Full wwPDB X-ray Structure Validation Report (i)

Sep 12, 2023 – 12:29 AM EDT

PDB ID	:	4LHX
Title	:	Crystal structure of nucleotide-free Rab8:Rabin8
Authors	:	Guo, Z.; Hou, X.M.; Goody, R.S.; Itzen, A.
Deposited on	:	2013-07-01
Resolution	:	3.05 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 (i) 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 (1)) were used in the production of this report:

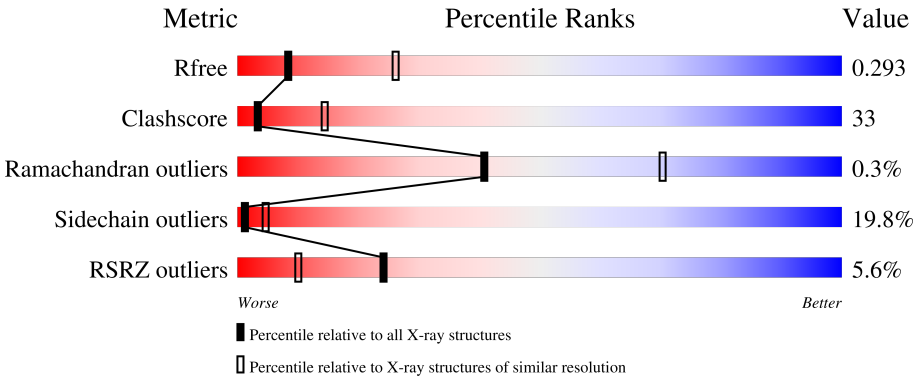
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.05 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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	186	42% 41% 11% • 6%
1	B	186	40% 37% 16% • 6%
2	C	78	8% 69% 21% • 8%
2	D	78	3% 72% 17% • 9%
2	E	78	14% 65% 26% 6% •

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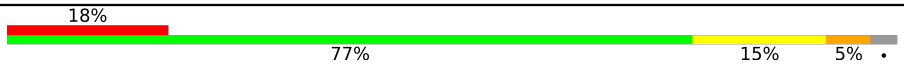
Mol	Chain	Length	Quality of chain
2	F	78	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	201	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4750 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 Ras-related protein Rab-8A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	0	0
			1390	888	235	260	7			
1	B	175	Total	C	N	O	S	0	0	0
			1389	885	233	264	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P61006
A	0	HIS	-	expression tag	UNP P61006
B	-1	GLY	-	expression tag	UNP P61006
B	0	HIS	-	expression tag	UNP P61006

- Molecule 2 is a protein called Rab-3A-interacting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	72	Total	C	N	O	S	0	0	0
			481	293	89	97	2			
2	D	71	Total	C	N	O	S	0	0	0
			469	284	83	100	2			
2	E	76	Total	C	N	O	S	0	0	0
			498	303	92	101	2			
2	F	76	Total	C	N	O	S	0	0	0
			508	307	96	103	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	155	GLY	-	expression tag	UNP Q96QF0
C	156	PRO	-	expression tag	UNP Q96QF0
D	155	GLY	-	expression tag	UNP Q96QF0
D	156	PRO	-	expression tag	UNP Q96QF0

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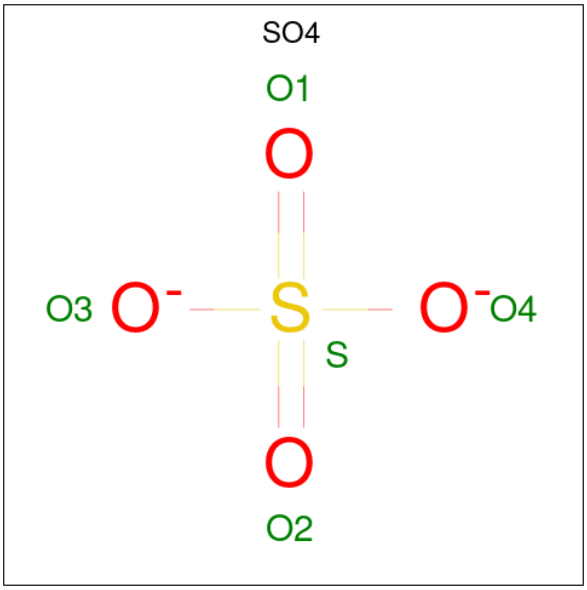
Chain	Residue	Modelled	Actual	Comment	Reference
E	155	GLY	-	expression tag	UNP Q96QF0
E	156	PRO	-	expression tag	UNP Q96QF0
F	155	GLY	-	expression tag	UNP Q96QF0
F	156	PRO	-	expression tag	UNP Q96QF0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



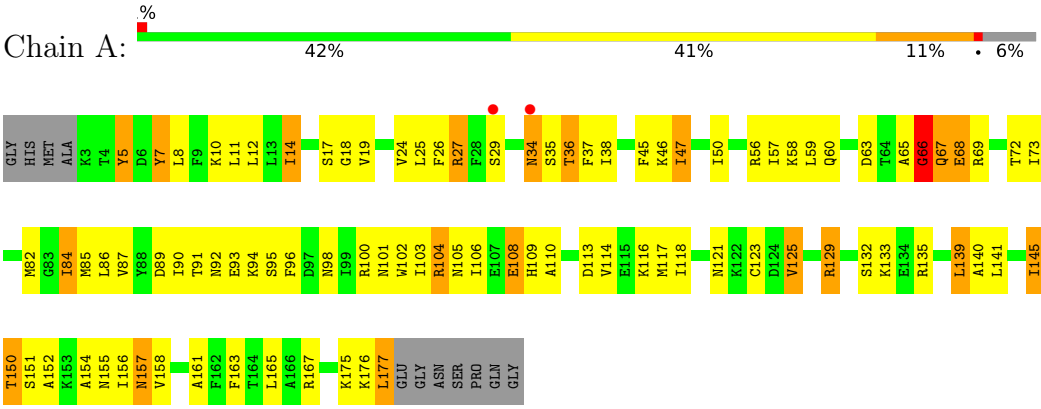
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

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.

