Full wwPDB X-ray Structure Validation Report (i)

May 29, 2020 – 03:40 pm BST

PDB ID	:	2QPQ
Title	:	Structure of Bug27 from Bordetella pertussis
Authors	:	Herrou, J.; Bompard, C.
Deposited on	:	2007-07-25
Resolution	:	1.92 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 following versions of software and data (see references (i)) were used in the production of this report:

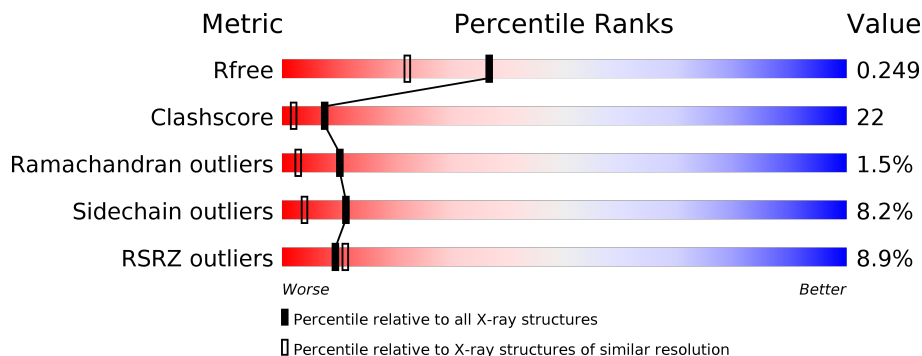|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.92 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	Percentile Ranks	Value
Rfree		0.249
Clashscore		22
Ramachandran outliers		1.5%
Sidechain outliers		8.2%
RSRZ outliers		8.9%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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.

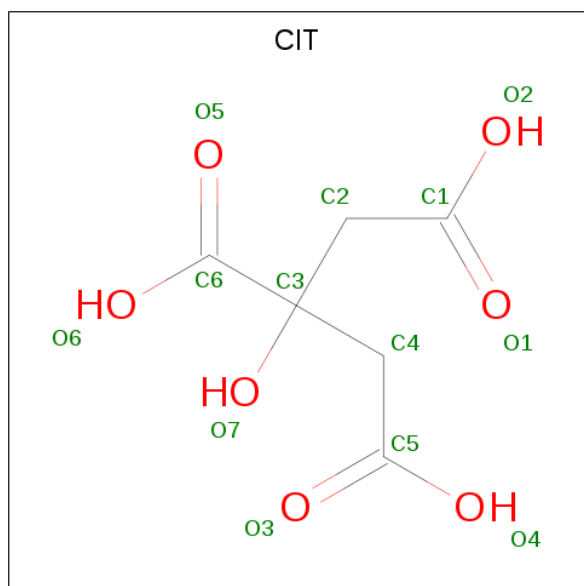| Mol	Chain	Length	Quality of chain
1	A	301	4% 80% 14% · · ·
1	B	301	19% 50% 39% 5% · ·
1	C	301	4% 73% 21% · · ·

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7184 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 protein Bug27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2191	1392	376	414	9			
1	B	291	Total	C	N	O	S	0	0	0
			2168	1382	371	406	9			
1	C	296	Total	C	N	O	S	0	0	0
			2189	1390	376	414	9			

