



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:44 AM UTC

PDB ID : 3UTT / pdb_00003utt
Title : 1E6-A*0201-ALWGPDPA AAA Complex, Triclinic
Authors : Rizkallah, P.J.; Cole, D.K.; Sewell, A.K.; Bulek, A.M.; Rossjohn, J.; Gras, S.
Deposited on : 2011-11-26
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

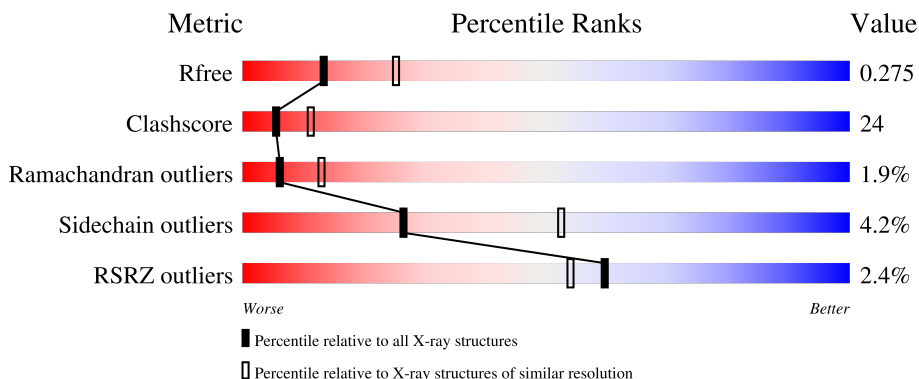
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.



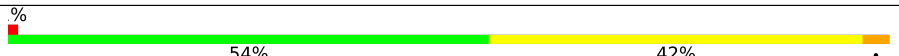
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	275	
1	F	275	
2	B	100	
2	G	100	
3	C	10	

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Mol	Chain	Length	Quality of chain
3	H	10	
4	D	199	
4	I	199	
5	E	245	
5	J	245	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13562 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	275	Total	C	N	O	S	0	1	0
			2257	1409	413	426	9			
1	F	275	Total	C	N	O	S	0	3	0
			2277	1420	418	430	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	G	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
G	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Insulin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	10	Total	C	N	O	0	0	0
			69	45	11	13			
3	H	10	Total	C	N	O	0	0	0
			69	45	11	13			

- Molecule 4 is a protein called 1E6 TCR Alpha Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	199	Total	C	N	O	S	0	0	0
			1570	983	258	319	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	199	Total	C	N	O	S	0	0	0
			1570	983	258	319	10			

- Molecule 5 is a protein called 1E6 TCR Beta Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	244	Total	C	N	O	S	0	0	0
			1960	1242	339	369	10			
5	J	245	Total	C	N	O	S	0	0	0
			1965	1245	340	370	10			

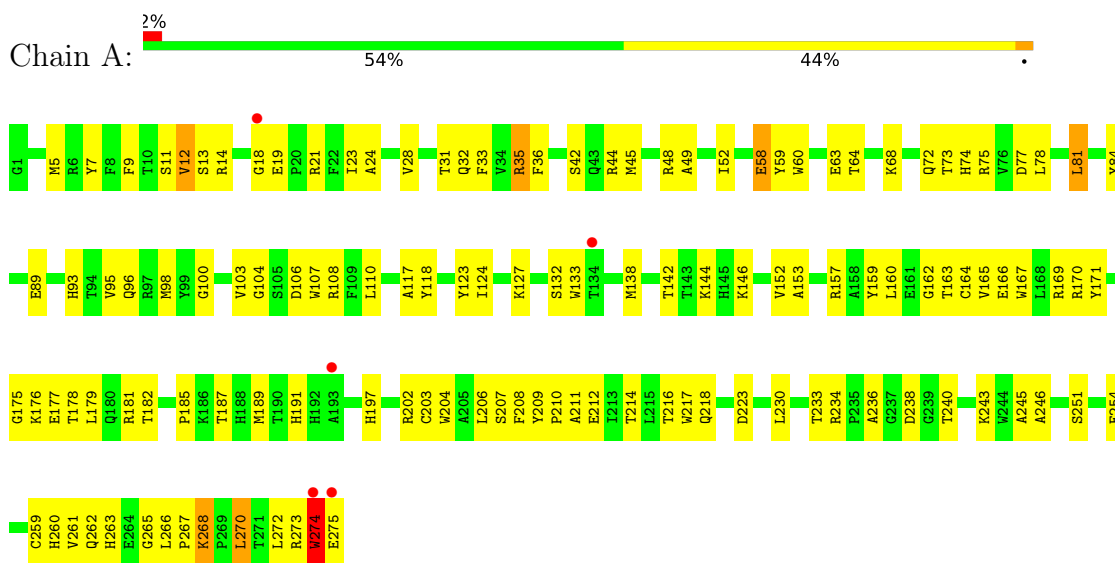
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	23	Total	O	0	0
			23	23		
6	B	11	Total	O	0	0
			11	11		
6	D	10	Total	O	0	0
			10	10		
6	E	26	Total	O	0	0
			26	26		
6	F	28	Total	O	0	0
			28	28		
6	G	19	Total	O	0	0
			19	19		
6	H	1	Total	O	0	0
			1	1		
6	I	15	Total	O	0	0
			15	15		
6	J	18	Total	O	0	0
			18	18		

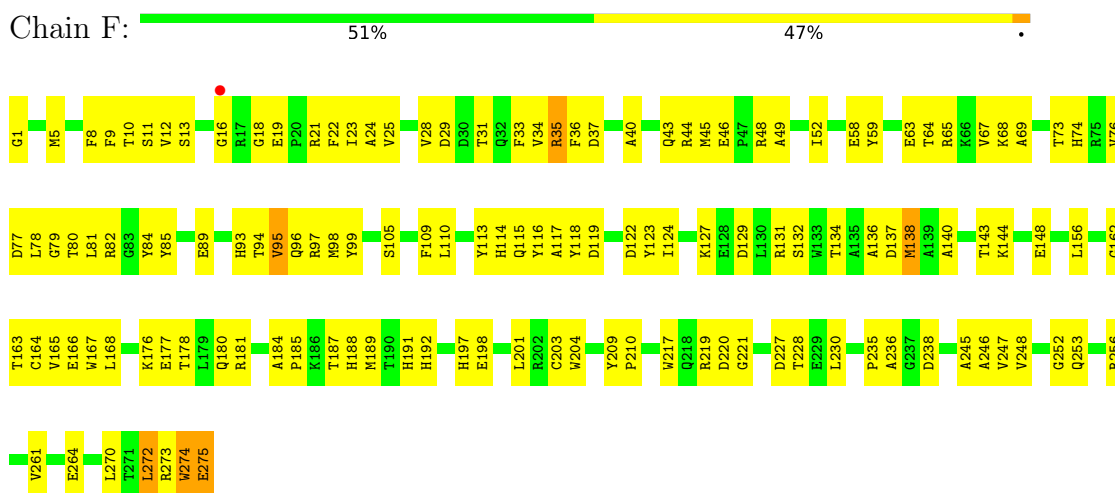
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: HLA class I histocompatibility antigen, A-2 alpha chain

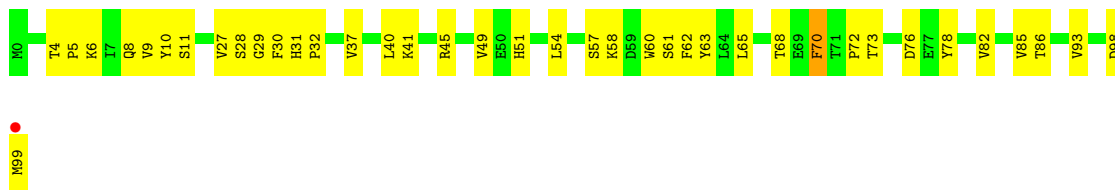


- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



- Molecule 2: Beta-2-microglobulin





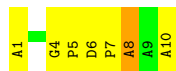
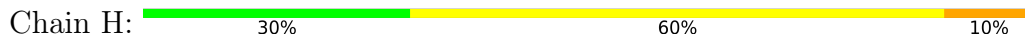
• Molecule 2: Beta-2-microglobulin



