Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 11:34 PM EDT

PDB ID	:	2B2X
Title	:	VLA1 RdeltaH I-domain complexed with a quadruple mutant of the AQC2 Fab
Authors	:	Clark, L.A.; Boriack-Sjodin, P.A.; Eldredge, J.; Fitch, C.; Friedman, B.; Hanf, K.J.; Jarpe, M.; Liparoto, S.F.; Li, Y.; Lugovskoy, A.
Deposited on	:	2005-09-19
Resolution	:	2.20 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:

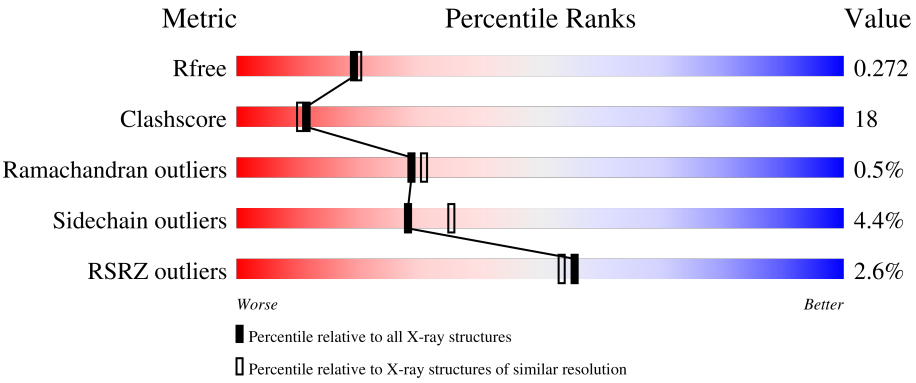
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	223	4% 48% 33% · 16%
1	B	223	6% 48% 29% · 21%
2	H	226	72% 21% 7%
2	I	226	72% 18% · 7%
3	L	213	2% 67% 28% · ·

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Mol	Chain	Length	Quality of chain
3	M	213	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9537 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 Integrin alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	0	0
			1490	940	258	288	4			
1	B	176	Total	C	N	O	S	0	0	0
			1397	884	240	270	3			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	125	GLY	-	cloning artifact	UNP P18614
A	126	SER	-	cloning artifact	UNP P18614
A	217	VAL	GLY	engineered mutation	UNP P18614
A	218	GLN	ARG	engineered mutation	UNP P18614
A	219	ARG	GLN	engineered mutation	UNP P18614
A	222	ARG	LEU	engineered mutation	UNP P18614
A	341	LEU	-	cloning artifact	UNP P18614
A	342	GLU	-	cloning artifact	UNP P18614
A	343	ARG	-	cloning artifact	UNP P18614
A	344	PRO	-	cloning artifact	UNP P18614
A	345	HIS	-	cloning artifact	UNP P18614
A	346	ARG	-	cloning artifact	UNP P18614
A	347	ASP	-	cloning artifact	UNP P18614
B	125	GLY	-	cloning artifact	UNP P18614
B	126	SER	-	cloning artifact	UNP P18614
B	217	VAL	GLY	engineered mutation	UNP P18614
B	218	GLN	ARG	engineered mutation	UNP P18614
B	219	ARG	GLN	engineered mutation	UNP P18614
B	222	ARG	LEU	engineered mutation	UNP P18614
B	341	LEU	-	cloning artifact	UNP P18614
B	342	GLU	-	cloning artifact	UNP P18614
B	343	ARG	-	cloning artifact	UNP P18614
B	344	PRO	-	cloning artifact	UNP P18614
B	345	HIS	-	cloning artifact	UNP P18614
B	346	ARG	-	cloning artifact	UNP P18614

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Chain	Residue	Modelled	Actual	Comment	Reference
B	347	ASP	-	cloning artifact	UNP P18614

- Molecule 2 is a protein called Antibody AQC2 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	210	Total	C	N	O	S	0	0	0
			1575	1000	260	308	7			
2	I	210	Total	C	N	O	S	0	0	0
			1575	1000	260	308	7			

- Molecule 3 is a protein called Antibody AQC2 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	210	Total	C	N	O	S	0	0	0
			1636	1026	274	330	6			
3	M	210	Total	C	N	O	S	0	0	0
			1636	1026	274	330	6			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

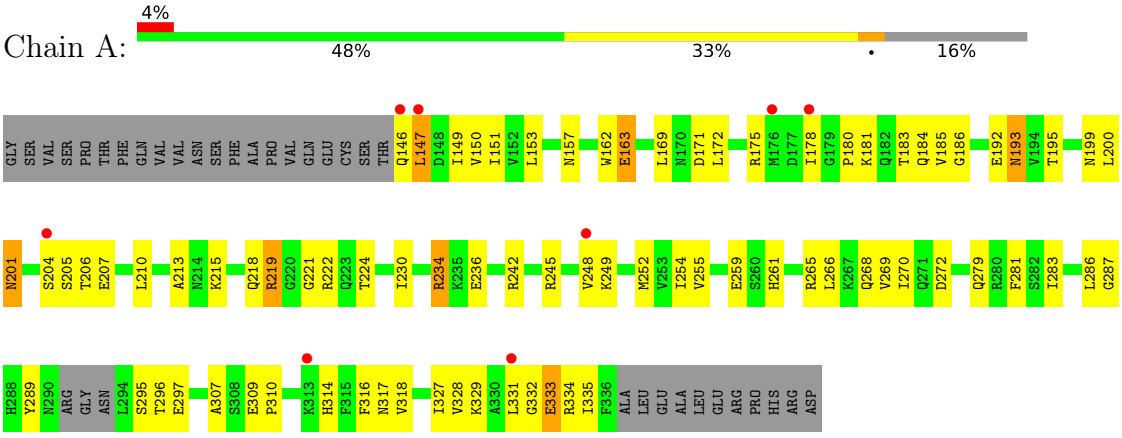
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	13	Total	O	0	0
			13	13		
5	H	73	Total	O	0	0
			73	73		
5	L	30	Total	O	0	0
			30	30		
5	B	5	Total	O	0	0
			5	5		
5	I	77	Total	O	0	0
			77	77		
5	M	28	Total	O	0	0
			28	28		

3 Residue-property plots (i)

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.