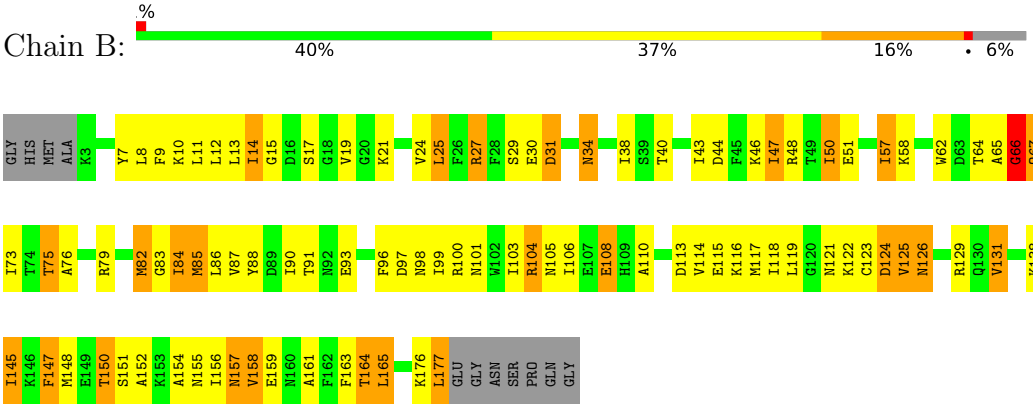
• Molecule 1: Ras-related protein Rab-8A

Chain A:



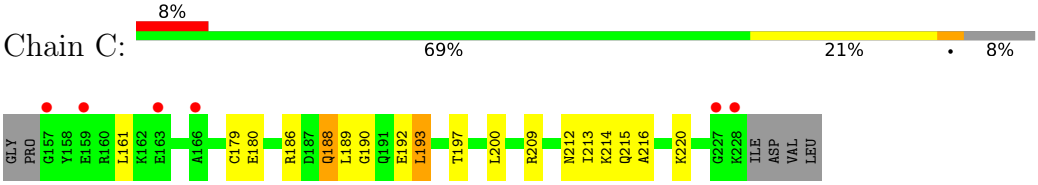
• Molecule 1: Ras-related protein Rab-8A

Chain B:



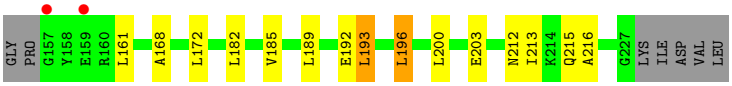
• Molecule 2: Rab-3A-interacting protein

Chain C:

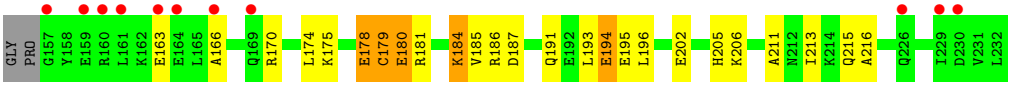


• Molecule 2: Rab-3A-interacting protein

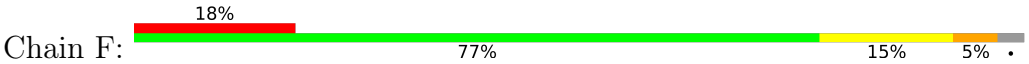
Chain D:

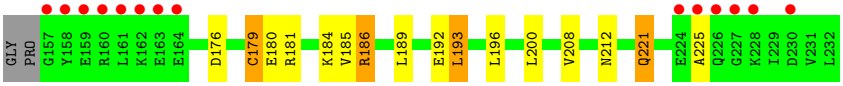


• Molecule 2: Rab-3A-interacting protein



• Molecule 2: Rab-3A-interacting protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	81.64Å 165.30Å 166.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 3.05 19.94 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.94-3.05) 99.2 (19.94-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.40 (at 3.04Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.264 , 0.300 0.259 , 0.293	Depositor DCC
R_{free} test set	1076 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	76.1	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 78.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4750	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: SO4

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	0.98	0/1411	1.04	3/1895 (0.2%)
1	B	0.89	0/1410	0.97	1/1896 (0.1%)
2	C	0.67	0/482	0.68	1/651 (0.2%)
2	D	0.67	0/470	0.68	0/638
2	E	0.58	0/499	0.66	0/674
2	F	0.68	1/509 (0.2%)	0.61	0/687
All	All	0.83	1/4781 (0.0%)	0.88	5/6441 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	179	CYS	CB-SG	-5.05	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	7	TYR	CB-CA-C	-5.49	99.41	110.40
1	A	5	TYR	CB-CA-C	-5.38	99.65	110.40
1	A	66	GLY	N-CA-C	5.32	126.40	113.10
1	B	66	GLY	N-CA-C	5.31	126.38	113.10
2	C	209	ARG	NE-CZ-NH1	5.22	122.91	120.30

