE2	2.18	0.43
1:D:178:ALA:O	1:D:179:MET:CB	2.66	0.43
2:H:118:ARG:HA	2:H:148:ALA:HB2	2.00	0.43
1:G:12:LYS:HE3	1:G:64:TRP:CE2	2.54	0.43
3:I:206:HIS:HD2	6:I:439:HOH:O	2.01	0.43
3:C:165:ILE:CD1	6:C:445:HOH:O	2.64	0.43
3:L:176:MET:HE3	3:L:207:LEU:HD13	1.99	0.43
2:E:59:ALA:O	2:E:60:SER:CB	2.62	0.43
3:F:21:GLU:O	3:F:24:VAL:HB	2.19	0.43
2:K:102:HIS:HB3	2:K:127:ASP:HA	1.99	0.43
3:I:18:THR:O	3:I:20:ASP:O	2.36	0.43
2:E:38:ILE:O	2:E:38:ILE:HG13	2.17	0.43
1:A:16:VAL:CG1	1:A:17:GLY:N	2.81	0.43
2:H:84:GLY:H	2:H:165:ARG:NH2	2.17	0.43
1:G:195:ALA:O	1:G:197:TYR:N	2.51	0.43
3:I:176:MET:CE	3:I:207:LEU:HD13	2.49	0.43
2:E:51:MET:HE2	2:E:142:PHE:CE1	2.54	0.43
2:E:58:PHE:O	2:E:59:ALA:C	2.57	0.43
2:B:102:HIS:HB3	2:B:127:ASP:HA	2.01	0.43
3:L:344:GLU:CG	3:L:345:GLU:N	2.81	0.43
2:K:80:HIS:O	2:K:83:LYS:O	2.37	0.43
1:A:67:ALA:HA	6:A:1252:HOH:O	2.18	0.43
3:C:329:PHE:CG	3:C:335:GLY:HA3	2.53	0.43
3:C:295:LYS:HG3	3:C:325:ILE:HG13	2.00	0.43
3:L:31:ASP:O	3:L:34:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:309:GLU:HA	3:I:338:ASP:OD1	2.18	0.43
1:G:93:THR:HG21	1:G:126:ILE:HG21	2.00	0.43
3:L:173:ASN:HD21	3:L:200:ARG:N	2.13	0.43
3:L:329:PHE:CG	3:L:335:GLY:HA3	2.54	0.43
3:I:66:GLU:HG2	3:I:100:ARG:HD2	2.01	0.43
2:H:95:THR:HG23	2:H:97:LYS:H	1.84	0.43
3:L:16:ILE:HG22	3:L:16:ILE:O	2.18	0.43
3:L:144:ARG:HG2	3:L:178:GLU:CG	2.48	0.43
6:G:3274:HOH:O	3:I:170:ARG:HG3	2.19	0.43
3:C:274:ILE:HG22	3:C:276:LEU:H	1.84	0.43
3:I:183:PHE:CE1	3:I:207:LEU:HD11	2.53	0.42
3:F:207:LEU:HG	3:F:212:LEU:HD22	2.01	0.42
3:L:259:ARG:HB3	3:L:259:ARG:CZ	2.49	0.42
1:G:126:ILE:CD1	5:G:3250:GNP:N2	2.82	0.42
2:B:51:MET:HE3	2:B:142:PHE:CD1	2.54	0.42
3:C:18:THR:HG22	3:C:21:GLU:HG3	2.00	0.42
2:B:163:GLU:O	2:B:166:GLU:OE2	2.37	0.42
3:I:207:LEU:HG	3:I:212:LEU:HD22	2.01	0.42
2:B:70:ARG:HD2	2:B:70:ARG:HA	1.86	0.42
1:J:13:LEU:HD13	1:J:86:ALA:HA	2.01	0.42
2:B:67:TRP:CH2	2:B:139:ALA:HB2	2.54	0.42
3:F:84:ARG:O	3:F:88:GLN:HB2	2.19	0.42
3:I:339:GLU:OE1	3:I:339:GLU:HA	2.19	0.42
3:C:339:GLU:HA	3:C:339:GLU:OE1	2.19	0.42
3:L:259:ARG:CB	3:L:259:ARG:NH1	2.78	0.42
2:H:144:ASN:HD22	2:H:147:ASN:ND2	2.17	0.42
6:D:2277:HOH:O	3:F:109:THR:HG22	2.16	0.42
2:K:149:GLN:O	2:K:153:THR:HG22	2.19	0.42
3:F:266:ASP:O	3:F:269:SER:HB3	2.20	0.42
2:K:58:PHE:O	2:K:59:ALA:C	2.58	0.42
3:I:18:THR:HG23	3:I:20:ASP:C	2.40	0.42
1:G:202:GLU:HA	1:G:205:GLN:HG2	2.01	0.42
2:H:93:ASP:O	2:H:95:THR:N	2.45	0.42
1:J:202:GLU:C	1:J:204:ALA:N	2.73	0.42
1:J:189:MET:O	1:J:190:ASP:CB	2.63	0.42
3:C:298:ILE:HD13	3:C:305:LEU:CD2	2.49	0.42
2:K:160:LYS:HG2	2:K:164:GLU:OE2	2.20	0.42
2:E:102:HIS:HB3	2:E:127:ASP:HA	2.02	0.42
2:E:80:HIS:O	2:E:83:LYS:O	2.37	0.42
3:F:339:GLU:OE1	3:F:339:GLU:HA	2.20	0.42
3:C:291:VAL:HG21	3:C:315:PHE:CD2	2.54	0.42
3:F:183:PHE:CE1	3:F:207:LEU:HD11	2.53	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:18:THR:HG23	3:I:20:ASP:O	2.20	0.42
3:L:252:ASN:ND2	3:L:280:ARG:HB3	2.35	0.42
3:L:72:THR:HG23	6:L:409:HOH:O	2.18	0.42
2:B:102:HIS:CE1	2:B:122:TRP:HE1	2.37	0.42
3:I:18:THR:HG22	3:I:21:GLU:HG3	2.01	0.42
3:I:344:GLU:CG	3:I:345:GLU:N	2.82	0.42
3:F:344:GLU:CG	3:F:345:GLU:N	2.83	0.42
1:A:177:VAL:HG23	2:B:38:ILE:CD1	2.49	0.42
2:E:88:LEU:HD23	2:E:89:LEU:N	2.35	0.42
2:K:102:HIS:CE1	2:K:122:TRP:HE1	2.37	0.42
3:I:66:GLU:OE1	3:I:100:ARG:HB2	2.20	0.42
1:A:178:ALA:O	1:A:179:MET:CB	2.67	0.42
1:D:171:ASP:OD1	1:D:173:ASN:N	2.49	0.42
2:H:40:THR:HB	2:H:43:GLU:OE2	2.19	0.42
2:K:51:MET:HE3	2:K:142:PHE:CD1	2.55	0.42
2:B:59:ALA:CB	2:B:65:PRO:HA	2.48	0.42
2:H:57:ARG:HD3	2:H:136:GLU:OE2	2.20	0.42
2:E:164:GLU:O	2:E:165:ARG:C	2.58	0.42
3:F:231:LEU:HA	3:F:231:LEU:HD12	1.91	0.42
1:J:205:GLN:OE1	2:K:111:LYS:HE2	2.20	0.41
2:H:33:LEU:HA	2:H:34:PRO:HD3	1.89	0.41
2:B:33:LEU:HA	2:B:34:PRO:HD3	1.90	0.41
2:B:84:GLY:H	2:B:165:ARG:NH2	2.17	0.41
2:K:70:ARG:HH11	2:K:70:ARG:HG2	1.86	0.41
2:B:88:LEU:HD23	2:B:89:LEU:N	2.34	0.41
1:A:124:VAL:HG22	1:A:149:ILE:O	2.19	0.41
3:F:294:LEU:O	3:F:298:ILE:HG13	2.20	0.41
3:I:256:LEU:O	3:I:257:SER:CB	2.69	0.41
2:K:93:ASP:O	2:K:95:THR:N	2.47	0.41
1:D:143:ASN:HA	2:E:22:ASN:HD22	1.81	0.41
1:J:137:VAL:O	1:J:140:ARG:HB2	2.20	0.41
1:D:189:MET:CG	1:D:193:LEU:HD22	2.51	0.41
3:F:242:SER:C	3:F:244:PRO:HD3	2.41	0.41
1:A:183:ALA:HA	1:A:184:PRO:HD3	1.83	0.41
3:I:238:ILE:HG21	3:L:238:ILE:HG21	2.02	0.41
1:J:93:THR:HG21	1:J:126:ILE:HG21	2.02	0.41
2:H:46:GLU:O	2:H:47:GLU:CB	2.69	0.41
3:L:18:THR:HG23	3:L:20:ASP:C	2.41	0.41
3:L:18:THR:HG23	3:L:20:ASP:O	2.20	0.41