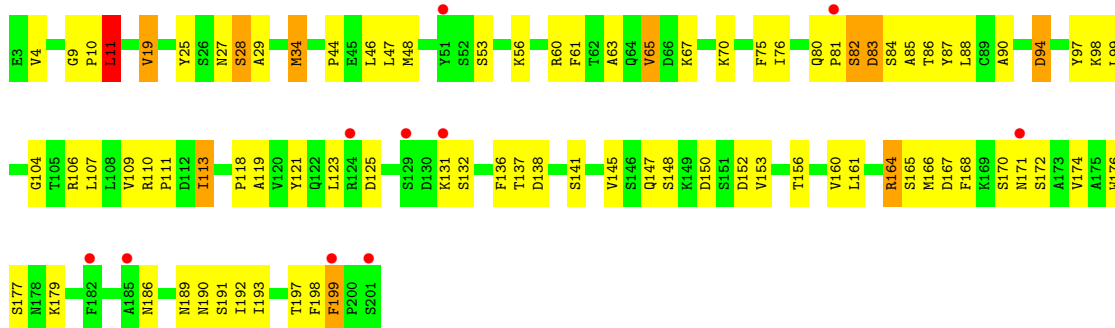
• Molecule 3: Insulin



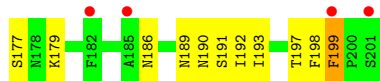
• Molecule 3: Insulin



• Molecule 4: 1E6 TCR Alpha Chain



• Molecule 4: 1E6 TCR Alpha Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	41.48Å 98.44Å 121.30Å 97.27° 98.16° 93.38°	Depositor
Resolution (Å)	29.34 – 2.60 29.34 – 2.60	Depositor EDS
% Data completeness (in resolution range)	89.9 (29.34-2.60) 96.9 (29.34-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.61Å)	Xtrriage
Refinement program	PHENIX 1.6.1_357, REFMAC	Depositor
R, R_{free}	0.195 , 0.274 0.200 , 0.275	Depositor DCC
R_{free} test set	2840 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	43.5	Xtrriage
Anisotropy	0.604	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13562	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.29	0/2322	0.68	0/3151
1	F	0.28	0/2342	0.67	0/3177
2	B	0.30	0/860	0.66	0/1162
2	G	0.31	0/860	0.67	0/1162
3	C	0.27	0/72	0.74	0/99
3	H	0.27	0/72	1.08	0/99
4	D	0.27	0/1606	0.67	0/2174
4	I	0.28	0/1606	0.72	1/2174 (0.0%)
5	E	0.30	0/2015	0.71	0/2741
5	J	0.29	0/2020	0.72	2/2748 (0.1%)
All	All	0.29	0/13775	0.69	3/18687 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	94	ASP	N-CA-C	6.74	122.30	114.62
5	J	69	MET	CA-C-N	5.12	124.73	119.05
5	J	69	MET	C-N-CA	5.12	124.73	119.05