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	1390	0	1388	112	0
1	B	1389	0	1372	138	0
2	C	481	0	409	14	0
2	D	469	0	380	27	0
2	E	498	0	411	23	0
2	F	508	0	423	26	0
3	A	5	0	0	2	0
3	B	10	0	0	0	0
All	All	4750	0	4383	299	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (299) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ILE:CG2	1:A:84:ILE:HD11	1.44	1.46
1:B:72:THR:CG2	2:D:189:LEU:HD12	1.72	1.18
1:A:14:ILE:CG2	1:A:84:ILE:CD1	2.22	1.17
1:B:72:THR:HG23	2:D:189:LEU:CD1	1.74	1.16
1:B:14:ILE:CG2	1:B:84:ILE:HD13	1.73	1.15
2:F:221:GLN:HE21	2:F:221:GLN:N	1.52	1.08
1:B:14:ILE:HG21	1:B:84:ILE:HD13	1.30	1.07
1:B:176:LYS:C	1:B:177:LEU:HD22	1.73	1.06
1:B:86:LEU:HD21	1:B:106:ILE:HD12	1.36	1.06
1:B:72:THR:HG23	2:D:189:LEU:HD12	1.23	1.03
1:A:121:ASN:OD1	1:A:150:THR:CG2	2.07	1.02
1:A:125:VAL:O	1:A:125:VAL:HG22	1.60	1.01
1:A:56:ARG:O	1:A:57:ILE:HD13	1.59	1.01
1:A:90:ILE:CD1	1:A:123:CYS:HA	1.93	0.98
1:A:19:VAL:CG1	1:A:87:VAL:HG12	1.96	0.95
1:A:72:THR:CG2	2:F:189:LEU:HD13	1.96	0.94
1:A:14:ILE:HG23	1:A:84:ILE:HD11	0.98	0.94
1:B:84:ILE:C	1:B:84:ILE:HD12	1.88	0.93
1:A:72:THR:HG22	2:F:189:LEU:HD13	1.51	0.92
1:A:121:ASN:OD1	1:A:150:THR:HG22	1.68	0.91
1:B:161:ALA:O	1:B:164:THR:HG22	1.73	0.88
1:A:14:ILE:HG22	1:A:84:ILE:CD1	2.00	0.87
1:A:56:ARG:C	1:A:57:ILE:HD13	1.94	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ILE:HG22	1:A:84:ILE:HD11	1.52	0.86
1:B:117:MET:HE2	1:B:119:LEU:HD11	1.56	0.86
1:B:121:ASN:HA	1:B:150:THR:HG22	1.57	0.84
2:C:186:ARG:HD2	2:D:185:VAL:HG11	1.61	0.83
1:B:19:VAL:CG1	1:B:87:VAL:HG12	2.09	0.82
1:B:84:ILE:HD12	1:B:85:MET:N	1.95	0.82
1:A:89:ASP:OD1	1:A:91:THR:HB	1.80	0.81
1:B:148:MET:HE1	1:B:164:THR:HG21	1.62	0.80
1:B:117:MET:CE	1:B:119:LEU:HD11	2.10	0.79
2:F:221:GLN:N	2:F:221:GLN:NE2	2.31	0.79
1:A:14:ILE:HG23	1:A:84:ILE:CD1	1.94	0.78
1:B:177:LEU:HD22	1:B:177:LEU:N	1.97	0.78
1:B:125:VAL:HG22	1:B:125:VAL:O	1.82	0.78
1:B:19:VAL:HG11	1:B:87:VAL:HG12	1.64	0.77
1:B:25:LEU:HD11	1:B:46:LYS:HB2	1.65	0.77
1:B:117:MET:CE	1:B:161:ALA:HB1	2.14	0.77
1:B:14:ILE:CD1	1:B:106:ILE:HD11	2.14	0.77
1:A:72:THR:HG22	2:F:189:LEU:CD1	2.15	0.76
1:B:14:ILE:HG21	1:B:84:ILE:CD1	2.12	0.76
1:B:164:THR:CG2	1:B:165:LEU:N	2.48	0.76
1:B:72:THR:HG22	1:B:73:ILE:N	2.00	0.75
1:B:38:ILE:HD11	1:B:65:ALA:HB2	1.68	0.75
1:A:125:VAL:O	1:A:125:VAL:CG2	2.29	0.74
1:A:19:VAL:HG11	1:A:87:VAL:HG12	1.66	0.74
1:A:8:LEU:HD11	1:A:60:GLN:NE2	2.02	0.74
1:A:93:GLU:OE2	1:A:135:ARG:NH2	2.21	0.74
1:B:25:LEU:HD22	1:B:25:LEU:O	1.87	0.73
2:E:187:ASP:O	2:E:191:GLN:HG3	1.89	0.72
1:A:90:ILE:HD11	1:A:123:CYS:HA	1.72	0.71
1:B:50:ILE:HG12	1:B:163:PHE:CZ	2.24	0.71
1:B:24:VAL:HG13	1:B:158:VAL:HG12	1.71	0.71
1:B:72:THR:HG21	2:D:189:LEU:HD12	1.68	0.71
1:B:72:THR:CG2	1:B:73:ILE:N	2.54	0.71
2:D:196:LEU:HD12	2:D:196:LEU:O	1.92	0.70
1:A:12:LEU:O	1:A:84:ILE:HD12	1.92	0.70
1:B:27:ARG:CZ	1:B:155:ASN:HB2	2.22	0.69
1:B:125:VAL:O	1:B:125:VAL:CG2	2.40	0.69
1:B:108:GLU:C	1:B:108:GLU:OE2	2.30	0.69
1:A:29:SER:CB	1:A:46:LYS:HG2	2.22	0.69
1:A:72:THR:HB	2:F:192:GLU:CD	2.13	0.69
2:E:175:LYS:NZ	2:F:176:ASP:CB	2.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:LYS:NZ	2:E:194:GLU:OE2	2.25	0.69
1:A:18:GLY:N	3:A:201:SO4:O1	2.25	0.69
2:E:175:LYS:O	2:E:179:CYS:N	2.24	0.69
1:A:63:ASP:C	1:A:63:ASP:OD1	2.29	0.69
1:A:47:ILE:HD13	2:E:202:GLU:OE2	1.92	0.68
1:B:66:GLY:O	1:B:67:GLN:C	2.31	0.68
1:B:14:ILE:CG2	1:B:84:ILE:CD1	2.62	0.68
1:A:7:TYR:CD2	1:A:57:ILE:HD12	2.29	0.68
1:A:27:ARG:CZ	1:A:155:ASN:HB2	2.24	0.68
1:B:117:MET:HE1	1:B:161:ALA:HB1	1.75	0.67
1:B:86:LEU:HD21	1:B:106:ILE:CD1	2.18	0.67
1:A:72:THR:HB	2:F:192:GLU:OE2	1.95	0.67
1:A:106:ILE:O	1:A:110:ALA:HB3	1.95	0.67
1:B:106:ILE:O	1:B:110:ALA:HB3	1.94	0.67
1:B:121:ASN:OD1	1:B:150:THR:CG2	2.42	0.67
1:A:86:LEU:HD21	1:A:106:ILE:HD12	1.76	0.66
1:A:118:ILE:HG13	1:A:145:ILE:HD11	1.77	0.66
1:B:13:LEU:O	1:B:64:THR:HG22	1.96	0.66
1:A:132:SER:OG	1:A:135:ARG:HB2	1.96	0.66
1:B:27:ARG:NE	1:B:155:ASN:HB2	2.11	0.66
2:D:168:ALA:O	2:D:172:LEU:CB	2.44	0.66
1:A:93:GLU:O	1:A:96:PHE:N	2.28	0.66
2:E:175:LYS:HZ2	2:F:176:ASP:CB	2.08	0.65
1:A:14:ILE:HG22	1:A:84:ILE:HD13	1.78	0.65
1:B:88:TYR:HB3	1:B:99:ILE:HD11	1.77	0.65
1:B:164:THR:HG22	1:B:165:LEU:N	2.12	0.65
1:B:164:THR:HG22	1:B:165:LEU:H	1.61	0.65
2:F:221:GLN:HE21	2:F:221:GLN:H	1.42	0.64
2:D:193:LEU:HD22	2:D:193:LEU:O	1.97	0.64
1:A:37:PHE:CE1	2:E:205:HIS:CE1	2.85	0.64
1:A:72:THR:HB	2:F:192:GLU:OE1	1.97	0.64
1:B:31:ASP:OD2	1:B:46:LYS:CE	2.46	0.64
1:B:159:GLU:O	1:B:163:PHE:HD1	1.81	0.64