2:H:167:LYS:HD2	2:H:167:LYS:H	1.85	0.41
1:A:81:ILE:HD13	1:A:82:GLN:HG3	2.01	0.41
3:C:96:LEU:O	3:C:121:HIS:HE1	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:84:ARG:O	3:C:88:GLN:HB2	2.20	0.41
3:C:138:ALA:O	3:C:142:ILE:HG12	2.21	0.41
2:E:134:LYS:HA	2:E:135:PRO:HD3	1.96	0.41
3:C:146:LEU:HD12	3:C:146:LEU:HA	1.91	0.41
2:E:86:ILE:HD12	2:E:162:ILE:HD11	2.02	0.41
2:B:123:ASN:HD22	2:B:124:THR:N	2.12	0.41
2:E:59:ALA:CB	2:E:65:PRO:HA	2.48	0.41
1:J:43:LEU:HD22	3:L:76:LYS:HA	2.02	0.41
2:E:46:GLU:HB3	2:E:47:GLU:H	1.69	0.41
2:E:144:ASN:HD22	2:E:147:ASN:HD21	1.69	0.41
3:C:72:THR:HG22	6:C:427:HOH:O	2.20	0.41
3:L:329:PHE:CD2	3:L:335:GLY:HA3	2.56	0.41
1:D:177:VAL:HG23	2:E:38:ILE:CD1	2.50	0.41
1:D:16:VAL:CG1	1:D:17:GLY:N	2.83	0.41
3:L:99:VAL:HG12	3:L:124:LEU:CD1	2.50	0.41
3:C:231:LEU:HD12	3:C:231:LEU:HA	1.93	0.41
3:F:96:LEU:O	3:F:121:HIS:HE1	2.04	0.41
2:B:144:ASN:HD22	2:B:147:ASN:HD21	1.69	0.41
1:A:189:MET:O	1:A:190:ASP:CB	2.62	0.41
3:L:199:ILE:HG22	3:L:204:ILE:HD12	2.02	0.41
2:H:109:GLU:O	2:H:110:LEU:HD23	2.20	0.41
3:F:91:LEU:HA	3:F:91:LEU:HD23	1.92	0.41
1:J:202:GLU:HA	1:J:205:GLN:HG2	2.02	0.41
2:E:113:ASN:O	2:E:114:ALA:C	2.58	0.41
2:H:113:ASN:O	2:H:114:ALA:C	2.58	0.41
3:L:242:SER:C	3:L:244:PRO:HD3	2.40	0.41
1:G:137:VAL:O	1:G:140:ARG:HB2	2.20	0.41
2:B:95:THR:HG23	2:B:97:LYS:H	1.86	0.41
3:C:317:GLU:CB	6:C:441:HOH:O	2.67	0.41
2:K:144:ASN:HD22	2:K:147:ASN:HD21	1.68	0.41
2:H:102:HIS:HB3	2:H:127:ASP:HA	2.02	0.41
2:B:57:ARG:HD3	2:B:136:GLU:OE2	2.21	0.41
3:C:329:PHE:CD2	3:C:335:GLY:HA3	2.56	0.41
2:H:67:TRP:CH2	2:H:139:ALA:HB2	2.56	0.41
1:D:28:LYS:O	1:D:31:LEU:HD12	2.21	0.41
3:C:242:SER:C	3:C:244:PRO:HD3	2.41	0.41
1:J:195:ALA:C	1:J:197:TYR:H	2.23	0.41
1:A:137:VAL:O	1:A:140:ARG:HB2	2.21	0.41
3:C:170:ARG:HG2	6:C:412:HOH:O	2.21	0.41
3:L:274:ILE:HG22	3:L:276:LEU:H	1.86	0.41
1:D:72:PHE:HE2	1:D:104:TRP:CD2	2.39	0.41
2:B:113:ASN:O	2:B:114:ALA:C	2.59	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:144:ASN:HD22	2:B:147:ASN:ND2	2.19	0.41
1:D:178:ALA:HB3	2:E:38:ILE:HD11	2.03	0.41
3:I:128:TYR:CE2	3:I:165:ILE:HG13	2.56	0.41
1:J:182:LEU:HD12	1:J:182:LEU:N	2.36	0.41
3:L:183:PHE:CE1	3:L:207:LEU:HD11	2.56	0.40
2:E:67:TRP:CH2	2:E:139:ALA:HB2	2.56	0.40
1:D:13:LEU:HD13	1:D:86:ALA:HA	2.04	0.40
2:K:109:GLU:CD	2:K:109:GLU:N	2.67	0.40
1:A:28:LYS:O	1:A:31:LEU:HD12	2.21	0.40
3:I:329:PHE:CG	3:I:335:GLY:HA3	2.56	0.40
1:J:146:TYR:CG	1:J:147:TYR:N	2.89	0.40
3:C:114:LEU:HD12	3:C:114:LEU:HA	1.94	0.40
2:B:46:GLU:HB3	2:B:47:GLU:H	1.69	0.40
2:K:62:ASN:HB3	2:K:64:LEU:CD2	2.51	0.40
1:G:195:ALA:C	1:G:197:TYR:H	2.25	0.40
3:I:84:ARG:O	3:I:88:GLN:HB2	2.21	0.40
3:F:146:LEU:HA	3:F:146:LEU:HD12	1.91	0.40
3:I:184:GLN:NE2	3:L:270:LYS:NZ	2.66	0.40
1:D:31:LEU:HB3	1:D:50:LEU:HD21	2.04	0.40
1:A:202:GLU:HA	1:A:205:GLN:HG2	2.03	0.40
3:I:138:ALA:O	3:I:142:ILE:HG12	2.21	0.40
3:I:114:LEU:HA	3:I:114:LEU:HD12	1.95	0.40
3:L:207:LEU:HG	3:L:212:LEU:HD22	2.04	0.40
2:E:123:ASN:HD22	2:E:124:THR:N	2.11	0.40
2:E:63:ASP:O	2:E:65:PRO:HD3	2.22	0.40
3:F:18:THR:HG22	3:F:21:GLU:HG3	2.02	0.40
3:C:344:GLU:CG	3:C:345:GLU:N	2.83	0.40
1:A:55:ASN:OD1	1:A:174:LEU:HD12	2.22	0.40
3:I:231:LEU:HA	3:I:231:LEU:HD12	1.90	0.40
1:J:202:GLU:O	1:J:206:THR:HG23	2.22	0.40
3:C:207:LEU:HG	3:C:212:LEU:HD22	2.03	0.40
3:I:259:ARG:NH1	3:I:259:ARG:CB	2.80	0.40
3:C:259:ARG:CZ	3:C:259:ARG:HB3	2.51	0.40
3:C:18:THR:HG23	3:C:20:ASP:C	2.42	0.40
3:L:21:GLU:O	3:L:24:VAL:HB	2.22	0.40
1:G:13:LEU:HD13	1:G:86:ALA:HA	2.04	0.40
2:E:70:ARG:HG2	2:E:70:ARG:HH11	1.87	0.40
3:C:331:THR:CG2	1:J:142:LYS:HA	2.50	0.40
3:F:334:ARG:CZ	3:F:334:ARG:HB3	2.52	0.40
1:G:203:VAL:O	1:G:203:VAL:HG12	2.22	0.40
2:K:70:ARG:HA	2:K:70:ARG:HD2	1.82	0.40
1:G:178:ALA:O	1:G:179:MET:CB	2.69	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	204/216 (94%)	174 (85%)	17 (8%)	13 (6%)	2	3
1	D	204/216 (94%)	176 (86%)	15 (7%)	13 (6%)	2	3
1	G	204/216 (94%)	174 (85%)	17 (8%)	13 (6%)	2	3
1	J	204/216 (94%)	175 (86%)	16 (8%)	13 (6%)	2	3
2	B	144/201 (72%)	121 (84%)	15 (10%)	8 (6%)	3	4
2	E	144/201 (72%)	119 (83%)	17 (12%)	8 (6%)	3	4
2	H	144/201 (72%)	121 (84%)	15 (10%)	8 (6%)	3	4
2	K	144/201 (72%)	121 (84%)	15 (10%)	8 (6%)	3	4
3	C	342/386 (89%)	301 (88%)	38 (11%)	3 (1%)	25	55
3	F	342/386 (89%)	302 (88%)	37 (11%)	3 (1%)	25	55
3	I	342/386 (89%)	305 (89%)	34 (10%)	3 (1%)	25	55
3	L	342/386 (89%)	305 (89%)	34 (10%)	3 (1%)	25	55
All	All	2760/3212 (86%)	2394 (87%)	270 (10%)	96 (4%)	6	12