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2257	0	2108	104	0
1	F	2277	0	2125	128	0
2	B	837	0	803	26	0
2	G	837	0	803	43	0
3	C	69	0	64	14	0
3	H	69	0	64	14	0
4	D	1570	0	1481	79	0
4	I	1570	0	1481	76	0
5	E	1960	0	1875	101	0
5	J	1965	0	1880	105	0
6	A	23	0	0	1	0
6	B	11	0	0	0	0
6	D	10	0	0	2	0
6	E	26	0	0	0	0
6	F	28	0	0	1	0
6	G	19	0	0	0	0
6	H	1	0	0	0	0
6	I	15	0	0	1	0
6	J	18	0	0	2	0
All	All	13562	0	12684	619	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (619) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:80:GLN:HB3	5:E:81:PRO:HD2	1.45	0.98
3:C:7:PRO:HA	3:C:8:ALA:HB3	1.45	0.97
5:J:46:LEU:HB3	5:J:60:MET:HE3	1.46	0.97
1:A:274:TRP:HE3	1:A:275:GLU:H	1.08	0.96
5:E:46:LEU:HB3	5:E:60:MET:HE3	1.47	0.95
1:A:191:HIS:HB2	1:A:275:GLU:HB3	1.51	0.92
4:D:34:MET:HB2	4:D:46:LEU:HD11	1.51	0.91
1:A:274:TRP:HE3	1:A:275:GLU:N	1.71	0.88
4:I:94:ASP:H	4:I:95:SER:HB3	1.40	0.86
1:F:69:ALA:HB1	3:H:6:ASP:HB3	1.59	0.85
1:F:11:SER:HB3	1:F:95:VAL:HG13	1.59	0.84
1:A:266:LEU:HD22	1:A:270:LEU:HD13	1.59	0.83
4:D:111:PRO:HG2	4:D:160:VAL:HG11	1.60	0.83
1:A:12:VAL:HG13	1:A:21:ARG:HB3	1.61	0.81
5:J:155:ASP:HB2	5:J:178:PRO:HG2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:274:TRP:O	1:F:275:GLU:HB2	1.80	0.80
5:J:43:LEU:HD23	5:J:43:LEU:H	1.46	0.79
5:E:120:LYS:HB2	5:E:227:GLN:HE21	1.49	0.78
4:D:121:TYR:HB3	5:E:133:SER:HB3	1.67	0.77
3:H:7:PRO:HA	3:H:8:ALA:HB3	1.67	0.76
1:A:127:LYS:HD2	1:A:132:SER:HB2	1.66	0.76
5:J:46:LEU:O	5:J:60:MET:HG2	1.86	0.76
4:I:46:LEU:HD23	5:J:104:ILE:HD13	1.68	0.76
1:A:187:THR:HG21	1:A:261:VAL:HG21	1.66	0.75
4:I:94:ASP:N	4:I:95:SER:HB3	2.02	0.75
1:A:133:TRP:HB2	1:A:144:LYS:HE2	1.68	0.74
5:E:33:PHE:HB2	5:E:93:ALA:HB3	1.68	0.74
1:F:189:MET:HB2	1:F:272:LEU:HD23	1.68	0.73
5:J:213:GLN:HG3	5:J:236:ILE:HG23	1.71	0.72
1:A:73:THR:HG21	3:C:7:PRO:HB2	1.71	0.72
5:E:15:MET:HE3	5:E:117:GLU:HA	1.71	0.71
4:D:19:VAL:HG13	4:D:76:ILE:HB	1.72	0.71
1:F:117:ALA:HB2	2:G:60:TRP:CE2	2.26	0.71
4:D:82:SER:O	4:D:84:SER:N	2.22	0.71
5:E:80:GLN:HB3	5:E:81:PRO:CD	2.20	0.71
1:A:204:TRP:CZ2	2:B:99:MET:HA	2.25	0.71
3:H:7:PRO:CA	3:H:8:ALA:HB3	2.21	0.71
1:F:12:VAL:HG12	1:F:21:ARG:HB3	1.72	0.70
4:D:10:PRO:HB3	4:D:106:ARG:NH1	2.07	0.70
5:J:41:ARG:HG2	5:J:42:GLY:N	2.07	0.69
4:D:152:ASP:HB3	4:D:179:LYS:HD2	1.73	0.69
4:I:53:SER:HA	4:I:65:VAL:HG13	1.73	0.69
1:F:187:THR:HG21	1:F:261:VAL:HG21	1.73	0.69
3:C:7:PRO:CA	3:C:8:ALA:HB3	2.22	0.69
3:C:7:PRO:HA	3:C:8:ALA:CB	2.22	0.69
4:D:44:PRO:HG2	5:E:43:LEU:HD11	1.75	0.69
5:J:225:TRP:CE2	5:J:227:GLN:HB2	2.29	0.68
2:B:41:LYS:HG3	2:B:78:TYR:CE1	2.29	0.68
4:I:8:PRO:CB	4:I:9:GLY:HA2	2.24	0.68
1:F:44:ARG:HA	1:F:64:THR:HG23	1.76	0.66
1:F:65[A]:ARG:NE	4:I:96:SER:HB2	2.11	0.66
1:F:235:PRO:HG2	2:G:65:LEU:HD22	1.77	0.66
1:A:273:ARG:HG2	1:A:274:TRP:H	1.60	0.66
1:A:211:ALA:HB1	1:A:233:THR:HG21	1.77	0.66
5:J:19:VAL:HG22	5:J:79:ILE:HB	1.77	0.66
2:B:5:PRO:HA	2:B:30:PHE:HB3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:80:GLN:HG3	5:J:81:PRO:HD2	1.77	0.66
1:F:12:VAL:CG1	1:F:21:ARG:HB3	2.26	0.65
4:I:8:PRO:HB2	4:I:9:GLY:HA2	1.78	0.65
3:H:7:PRO:HA	3:H:8:ALA:CB	2.26	0.65
1:F:191:HIS:CB	1:F:275:GLU:HG2	2.26	0.64
1:F:35:ARG:NH1	1:F:48:ARG:HH12	1.94	0.64
1:A:152:VAL:HG22	5:E:97:TRP:CH2	2.32	0.64
4:I:92:ARG:HB3	4:I:99:LEU:HD12	1.79	0.64
4:I:34:MET:HG2	4:I:90:ALA:HB3	1.80	0.64
1:A:32:GLN:NE2	1:A:48:ARG:HG3	2.13	0.64
5:E:99:LYS:HB3	5:E:104:ILE:HB	1.80	0.64
1:F:82[A]:ARG:HD2	1:F:89:GLU:HA	1.78	0.64
4:I:161:LEU:HB2	4:I:170:SER:O	1.98	0.64
5:E:122:VAL:HG12	5:E:232:PRO:HB2	1.81	0.63
1:A:138:MET:HE2	1:A:138:MET:HA	1.81	0.63
5:J:132:PRO:HD2	5:J:203:TRP:CZ2	2.34	0.63
5:E:120:LYS:HB2	5:E:227:GLN:NE2	2.13	0.63
5:E:129:VAL:HG23	5:E:239:ALA:HB3	1.81	0.63
4:I:103:SER:HA	5:J:42:GLY:H	1.63	0.63
1:F:64:THR:HG22	1:F:68:LYS:HE3	1.81	0.63
1:A:58:GLU:CD	1:A:58:GLU:H	2.06	0.62
5:E:76:THR:HG23	5:E:78:LYS:HG3	1.80	0.62
1:F:177:GLU:HG2	1:F:178:THR:HG23	1.80	0.62
4:I:138:ASP:HA	4:I:170:SER:HB2	1.81	0.62
4:I:5:GLU:HB3	4:I:24:THR:HG23	1.81	0.62
4:D:113:ILE:HD13	4:D:113:ILE:N	2.15	0.62
1:A:89:GLU:HB3	5:J:24:LYS:NZ	2.15	0.61
4:D:186:ASN:HB2	4:D:189:ASN:HD21	1.65	0.61
1:A:204:TRP:HZ2	2:B:99:MET:HA	1.65	0.61
4:D:123:LEU:HG	5:E:132:PRO:HA	1.80	0.61
1:A:214:THR:HB	1:A:262:GLN:HB2	1.83	0.61
1:F:189:MET:HE3	1:F:201:LEU:HB3	1.82	0.61
5:J:124:PRO:HD3	5:J:232:PRO:HB3	1.83	0.61
5:E:204:GLN:HB3	5:E:245:ALA:HA	1.82	0.61
1:F:273:ARG:HG2	1:F:274:TRP:H	1.65	0.61
1:A:267:PRO:HG2	1:A:268:LYS:HG3	1.83	0.61
1:F:69:ALA:CB	3:H:6:ASP:HB3	2.28	0.61
4:I:43:GLY:HA2	5:J:91:PHE:CE1	2.34	0.61
5:E:219:LEU:HD13	5:E:232:PRO:HG2	1.80	0.61
4:I:48:MET:SD	4:I:58:ASP:HB3	2.41	0.61
1:F:123:TYR:CZ	1:F:140:ALA:HA	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:161:LEU:HD21	5:E:171:GLY:O	2.02	0.60
1:F:82[A]:ARG:HE	1:F:89:GLU:HG2	1.67	0.60
1:F:178:THR:O	1:F:181:ARG:HG2	2.01	0.60
4:I:11:LEU:HD12	4:I:11:LEU:O	2.01	0.60
5:J:61:PRO:O	5:J:62:GLU:HB2	2.00	0.60
4:D:98:LYS:HA	5:E:45:LEU:HD22	1.84	0.60
5:E:69:MET:HE2	5:E:71:ASN:O	2.01	0.60
1:A:133:TRP:HE1	1:A:153:ALA:HB2	1.67	0.60
4:I:113:ILE:HD13	4:I:116:PRO:HD3	1.84	0.60
2:G:7:ILE:HB	2:G:93:VAL:HG21	1.82	0.60
5:J:127:VAL:HG13	5:J:147:CYS:SG	2.41	0.60
1:A:12:VAL:CG1	1:A:21:ARG:HB3	2.31	0.59
1:A:9:PHE:HZ	3:C:2:LEU:HD11	1.67	0.59
1:F:35:ARG:HD3	1:F:35:ARG:C	2.27	0.59
1:F:23:ILE:HG12	1:F:37:ASP:OD1	2.03	0.59
1:F:238:ASP:HB3	2:G:12:ARG:HD3	1.84	0.59
5:J:227:GLN:HG2	6:J:248:HOH:O	2.01	0.59
1:A:95:VAL:HG12	1:A:118:TYR:HD1	1.68	0.59
4:D:110:ARG:HB3	4:D:141:SER:HB3	1.85	0.59
4:D:136:PHE:O	4:D:172:SER:HA	2.02	0.59
2:G:24:ASN:HB3	2:G:65:LEU:HD11	1.85	0.58
4:D:25:TYR:CE1	4:D:70:LYS:HG3	2.37	0.58
1:A:81:LEU:HD23	1:A:118:TYR:CD1	2.38	0.58
4:I:33:PHE:CE2	4:I:65:VAL:HG21	2.38	0.58
5:J:80:GLN:CB	5:J:81:PRO:HD2	2.33	0.58
1:A:63:GLU:OE1	3:C:2:LEU:HB2	2.04	0.58
5:J:219:LEU:HD13	5:J:232:PRO:HG2	1.85	0.58
4:D:80:GLN:HB3	4:D:81:PRO:HD2	1.85	0.58
5:J:41:ARG:HG2	5:J:42:GLY:H	1.68	0.58
4:D:125:ASP:HA	5:E:130:PHE:HD2	1.69	0.57
2:B:98:ASP:O	2:B:99:MET:HB3	2.04	0.57
4:I:33:PHE:CD1	4:I:72:ILE:HD11	2.40	0.57
1:A:274:TRP:CE3	1:A:275:GLU:N	2.56	0.57
4:I:25:TYR:O	4:I:70:LYS:HB3	2.04	0.57
5:E:173:CYS:HB3	5:E:195:ARG:HD2	1.87	0.57
4:I:35:TRP:CE2	4:I:74:LEU:HB2	2.40	0.57
5:E:80:GLN:O	5:E:81:PRO:C	2.48	0.57
1:A:203:CYS:HB2	1:A:217:TRP:CZ2	2.40	0.57
1:F:189:MET:HB2	1:F:272:LEU:CD2	2.34	0.56
4:I:81:PRO:HA	4:I:109:VAL:HG13	1.87	0.56
1:A:11:SER:HB3	1:A:95:VAL:CG2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:8:PRO:HB2	4:I:10:PRO:HD2	1.87	0.56
5:J:80:GLN:O	5:J:81:PRO:C	2.48	0.56
1:A:103:VAL:HB	1:A:107:TRP:HA	1.86	0.56
1:A:12:VAL:HA	1:A:93:HIS:O	2.06	0.56
1:A:68:LYS:O	1:A:72:GLN:HG2	2.06	0.56
4:D:28:SER:O	4:D:29:ALA:HB3	2.05	0.56
1:F:176:LYS:HA	1:F:180:GLN:HG3	1.88	0.56
4:I:7:ASP:HB2	4:I:105:THR:OG1	2.05	0.56
3:C:5:PRO:HA	4:D:94:ASP:O	2.05	0.56
5:J:93:ALA:HA	5:J:106:TYR:O	2.06	0.56