1:A:66:GLY:O	1:A:67:GLN:C	2.31	0.64
1:B:72:THR:HG21	2:D:189:LEU:HA	1.79	0.63
1:B:148:MET:CE	1:B:164:THR:HG21	2.28	0.63
1:A:90:ILE:HD13	1:A:123:CYS:HA	1.76	0.62
1:A:27:ARG:NE	1:A:155:ASN:HB2	2.14	0.62
1:A:38:ILE:HD11	1:A:65:ALA:HB2	1.81	0.62
1:A:101:ASN:O	1:A:104:ARG:HB2	1.98	0.61
1:B:72:THR:HG22	2:D:192:GLU:OE2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:VAL:HG12	1:B:87:VAL:HG12	1.83	0.61
1:A:121:ASN:HA	1:A:150:THR:HG22	1.81	0.61
1:A:37:PHE:HE1	2:E:205:HIS:CE1	2.19	0.60
1:A:129:ARG:NH2	1:A:149:GLU:OE2	2.35	0.59
1:B:117:MET:HE1	1:B:161:ALA:CB	2.32	0.59
1:B:117:MET:HE1	1:B:161:ALA:CA	2.32	0.59
1:B:176:LYS:O	1:B:177:LEU:C	2.41	0.59
1:B:121:ASN:OD1	1:B:150:THR:HG22	2.03	0.58
1:B:72:THR:CG2	2:D:189:LEU:CD1	2.49	0.58
1:A:163:PHE:O	1:A:167:ARG:HG3	2.04	0.58
1:B:96:PHE:CG	1:B:131:VAL:HG11	2.39	0.58
1:A:36:THR:OG1	1:A:37:PHE:N	2.34	0.58
2:E:180:GLU:O	2:E:184:LYS:HB2	2.03	0.58
2:E:175:LYS:HZ3	2:F:176:ASP:HA	1.69	0.58
1:A:50:ILE:HD13	1:A:59:LEU:HD11	1.85	0.57
1:B:7:TYR:HB3	1:B:57:ILE:HD13	1.86	0.57
1:B:118:ILE:HG13	1:B:145:ILE:HD11	1.85	0.57
2:D:213:ILE:O	2:D:216:ALA:HB3	2.04	0.57
2:C:200:LEU:HB3	2:D:200:LEU:HD23	1.85	0.57
1:B:122:LYS:HB3	1:B:125:VAL:CG1	2.35	0.57
1:A:45:PHE:CE1	1:A:47:ILE:HD12	2.40	0.56
1:A:68:GLU:OE1	1:A:69:ARG:N	2.36	0.56
1:A:19:VAL:HG11	1:A:87:VAL:O	2.06	0.55
1:B:68:GLU:OE1	1:B:69:ARG:N	2.36	0.55
1:B:31:ASP:OD2	1:B:46:LYS:HE3	2.07	0.55
1:B:9:PHE:CD2	1:B:57:ILE:HD11	2.42	0.55
1:B:126:ASN:ND2	1:B:129:ARG:HH11	2.05	0.55
2:C:193:LEU:HD13	2:C:197:THR:HG23	1.88	0.55
1:A:117:MET:HE1	1:A:148:MET:SD	2.46	0.54
1:B:29:SER:O	1:B:30:GLU:HB2	2.07	0.54
1:B:155:ASN:CG	1:B:155:ASN:O	2.45	0.54
1:A:121:ASN:OD1	1:A:150:THR:HG21	2.03	0.54
1:A:150:THR:HG23	1:A:151:SER:N	2.22	0.54
1:B:72:THR:HG22	1:B:73:ILE:H	1.71	0.54
1:A:5:TYR:CD1	1:A:58:LYS:HE3	2.43	0.54
1:B:159:GLU:O	1:B:163:PHE:CD1	2.60	0.54
2:E:175:LYS:NZ	2:F:176:ASP:HA	2.23	0.54
1:B:126:ASN:HD21	1:B:129:ARG:HH11	1.54	0.54
1:B:177:LEU:HD13	1:B:177:LEU:H	1.73	0.54
2:D:196:LEU:HD12	2:D:196:LEU:C	2.27	0.53
1:A:12:LEU:HG	1:A:84:ILE:HD13	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ASN:H	1:A:34:ASN:ND2	2.07	0.53
1:B:8:LEU:HD12	1:B:58:LYS:CB	2.38	0.53
2:F:221:GLN:NE2	2:F:221:GLN:CA	2.72	0.53
1:A:155:ASN:CG	1:A:155:ASN:O	2.46	0.53
1:B:34:ASN:ND2	1:B:34:ASN:H	2.07	0.53
1:B:82:MET:O	1:B:114:VAL:HG23	2.09	0.53
2:C:186:ARG:HD2	2:D:185:VAL:HG21	1.91	0.53
1:A:5:TYR:HD1	1:A:58:LYS:HE3	1.74	0.53
1:B:114:VAL:O	1:B:114:VAL:HG13	2.09	0.53
1:A:133:LYS:HD3	1:A:149:GLU:CD	2.29	0.53
1:B:148:MET:SD	1:B:157:ASN:OD1	2.67	0.53
1:A:10:LYS:CE	2:E:194:GLU:OE2	2.56	0.52
1:A:148:MET:HG2	1:A:157:ASN:OD1	2.08	0.52
1:B:38:ILE:CD1	1:B:65:ALA:HB2	2.39	0.52
2:F:180:GLU:O	2:F:184:LYS:HG3	2.08	0.52
1:B:90:ILE:CD1	1:B:123:CYS:HA	2.39	0.52
1:A:26:PHE:CZ	1:A:36:THR:HB	2.45	0.52
2:E:175:LYS:NZ	2:F:176:ASP:CA	2.72	0.52
1:B:14:ILE:HG23	1:B:84:ILE:HD13	1.83	0.52
1:A:129:ARG:O	1:A:129:ARG:HG2	2.08	0.52
1:A:140:ALA:HB2	1:A:147:PHE:HB2	1.92	0.52
1:B:164:THR:HG23	1:B:165:LEU:N	2.23	0.52
1:A:114:VAL:HG13	1:A:114:VAL:O	2.09	0.52
1:A:177:LEU:N	1:A:177:LEU:HD22	2.25	0.52
1:B:177:LEU:N	1:B:177:LEU:HD13	2.25	0.52
1:B:86:LEU:HD11	1:B:106:ILE:CD1	2.40	0.52
2:D:212:ASN:O	2:D:215:GLN:HB2	2.09	0.52
2:F:179:CYS:O	2:F:180:GLU:C	2.47	0.51
1:A:14:ILE:CG2	1:A:84:ILE:HD13	2.30	0.51
1:A:47:ILE:HD13	2:E:202:GLU:CD	2.32	0.51
1:B:50:ILE:HG12	1:B:163:PHE:HZ	1.76	0.51
1:B:124:ASP:HB3	1:B:151:SER:OG	2.11	0.51
1:A:34:ASN:H	1:A:34:ASN:HD22	1.59	0.50
1:A:150:THR:HG22	1:A:150:THR:O	2.12	0.50
1:B:14:ILE:HD13	1:B:86:LEU:HG	1.94	0.50
1:B:159:GLU:HG3	1:B:163:PHE:CE1	2.46	0.50
2:D:193:LEU:O	2:D:193:LEU:CD2	2.60	0.50
1:A:36:THR:OG1	1:A:38:ILE:HG22	2.12	0.50
1:A:118:ILE:CG1	1:A:145:ILE:HD11	2.41	0.50
1:A:154:ALA:HB3	1:A:156:ILE:HG13	1.94	0.50
2:C:212:ASN:O	2:C:215:GLN:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ALA:HB3	1:B:156:ILE:HG13	1.94	0.50
1:B:12:LEU:HD12	1:B:62:TRP:O	2.12	0.50
2:F:196:LEU:HD12	2:F:196:LEU:O	2.12	0.50
1:B:86:LEU:HD11	1:B:106:ILE:HD13	1.94	0.50
1:B:117:MET:HE1	1:B:148:MET:HE1	1.94	0.49
1:B:98:ASN:O	1:B:99:ILE:C	2.49	0.49
1:B:116:LYS:HZ3	1:B:116:LYS:HB2	1.77	0.49
1:B:34:ASN:H	1:B:34:ASN:HD22	1.59	0.49
1:A:108:GLU:OE2	1:A:109:HIS:ND1	2.46	0.49
1:B:108:GLU:OE2	1:B:108:GLU:O	2.30	0.49
1:B:117:MET:HE1	1:B:161:ALA:HA	1.94	0.49
1:B:14:ILE:HD13	1:B:84:ILE:HD11	1.96	0.48
1:B:117:MET:HE3	1:B:119:LEU:HD11	1.94	0.48
1:B:117:MET:CE	1:B:148:MET:CE	2.90	0.48
1:A:7:TYR:CD2	1:A:57:ILE:CD1	2.97	0.48