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	ARG
1	A	179	MET
1	A	189	MET
1	A	190	ASP
1	A	191	PRO
2	B	45	GLU
2	B	46	GLU
2	B	59	ALA
2	B	60	SER
2	B	165	ARG

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Mol	Chain	Res	Type
1	D	179	MET
1	D	189	MET
1	D	190	ASP
1	D	191	PRO
2	E	45	GLU
2	E	46	GLU
2	E	59	ALA
2	E	60	SER
2	E	165	ARG
1	G	106	ARG
1	G	179	MET
1	G	189	MET
1	G	190	ASP
1	G	191	PRO
2	H	45	GLU
2	H	46	GLU
2	H	59	ALA
2	H	60	SER
2	H	165	ARG
1	J	106	ARG
1	J	179	MET
1	J	189	MET
1	J	190	ASP
1	J	191	PRO
2	K	45	GLU
2	K	46	GLU
2	K	59	ALA
2	K	60	SER
2	K	165	ARG
1	A	178	ALA
1	A	196	GLN
2	B	116	SER
1	D	106	ARG
1	D	178	ALA
1	D	196	GLN
2	E	116	SER
3	F	172	GLU
1	G	178	ALA
1	G	196	GLN
2	H	116	SER
1	J	178	ALA
1	J	196	GLN