1:A:23:ILE:HA	1:A:36:PHE:O	2.06	0.56
5:E:24:LYS:CE	1:F:89:GLU:HB3	2.36	0.56
5:E:149:ALA:HB2	5:E:214:VAL:HG21	1.88	0.56
4:D:118:PRO:HB2	4:D:197:THR:HA	1.88	0.55
5:E:19:VAL:HG22	5:E:79:ILE:HB	1.88	0.55
1:F:73:THR:HG21	3:H:7:PRO:HB2	1.88	0.55
1:F:144:LYS:O	1:F:148:GLU:HG2	2.06	0.55
4:D:81:PRO:O	4:D:82:SER:O	2.25	0.55
5:E:24:LYS:HE2	1:F:89:GLU:HB3	1.88	0.55
4:I:87:TYR:O	4:I:104:GLY:HA2	2.07	0.55
4:D:53:SER:HA	4:D:65:VAL:HG13	1.89	0.55
5:E:64:ARG:HH21	5:E:85:ARG:NH2	2.05	0.55
1:F:8:PHE:HB2	1:F:25:VAL:HG22	1.88	0.55
5:J:84:PRO:HA	5:J:115:VAL:O	2.06	0.55
2:B:73:THR:OG1	2:B:76:ASP:HB2	2.06	0.55
1:A:187:THR:HB	1:A:272:LEU:HD21	1.88	0.55
1:A:7:TYR:O	1:A:98:MET:HA	2.07	0.55
4:D:97:TYR:HH	5:E:97:TRP:CD1	2.25	0.55
5:E:21:LEU:HD22	5:E:111:THR:HG21	1.89	0.55
5:E:47:ILE:HD11	5:E:54:PRO:HB3	1.89	0.55
1:F:93:HIS:HE1	6:F:303:HOH:O	1.88	0.55
5:J:80:GLN:CG	5:J:81:PRO:HD2	2.36	0.55
4:D:176:TRP:CE3	5:E:148:LEU:HD11	2.42	0.54
1:F:188:HIS:C	1:F:272:LEU:HD21	2.32	0.54
5:J:129:VAL:HG23	5:J:239:ALA:HB3	1.89	0.54
4:D:150:ASP:OD1	4:D:153:VAL:HG23	2.08	0.54
4:I:164:ARG:HA	4:I:164:ARG:NE	2.22	0.54
4:I:37:ARG:HB2	4:I:47:LEU:HD11	1.87	0.54
4:I:106:ARG:HD2	5:J:40:MET:HE1	1.88	0.54
5:E:41:ARG:HG2	5:E:42:GLY:N	2.21	0.54
1:F:49:ALA:O	1:F:52:ILE:HG22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:7:PRO:CA	3:H:8:ALA:CB	2.85	0.54
4:I:94:ASP:H	4:I:95:SER:CB	2.15	0.54
4:I:98:LYS:HA	5:J:45:LEU:HD22	1.87	0.54
1:A:89:GLU:HB3	5:J:24:LYS:HZ3	1.71	0.54
5:J:19:VAL:CG2	5:J:79:ILE:HB	2.37	0.54
5:J:29:HIS:HD2	5:J:94:SER:OG	1.91	0.54
2:B:58:LYS:HD3	2:B:58:LYS:C	2.31	0.54
1:F:219:ARG:C	1:F:219:ARG:HD2	2.32	0.54
4:D:131:LYS:HD3	4:D:176:TRP:CD1	2.43	0.54
2:B:31:HIS:ND1	2:B:32:PRO:HA	2.23	0.54
4:D:125:ASP:HA	5:E:130:PHE:CD2	2.43	0.54
2:B:49:VAL:HG22	2:B:68:THR:HB	1.90	0.53
1:F:124:ILE:HA	1:F:134:THR:O	2.08	0.53
4:I:4:VAL:HG11	4:I:91:MET:HE3	1.90	0.53
1:F:65[B]:ARG:NH1	5:J:56:ASP:HA	2.24	0.53
1:A:160:LEU:O	1:A:165:VAL:HG23	2.08	0.53
4:D:113:ILE:HD12	4:D:141:SER:H	1.72	0.53
1:A:73:THR:HG21	3:C:7:PRO:CB	2.39	0.53
4:D:148:SER:HA	4:D:190:ASN:ND2	2.24	0.53
4:D:121:TYR:HB3	5:E:133:SER:CB	2.36	0.53
4:I:28:SER:O	4:I:29:ALA:HB3	2.08	0.53
1:A:268:LYS:HD2	1:A:268:LYS:O	2.08	0.53
2:G:2:GLN:HB3	2:G:86:THR:HG22	1.90	0.53
2:G:25:CYS:HB2	2:G:39:LEU:HD21	1.91	0.53
4:I:113:ILE:HD11	4:I:140:ASP:OD1	2.09	0.53
5:E:132:PRO:HD2	5:E:203:TRP:CZ2	2.44	0.52
4:D:148:SER:HA	4:D:190:ASN:HD22	1.75	0.52
5:E:37:GLN:OE1	5:E:91:PHE:HE2	1.92	0.52
1:F:203:CYS:SG	1:F:272:LEU:HD22	2.48	0.52
1:F:138:MET:HA	1:F:138:MET:CE	2.40	0.52
1:F:230:LEU:HD13	1:F:245:ALA:HB2	1.92	0.52
1:A:162:GLY:O	1:A:166:GLU:HG3	2.08	0.52
1:F:82[B]:ARG:HD2	1:F:89:GLU:HG2	1.91	0.52
3:H:7:PRO:HB3	3:H:8:ALA:HB3	1.90	0.52
1:A:230:LEU:HD11	1:A:243:LYS:HE3	1.90	0.52
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.45	0.52
5:E:9:ARG:NH1	5:E:109:ALA:HB3	2.25	0.52
2:G:5:PRO:HA	2:G:30:PHE:HB3	1.92	0.52
2:G:98:ASP:O	2:G:99:MET:HG2	2.10	0.52
1:F:93:HIS:HD2	1:F:119:ASP:OD2	1.92	0.51
1:A:182:THR:HB	1:A:265:GLY:HA2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:TRP:CH2	2:B:99:MET:HA	2.44	0.51
4:D:176:TRP:CG	5:E:148:LEU:HD21	2.46	0.51
4:I:111:PRO:HG2	4:I:160:VAL:HG22	1.92	0.51
1:F:253:GLN:O	1:F:256:ARG:HB2	2.10	0.51
5:J:125:PRO:HD3	5:J:216:PHE:CD1	2.45	0.51
1:A:152:VAL:HG22	5:E:97:TRP:CZ3	2.46	0.51
1:A:204:TRP:CE3	1:A:206:LEU:HD21	2.46	0.51
5:E:155:ASP:HB2	5:E:178:PRO:HG2	1.93	0.51
4:D:166:MET:O	4:D:168:PHE:N	2.40	0.51
5:E:175:ASP:OD2	5:E:193:SER:HB3	2.11	0.51
1:F:94:THR:O	1:F:118:TYR:HA	2.11	0.51
2:G:16:GLU:O	2:G:17:ASN:C	2.54	0.51
1:A:45:MET:HG3	1:A:60:TRP:HZ3	1.76	0.51
5:J:137:ILE:O	5:J:141:GLN:HA	2.11	0.51
5:E:61:PRO:O	5:E:62:GLU:HB2	2.11	0.51
1:F:11:SER:HA	1:F:21:ARG:O	2.11	0.51
1:F:37:ASP:HB3	1:F:40:ALA:HB2	1.93	0.50
4:I:9:GLY:HA3	4:I:105:THR:HG23	1.92	0.50
5:E:76:THR:CG2	5:E:78:LYS:HG3	2.40	0.50
1:A:9:PHE:O	1:A:96:GLN:HA	2.11	0.50
1:A:266:LEU:HD12	1:A:266:LEU:O	2.11	0.50
4:I:60:ARG:HA	4:I:77:ARG:NH1	2.25	0.50
1:A:9:PHE:CZ	3:C:2:LEU:HD11	2.46	0.50
1:F:8:PHE:O	1:F:24:ALA:HA	2.12	0.50
1:F:95:VAL:HA	1:F:117:ALA:O	2.11	0.50
5:J:132:PRO:HD2	5:J:203:TRP:CH2	2.47	0.50
1:F:35:ARG:HG2	1:F:48:ARG:CZ	2.41	0.50
1:F:219:ARG:C	1:F:221:GLY:H	2.19	0.50
2:B:9:VAL:HG21	2:B:93:VAL:O	2.12	0.50
4:D:34:MET:HG2	4:D:90:ALA:HB3	1.93	0.50
4:D:125:ASP:OD2	4:D:132:SER:HA	2.11	0.50
1:F:69:ALA:HB1	3:H:6:ASP:CB	2.35	0.50
1:F:78:LEU:HD21	1:F:95:VAL:HG12	1.93	0.50
4:I:8:PRO:HB2	4:I:10:PRO:CD	2.42	0.50
5:J:122:VAL:HA	5:J:153:TYR:O	2.11	0.50
5:J:130:PHE:HD1	5:J:146:VAL:O	1.95	0.50
5:E:181:GLU:C	5:E:183:PRO:HD3	2.37	0.50
1:F:80:THR:HG22	1:F:84:TYR:CZ	2.47	0.50
1:F:192:HIS:CE1	2:G:98:ASP:HB3	2.47	0.50
3:H:7:PRO:CB	3:H:8:ALA:HB3	2.41	0.50
5:J:13:THR:HG21	5:J:19:VAL:CG1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:44:ARG:HA	1:F:64:THR:CG2	2.40	0.49
1:F:228:THR:HG22	1:F:247:VAL:HG23	1.94	0.49
5:J:203:TRP:O	5:J:243:GLY:HA2	2.12	0.49
4:D:119:ALA:HA	4:D:198:PHE:HB3	1.95	0.49
4:D:164:ARG:O	4:D:166:MET:N	2.45	0.49
1:F:191:HIS:HB2	1:F:275:GLU:HG2	1.94	0.49
1:F:274:TRP:O	1:F:275:GLU:CB	2.58	0.49
2:G:31:HIS:ND1	2:G:32:PRO:HA	2.27	0.49
5:J:18:GLN:OE1	5:J:78:LYS:HD3	2.11	0.49
4:D:113:ILE:HD13	4:D:113:ILE:H	1.77	0.49
4:D:168:PHE:CE2	4:D:170:SER:HB3	2.47	0.49
3:C:5:PRO:O	3:C:6:ASP:HB3	2.13	0.49
4:D:67:LYS:O	4:D:70:LYS:HD2	2.13	0.49
4:D:84:SER:HA	4:D:107:LEU:O	2.13	0.49
1:F:143:THR:HG23	3:H:10:ALA:HA	1.95	0.49
2:G:11:SER:HA	2:G:22:PHE:O	2.12	0.49
4:I:113:ILE:O	4:I:113:ILE:HD12	2.13	0.49
5:J:225:TRP:CZ2	5:J:227:GLN:HB2	2.47	0.49
5:J:123:PHE:HD1	5:J:229:ARG:NH2	2.10	0.49
1:F:76:VAL:HG22	5:J:51:ASN:HD21	1.78	0.49
1:F:138:MET:HA	1:F:138:MET:HE2	1.93	0.49
1:F:209:TYR:CD1	1:F:210:PRO:HA	2.48	0.49
2:G:96:ASP:O	2:G:99:MET:HE2	2.12	0.49
1:A:123:TYR:HD2	1:A:124:ILE:HG22	1.78	0.49
1:F:5:MET:HB2	1:F:168:LEU:HD13	1.93	0.49
1:F:129:ASP:O	1:F:131:ARG:HG2	2.13	0.49
1:A:11:SER:HB3	1:A:95:VAL:HG22	1.94	0.49
2:B:29:GLY:HA2	2:B:61:SER:OG	2.13	0.49
2:G:5:PRO:CA	2:G:30:PHE:HB3	2.42	0.49
5:J:13:THR:HG21	5:J:19:VAL:HG12	1.95	0.48
4:D:10:PRO:O	4:D:11:LEU:O	2.31	0.48
1:F:45:MET:HG2	1:F:63:GLU:HB3	1.95	0.48
5:J:47:ILE:HG12	5:J:48:TYR:N	2.29	0.48
1:A:230:LEU:HD13	1:A:245:ALA:HB2	1.95	0.48
4:D:90:ALA:HB1	4:D:99:LEU:HG	1.95	0.48
4:I:10:PRO:O	4:I:11:LEU:C	2.55	0.48
1:F:127:LYS:HD2	1:F:132:SER:HB2	1.95	0.48
2:G:25:CYS:CB	2:G:39:LEU:HD21	2.44	0.48
1:A:187:THR:CG2	1:A:261:VAL:HG21	2.37	0.48
4:D:80:GLN:O	4:D:109:VAL:HG11	2.14	0.48
4:D:138:ASP:H	4:D:170:SER:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:9:PHE:HB2	1:F:97:ARG:HB3	1.95	0.48
1:A:7:TYR:CE2	3:C:2:LEU:HD13	2.48	0.48
4:I:146:SER:H	4:I:191:SER:HB2	1.79	0.48
5:J:132:PRO:CG	5:J:143:ALA:HB1	2.44	0.48
5:J:149:ALA:HB2	5:J:214:VAL:HG21	1.95	0.48
5:E:206:PRO:HA	5:E:243:GLY:C	2.38	0.48
1:A:274:TRP:HE3	1:A:275:GLU:CA	2.26	0.48