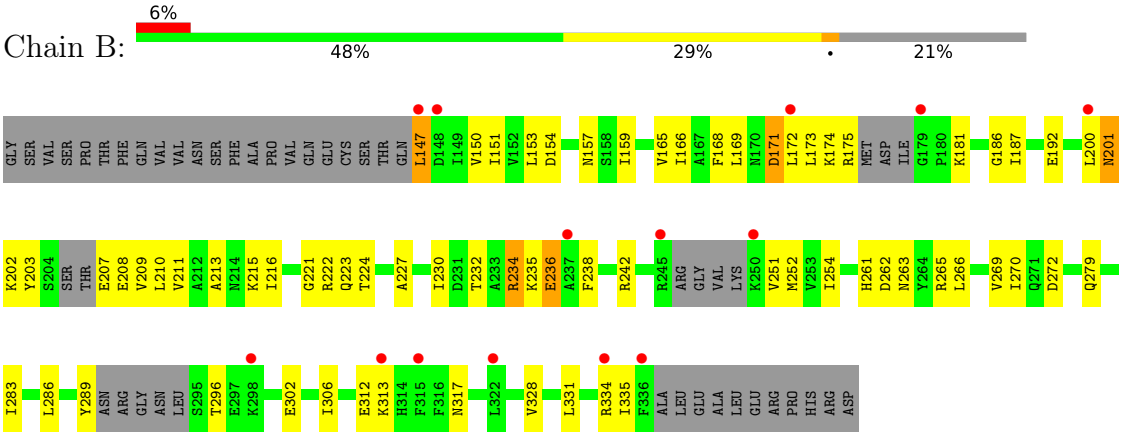
• Molecule 1: Integrin alpha-1

Chain A:



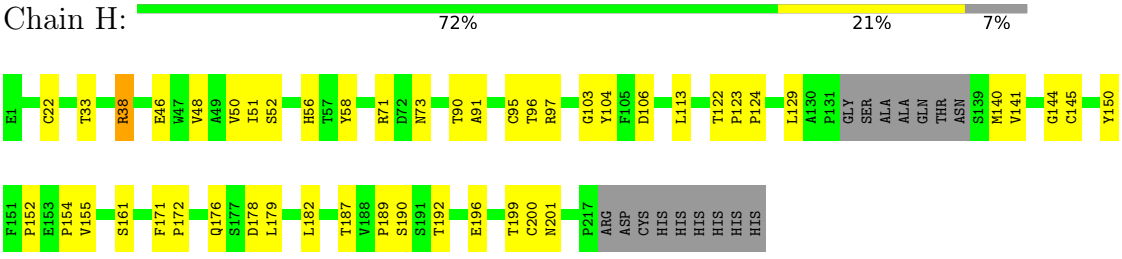
• Molecule 1: Integrin alpha-1

Chain B:



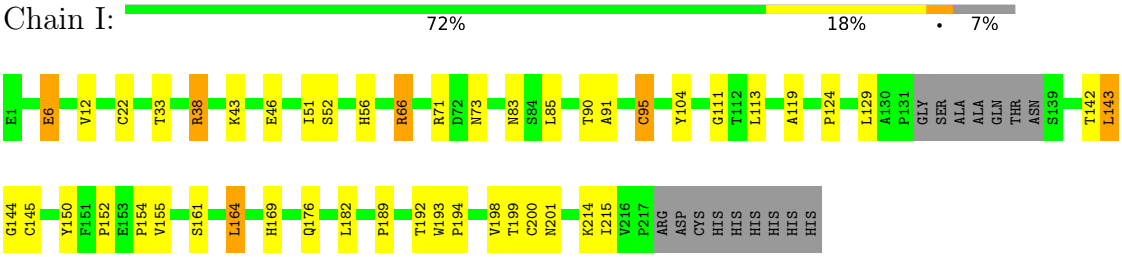
• Molecule 2: Antibody AQC2 Fab

Chain H:



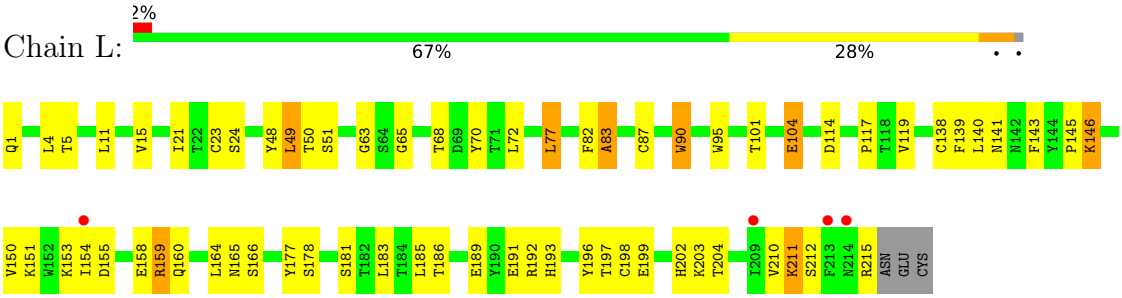
• Molecule 2: Antibody AQC2 Fab

Chain I:



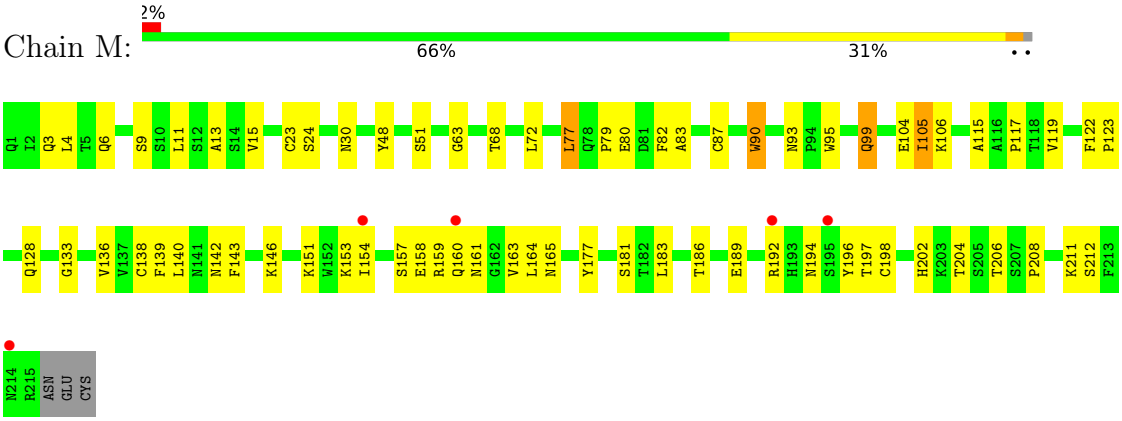
• Molecule 3: Antibody AQC2 Fab

Chain L:



• Molecule 3: Antibody AQC2 Fab

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	106.12Å 43.68Å 153.88Å 90.00° 104.10° 90.00°	Depositor
Resolution (Å)	35.00 – 2.20 49.75 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.3 (35.00-2.20) 94.2 (49.75-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.04 (at 2.20Å)	Xtriage
Refinement program	CNS, CNX	Depositor
R, R_{free}	0.238 , 0.272 0.238 , 0.272	Depositor DCC
R_{free} test set	3380 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	38.6	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9537	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.80 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7301e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.28	0/1510	0.56	0/2036
1	B	0.27	0/1414	0.55	0/1903
2	H	0.39	0/1616	0.71	0/2208
2	I	0.37	0/1616	0.70	0/2208
3	L	0.35	0/1680	0.63	0/2288
3	M	0.33	0/1680	0.61	0/2288
All	All	0.34	0/9516	0.63	0/12931

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1490	0	1497	67	0
1	B	1397	0	1395	75	0
2	H	1575	0	1537	39	0
2	I	1575	0	1537	38	0
3	L	1636	0	1561	53	0
3	M	1636	0	1561	56	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	13	0	0	0	0
5	B	5	0	0	0	0
5	H	73	0	0	0	0
5	I	77	0	0	1	0
5	L	30	0	0	1	0
5	M	28	0	0	0	0
All	All	9537	0	9088	315	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 18.