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Mol	Chain	Res	Type
1	A	194	ALA
3	C	172	GLU
1	D	194	ALA
2	E	47	GLU
1	G	194	ALA
2	H	47	GLU
3	I	172	GLU
1	J	194	ALA
2	K	47	GLU
2	K	116	SER
3	L	172	GLU
3	L	336	GLU
1	A	186	GLU
1	A	187	VAL
1	A	195	ALA
2	B	47	GLU
3	C	336	GLU
1	D	186	GLU
1	D	187	VAL
1	D	195	ALA
3	F	336	GLU
1	G	186	GLU
1	G	187	VAL
1	G	195	ALA
3	I	336	GLU
1	J	186	GLU
1	J	195	ALA
1	A	188	VAL
1	D	188	VAL
1	D	210	PRO
1	G	188	VAL
1	G	210	PRO
1	J	187	VAL
1	J	188	VAL
1	J	210	PRO
1	A	210	PRO
2	H	65	PRO
2	B	65	PRO
2	K	65	PRO
2	E	65	PRO
3	C	16	ILE
3	F	16	ILE

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Mol	Chain	Res	Type
3	I	16	ILE
3	L	16	ILE

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	178/185 (96%)	165 (93%)	13 (7%)	20	44
1	D	178/185 (96%)	165 (93%)	13 (7%)	20	44
1	G	178/185 (96%)	165 (93%)	13 (7%)	20	44
1	J	178/185 (96%)	166 (93%)	12 (7%)	23	49
2	B	131/176 (74%)	119 (91%)	12 (9%)	13	29
2	E	131/176 (74%)	119 (91%)	12 (9%)	13	29
2	H	131/176 (74%)	119 (91%)	12 (9%)	13	29
2	K	131/176 (74%)	119 (91%)	12 (9%)	13	29
3	C	295/334 (88%)	277 (94%)	18 (6%)	26	54
3	F	295/334 (88%)	277 (94%)	18 (6%)	26	54
3	I	295/334 (88%)	277 (94%)	18 (6%)	26	54
3	L	295/334 (88%)	277 (94%)	18 (6%)	26	54
All	All	2416/2780 (87%)	2245 (93%)	171 (7%)	21	46