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	261	Total O 261 261	0	0
3	B	153	Total O 153 153	0	0
3	C	196	Total O 196 196	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.
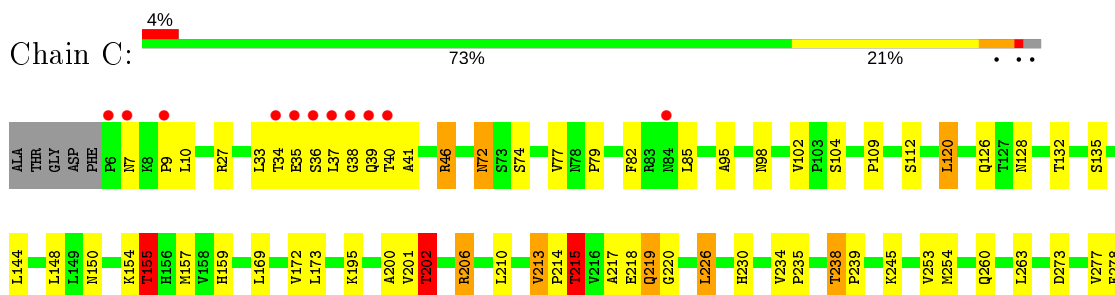
- Molecule 1: protein Bug27
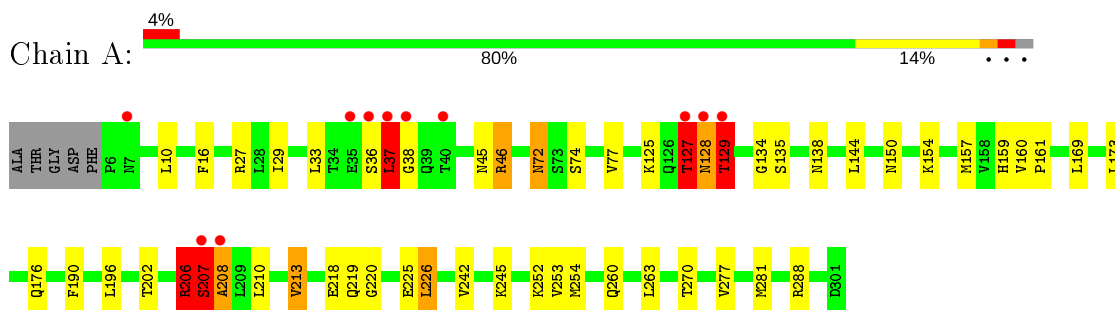
- Molecule 1: protein Bug27
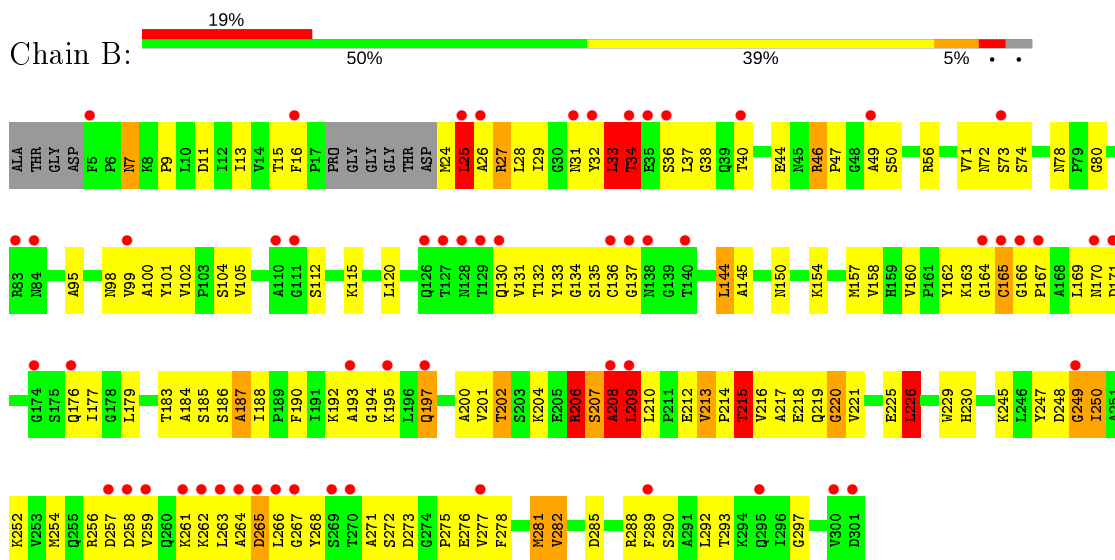
- Molecule 1: protein Bug27

Q279 K280 M281 T284 D285 R288 F289 T293 K299 V300 D301

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.39Å 82.31Å 87.47Å 90.00° 95.35° 90.00°	Depositor
Resolution (Å)	6.56 – 1.92 6.56 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.8 (6.56-1.92) 99.8 (6.56-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$<I/\sigma(I)>$ [1]	2.06 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.191 , 0.252 0.191 , 0.249	Depositor DCC
R_{free} test set	3852 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	26.4	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.61 , 69.3	EDS
L-test for twinning[2]	$<|L|> = 0.48, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7184	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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

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	0.80	0/2234	0.89	6/3038 (0.2%)
1	B	0.72	1/2210 (0.0%)	1.01	17/3004 (0.6%)
1	C	0.81	0/2232	1.04	15/3035 (0.5%)
All	All	0.78	1/6676 (0.0%)	0.98	38/9077 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	2	6
1	C	1	2
All	All	3	11