All (315) 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)
3:L:191:GLU:HA	3:L:215:ARG:HH12	1.25	0.98
1:B:234:ARG:HH11	1:B:234:ARG:HB3	1.27	0.97
2:H:161:SER:H	2:H:201:ASN:HD21	1.00	0.95
2:I:161:SER:H	2:I:201:ASN:HD21	1.08	0.94
3:M:6:GLN:H	3:M:99:GLN:NE2	1.64	0.94
3:M:6:GLN:N	3:M:99:GLN:HE22	1.69	0.91
3:M:23:CYS:HG	3:M:87:CYS:HG	1.03	0.91
1:B:286:LEU:HD11	1:B:317:ASN:HD21	1.36	0.89
2:H:140:MET:HG2	2:H:189:PRO:HA	1.55	0.89
1:B:224:THR:H	1:B:261:HIS:CD2	1.92	0.87
3:L:23:CYS:HG	3:L:87:CYS:HG	0.94	0.85
3:L:138:CYS:HG	3:L:198:CYS:HG	1.00	0.85
2:I:38:ARG:HD2	2:I:46:GLU:OE1	1.79	0.83
3:M:6:GLN:H	3:M:99:GLN:HE22	0.84	0.82
2:H:161:SER:H	2:H:201:ASN:ND2	1.78	0.81
1:B:224:THR:H	1:B:261:HIS:HD2	1.30	0.79
3:M:138:CYS:HG	3:M:198:CYS:HG	0.82	0.79
3:L:159:ARG:HG3	3:L:159:ARG:HH11	1.48	0.79
2:I:161:SER:H	2:I:201:ASN:ND2	1.82	0.76
1:A:224:THR:H	1:A:261:HIS:CD2	2.03	0.76
1:B:174:LYS:NZ	1:B:175:ARG:HH12	1.83	0.76
1:A:224:THR:H	1:A:261:HIS:HD2	1.32	0.76
1:A:181:LYS:HE2	1:A:181:LYS:HA	1.68	0.75
1:A:234:ARG:HE	1:A:272:ASP:HB3	1.50	0.75
1:A:157:ASN:HB3	2:H:33:THR:HG21	1.69	0.75
1:A:195:THR:HG21	1:A:219:ARG:HE	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:38:ARG:HD2	2:H:46:GLU:OE1	1.88	0.73
2:H:71:ARG:HD3	2:H:73:ASN:HD21	1.56	0.71
1:A:327:ILE:HG22	1:A:331:LEU:HB2	1.72	0.71
3:M:159:ARG:HD2	3:M:161:ASN:OD1	1.91	0.71
3:L:191:GLU:HA	3:L:215:ARG:NH1	2.05	0.70
2:H:22:CYS:HG	2:H:95:CYS:CB	2.04	0.69
1:B:234:ARG:HB3	1:B:234:ARG:NH1	2.07	0.68
1:B:251:VAL:HG11	1:B:335:ILE:HD11	1.74	0.68
3:L:104:GLU:HG3	3:L:177:TYR:OH	1.92	0.68
1:B:166:ILE:HD11	1:B:216:ILE:O	1.93	0.68
2:H:161:SER:N	2:H:201:ASN:HD21	1.84	0.68
1:B:266:LEU:O	1:B:270:ILE:HG12	1.95	0.67
2:H:145:CYS:CB	2:H:200:CYS:HG	2.07	0.67
2:I:145:CYS:HG	2:I:200:CYS:CB	2.08	0.66
1:B:252:MET:HG2	1:B:254:ILE:HD11	1.77	0.66
1:A:171:ASP:OD2	1:A:328:VAL:HG21	1.96	0.66
2:I:176:GLN:OE1	3:M:164:LEU:HD11	1.96	0.65
3:L:153:LYS:HB3	3:L:197:THR:HG23	1.78	0.65
1:A:236:GLU:O	1:A:242:ARG:HD2	1.97	0.65
2:H:189:PRO:HG2	2:H:192:THR:OG1	1.97	0.65
3:M:104:GLU:HG2	3:M:105:ILE:N	2.09	0.65
2:I:71:ARG:HD3	2:I:73:ASN:HD21	1.61	0.64
1:B:174:LYS:HZ1	1:B:175:ARG:HH12	1.45	0.64
3:M:153:LYS:HB3	3:M:197:THR:HG22	1.80	0.64
3:L:146:LYS:HB3	3:L:177:TYR:CD2	2.32	0.64
3:L:5:THR:HG23	5:L:226:HOH:O	1.97	0.63
1:A:192:GLU:HG3	1:A:221:GLY:HA2	1.81	0.63
2:I:22:CYS:HG	2:I:95:CYS:HG	1.06	0.63
3:L:21:ILE:HD12	3:L:101:THR:HG21	1.80	0.62
1:B:157:ASN:ND2	1:B:221:GLY:H	1.97	0.62
3:L:141:ASN:HD22	3:L:178:SER:HB3	1.63	0.62
3:L:154:ILE:O	3:L:154:ILE:HG13	1.98	0.62
1:B:313:LYS:HZ3	1:B:334:ARG:HD3	1.64	0.62
2:I:71:ARG:HD3	2:I:73:ASN:ND2	2.15	0.62
1:A:249:LYS:CE	1:A:279:GLN:HG2	2.30	0.62
1:B:236:GLU:O	1:B:242:ARG:HD2	2.00	0.62
2:I:22:CYS:HG	2:I:95:CYS:CB	2.13	0.62
1:B:289:TYR:CB	1:B:296:THR:HG22	2.29	0.62
1:A:195:THR:HG21	1:A:219:ARG:NE	2.15	0.61
1:B:254:ILE:HD12	1:B:254:ILE:N	2.16	0.61
1:B:207:GLU:HG3	1:B:208:GLU:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:71:ARG:HD3	2:H:73:ASN:ND2	2.14	0.60
1:B:312:GLU:HG3	1:B:313:LYS:HG2	1.83	0.60
2:H:182:LEU:HD12	2:H:182:LEU:C	2.21	0.60
2:H:71:ARG:CD	2:H:73:ASN:HD21	2.15	0.60
2:I:182:LEU:C	2:I:182:LEU:HD12	2.22	0.60
1:A:153:LEU:HD21	1:A:169:LEU:HD11	1.85	0.59
1:A:266:LEU:O	1:A:270:ILE:HG12	2.02	0.59
3:L:159:ARG:HG3	3:L:159:ARG:NH1	2.16	0.59
1:B:263:ASN:HB3	3:M:30:ASN:HD22	1.66	0.59
1:A:318:VAL:HG13	1:A:327:ILE:HD11	1.84	0.59
1:B:192:GLU:HG3	1:B:221:GLY:HA2	1.84	0.59
1:A:147:LEU:HA	1:A:248:VAL:HG12	1.85	0.59
1:B:331:LEU:O	1:B:331:LEU:HD23	2.02	0.59
1:B:203:TYR:HD2	1:B:208:GLU:HG2	1.68	0.58
2:I:6:GLU:HG3	2:I:111:GLY:CA	2.33	0.58
1:B:157:ASN:HB3	2:I:33:THR:HG21	1.84	0.58
2:I:199:THR:HG22	2:I:214:LYS:HA	1.86	0.57
1:B:147:LEU:HD12	1:B:147:LEU:O	2.04	0.57
3:L:146:LYS:HB3	3:L:177:TYR:CG	2.40	0.57
2:H:33:THR:HB	2:H:52:SER:HA	1.84	0.57
1:B:211:VAL:O	1:B:215:LYS:HE2	2.04	0.57
1:B:154:ASP:O	1:B:159:ILE:HG13	2.04	0.57
3:M:24:SER:HA	3:M:68:THR:O	2.04	0.56
2:I:189:PRO:O	2:I:192:THR:HB	2.04	0.56
1:A:147:LEU:HA	1:A:248:VAL:CG1	2.35	0.56
1:A:205:SER:OG	1:A:207:GLU:HG2	2.05	0.56
1:B:230:ILE:HG23	1:B:252:MET:SD	2.45	0.56
3:M:140:LEU:N	3:M:140:LEU:HD12	2.19	0.56
1:A:162:TRP:HB2	1:A:218:GLN:NE2	2.19	0.56
3:M:151:LYS:HD3	3:M:158:GLU:OE1	2.05	0.56
1:B:232:THR:O	1:B:236:GLU:HB2	2.05	0.56
1:A:149:ILE:O	1:A:185:VAL:HA	2.05	0.56
1:B:211:VAL:HG12	1:B:215:LYS:HE2	1.86	0.56
1:A:199:ASN:HB3	1:A:242:ARG:O	2.05	0.56
1:A:195:THR:CG2	1:A:219:ARG:HE	2.19	0.55
1:A:180:PRO:HD3	1:A:204:SER:HB2	1.88	0.55
3:L:82:PHE:O	3:L:83:ALA:HB2	2.05	0.55
3:M:153:LYS:HG2	3:M:157:SER:N	2.22	0.55
3:L:145:PRO:HG2	3:L:203:LYS:NZ	2.21	0.55
3:M:79:PRO:HA	3:M:105:ILE:HG21	1.89	0.55
3:M:163:VAL:O	3:M:164:LEU:HD23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:6:GLU:OE2	2:I:95:CYS:N	2.40	0.54