1:F:79:GLY:HA2	1:F:82[A]:ARG:NH1	2.28	0.48
1:F:10:THR:O	1:F:22:PHE:HA	2.14	0.48
5:J:145:LEU:HD12	5:J:145:LEU:N	2.29	0.47
1:F:82[A]:ARG:NE	1:F:89:GLU:HG2	2.28	0.47
1:A:127:LYS:HD2	1:A:132:SER:CB	2.40	0.47
1:A:251:SER:HA	1:A:254:GLU:OE2	2.14	0.47
1:A:165:VAL:O	1:A:169:ARG:HG3	2.15	0.47
5:E:29:HIS:HD2	5:E:94:SER:C	2.22	0.47
5:E:192:LEU:HG	5:E:193:SER:H	1.80	0.47
1:A:133:TRP:NE1	1:A:153:ALA:HB2	2.28	0.47
1:A:207:SER:HA	1:A:240:THR:HB	1.96	0.47
1:A:209:TYR:HA	1:A:210:PRO:C	2.39	0.47
1:A:236:ALA:HB3	1:A:238:ASP:OD1	2.14	0.47
5:E:64:ARG:HH21	5:E:85:ARG:HH21	1.62	0.47
1:A:187:THR:HA	1:A:204:TRP:O	2.14	0.47
4:D:60:ARG:HD2	6:D:211:HOH:O	2.14	0.47
1:F:33:PHE:O	1:F:48:ARG:N	2.44	0.47
4:I:135:LEU:HG	4:I:137:THR:HB	1.97	0.47
5:J:33:PHE:HZ	5:J:100:LEU:HD21	1.80	0.47
5:J:108:GLY:C	5:J:110:GLY:H	2.23	0.47
5:J:132:PRO:HB2	5:J:137:ILE:HD11	1.97	0.47
1:F:114:HIS:CD2	1:F:156:LEU:HD11	2.50	0.47
4:I:132:SER:O	4:I:176:TRP:HA	2.15	0.47
5:J:31:TYR:HB2	5:J:95:SER:O	2.15	0.47
1:A:5:MET:O	1:A:100:GLY:HA3	2.14	0.47
1:A:28:VAL:HG23	1:A:33:PHE:CE1	2.50	0.47
5:E:76:THR:O	5:E:76:THR:HG22	2.14	0.47
5:E:129:VAL:HG23	5:E:239:ALA:CB	2.45	0.47
2:G:37:VAL:HB	2:G:66:TYR:CZ	2.49	0.47
4:I:25:TYR:CE1	4:I:70:LYS:HG3	2.50	0.47
4:D:176:TRP:O	4:D:177:SER:HB2	2.15	0.47
1:F:5:MET:HE2	1:F:164:CYS:SG	2.55	0.47
4:D:11:LEU:HD11	4:D:107:LEU:HD13	1.96	0.46
4:D:60:ARG:NH2	4:D:83:ASP:OD2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:58[A]:GLU:CD	1:F:58[A]:GLU:H	2.22	0.46
1:F:74:HIS:CE1	1:F:97:ARG:HE	2.32	0.46
5:J:175:ASP:OD2	5:J:193:SER:HB3	2.15	0.46
5:E:127:VAL:HG13	5:E:147:CYS:SG	2.55	0.46
1:F:227:ASP:HB3	1:F:248:VAL:HB	1.96	0.46
3:H:4:GLY:C	4:I:94:ASP:O	2.58	0.46
5:J:20:THR:HG23	5:J:76:THR:CG2	2.46	0.46
5:J:83:GLU:O	5:J:86:ASP:HB2	2.15	0.46
1:F:85:TYR:HE1	1:F:137:ASP:OD2	1.98	0.46
1:F:96:GLN:O	1:F:116:TYR:HA	2.15	0.46
2:G:27:VAL:HG11	2:G:37:VAL:HG22	1.96	0.46
5:J:123:PHE:CD1	5:J:229:ARG:NH2	2.83	0.46
5:E:29:HIS:HA	5:E:96:LEU:CD2	2.46	0.46
5:E:159:LEU:C	5:E:159:LEU:HD23	2.41	0.46
4:I:19:VAL:HG21	4:I:107:LEU:HD13	1.96	0.46
5:J:63:ASP:O	5:J:64:ARG:HB2	2.16	0.46
2:B:37:VAL:HG22	2:B:82:VAL:HG22	1.97	0.46
4:D:156:THR:HG21	5:E:193:SER:HB3	1.98	0.46
1:F:273:ARG:HG2	1:F:274:TRP:N	2.30	0.46
4:I:111:PRO:CG	4:I:160:VAL:HG22	2.46	0.46
5:E:35:TYR:HE1	5:E:105:GLN:HE22	1.64	0.46
5:J:183:PRO:C	5:J:185:LEU:H	2.22	0.46
5:E:37:GLN:HB2	5:E:43:LEU:HD23	1.98	0.46
5:E:158:GLU:HB2	5:E:215:GLN:HB3	1.96	0.46
4:I:15:GLU:HB2	4:I:110:ARG:O	2.16	0.46
1:A:104:GLY:N	1:A:110:LEU:HG	2.31	0.46
5:J:43:LEU:H	5:J:43:LEU:CD2	2.23	0.46
1:F:28:VAL:HG23	1:F:33:PHE:CD1	2.51	0.45
1:F:177:GLU:CD	1:F:177:GLU:H	2.25	0.45
1:A:14:ARG:HD3	1:A:21:ARG:HB2	1.98	0.45
1:A:202:ARG:HA	1:A:246:ALA:HA	1.98	0.45
5:E:185:LEU:HB3	5:E:187:ASP:OD1	2.16	0.45
1:A:212:GLU:O	1:A:263:HIS:HD2	1.99	0.45
3:C:2:LEU:HD12	3:C:2:LEU:HA	1.73	0.45
4:D:83:ASP:HA	6:D:205:HOH:O	2.15	0.45
5:E:14:GLU:HB2	5:E:119:LEU:HG	1.98	0.45
1:F:167:TRP:CD1	3:H:1:ALA:HB3	2.51	0.45
5:J:100:LEU:HD12	5:J:100:LEU:HA	1.81	0.45
1:F:33:PHE:CD2	1:F:34:VAL:HG13	2.52	0.45
1:F:235:PRO:CG	2:G:65:LEU:HD22	2.45	0.45
5:J:29:HIS:CD2	5:J:94:SER:OG	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:SER:HB3	1:A:78:LEU:HD13	1.99	0.45
4:D:131:LYS:HE2	5:E:150:THR:HG21	1.98	0.45
5:E:95:SER:OG	5:E:100:LEU:HD13	2.16	0.45
1:A:171:TYR:O	1:A:175:GLY:N	2.50	0.45
2:G:4:THR:OG1	2:G:5:PRO:HD2	2.16	0.45
5:J:80:GLN:HB3	5:J:81:PRO:HD2	1.98	0.45
1:A:209:TYR:CD1	1:A:210:PRO:HA	2.52	0.45
5:E:119:LEU:HD13	5:E:219:LEU:HG	1.99	0.45
1:F:1:GLY:O	1:F:105:SER:HA	2.17	0.45
1:A:234:ARG:HD3	2:B:8:GLN:OE1	2.17	0.45
4:D:193:ILE:HD12	4:D:193:ILE:C	2.42	0.45
2:G:29:GLY:HA2	2:G:61:SER:HB2	2.00	0.45
1:A:254:GLU:HG2	1:A:275:GLU:O	2.16	0.44
1:F:116:TYR:HB3	1:F:124:ILE:O	2.17	0.44
1:F:122:ASP:CG	2:G:60:TRP:HE1	2.25	0.44
1:A:24:ALA:O	1:A:35:ARG:HA	2.17	0.44
1:A:74:HIS:HA	1:A:77:ASP:HB2	1.99	0.44
4:I:48:MET:HE2	4:I:56:LYS:O	2.17	0.44
4:I:113:ILE:HG12	4:I:140:ASP:HA	1.98	0.44
5:J:50:ASN:HB3	5:J:55:ILE:HD11	1.98	0.44
5:E:147:CYS:SG	5:E:148:LEU:N	2.91	0.44
1:F:35:ARG:CZ	1:F:48:ARG:HH12	2.30	0.44
4:I:32:TYR:O	4:I:91:MET:HA	2.18	0.44
5:J:60:MET:HE2	5:J:61:PRO:HD2	1.99	0.44
1:A:234:ARG:HD2	2:B:10:TYR:CE1	2.53	0.44
1:A:259:CYS:HB3	1:A:272:LEU:HB2	1.98	0.44
2:G:40:LEU:HD23	2:G:45:ARG:HA	1.98	0.44
5:J:219:LEU:N	5:J:219:LEU:HD12	2.32	0.44
1:A:59:TYR:O	1:A:63:GLU:HG2	2.18	0.44
3:C:5:PRO:HG2	4:D:97:TYR:CE1	2.53	0.44
4:D:48:MET:HE3	4:D:63:ALA:H	1.83	0.44
1:F:35:ARG:HD3	1:F:35:ARG:O	2.17	0.44
4:I:34:MET:HE2	5:J:103:ASN:CB	2.48	0.44
1:A:133:TRP:HB2	1:A:144:LYS:HG3	1.99	0.44
4:I:60:ARG:NH2	4:I:83:ASP:OD2	2.50	0.44
5:E:87:SER:HA	5:E:113:LEU:O	2.18	0.44
5:E:129:VAL:HG12	5:E:130:PHE:N	2.32	0.44
5:E:222:ASN:O	5:E:223:ASP:C	2.60	0.44
2:B:54:LEU:HD11	2:B:62:PHE:HB3	1.99	0.44
4:I:8:PRO:CG	4:I:9:GLY:HA2	2.48	0.44
5:J:140:THR:O	5:J:142:LYS:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:MET:SD	1:A:171:TYR:HE2	2.41	0.44
4:I:110:ARG:HA	4:I:111:PRO:HD3	1.82	0.44
5:J:31:TYR:HA	5:J:49:PHE:O	2.18	0.44
4:D:199:PHE:HD1	4:D:199:PHE:HA	1.70	0.43
4:I:34:MET:HB3	4:I:34:MET:HE3	1.73	0.43
4:I:124:ARG:HH22	5:J:244:ARG:CZ	2.29	0.43
1:A:81:LEU:HD12	1:A:84:TYR:HD2	1.83	0.43
2:G:51:HIS:HA	2:G:65:LEU:O	2.18	0.43
4:I:174:VAL:HG23	5:J:195:ARG:HH21	1.83	0.43
5:J:95:SER:HB3	5:J:100:LEU:HD13	2.00	0.43
5:J:127:VAL:HG21	5:J:237:VAL:O	2.18	0.43
2:B:6:LYS:O	2:B:27:VAL:HA	2.19	0.43
4:D:145:VAL:HA	4:D:191:SER:OG	2.19	0.43
5:E:141:GLN:C	5:E:200:ALA:HB2	2.42	0.43
5:J:11:GLU:HG2	5:J:113:LEU:HD13	2.00	0.43
2:B:5:PRO:CA	2:B:30:PHE:HB3	2.44	0.43
1:F:191:HIS:CG	1:F:275:GLU:HG2	2.53	0.43
1:F:204:TRP:HZ2	2:G:98:ASP:O	2.02	0.43
2:G:29:GLY:HA2	2:G:61:SER:CB	2.48	0.43
4:I:63:ALA:HB1	6:I:208:HOH:O	2.18	0.43
4:D:53:SER:OG	4:D:67:LYS:HB2	2.18	0.43
1:F:227:ASP:O	1:F:247:VAL:HA	2.19	0.43
2:B:70:PHE:CZ	2:B:72:PRO:HG3	2.54	0.43
5:E:152:PHE:CE2	5:E:190:TYR:HB2	2.54	0.43
1:F:228:THR:HA	1:F:246:ALA:O	2.18	0.43
5:J:151:GLY:HA3	5:J:189:ARG:NH1	2.33	0.43
1:A:106:ASP:OD1	1:A:108:ARG:HB2	2.19	0.43
4:D:19:VAL:CG1	4:D:76:ILE:HB	2.45	0.43
4:D:174:VAL:HG23	5:E:195:ARG:NH2	2.34	0.43
4:D:176:TRP:CZ3	5:E:148:LEU:HD11	2.54	0.43
5:E:118:ASP:CG	5:E:120:LYS:HG2	2.44	0.43
5:J:102:LYS:HB2	5:J:104:ILE:HG12	1.99	0.43
5:J:140:THR:O	5:J:141:GLN:HG2	2.18	0.43
1:A:42:SER:OG	1:A:44:ARG:HB2	2.18	0.43
4:I:110:ARG:HD3	4:I:158:LYS:NZ	2.34	0.43
5:J:61:PRO:HG2	5:J:65:PHE:CG	2.54	0.43
1:A:142:THR:O	1:A:146:LYS:HB2	2.19	0.43
1:A:176:LYS:HG3	1:A:177:GLU:N	2.34	0.43
1:F:13:SER:HB3	1:F:78:LEU:HD22	2.01	0.43
2:G:53:ASP:O	2:G:54:LEU:C	2.62	0.43
4:I:54:GLY:H	4:I:65:VAL:HG13	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:119:ALA:CB	4:I:198:PHE:HB3	2.49	0.43
5:E:3:GLY:O	5:E:5:ILE:HD12	2.19	0.43
5:E:9:ARG:HH12	5:E:109:ALA:HB3	1.84	0.43
1:F:201:LEU:HB2	1:F:247:VAL:HG12	2.01	0.43