1:B:117:MET:HE2	1:B:161:ALA:HB1	1.93	0.47
1:B:83:GLY:HA2	1:B:115:GLU:O	2.14	0.47
1:B:122:LYS:HB3	1:B:125:VAL:HG13	1.96	0.47
1:A:26:PHE:HZ	1:A:36:THR:HB	1.79	0.47
1:A:73:ILE:O	1:A:76:ALA:HB3	2.14	0.47
2:C:186:ARG:O	2:C:188:GLN:N	2.48	0.47
2:E:175:LYS:HZ2	2:F:176:ASP:CA	2.26	0.47
2:E:213:ILE:O	2:E:216:ALA:HB3	2.13	0.47
1:A:92:ASN:O	1:A:95:SER:OG	2.33	0.47
1:A:14:ILE:HD11	1:A:102:TRP:HB3	1.97	0.47
1:B:19:VAL:HG13	1:B:88:TYR:C	2.35	0.47
2:C:214:LYS:CB	2:D:215:GLN:NE2	2.78	0.47
2:F:196:LEU:HD12	2:F:196:LEU:C	2.35	0.47
1:A:34:ASN:O	1:A:36:THR:HG22	2.14	0.47
1:B:117:MET:CE	1:B:148:MET:HE1	2.45	0.47
1:A:7:TYR:HD2	1:A:57:ILE:CD1	2.28	0.46
1:A:89:ASP:CG	1:A:91:THR:HB	2.35	0.46
1:A:96:PHE:CZ	1:A:139:LEU:HD12	2.50	0.46
2:C:213:ILE:O	2:C:216:ALA:HB3	2.15	0.46
1:B:50:ILE:HD12	1:B:51:GLU:H	1.81	0.46
1:A:29:SER:OG	1:A:46:LYS:HG2	2.15	0.46
1:A:93:GLU:HG3	1:B:93:GLU:HG2	1.97	0.46
1:A:100:ARG:O	1:A:103:ILE:HB	2.16	0.46
1:A:10:LYS:H	1:A:82:MET:CE	2.29	0.46
1:A:19:VAL:HG12	1:A:87:VAL:HG12	1.91	0.46
1:B:14:ILE:HD13	1:B:106:ILE:HD11	1.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:214:LYS:HB3	2:D:215:GLN:NE2	2.31	0.46
1:B:104:ARG:O	1:B:105:ASN:C	2.55	0.46
1:B:147:PHE:C	1:B:147:PHE:CD2	2.90	0.46
1:A:96:PHE:CE1	1:A:139:LEU:HD12	2.51	0.45
1:A:84:ILE:HD12	1:A:85:MET:N	2.32	0.45
1:B:84:ILE:HD11	1:B:106:ILE:HD11	1.99	0.45
2:C:186:ARG:CD	2:D:185:VAL:HG21	2.47	0.45
2:E:170:ARG:O	2:E:174:LEU:N	2.44	0.45
1:B:43:ILE:HG22	1:B:44:ASP:N	2.31	0.45
2:E:175:LYS:HA	2:E:178:GLU:HB2	1.98	0.45
2:E:211:ALA:HB2	2:F:208:VAL:HG13	1.99	0.45
1:B:12:LEU:HB3	1:B:84:ILE:HB	1.99	0.44
1:B:15:GLY:O	1:B:21:LYS:HE2	2.17	0.44
1:B:47:ILE:CG2	1:B:48:ARG:N	2.79	0.44
1:B:93:GLU:OE1	1:B:97:ASP:OD1	2.35	0.44
1:A:104:ARG:O	1:A:105:ASN:C	2.55	0.44
1:A:45:PHE:HZ	1:A:60:GLN:HG2	1.83	0.44
1:A:114:VAL:HG13	1:A:116:LYS:HG3	2.00	0.44
1:B:84:ILE:HD11	1:B:86:LEU:HG	1.98	0.44
2:D:212:ASN:O	2:D:215:GLN:N	2.51	0.44
1:B:9:PHE:HA	1:B:82:MET:SD	2.58	0.44
2:E:163:GLU:O	2:E:166:ALA:HB3	2.17	0.44
1:B:87:VAL:HG22	1:B:119:LEU:HB2	2.00	0.44
1:B:121:ASN:OD1	1:B:150:THR:HG23	2.17	0.44
1:B:121:ASN:CA	1:B:150:THR:HG22	2.40	0.44
1:B:72:THR:CG2	2:D:192:GLU:OE2	2.65	0.43
2:C:161:LEU:CB	2:D:161:LEU:CB	2.96	0.43
1:B:72:THR:HB	2:D:192:GLU:OE1	2.18	0.43
1:B:139:LEU:O	1:B:142:ASP:HB2	2.18	0.43
1:A:79:ARG:NH2	2:E:186:ARG:CB	2.82	0.43
1:B:27:ARG:HD3	1:B:152:ALA:O	2.19	0.43
1:B:72:THR:HB	2:D:192:GLU:CD	2.39	0.43
1:A:72:THR:CG2	2:F:189:LEU:CD1	2.80	0.43
1:A:92:ASN:HD21	1:A:94:LYS:NZ	2.17	0.43
1:B:98:ASN:O	1:B:101:ASN:N	2.52	0.42
1:B:40:THR:OG1	2:D:203:GLU:HG2	2.20	0.42
2:E:205:HIS:O	2:E:206:LYS:C	2.57	0.42
1:B:86:LEU:HD22	1:B:103:ILE:HG13	2.02	0.42
1:A:18:GLY:CA	3:A:201:SO4:O1	2.67	0.42
1:A:140:ALA:HB1	1:A:145:ILE:O	2.19	0.42
2:C:214:LYS:HE2	2:D:215:GLN:HE22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:THR:O	1:A:91:THR:CG2	2.68	0.42
2:C:179:CYS:O	2:C:180:GLU:C	2.58	0.42
2:F:185:VAL:O	2:F:186:ARG:C	2.58	0.42
1:B:10:LYS:O	1:B:11:LEU:HD12	2.20	0.42
1:B:122:LYS:O	1:B:125:VAL:HG13	2.20	0.42
1:A:117:MET:HE2	1:A:161:ALA:HB1	2.00	0.42
1:B:91:THR:O	1:B:91:THR:CG2	2.68	0.42
1:A:117:MET:HE3	1:A:148:MET:HB2	2.02	0.42
1:A:145:ILE:HG21	1:A:145:ILE:HD13	1.84	0.41
1:A:176:LYS:O	1:A:176:LYS:HG3	2.20	0.41
1:B:114:VAL:O	1:B:114:VAL:CG1	2.68	0.41
1:A:98:ASN:O	1:A:101:ASN:HB2	2.21	0.41
1:A:176:LYS:O	1:A:176:LYS:CG	2.68	0.41
1:B:27:ARG:CD	1:B:152:ALA:O	2.69	0.41
1:B:114:VAL:HG13	1:B:116:LYS:HG3	2.01	0.41
1:B:75:THR:HG22	1:B:76:ALA:N	2.33	0.41
2:F:208:VAL:HG12	2:F:212:ASN:HD21	1.86	0.41
1:B:19:VAL:HG11	1:B:87:VAL:C	2.41	0.41
2:F:221:GLN:O	2:F:225:ALA:HB3	2.20	0.41
1:B:176:LYS:O	1:B:177:LEU:HD22	2.14	0.41
1:A:5:TYR:HD2	1:A:7:TYR:N	2.18	0.41
1:A:114:VAL:O	1:A:114:VAL:CG1	2.68	0.41
1:B:148:MET:HE1	1:B:161:ALA:HA	2.02	0.41
2:E:193:LEU:O	2:E:193:LEU:HD23	2.22	0.41
1:B:31:ASP:OD2	1:B:46:LYS:HE2	2.21	0.40
1:B:122:LYS:O	1:B:123:CYS:C	2.60	0.40
1:A:27:ARG:HD3	1:A:152:ALA:O	2.21	0.40
2:C:186:ARG:O	2:C:190:GLY:N	2.45	0.40
2:F:192:GLU:O	2:F:193:LEU:C	2.59	0.40
1:B:50:ILE:O	1:B:57:ILE:HG23	2.20	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	173/186 (93%)	164 (95%)	8 (5%)	1 (1%)	25 55
1	B	173/186 (93%)	158 (91%)	14 (8%)	1 (1%)	25 55
2	C	70/78 (90%)	61 (87%)	9 (13%)	0	100 100
2	D	69/78 (88%)	65 (94%)	4 (6%)	0	100 100
2	E	74/78 (95%)	70 (95%)	4 (5%)	0	100 100
2	F	74/78 (95%)	69 (93%)	5 (7%)	0	100 100
All	All	633/684 (92%)	587 (93%)	44 (7%)	2 (0%)	41 70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	GLY
1	B	66	GLY