1:B:151:ILE:HB	1:B:187:ILE:CD1	2.37	0.54
3:L:119:VAL:HG23	3:L:211:LYS:HD3	1.90	0.54
3:L:140:LEU:HD12	3:L:140:LEU:N	2.23	0.54
1:A:286:LEU:HD11	1:A:317:ASN:HD21	1.73	0.54
2:I:90:THR:O	2:I:91:ALA:HB2	2.09	0.53
3:M:136:VAL:CG1	3:M:183:LEU:HB3	2.37	0.53
2:H:141:VAL:HG23	2:H:190:SER:HA	1.89	0.53
3:L:165:ASN:HD22	3:L:181:SER:HA	1.73	0.53
1:B:174:LYS:HZ3	1:B:175:ARG:HH12	1.56	0.53
2:I:199:THR:HG22	2:I:214:LYS:HG3	1.90	0.53
1:B:289:TYR:HB2	1:B:296:THR:HG22	1.90	0.53
3:M:192:ARG:HA	3:M:192:ARG:NE	2.23	0.53
1:B:251:VAL:HG22	1:B:279:GLN:HB2	1.91	0.53
3:M:104:GLU:HG3	3:M:177:TYR:OH	2.08	0.53
3:L:153:LYS:HB3	3:L:197:THR:CG2	2.39	0.53
3:L:199:GLU:HG2	3:L:210:VAL:HG22	1.90	0.52
3:M:154:ILE:O	3:M:154:ILE:HG13	2.09	0.52
1:A:146:GLN:O	1:A:146:GLN:HG3	2.08	0.52
1:B:234:ARG:HH11	1:B:234:ARG:CB	2.12	0.52
1:B:181:LYS:HE2	1:B:181:LYS:HA	1.92	0.52
1:A:234:ARG:NE	1:A:272:ASP:HB3	2.21	0.52
2:I:71:ARG:CD	2:I:73:ASN:HD21	2.23	0.52
3:L:117:PRO:HB3	3:L:143:PHE:HB3	1.92	0.51
1:B:165:VAL:O	1:B:168:PHE:HB3	2.09	0.51
2:H:50:VAL:HG12	2:H:58:TYR:HB2	1.93	0.51
3:L:49:LEU:O	3:L:50:THR:HB	2.10	0.50
1:A:328:VAL:HG23	1:A:329:LYS:N	2.26	0.50
3:M:197:THR:OG1	3:M:212:SER:HB3	2.11	0.50
3:L:186:THR:OG1	3:L:189:GLU:HG3	2.12	0.50
1:B:174:LYS:HG3	1:B:174:LYS:O	2.12	0.50
2:H:38:ARG:HG2	2:H:48:VAL:CG2	2.42	0.50
1:B:151:ILE:HG22	1:B:153:LEU:HD12	1.94	0.50
3:M:136:VAL:HG12	3:M:183:LEU:HB3	1.94	0.50
3:L:65:GLY:HA3	3:L:70:TYR:HA	1.93	0.49
2:H:33:THR:CB	2:H:52:SER:HA	2.41	0.49
2:H:90:THR:O	2:H:91:ALA:HB2	2.12	0.49
1:A:265:ARG:O	1:A:269:VAL:HG23	2.12	0.49
3:M:99:GLN:NE2	3:M:99:GLN:H	2.09	0.49
3:M:119:VAL:HA	3:M:139:PHE:O	2.13	0.49
1:B:202:LYS:HG3	1:B:203:TYR:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:GLU:HG3	1:B:208:GLU:H	1.74	0.49
1:A:259:GLU:HG3	1:A:289:TYR:OH	2.12	0.49
3:L:202:HIS:CE1	3:L:204:THR:HG23	2.48	0.49
1:B:171:ASP:OD2	1:B:328:VAL:HG21	2.12	0.49
1:B:283:ILE:HD11	1:B:331:LEU:CD1	2.42	0.49
3:L:139:PHE:C	3:L:140:LEU:HD12	2.33	0.49
1:A:150:VAL:HA	1:A:186:GLY:O	2.13	0.49
3:L:119:VAL:CG2	3:L:211:LYS:HD3	2.43	0.48
3:L:189:GLU:O	3:L:192:ARG:HB3	2.14	0.48
3:M:13:ALA:HB3	3:M:77:LEU:HD12	1.96	0.48
1:A:157:ASN:ND2	1:A:221:GLY:H	2.12	0.48
1:B:265:ARG:O	1:B:269:VAL:HG23	2.12	0.48
1:A:289:TYR:CB	1:A:296:THR:HG22	2.43	0.48
2:I:12:VAL:HG11	2:I:85:LEU:HD13	1.95	0.48
2:I:143:LEU:HD23	2:I:198:VAL:HG11	1.95	0.48
2:H:124:PRO:HB3	2:H:150:TYR:HB3	1.96	0.48
1:B:252:MET:HG2	1:B:254:ILE:CD1	2.43	0.48
3:M:128:GLN:HG2	3:M:133:GLY:O	2.14	0.48
1:A:230:ILE:HG23	1:A:252:MET:SD	2.54	0.48
2:H:192:THR:O	2:H:196:GLU:HB2	2.13	0.48
2:I:143:LEU:HG	2:I:215:ILE:HG21	1.95	0.47
3:M:119:VAL:HG12	3:M:140:LEU:HG	1.95	0.47
3:M:153:LYS:HB3	3:M:197:THR:CG2	2.43	0.47
3:L:183:LEU:HD11	3:L:185:LEU:HD21	1.96	0.47
1:B:235:LYS:O	1:B:236:GLU:HG3	2.15	0.47
1:B:286:LEU:HD11	1:B:317:ASN:ND2	2.16	0.47
1:B:171:ASP:HB3	1:B:328:VAL:HG21	1.97	0.47
3:M:105:ILE:HG12	3:M:105:ILE:O	2.13	0.47
1:A:147:LEU:HD23	1:A:183:THR:HG22	1.96	0.47
3:L:11:LEU:HD12	3:L:11:LEU:C	2.35	0.47
1:B:331:LEU:O	1:B:335:ILE:HG22	2.15	0.47
2:I:169:HIS:HE1	3:M:142:ASN:OD1	1.97	0.47
3:M:138:CYS:CB	3:M:198:CYS:HG	2.26	0.47
3:M:146:LYS:HB3	3:M:177:TYR:CD2	2.50	0.47
3:L:150:VAL:HA	3:L:199:GLU:O	2.15	0.47
1:A:327:ILE:CG2	1:A:331:LEU:HB2	2.43	0.47
3:L:153:LYS:O	3:L:197:THR:HG22	2.15	0.46
1:A:163:GLU:N	1:A:163:GLU:OE1	2.48	0.46
2:H:129:LEU:HB2	2:H:144:GLY:O	2.14	0.46
3:M:51:SER:HB3	3:M:63:GLY:O	2.16	0.46
3:M:122:PHE:HA	3:M:123:PRO:HD3	1.75	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:11:LEU:HD21	3:L:21:ILE:HD11	1.97	0.46
3:M:165:ASN:HD22	3:M:181:SER:HA	1.80	0.46
2:I:119:ALA:HB1	5:I:277:HOH:O	2.15	0.46
1:A:151:ILE:HG22	1:A:153:LEU:HD13	1.98	0.46
1:B:192:GLU:HG3	1:B:221:GLY:CA	2.46	0.46
2:I:6:GLU:HG3	2:I:111:GLY:HA2	1.98	0.46
1:A:172:LEU:HD11	1:A:331:LEU:HD22	1.98	0.46
1:A:332:GLY:C	1:A:334:ARG:H	2.19	0.46
1:A:172:LEU:HD23	1:A:172:LEU:O	2.16	0.45
1:A:254:ILE:N	1:A:254:ILE:HD12	2.31	0.45
2:H:176:GLN:CD	3:L:164:LEU:HD11	2.36	0.45
3:L:119:VAL:HG12	3:L:140:LEU:HG	1.99	0.45
3:M:72:LEU:C	3:M:72:LEU:HD23	2.36	0.45
1:A:193:ASN:C	1:A:193:ASN:HD22	2.19	0.45
1:A:201:ASN:C	1:A:201:ASN:HD22	2.19	0.45
1:A:329:LYS:O	1:A:333:GLU:HG2	2.16	0.45
2:I:142:THR:O	3:M:122:PHE:HZ	2.00	0.45
3:L:90:TRP:HA	3:L:95:TRP:CD1	2.51	0.45
1:B:313:LYS:HZ3	1:B:313:LYS:HB3	1.80	0.45
1:A:178:ILE:HG23	1:A:183:THR:O	2.17	0.45
3:L:141:ASN:ND2	3:L:178:SER:HB3	2.30	0.45
2:I:33:THR:HB	2:I:52:SER:HA	1.98	0.45
3:L:151:LYS:HE3	3:L:158:GLU:OE2	2.16	0.45
1:B:211:VAL:HG12	1:B:215:LYS:CE	2.47	0.45
1:B:251:VAL:HG11	1:B:335:ILE:CD1	2.44	0.45
1:B:313:LYS:HB3	1:B:313:LYS:NZ	2.32	0.45
3:M:106:LYS:HB2	3:M:106:LYS:HE3	1.83	0.45