1:F:273:ARG:O	1:F:274:TRP:CB	2.67	0.43
2:G:36:GLU:O	2:G:82:VAL:HA	2.19	0.43
1:A:49:ALA:O	1:A:52:ILE:HG22	2.20	0.42
4:D:47:LEU:HD11	4:D:87:TYR:HE1	1.83	0.42
1:F:64:THR:O	1:F:67:VAL:HG12	2.18	0.42
5:J:194:SER:C	5:J:195:ARG:HG3	2.44	0.42
1:A:19:GLU:HG2	1:A:75:ARG:CZ	2.49	0.42
5:E:22:ARG:HB3	1:F:16:GLY:O	2.19	0.42
1:F:184:ALA:HA	1:F:185:PRO:HD3	1.90	0.42
2:G:70:PHE:HD2	2:G:78:TYR:CZ	2.38	0.42
5:J:225:TRP:NE1	5:J:227:GLN:HB2	2.33	0.42
4:D:86:THR:OG1	4:D:106:ARG:HG2	2.19	0.42
1:F:201:LEU:O	1:F:246:ALA:HA	2.18	0.42
2:G:33:SER:HB3	2:G:62:PHE:CZ	2.54	0.42
4:I:35:TRP:CH2	4:I:89:CYS:HB3	2.54	0.42
5:J:158:GLU:CD	5:J:217:TYR:HE1	2.27	0.42
1:F:109:PHE:HB2	1:F:165:VAL:HG21	2.02	0.42
2:G:70:PHE:CZ	2:G:72:PRO:HG3	2.54	0.42
1:A:157:ARG:C	1:A:157:ARG:HD3	2.45	0.42
5:E:157:VAL:HA	5:E:215:GLN:O	2.19	0.42
1:F:28:VAL:HG23	1:F:33:PHE:CE1	2.53	0.42
1:F:78:LEU:CD2	1:F:95:VAL:HG12	2.49	0.42
1:F:98:MET:SD	1:F:98:MET:C	3.02	0.42
2:G:41:LYS:HG2	2:G:42:ASN:ND2	2.35	0.42
4:I:164:ARG:O	4:I:166:MET:N	2.53	0.42
5:J:15:MET:CE	5:J:117:GLU:HA	2.50	0.42
4:D:98:LYS:HG3	5:E:45:LEU:HD23	2.00	0.42
5:E:96:LEU:O	5:E:100:LEU:HB2	2.20	0.42
5:E:112:ARG:HB3	5:E:156:HIS:CE1	2.55	0.42
4:I:35:TRP:CZ3	4:I:89:CYS:HB3	2.55	0.42
1:A:159:TYR:CD1	1:A:163:THR:HB	2.55	0.42
4:D:10:PRO:HB3	4:D:106:ARG:HH12	1.82	0.42
4:D:34:MET:HE2	5:E:103:ASN:CB	2.50	0.42
1:F:217:TRP:HE1	1:F:245:ALA:C	2.26	0.42
2:G:96:ASP:CG	2:G:99:MET:H	2.28	0.42
4:I:46:LEU:CD2	5:J:104:ILE:HD13	2.43	0.42
4:I:49:TYR:O	4:I:49:TYR:CG	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:TRP:O	1:A:170:ARG:HB3	2.20	0.42
2:B:4:THR:HA	2:B:86:THR:OG1	2.20	0.42
5:E:182:GLN:HB3	5:E:185:LEU:HD12	2.01	0.42
1:F:77:ASP:O	1:F:81:LEU:HD13	2.20	0.42
1:F:219:ARG:O	1:F:220:ASP:HB2	2.20	0.42
5:J:48:TYR:CE1	5:J:55:ILE:HB	2.55	0.42
5:E:178:PRO:HB2	5:E:190:TYR:HB3	2.02	0.42
1:F:34:VAL:HA	1:F:46:GLU:O	2.20	0.42
1:F:99:TYR:HA	1:F:113:TYR:O	2.20	0.42
3:H:4:GLY:HA2	3:H:5:PRO:C	2.44	0.42
4:I:33:PHE:CD1	4:I:72:ILE:CD1	3.02	0.42
5:J:61:PRO:HG2	5:J:65:PHE:CD1	2.54	0.42
5:J:235:GLN:HE21	5:J:237:VAL:HG22	1.84	0.42
1:A:52:ILE:HD12	1:A:52:ILE:HA	1.92	0.42
5:J:91:PHE:HB3	5:J:107:PHE:HD1	1.85	0.42
5:E:24:LYS:HE3	1:F:89:GLU:HB3	2.02	0.41
1:F:59:TYR:O	1:F:63:GLU:HG2	2.20	0.41
1:F:156:LEU:HD23	1:F:156:LEU:HA	1.89	0.41
5:J:142:LYS:HZ2	5:J:142:LYS:HB3	1.84	0.41
5:J:146:VAL:HG22	5:J:195:ARG:HG2	2.01	0.41
4:D:10:PRO:HA	4:D:106:ARG:HB2	2.01	0.41
4:D:84:SER:O	4:D:85:ALA:HB2	2.21	0.41
5:E:60:MET:HE2	5:E:61:PRO:CD	2.50	0.41
5:E:144:THR:HA	5:E:196:LEU:O	2.20	0.41
5:E:185:LEU:C	5:E:187:ASP:H	2.28	0.41
2:B:51:HIS:HA	2:B:65:LEU:O	2.20	0.41
4:D:48:MET:HE3	4:D:63:ALA:N	2.35	0.41
4:D:61:PHE:HA	4:D:75:PHE:O	2.19	0.41
1:F:97:ARG:HA	1:F:115:GLN:O	2.20	0.41
2:G:23:LEU:HD22	2:G:78:TYR:CD1	2.56	0.41
5:E:29:HIS:HA	5:E:96:LEU:HD21	2.02	0.41
1:F:163:THR:O	1:F:167:TRP:HD1	2.03	0.41
4:I:35:TRP:CD2	4:I:74:LEU:HB2	2.55	0.41
5:J:68:LYS:HB2	5:J:68:LYS:HE2	1.79	0.41
5:J:132:PRO:HG2	5:J:143:ALA:HB1	2.02	0.41
1:A:153:ALA:O	1:A:157:ARG:HB2	2.21	0.41
2:B:40:LEU:HD23	2:B:45:ARG:HA	2.01	0.41
5:E:36:ARG:HG2	5:E:46:LEU:HD21	2.02	0.41
2:G:6:LYS:O	2:G:27:VAL:HA	2.20	0.41
5:J:161:TRP:CD1	5:J:172:VAL:HG13	2.55	0.41
1:A:236:ALA:HB2	6:A:279:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:179:LEU:HD23	5:E:191:ALA:O	2.21	0.41
5:E:209:HIS:HE1	5:E:240:GLU:HB2	1.85	0.41
1:F:43:GLN:O	1:F:68:LYS:HE2	2.20	0.41
2:G:54:LEU:HD11	2:G:62:PHE:CD1	2.56	0.41
4:I:38:GLN:NE2	5:J:37:GLN:OE1	2.53	0.41
5:J:15:MET:HE3	5:J:117:GLU:HA	2.02	0.41
5:J:61:PRO:O	5:J:62:GLU:CB	2.67	0.41
5:J:66:SER:O	5:J:77:LEU:HD12	2.20	0.41
5:J:96:LEU:HD13	5:J:98:GLU:OE1	2.20	0.41
1:A:178:THR:O	1:A:181:ARG:HG2	2.21	0.41
1:A:209:TYR:CG	1:A:210:PRO:HA	2.55	0.41
2:B:32:PRO:HD2	2:B:85:VAL:HG11	2.03	0.41
3:C:7:PRO:HB3	3:C:8:ALA:O	2.19	0.41
4:D:28:SER:O	4:D:29:ALA:CB	2.69	0.41
1:F:44:ARG:HD2	1:F:64:THR:HG21	2.01	0.41
1:F:98:MET:O	1:F:114:HIS:HA	2.21	0.41
4:I:28:SER:C	4:I:30:PHE:H	2.28	0.41
4:I:120:VAL:HG12	4:I:184:CYS:HB3	2.03	0.41
4:D:25:TYR:CZ	4:D:70:LYS:HG3	2.56	0.41
5:E:60:MET:C	5:E:62:GLU:H	2.29	0.41
5:E:137:ILE:HD13	5:E:203:TRP:CD1	2.56	0.41
1:F:191:HIS:ND1	1:F:275:GLU:HG2	2.36	0.41
1:F:197:HIS:ND1	1:F:198:GLU:HG3	2.35	0.41
1:A:81:LEU:HD12	1:A:84:TYR:CD2	2.56	0.41
1:A:106:ASP:C	1:A:108:ARG:H	2.29	0.41
2:B:28:SER:HA	2:B:63:TYR:HA	2.03	0.41
2:B:54:LEU:HD11	2:B:62:PHE:CD1	2.56	0.41
4:D:85:ALA:O	4:D:107:LEU:N	2.54	0.41
4:D:88:LEU:HD23	4:D:104:GLY:CA	2.51	0.41
4:D:137:THR:HA	4:D:171:ASN:O	2.21	0.41
5:E:6:GLN:CD	5:E:92:CYS:H	2.29	0.41
1:F:28:VAL:O	1:F:29:ASP:HB2	2.21	0.41
1:F:31:THR:HG22	1:F:209:TYR:OH	2.21	0.41
1:F:65[B]:ARG:HH11	5:J:56:ASP:HA	1.85	0.41
2:G:25:CYS:HB2	2:G:39:LEU:CD2	2.51	0.41
2:G:96:ASP:HB3	2:G:99:MET:HA	2.03	0.41
4:I:14:PRO:HG3	4:I:110:ARG:HH12	1.85	0.41
4:I:163:MET:HG2	5:J:171:GLY:HA2	2.02	0.41
5:J:182:GLN:HA	5:J:183:PRO:HD2	1.94	0.41
5:E:137:ILE:O	5:E:141:GLN:HA	2.20	0.41
4:D:113:ILE:N	4:D:113:ILE:CD1	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:19:VAL:HG13	5:E:82:SER:HB3	2.03	0.40
1:F:36:PHE:HB3	1:F:67:VAL:HG21	2.03	0.40
1:F:117:ALA:HB2	2:G:60:TRP:CD2	2.55	0.40
4:I:4:VAL:HG21	4:I:89:CYS:SG	2.61	0.40
5:J:60:MET:HA	5:J:61:PRO:HD3	1.87	0.40
1:A:189:MET:HE3	1:A:189:MET:HB2	1.93	0.40
1:F:82[B]:ARG:CD	1:F:89:GLU:HG2	2.52	0.40
2:G:2:GLN:HB3	2:G:86:THR:CG2	2.50	0.40
5:J:125:PRO:HA	5:J:152:PHE:HB3	2.03	0.40
5:J:125:PRO:CD	5:J:216:PHE:HB2	2.51	0.40
1:A:216:THR:HB	1:A:260:HIS:HB2	2.03	0.40
4:D:44:PRO:HD2	5:E:107:PHE:CG	2.56	0.40
5:E:148:LEU:O	5:E:150:THR:HG23	2.22	0.40
5:E:159:LEU:HD23	5:E:160:SER:N	2.35	0.40
5:E:166:LYS:HB3	5:E:166:LYS:HE3	1.88	0.40
2:G:5:PRO:HB3	2:G:30:PHE:HB3	2.04	0.40
1:A:185:PRO:HA	1:A:208:PHE:HB3	2.01	0.40
1:F:162:GLY:O	1:F:166:GLU:HG3	2.22	0.40
1:F:236:ALA:HB1	2:G:12:ARG:HG3	2.02	0.40
2:G:17:ASN:HA	2:G:72:PRO:O	2.21	0.40
4:I:60:ARG:HA	4:I:77:ARG:HH12	1.86	0.40
5:J:155:ASP:HB2	5:J:178:PRO:CG	2.43	0.40
1:A:28:VAL:HG11	1:A:179:LEU:HD13	2.04	0.40
1:A:218:GLN:HG2	1:A:223:ASP:HA	2.03	0.40
4:D:198:PHE:CG	4:D:199:PHE:N	2.90	0.40
5:E:100:LEU:HD12	5:E:100:LEU:HA	1.84	0.40
5:E:219:LEU:N	5:E:219:LEU:HD12	2.36	0.40
4:I:152:ASP:HB3	4:I:179:LYS:HD2	2.03	0.40
5:J:38:THR:HG22	6:J:257:HOH:O	2.22	0.40
5:J:68:LYS:HD3	5:J:68:LYS:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	274/275 (100%)	251 (92%)	21 (8%)	2 (1%)	18	38
1	F	276/275 (100%)	259 (94%)	13 (5%)	4 (1%)	9	19
2	B	98/100 (98%)	90 (92%)	8 (8%)	0	100	100
2	G	98/100 (98%)	91 (93%)	6 (6%)	1 (1%)	12	28
3	C	8/10 (80%)	6 (75%)	1 (12%)	1 (12%)	0	0
3	H	8/10 (80%)	6 (75%)	1 (12%)	1 (12%)	0	0
4	D	197/199 (99%)	160 (81%)	26 (13%)	11 (6%)	1	1
4	I	197/199 (99%)	165 (84%)	27 (14%)	5 (2%)	4	8
5	E	242/245 (99%)	217 (90%)	22 (9%)	3 (1%)	10	23
5	J	243/245 (99%)	220 (90%)	20 (8%)	3 (1%)	10	23
All	All	1641/1658 (99%)	1465 (89%)	145 (9%)	31 (2%)	6	13