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	16	VAL
1	A	28	LYS
1	A	31	LEU
1	A	81	ILE
1	A	97	THR
1	A	111	VAL
1	A	118	VAL
1	A	140	ARG

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Mol	Chain	Res	Type
1	A	141	LYS
1	A	157	PHE
1	A	158	GLU
1	A	186	GLU
2	B	26	GLN
2	B	46	GLU
2	B	57	ARG
2	B	63	ASP
2	B	64	LEU
2	B	75	VAL
2	B	109	GLU
2	B	118	ARG
2	B	123	ASN
2	B	146	GLU
2	B	156	GLU
2	B	166	GLU
3	C	19	GLU
3	C	29	LEU
3	C	43	THR
3	C	66	GLU
3	C	78	GLU
3	C	81	GLU
3	C	109	THR
3	C	112	GLU
3	C	114	LEU
3	C	146	LEU
3	C	192	VAL
3	C	196	GLN
3	C	208	LEU
3	C	212	LEU
3	C	247	ARG
3	C	278	THR
3	C	293	THR
3	C	296	THR
1	D	13	LEU
1	D	16	VAL
1	D	28	LYS
1	D	31	LEU
1	D	81	ILE
1	D	97	THR
1	D	111	VAL
1	D	118	VAL

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Mol	Chain	Res	Type
1	D	140	ARG
1	D	141	LYS
1	D	157	PHE
1	D	158	GLU
1	D	186	GLU
2	E	26	GLN
2	E	46	GLU
2	E	57	ARG
2	E	63	ASP
2	E	64	LEU
2	E	75	VAL
2	E	109	GLU
2	E	118	ARG
2	E	123	ASN
2	E	146	GLU
2	E	156	GLU
2	E	166	GLU
3	F	19	GLU
3	F	29	LEU
3	F	43	THR
3	F	66	GLU
3	F	78	GLU
3	F	81	GLU
3	F	109	THR
3	F	112	GLU
3	F	114	LEU
3	F	146	LEU
3	F	192	VAL
3	F	196	GLN
3	F	208	LEU
3	F	212	LEU
3	F	247	ARG
3	F	278	THR
3	F	293	THR
3	F	296	THR
1	G	13	LEU
1	G	16	VAL
1	G	28	LYS
1	G	31	LEU
1	G	81	ILE
1	G	97	THR
1	G	111	VAL

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Mol	Chain	Res	Type
1	G	118	VAL
1	G	140	ARG
1	G	141	LYS
1	G	157	PHE
1	G	158	GLU
1	G	186	GLU
2	H	26	GLN
2	H	46	GLU
2	H	57	ARG
2	H	63	ASP
2	H	64	LEU
2	H	75	VAL
2	H	109	GLU
2	H	118	ARG
2	H	123	ASN
2	H	146	GLU
2	H	156	GLU
2	H	166	GLU
3	I	19	GLU
3	I	29	LEU
3	I	43	THR
3	I	66	GLU
3	I	78	GLU
3	I	81	GLU
3	I	109	THR
3	I	112	GLU
3	I	114	LEU
3	I	146	LEU
3	I	192	VAL
3	I	196	GLN
3	I	208	LEU
3	I	212	LEU
3	I	247	ARG
3	I	278	THR
3	I	293	THR
3	I	296	THR
1	J	13	LEU
1	J	16	VAL
1	J	28	LYS
1	J	31	LEU
1	J	81	ILE
1	J	97	THR

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Mol	Chain	Res	Type
1	J	118	VAL
1	J	140	ARG
1	J	141	LYS
1	J	157	PHE
1	J	158	GLU
1	J	186	GLU
2	K	26	GLN
2	K	46	GLU
2	K	57	ARG
2	K	63	ASP
2	K	64	LEU
2	K	75	VAL
2	K	109	GLU
2	K	118	ARG
2	K	123	ASN
2	K	146	GLU
2	K	156	GLU
2	K	166	GLU
3	L	19	GLU
3	L	29	LEU
3	L	43	THR
3	L	66	GLU
3	L	78	GLU
3	L	81	GLU
3	L	109	THR
3	L	112	GLU
3	L	114	LEU
3	L	146	LEU
3	L	192	VAL
3	L	196	GLN
3	L	208	LEU
3	L	212	LEU
3	L	247	ARG
3	L	278	THR
3	L	293	THR
3	L	296	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	30	HIS

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Mol	Chain	Res	Type
1	A	100	ASN
1	A	143	ASN
1	A	156	ASN
2	B	22	ASN
2	B	102	HIS
2	B	113	ASN
2	B	123	ASN
2	B	147	ASN
3	C	111	GLN
3	C	121	HIS
3	C	130	HIS
3	C	131	ASN
3	C	173	ASN
3	C	186	HIS
3	C	206	HIS
3	C	252	ASN
1	D	10	GLN
1	D	30	HIS
1	D	143	ASN
1	D	156	ASN
2	E	22	ASN
2	E	102	HIS
2	E	113	ASN
2	E	123	ASN
2	E	147	ASN
3	F	111	GLN
3	F	121	HIS
3	F	130	HIS
3	F	131	ASN
3	F	173	ASN
3	F	186	HIS
3	F	206	HIS
3	F	245	ASN
3	F	252	ASN
1	G	10	GLN
1	G	30	HIS
1	G	100	ASN
1	G	143	ASN
1	G	156	ASN
2	H	22	ASN
2	H	102	HIS
2	H	113	ASN