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	146/159 (92%)	118 (81%)	28 (19%)	1 5
1	B	146/159 (92%)	111 (76%)	35 (24%)	0 2
2	C	36/66 (54%)	31 (86%)	5 (14%)	3 13
2	D	35/66 (53%)	32 (91%)	3 (9%)	10 33
2	E	35/66 (53%)	25 (71%)	10 (29%)	0 1
2	F	37/66 (56%)	32 (86%)	5 (14%)	4 14
All	All	435/582 (75%)	349 (80%)	86 (20%)	1 5

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	14	ILE
1	A	17	SER
1	A	24	VAL
1	A	25	LEU
1	A	27	ARG
1	A	34	ASN
1	A	35	SER
1	A	36	THR
1	A	47	ILE
1	A	67	GLN
1	A	68	GLU
1	A	84	ILE
1	A	104	ARG
1	A	108	GLU
1	A	113	ASP
1	A	125	VAL
1	A	129	ARG
1	A	139	LEU
1	A	141	LEU
1	A	145	ILE
1	A	147	PHE
1	A	150	THR
1	A	157	ASN
1	A	158	VAL
1	A	165	LEU
1	A	175	LYS
1	A	177	LEU
1	B	14	ILE
1	B	17	SER
1	B	25	LEU
1	B	27	ARG
1	B	31	ASP
1	B	34	ASN
1	B	47	ILE
1	B	50	ILE
1	B	57	ILE
1	B	67	GLN
1	B	68	GLU
1	B	72	THR
1	B	75	THR
1	B	79	ARG
1	B	82	MET