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	11	LEU
4	D	82	SER
5	E	81	PRO
5	J	81	PRO
1	A	18	GLY
1	A	274	TRP
4	D	27	ASN
4	D	28	SER
4	D	165	SER
4	D	167	ASP
5	E	222	ASN
1	F	274	TRP
3	H	8	ALA
4	I	11	LEU
4	I	28	SER
4	I	167	ASP
4	D	9	GLY
4	D	147	GLN
4	I	165	SER
4	D	94	ASP
5	E	148	LEU
1	F	18	GLY

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Mol	Chain	Res	Type
4	I	95	SER
5	J	18	GLN
5	J	141	GLN
4	D	83	ASP
1	F	136	ALA
2	G	17	ASN
3	C	6	ASP
1	F	252	GLY
4	D	192	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/231 (100%)	221 (95%)	11 (5%)	23	48
1	F	234/231 (101%)	225 (96%)	9 (4%)	29	56
2	B	95/95 (100%)	92 (97%)	3 (3%)	34	62
2	G	95/95 (100%)	92 (97%)	3 (3%)	34	62
3	C	5/5 (100%)	4 (80%)	1 (20%)	1	2
3	H	5/5 (100%)	5 (100%)	0	100	100
4	D	180/180 (100%)	171 (95%)	9 (5%)	22	46
4	I	180/180 (100%)	172 (96%)	8 (4%)	25	50
5	E	215/215 (100%)	206 (96%)	9 (4%)	26	52
5	J	215/215 (100%)	207 (96%)	8 (4%)	30	57
All	All	1456/1452 (100%)	1395 (96%)	61 (4%)	26	52