1:B:151:ILE:HG22	1:B:153:LEU:CD1	2.47	0.45
3:M:202:HIS:CE1	3:M:204:THR:HG23	2.52	0.45
1:A:307:ALA:HB1	1:A:314:HIS:HB3	1.99	0.45
2:H:50:VAL:CG1	2:H:58:TYR:HB2	2.47	0.45
2:I:104:TYR:CZ	3:M:48:TYR:HB3	2.51	0.45
3:M:90:TRP:HA	3:M:95:TRP:CD1	2.51	0.45
3:M:165:ASN:ND2	3:M:181:SER:HA	2.31	0.45
3:L:155:ASP:OD2	3:L:193:HIS:HB3	2.17	0.44
1:B:234:ARG:NE	1:B:272:ASP:HB3	2.32	0.44
1:B:302:GLU:O	1:B:306:ILE:HG13	2.18	0.44
1:A:184:GLN:HB3	1:A:200:LEU:O	2.18	0.44
1:B:283:ILE:HD11	1:B:331:LEU:HD12	2.00	0.44
2:H:71:ARG:CD	2:H:73:ASN:ND2	2.79	0.44
2:I:66:ARG:HG2	2:I:83:ASN:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:71:ARG:CD	2:I:73:ASN:ND2	2.81	0.44
2:I:193:TRP:CD1	2:I:194:PRO:HA	2.53	0.44
1:B:192:GLU:CG	1:B:222:ARG:H	2.31	0.43
3:M:82:PHE:O	3:M:83:ALA:HB2	2.17	0.43
1:A:249:LYS:HE3	1:A:279:GLN:HG2	1.99	0.43
1:A:295:SER:HB2	1:A:297:GLU:HG3	2.01	0.43
1:B:151:ILE:HB	1:B:187:ILE:HD12	2.00	0.43
1:B:235:LYS:O	1:B:235:LYS:HG3	2.19	0.43
2:I:6:GLU:HG3	2:I:111:GLY:N	2.34	0.43
1:A:213:ALA:C	1:A:215:LYS:H	2.21	0.43
1:B:151:ILE:HD12	1:B:187:ILE:HD11	2.00	0.43
1:B:211:VAL:C	1:B:215:LYS:HE2	2.39	0.43
3:M:206:THR:O	3:M:208:PRO:HD3	2.19	0.43
1:A:289:TYR:HB3	1:A:296:THR:HG22	1.99	0.43
3:M:3:GLN:HE21	3:M:3:GLN:HB2	1.65	0.43
3:M:139:PHE:C	3:M:140:LEU:HD12	2.39	0.43
3:M:154:ILE:HG22	3:M:196:TYR:CD1	2.53	0.43
1:A:309:GLU:OE2	1:A:310:PRO:HA	2.18	0.43
1:B:153:LEU:HD21	1:B:169:LEU:HD11	2.01	0.43
2:I:164:LEU:HA	2:I:164:LEU:HD23	1.82	0.43
1:B:223:GLN:HE22	3:M:93:ASN:HD21	1.67	0.42
2:H:122:THR:HG23	2:H:123:PRO:HD2	2.01	0.42
2:H:129:LEU:HB2	2:H:144:GLY:C	2.39	0.42
3:L:51:SER:HB3	3:L:63:GLY:O	2.20	0.42
1:B:153:LEU:HD13	1:B:187:ILE:HG23	2.01	0.42
1:B:289:TYR:HB3	1:B:296:THR:HG22	2.00	0.42
1:A:331:LEU:C	1:A:331:LEU:HD23	2.39	0.42
2:H:140:MET:HE2	2:H:187:THR:HG22	2.01	0.42
1:B:286:LEU:CD1	1:B:317:ASN:HD21	2.20	0.42
2:I:193:TRP:CG	2:I:194:PRO:HA	2.54	0.42
1:A:151:ILE:HG22	1:A:153:LEU:CD1	2.48	0.42
1:A:281:PHE:CZ	1:A:335:ILE:HG12	2.54	0.42
3:L:1:GLN:CD	3:L:1:GLN:H3	2.22	0.42
2:I:6:GLU:HG3	2:I:111:GLY:H	1.84	0.42
1:A:147:LEU:HD23	1:A:147:LEU:N	2.35	0.42
1:A:206:THR:O	1:A:210:LEU:HG	2.19	0.42
2:H:51:ILE:HA	2:H:56:HIS:O	2.20	0.42
3:M:119:VAL:HG23	3:M:119:VAL:O	2.19	0.42
2:H:161:SER:N	2:H:201:ASN:ND2	2.54	0.42
3:M:186:THR:OG1	3:M:189:GLU:HG3	2.19	0.42
2:H:22:CYS:SG	2:H:95:CYS:CB	3.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:171:PHE:CD1	2:H:171:PHE:N	2.87	0.42
3:M:117:PRO:HB3	3:M:143:PHE:HB3	2.02	0.42
1:A:215:LYS:HE3	1:A:215:LYS:HB2	1.93	0.42
1:A:192:GLU:CG	1:A:222:ARG:H	2.32	0.42
3:M:80:GLU:O	3:M:80:GLU:HG3	2.20	0.42
2:H:103:GLY:HA3	3:L:90:TRP:HB2	2.01	0.42
3:L:114:ASP:OD2	3:L:203:LYS:HD2	2.20	0.42
1:B:186:GLY:N	1:B:200:LEU:HD23	2.35	0.42
1:B:227:ALA:HB3	1:B:262:ASP:CG	2.41	0.42
2:H:104:TYR:CZ	3:L:48:TYR:HB3	2.55	0.41
1:B:201:ASN:C	1:B:201:ASN:ND2	2.74	0.41
3:M:119:VAL:HG23	3:M:211:LYS:HD3	2.01	0.41
1:A:192:GLU:HG3	1:A:221:GLY:CA	2.49	0.41
1:A:175:ARG:HG3	1:A:175:ARG:HH11	1.85	0.41
2:I:6:GLU:H	2:I:6:GLU:HG2	1.30	0.41
1:A:252:MET:SD	1:A:254:ILE:HD11	2.60	0.41
2:I:124:PRO:HB3	2:I:150:TYR:HB3	2.01	0.41
1:B:209:VAL:O	1:B:210:LEU:C	2.59	0.41
2:I:51:ILE:HA	2:I:56:HIS:O	2.21	0.41
3:M:79:PRO:O	3:M:105:ILE:HD12	2.20	0.41
2:H:178:ASP:O	2:H:179:LEU:HD23	2.20	0.41
3:L:24:SER:HA	3:L:68:THR:O	2.21	0.41
1:B:150:VAL:O	1:B:252:MET:HA	2.21	0.41
1:A:222:ARG:HB3	3:L:95:TRP:CZ2	2.56	0.41
3:L:90:TRP:C	3:L:90:TRP:CD1	2.94	0.41
1:A:255:VAL:HG22	1:A:283:ILE:HD12	2.02	0.41
3:L:196:TYR:O	3:L:212:SER:HB2	2.21	0.41
1:B:172:LEU:C	1:B:174:LYS:H	2.24	0.41
1:B:213:ALA:C	1:B:215:LYS:H	2.25	0.41
3:M:11:LEU:C	3:M:11:LEU:HD12	2.40	0.41
1:A:316:PHE:HB3	1:A:327:ILE:HD13	2.03	0.41
2:H:172:PRO:HG2	3:L:166:SER:OG	2.20	0.41
1:A:245:ARG:HB2	1:A:248:VAL:HG21	2.03	0.40
3:L:15:VAL:HA	3:L:77:LEU:O	2.21	0.40
2:H:97:ARG:HH21	2:H:106:ASP:CG	2.25	0.40
2:H:182:LEU:HD12	2:H:182:LEU:O	2.21	0.40
3:L:72:LEU:C	3:L:72:LEU:HD23	2.41	0.40
3:L:158:GLU:CD	3:L:160:GLN:HE21	2.24	0.40
1:A:248:VAL:HG12	1:A:249:LYS:N	2.36	0.40
1:B:201:ASN:C	1:B:201:ASN:HD22	2.25	0.40
3:M:115:ALA:O	3:M:143:PHE:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:189:PRO:O	2:H:192:THR:HB	2.22	0.40
2:I:129:LEU:HB2	2:I:144:GLY:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	184/223 (82%)	164 (89%)	18 (10%)	2 (1%)	14	12
1	B	166/223 (74%)	147 (89%)	17 (10%)	2 (1%)	13	10
2	H	206/226 (91%)	201 (98%)	5 (2%)	0	100	100
2	I	206/226 (91%)	202 (98%)	4 (2%)	0	100	100
3	L	208/213 (98%)	198 (95%)	9 (4%)	1 (0%)	29	31
3	M	208/213 (98%)	195 (94%)	12 (6%)	1 (0%)	29	31
All	All	1178/1324 (89%)	1107 (94%)	65 (6%)	6 (0%)	29	31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	GLY
1	B	236	GLU
1	A	333	GLU
3	L	83	ALA
1	B	173	LEU
3	M	160	GLN