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Mol	Chain	Res	Type
1	B	84	ILE
1	B	85	MET
1	B	100	ARG
1	B	104	ARG
1	B	108	GLU
1	B	113	ASP
1	B	124	ASP
1	B	125	VAL
1	B	126	ASN
1	B	131	VAL
1	B	138	LYS
1	B	139	LEU
1	B	145	ILE
1	B	147	PHE
1	B	150	THR
1	B	157	ASN
1	B	158	VAL
1	B	164	THR
1	B	165	LEU
1	B	177	LEU
2	C	188	GLN
2	C	189	LEU
2	C	192	GLU
2	C	193	LEU
2	C	220	LYS
2	D	182	LEU
2	D	193	LEU
2	D	196	LEU
2	E	178	GLU
2	E	179	CYS
2	E	180	GLU
2	E	181	ARG
2	E	184	LYS
2	E	185	VAL
2	E	194	GLU
2	E	195	GLU
2	E	196	LEU
2	E	215	GLN
2	F	181	ARG
2	F	186	ARG
2	F	193	LEU
2	F	200	LEU

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Mol	Chain	Res	Type
2	F	221	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	60	GLN
1	A	67	GLN
1	B	34	ASN
1	B	67	GLN
1	B	101	ASN
1	B	126	ASN
2	D	215	GLN
2	F	212	ASN
2	F	215	GLN
2	F	221	GLN