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	31	THR
1	A	35	ARG
1	A	58	GLU

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Mol	Chain	Res	Type
1	A	64	THR
1	A	81	LEU
1	A	164	CYS
1	A	197	HIS
1	A	268	LYS
1	A	270	LEU
1	A	274	TRP
2	B	11	SER
2	B	57	SER
2	B	70	PHE
3	C	2	LEU
4	D	4	VAL
4	D	11	LEU
4	D	19	VAL
4	D	34	MET
4	D	56	LYS
4	D	65	VAL
4	D	113	ILE
4	D	164	ARG
4	D	199	PHE
5	E	19	VAL
5	E	60	MET
5	E	76	THR
5	E	100	LEU
5	E	126	GLU
5	E	141	GLN
5	E	187	ASP
5	E	195	ARG
5	E	201	THR
1	F	19	GLU
1	F	35	ARG
1	F	95	VAL
1	F	110	LEU
1	F	138	MET
1	F	264	GLU
1	F	270	LEU
1	F	272	LEU
1	F	275	GLU
2	G	6	LYS
2	G	58	LYS
2	G	70	PHE
4	I	4	VAL

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Mol	Chain	Res	Type
4	I	24	THR
4	I	65	VAL
4	I	99	LEU
4	I	109	VAL
4	I	160	VAL
4	I	161	LEU
4	I	164	ARG
5	J	43	LEU
5	J	53	VAL
5	J	60	MET
5	J	68	LYS
5	J	80	GLN
5	J	100	LEU
5	J	141	GLN
5	J	166	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	86	ASN
1	A	155	GLN
1	A	260	HIS
1	A	262	GLN
4	D	64	GLN
4	D	122	GLN
4	D	190	ASN
5	E	10	HIS
5	E	29	HIS
5	E	51	ASN
5	E	105	GLN
5	E	156	HIS
5	E	209	HIS
5	E	215	GLN
5	E	227	GLN
1	F	93	HIS
1	F	155	GLN
1	F	260	HIS
4	I	122	GLN
4	I	142	GLN
5	J	29	HIS
5	J	156	HIS

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Mol	Chain	Res	Type
5	J	209	HIS
5	J	222	ASN
5	J	235	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	275/275 (100%)	0.00	5 (1%) 67 63	18, 52, 97, 132	1 (0%)
1	F	275/275 (100%)	-0.29	1 (0%) 88 86	13, 46, 82, 98	3 (1%)
2	B	100/100 (100%)	-0.17	1 (1%) 79 76	24, 51, 86, 102	0
2	G	100/100 (100%)	-0.29	0 100 100	19, 41, 76, 87	0
3	C	10/10 (100%)	0.34	1 (10%) 12 9	26, 42, 59, 60	0
3	H	10/10 (100%)	-0.21	0 100 100	25, 38, 40, 43	0
4	D	199/199 (100%)	0.41	10 (5%) 34 28	26, 75, 140, 184	0
4	I	199/199 (100%)	0.54	13 (6%) 25 19	25, 77, 144, 183	0
5	E	244/245 (99%)	0.06	6 (2%) 58 52	21, 56, 111, 146	0
5	J	245/245 (100%)	0.05	2 (0%) 82 80	24, 58, 112, 148	0
All	All	1657/1658 (99%)	0.06	39 (2%) 59 54	13, 55, 120, 184	4 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	I	160	VAL	4.7
4	D	81	PRO	4.1
5	E	138	SER	3.7
4	I	169	LYS	3.3
5	E	185	LEU	3.2
4	D	129	SER	3.2
4	I	8	PRO	3.0
1	A	274	TRP	3.0
4	D	185	ALA	2.9
5	J	245	ALA	2.9
5	J	229	ARG	2.8
4	I	7	ASP	2.8
5	E	184	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
4	I	41	ARG	2.8
3	C	8	ALA	2.7
1	A	18	GLY	2.7
1	A	193	ALA	2.7
4	D	131	LYS	2.5
4	I	131	LYS	2.5
4	D	51	TYR	2.4
4	I	123	LEU	2.4
4	I	200	PRO	2.4
4	I	133	VAL	2.4
1	A	275	GLU	2.3
2	B	99	MET	2.3
4	I	171	ASN	2.3
4	D	199	PHE	2.3
4	D	171	ASN	2.2
4	I	196	ASP	2.2
4	D	201	SER	2.2
4	I	163	MET	2.1
5	E	129	VAL	2.1
5	E	187	ASP	2.1
4	D	124	ARG	2.1
1	A	134	THR	2.1
1	F	16	GLY	2.1
4	D	182	PHE	2.1
5	E	203	TRP	2.0
4	I	135	LEU	2.0

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

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

6.3 Carbohydrates [\(i\)](#)

There are no oligosaccharides in this entry.

6.4 Ligands [\(i\)](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.