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	164/194 (84%)	157 (96%)	7 (4%)	29	36
1	B	153/194 (79%)	148 (97%)	5 (3%)	38	49
2	H	177/190 (93%)	170 (96%)	7 (4%)	31	40
2	I	177/190 (93%)	166 (94%)	11 (6%)	18	21
3	L	187/190 (98%)	179 (96%)	8 (4%)	29	36
3	M	187/190 (98%)	179 (96%)	8 (4%)	29	36
All	All	1045/1148 (91%)	999 (96%)	46 (4%)	28	35

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	LEU
1	A	163	GLU
1	A	193	ASN
1	A	201	ASN
1	A	219	ARG
1	A	234	ARG
1	A	268	GLN
2	H	38	ARG
2	H	96	THR
2	H	113	LEU
2	H	152	PRO
2	H	154	PRO
2	H	155	VAL
2	H	199	THR
3	L	4	LEU
3	L	49	LEU
3	L	77	LEU
3	L	90	TRP
3	L	104	GLU
3	L	146	LYS
3	L	159	ARG
3	L	211	LYS

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Mol	Chain	Res	Type
1	B	147	LEU
1	B	171	ASP
1	B	201	ASN
1	B	234	ARG
1	B	238	PHE
2	I	6	GLU
2	I	38	ARG
2	I	43	LYS
2	I	66	ARG
2	I	95	CYS
2	I	113	LEU
2	I	143	LEU
2	I	152	PRO
2	I	154	PRO
2	I	155	VAL
2	I	164	LEU
3	M	4	LEU
3	M	9	SER
3	M	15	VAL
3	M	77	LEU
3	M	90	TRP
3	M	99	GLN
3	M	105	ILE
3	M	194	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	157	ASN
1	A	170	ASN
1	A	193	ASN
1	A	201	ASN
1	A	214	ASN
1	A	218	GLN
1	A	261	HIS
1	A	268	GLN
1	A	271	GLN
1	A	279	GLN
1	A	314	HIS
2	H	3	GLN
2	H	73	ASN