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Mol	Chain	Res	Type
2	H	123	ASN
2	H	147	ASN
3	I	111	GLN
3	I	121	HIS
3	I	130	HIS
3	I	131	ASN
3	I	147	GLN
3	I	173	ASN
3	I	184	GLN
3	I	186	HIS
3	I	252	ASN
1	J	10	GLN
1	J	30	HIS
1	J	100	ASN
1	J	143	ASN
1	J	156	ASN
2	K	22	ASN
2	K	102	HIS
2	K	113	ASN
2	K	123	ASN
2	K	147	ASN
3	L	111	GLN
3	L	121	HIS
3	L	130	HIS
3	L	131	ASN
3	L	173	ASN
3	L	186	HIS
3	L	206	HIS
3	L	252	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	GNP	A	1250	4	34,34,34	1.54	8 (23%)	50,54,54	3.22	9 (18%)
5	GNP	D	2250	4	34,34,34	1.79	10 (29%)	50,54,54	2.83	9 (18%)
5	GNP	G	3250	4	34,34,34	1.71	7 (20%)	50,54,54	3.24	10 (20%)
5	GNP	J	4250	4	34,34,34	1.71	9 (26%)	50,54,54	2.71	10 (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
5	GNP	A	1250	4	-	1/18/38/38	0/1/3/3
5	GNP	D	2250	4	-	1/18/38/38	0/1/3/3
5	GNP	G	3250	4	-	1/18/38/38	0/1/3/3
5	GNP	J	4250	4	-	1/18/38/38	0/1/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	3250	GNP	PB-N3B	4.60	1.68	1.64
5	D	2250	GNP	PB-N3B	4.34	1.68	1.64
5	D	2250	GNP	C6-C5	3.59	1.47	1.41
5	D	2250	GNP	C2-N3	3.57	1.38	1.33
5	J	4250	GNP	PB-N3B	3.51	1.67	1.64
5	D	2250	GNP	PG-N3B	3.42	1.67	1.64
5	J	4250	GNP	C6-C5	3.37	1.46	1.41
5	G	3250	GNP	C2-N3	3.25	1.37	1.33
5	D	2250	GNP	PG-O2G	-3.25	1.45	1.55
5	G	3250	GNP	C6-C5	3.18	1.46	1.41
5	D	2250	GNP	PB-O2B	-3.15	1.46	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1250	GNP	C2-N3	3.14	1.37	1.33
5	J	4250	GNP	C2-N3	3.10	1.37	1.33
5	A	1250	GNP	PG-O2G	-3.10	1.46	1.55
5	G	3250	GNP	PG-O2G	-3.08	1.46	1.55
5	J	4250	GNP	PB-O3A	3.07	1.63	1.59
5	G	3250	GNP	PG-N3B	3.00	1.66	1.64
5	G	3250	GNP	PB-O2B	-2.94	1.46	1.55
5	J	4250	GNP	PB-O2B	-2.91	1.46	1.55
5	A	1250	GNP	PG-N3B	2.90	1.66	1.64
5	G	3250	GNP	C8-N9	2.89	1.40	1.36
5	A	1250	GNP	PB-N3B	2.82	1.66	1.64
5	J	4250	GNP	PA-O3A	2.77	1.64	1.59
5	A	1250	GNP	C6-C5	2.74	1.45	1.41
5	J	4250	GNP	PG-O2G	-2.64	1.47	1.55
5	A	1250	GNP	PA-O3A	2.60	1.64	1.59
5	J	4250	GNP	C8-N9	2.55	1.40	1.36
5	A	1250	GNP	PB-O3A	2.42	1.62	1.59
5	D	2250	GNP	C8-N9	2.39	1.40	1.36
5	A	1250	GNP	PB-O2B	-2.35	1.48	1.55
5	D	2250	GNP	C8-N7	-2.15	1.30	1.34
5	D	2250	GNP	PB-O3A	2.15	1.62	1.59
5	J	4250	GNP	PG-N3B	2.05	1.66	1.64
5	D	2250	GNP	PA-O3A	2.02	1.63	1.59