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

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	A	201	-	4,4,4	0.14	0	6,6,6	0.53	0
3	SO4	B	202	-	4,4,4	0.18	0	6,6,6	0.33	0
3	SO4	B	201	-	4,4,4	0.32	0	6,6,6	0.59	0

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	201	SO4	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	175/186 (94%)	-0.28	2 (1%) 80 60	38, 67, 115, 139	0
1	B	175/186 (94%)	-0.25	1 (0%) 89 76	43, 73, 115, 153	0
2	C	72/78 (92%)	0.11	6 (8%) 11 4	52, 118, 180, 198	0
2	D	71/78 (91%)	0.12	2 (2%) 53 28	54, 128, 210, 220	0
2	E	76/78 (97%)	0.49	11 (14%) 2 1	52, 127, 231, 245	0
2	F	76/78 (97%)	0.78	14 (18%) 1 0	59, 139, 261, 273	0
All	All	645/684 (94%)	0.03	36 (5%) 24 10	38, 81, 206, 273	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	158	TYR	6.8
2	F	159	GLU	6.8
2	F	160	ARG	6.1
2	F	161	LEU	4.4
2	F	157	GLY	4.1
2	E	229	ILE	3.8
2	D	157	GLY	3.8
2	E	161	LEU	3.4
2	F	224	GLU	3.3
2	C	157	GLY	3.3
2	F	162	LYS	3.3
2	F	227	GLY	3.2
2	D	159	GLU	3.1
2	E	160	ARG	3.1
2	F	228	LYS	3.1
1	A	29	SER	3.1
1	A	34	ASN	3.0
2	C	163	GLU	2.9
2	E	159	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
2	C	166	ALA	2.7
2	E	164	GLU	2.6
2	F	163	GLU	2.6
2	E	230	ASP	2.6
2	E	226	GLN	2.5
2	E	157	GLY	2.5
2	E	166	ALA	2.5
1	B	68	GLU	2.5
2	F	164	GLU	2.5
2	E	163	GLU	2.4
2	F	230	ASP	2.4
2	C	228	LYS	2.3
2	E	169	GLN	2.2
2	F	226	GLN	2.2
2	C	227	GLY	2.1
2	F	225	ALA	2.1
2	C	159	GLU	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
3	SO4	B	202	5/5	0.84	0.28	114,115,115,115	0
3	SO4	B	201	5/5	0.99	0.07	29,31,34,35	0
3	SO4	A	201	5/5	0.99	0.08	45,46,49,50	0

6.5 Other polymers (i)

There are no such residues in this entry.