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Mol	Chain	Res	Type
2	H	76	ASN
2	H	169	HIS
2	H	201	ASN
3	L	1	GLN
3	L	3	GLN
3	L	93	ASN
3	L	141	ASN
3	L	160	GLN
3	L	165	ASN
1	B	157	ASN
1	B	201	ASN
1	B	218	GLN
1	B	261	HIS
1	B	268	GLN
1	B	288	HIS
1	B	314	HIS
1	B	317	ASN
2	I	73	ASN
2	I	169	HIS
2	I	201	ASN
3	M	3	GLN
3	M	36	GLN
3	M	93	ASN
3	M	99	GLN
3	M	141	ASN
3	M	160	GLN
3	M	165	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	188/223 (84%)	0.40	8 (4%) 35 33	28, 59, 77, 83	0
1	B	176/223 (78%)	0.66	14 (7%) 12 11	33, 66, 91, 96	0
2	H	210/226 (92%)	0.06	0 100 100	22, 31, 49, 58	0
2	I	210/226 (92%)	0.01	0 100 100	24, 34, 50, 61	0
3	L	210/213 (98%)	0.17	4 (1%) 66 65	22, 42, 74, 86	0
3	M	210/213 (98%)	0.16	5 (2%) 59 56	24, 41, 68, 86	0
All	All	1204/1324 (90%)	0.23	31 (2%) 56 53	22, 42, 78, 96	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	200	LEU	4.3
1	B	179	GLY	3.7
1	B	147	LEU	3.4
3	M	192	ARG	3.4
1	B	334	ARG	3.3
3	M	214	ASN	3.2
1	A	146	GLN	3.0
3	L	209	ILE	3.0
3	M	154	ILE	2.9
3	L	213	PHE	2.8
3	L	154	ILE	2.8
1	A	178	ILE	2.7
1	B	237	ALA	2.7
1	A	147	LEU	2.7
1	B	313	LYS	2.7
3	M	195	SER	2.7
1	B	336	PHE	2.6
3	L	214	ASN	2.6
1	A	331	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	245	ARG	2.5
1	B	298	LYS	2.5
1	A	248	VAL	2.4
1	B	322	LEU	2.4
1	B	148	ASP	2.4
1	B	315	PHE	2.3
1	A	313	LYS	2.3
1	A	204	SER	2.2
1	B	250	LYS	2.2
1	A	176	MET	2.1
3	M	160	GLN	2.0
1	B	172	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	B	401	1/1	0.88	0.16	54,54,54,54	0
4	MG	A	400	1/1	0.92	0.14	47,47,47,47	0

6.5 Other polymers (i)

There are no such residues in this entry.