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	3250	GNP	C6-C5-N7	-20.52	131.38	134.14
5	A	1250	GNP	C6-C5-N7	-20.40	131.39	134.14
5	D	2250	GNP	C6-C5-N7	-17.39	131.80	134.14
5	J	4250	GNP	C6-C5-N7	-16.45	131.93	134.14
5	J	4250	GNP	O2B-PB-N3B	3.58	116.33	106.61
5	G	3250	GNP	O3G-PG-O1G	-3.56	104.46	113.60
5	A	1250	GNP	O3G-PG-O1G	-3.54	104.50	113.60
5	D	2250	GNP	O2B-PB-N3B	3.53	116.20	106.61
5	G	3250	GNP	O2G-PG-N3B	3.53	116.20	106.61
5	G	3250	GNP	C8-N9-C4	-3.50	104.23	106.90
5	J	4250	GNP	O2G-PG-N3B	3.47	116.04	106.61
5	D	2250	GNP	O3G-PG-O1G	-3.46	104.72	113.60
5	D	2250	GNP	O2G-PG-N3B	3.45	115.98	106.61
5	D	2250	GNP	C8-N9-C4	-3.44	104.27	106.90
5	A	1250	GNP	O2G-PG-N3B	3.43	115.93	106.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	3250	GNP	O2B-PB-N3B	3.43	115.92	106.61
5	A	1250	GNP	C6-N1-C2	3.38	125.43	119.51
5	G	3250	GNP	C6-N1-C2	3.34	125.35	119.51
5	A	1250	GNP	C8-N9-C4	-3.29	104.39	106.90
5	D	2250	GNP	C6-N1-C2	3.26	125.21	119.51
5	J	4250	GNP	C6-N1-C2	3.19	125.09	119.51
5	J	4250	GNP	O3G-PG-O1G	-3.18	105.45	113.60
5	J	4250	GNP	C8-N9-C4	-3.13	104.51	106.90
5	A	1250	GNP	O2B-PB-N3B	3.07	114.96	106.61
5	A	1250	GNP	PB-N3B-PG	-2.77	125.41	130.07
5	J	4250	GNP	PB-N3B-PG	-2.54	125.80	130.07
5	G	3250	GNP	PB-N3B-PG	-2.49	125.89	130.07
5	A	1250	GNP	O1G-PG-N3B	2.47	115.56	111.83
5	D	2250	GNP	O1G-PG-N3B	2.38	115.42	111.83
5	A	1250	GNP	O4'-C1'-C2'	-2.33	103.20	106.77
5	G	3250	GNP	O4'-C1'-C2'	-2.24	103.33	106.77
5	G	3250	GNP	O1G-PG-N3B	2.23	115.20	111.83
5	D	2250	GNP	O2G-PG-O1G	-2.18	108.00	113.60
5	J	4250	GNP	O1G-PG-N3B	2.13	115.05	111.83
5	J	4250	GNP	O2G-PG-O1G	-2.08	108.25	113.60
5	D	2250	GNP	O4'-C1'-C2'	-2.08	103.58	106.77
5	G	3250	GNP	O4'-C1'-N9	2.02	110.32	108.44
5	J	4250	GNP	O1B-PB-N3B	2.02	114.88	111.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	4250	GNP	O1B-PB-N3B-PG
5	A	1250	GNP	O1B-PB-N3B-PG
5	D	2250	GNP	O1B-PB-N3B-PG
5	G	3250	GNP	O1B-PB-N3B-PG

There are no ring outliers.

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	206/216 (95%)	0.08	18 (8%) 10 10	27, 46, 132, 170	0
1	D	206/216 (95%)	0.32	20 (9%) 8 8	21, 46, 146, 188	0
1	G	206/216 (95%)	0.18	19 (9%) 9 9	28, 49, 127, 168	0
1	J	206/216 (95%)	0.04	11 (5%) 25 28	24, 47, 117, 170	0
2	B	146/201 (72%)	0.54	21 (14%) 3 4	36, 72, 130, 159	0
2	E	146/201 (72%)	1.02	32 (21%) 1 2	41, 88, 138, 159	0
2	H	146/201 (72%)	0.70	19 (13%) 4 4	41, 71, 138, 176	0
2	K	146/201 (72%)	0.36	14 (9%) 8 8	28, 73, 126, 149	0
3	C	344/386 (89%)	-0.27	2 (0%) 86 90	21, 42, 76, 135	0
3	F	344/386 (89%)	-0.24	6 (1%) 67 73	24, 45, 83, 135	0
3	I	344/386 (89%)	-0.23	3 (0%) 81 85	23, 45, 81, 114	0
3	L	344/386 (89%)	-0.19	6 (1%) 67 73	22, 45, 90, 143	0
All	All	2784/3212 (86%)	0.07	171 (6%) 21 22	21, 49, 120, 188	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	189	MET	14.0
1	D	191	PRO	11.0
1	D	188	VAL	10.8
1	D	195	ALA	10.7
1	G	192	ALA	9.3
1	D	187	VAL	9.1
2	H	63	ASP	9.0
1	G	191	PRO	8.8
1	D	192	ALA	8.6
1	D	194	ALA	8.3
2	H	23	HIS	6.8

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Mol	Chain	Res	Type	RSRZ
2	H	22	ASN	6.7
2	B	63	ASP	6.6
1	A	197	TYR	6.4
1	A	188	VAL	6.4
1	A	190	ASP	6.3
1	D	190	ASP	6.2
1	A	192	ALA	6.2
2	B	23	HIS	6.1
1	G	197	TYR	6.1
1	D	197	TYR	5.9
1	D	141	LYS	5.9
1	A	187	VAL	5.8
1	J	190	ASP	5.7
2	E	107	MET	5.6
1	J	189	MET	5.5
1	A	191	PRO	5.5
1	G	196	GLN	5.2
1	A	212	GLU	5.1
1	G	186	GLU	5.0
2	B	65	PRO	4.9
2	E	61	GLU	4.8
1	A	186	GLU	4.8
2	E	23	HIS	4.8
1	D	193	LEU	4.8
2	E	145	ALA	4.8
2	H	65	PRO	4.7
1	G	141	LYS	4.7
1	A	141	LYS	4.7
2	E	22	ASN	4.7
1	D	199	HIS	4.7
1	D	196	GLN	4.6
1	A	195	ALA	4.5
1	D	198	GLU	4.5
1	G	195	ALA	4.4
1	A	194	ALA	4.3
2	E	82	GLU	4.3
2	E	63	ASP	4.3
2	E	116	SER	4.2
1	D	186	GLU	4.2
1	G	193	LEU	4.1
2	H	116	SER	4.1
3	F	20	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	199	HIS	4.0
2	H	61	GLU	4.0
1	A	193	LEU	4.0
2	E	160	LYS	3.9
2	H	114	ALA	3.8
2	E	144	ASN	3.8
1	A	213	ASP	3.8
2	K	61	GLU	3.7
2	B	22	ASN	3.7
1	J	197	TYR	3.6
2	B	82	GLU	3.6
2	H	37	GLU	3.6
2	H	82	GLU	3.6
2	K	23	HIS	3.6
2	E	49	PHE	3.6
1	J	191	PRO	3.5
2	B	61	GLU	3.5
3	L	345	GLU	3.5
2	B	167	LYS	3.5
1	G	212	GLU	3.5
2	B	24	ASP	3.4
2	H	24	ASP	3.4
2	H	115	GLY	3.4
2	B	117	ASP	3.4
1	A	189	MET	3.4
1	G	189	MET	3.4
1	A	211	ASP	3.3
2	H	167	LYS	3.3
3	I	333	GLY	3.3
2	E	165	ARG	3.2
1	D	202	GLU	3.2
3	I	334	ARG	3.2
2	K	82	GLU	3.2
1	G	140	ARG	3.2
3	I	345	GLU	3.1
1	G	190	ASP	3.1
2	E	167	LYS	3.0
1	A	202	GLU	3.0
2	H	28	GLU	3.0
2	B	45	GLU	3.0
2	E	67	TRP	3.0
2	E	143	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	194	ALA	3.0
2	B	166	GLU	3.0
2	K	65	PRO	3.0
1	J	193	LEU	3.0
1	G	198	GLU	2.9
2	E	119	ALA	2.9
2	E	117	ASP	2.9
1	D	212	GLU	2.9
2	H	64	LEU	2.9
1	A	199	HIS	2.9
2	K	115	GLY	2.8
3	C	341	ASP	2.8
2	B	115	GLY	2.8
1	J	196	GLN	2.7
2	E	121	VAL	2.7
2	B	28	GLU	2.7
1	G	213	ASP	2.7
2	K	63	ASP	2.7
1	G	187	VAL	2.7
1	G	188	VAL	2.7
2	H	117	ASP	2.6
3	L	327	GLU	2.6
1	G	211	ASP	2.6
1	J	192	ALA	2.6
2	B	64	LEU	2.6
2	H	140	ILE	2.5
3	F	157	ASN	2.5
1	D	213	ASP	2.5
3	L	20	ASP	2.5
2	B	116	SER	2.5
2	E	24	ASP	2.4
2	E	132	CYS	2.4
2	B	59	ALA	2.4
2	B	37	GLU	2.4
2	E	65	PRO	2.4
2	K	84	GLY	2.4
3	L	230	HIS	2.4
2	E	60	SER	2.4
3	L	30	GLU	2.3
2	E	149	GLN	2.3
2	E	66	GLU	2.3
2	H	164	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	K	110	LEU	2.3
2	K	38	ILE	2.3
3	F	345	GLU	2.3
3	F	32	ASP	2.3
2	E	111	LYS	2.3
3	F	19	GLU	2.3
2	B	140	ILE	2.3
2	B	62	ASN	2.3
2	E	62	ASN	2.3
3	L	320	ASP	2.2
2	E	115	GLY	2.2
2	B	60	SER	2.2
1	A	198	GLU	2.2
2	E	46	GLU	2.2
2	B	26	GLN	2.2
2	H	107	MET	2.1
3	C	230	HIS	2.1
1	J	195	ALA	2.1
2	E	45	GLU	2.1
1	J	200	ASP	2.1
3	F	31	ASP	2.1
2	K	107	MET	2.1
1	D	140	ARG	2.1
2	E	122	TRP	2.1
1	D	127	LYS	2.1
1	J	206	THR	2.1
2	H	145	ALA	2.1
2	E	64	LEU	2.1
2	K	22	ASN	2.1
2	K	144	ASN	2.1
2	K	132	CYS	2.0
2	E	163	GLU	2.0
1	J	213	ASP	2.0
2	K	117	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
5	GNP	G	3250	32/32	0.15	-0.42	37,37,37,37	0
5	GNP	A	1250	32/32	0.13	-0.42	37,37,37,37	0
4	MG	G	3251	1/1	0.14	-0.49	36,36,36,36	0
5	GNP	D	2250	32/32	0.12	-0.85	37,37,37,37	0
5	GNP	J	4250	32/32	0.12	-1.18	36,36,36,36	0
4	MG	J	4251	1/1	0.10	-1.45	44,44,44,44	0
4	MG	A	1251	1/1	0.08	-1.82	29,29,29,29	0
4	MG	D	2251	1/1	0.06	-2.07	44,44,44,44	0

6.5 Other polymers ⓘ

There are no such residues in this entry.