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	202	THR	CB-CG2	-5.29	1.34	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	206	ARG	NE-CZ-NH1	17.05	128.82	120.30
1	C	206	ARG	NE-CZ-NH2	-14.19	113.21	120.30
1	B	207	SER	N-CA-C	-12.78	76.48	111.00
1	C	288	ARG	NE-CZ-NH2	-10.37	115.12	120.30
1	A	206	ARG	NE-CZ-NH1	9.20	124.90	120.30
1	B	208	ALA	N-CA-C	8.43	133.76	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	34	THR	N-CA-C	-8.36	88.43	111.00
1	B	250	ILE	N-CA-C	-8.21	88.85	111.00
1	B	206	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	A	46	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	B	209	LEU	N-CA-C	7.67	131.70	111.00
1	B	220	GLY	N-CA-C	-7.66	93.95	113.10
1	B	25	LEU	CA-CB-CG	7.41	132.35	115.30
1	B	187	ALA	N-CA-C	-7.34	91.18	111.00
1	C	288	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	C	27	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	B	219	GLN	CA-C-N	7.05	130.30	116.20
1	B	219	GLN	C-N-CA	7.03	137.06	122.30
1	C	38	GLY	N-CA-C	6.99	130.57	113.10
1	C	27	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	C	202	THR	OG1-CB-CG2	6.50	124.95	110.00
1	C	206	ARG	CB-CG-CD	6.40	128.23	111.60
1	B	209	LEU	CA-CB-CG	-6.27	100.88	115.30
1	A	129	THR	N-CA-CB	6.26	122.20	110.30
1	B	219	GLN	O-C-N	-6.23	112.61	123.20
1	B	215	THR	N-CA-CB	-6.07	98.77	110.30
1	A	46	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	C	215	THR	N-CA-CB	-5.61	99.64	110.30
1	C	219	GLN	CA-C-N	5.55	127.30	116.20
1	B	226	LEU	CA-CB-CG	5.41	127.74	115.30
1	A	206	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	128	ASN	N-CA-C	-5.35	96.56	111.00
1	C	46	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	C	155	THR	N-CA-CB	-5.13	100.55	110.30
1	B	219	GLN	N-CA-C	5.11	124.80	111.00
1	C	202	THR	N-CA-CB	-5.07	100.66	110.30
1	B	136	CYS	CA-CB-SG	-5.03	104.94	114.00
1	C	202	THR	CA-CB-CG2	5.03	119.44	112.40

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	202	THR	CB
1	B	209	LEU	CA
1	C	202	THR	CB

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	206	ARG	Peptide
1	A	207	SER	Peptide
1	A	219	GLN	Peptide
1	B	186	SER	Peptide
1	B	206	ARG	Peptide
1	B	207	SER	Peptide
1	B	208	ALA	Peptide
1	B	249	GLY	Peptide
1	B	33	LEU	Peptide
1	C	219	GLN	Peptide
1	C	37	LEU	Peptide

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	2191	0	2228	55	0
1	B	2168	0	2208	161	0
1	C	2189	0	2221	80	0
2	A	13	0	5	0	0
2	C	13	0	5	0	0
3	A	261	0	0	23	1
3	B	153	0	0	77	0
3	C	196	0	0	24	1
All	All	7184	0	6667	293	1

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 22.

All (293) 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:C:109:PRO:HD2	3:C:484:HOH:O	1.24	1.31
1:B:293:THR:HB	3:B:430:HOH:O	1.23	1.26
1:A:169:LEU:HB3	3:A:554:HOH:O	1.37	1.22
1:B:218:GLU:HB2	3:B:449:HOH:O	1.43	1.18
1:C:226:LEU:HB2	3:C:482:HOH:O	1.41	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:MET:CE	3:C:493:HOH:O	1.95	1.11
1:A:128:ASN:HB2	3:A:504:HOH:O	1.52	1.10
1:C:281:MET:HE2	3:C:493:HOH:O	1.51	1.08
1:B:292:LEU:HB3	3:B:426:HOH:O	1.53	1.06
1:C:215:THR:HG21	3:C:307:HOH:O	1.54	1.04
1:B:262:LYS:HB3	3:B:400:HOH:O	1.56	1.02
1:A:210:LEU:HB3	1:A:213:VAL:CG1	1.89	1.01
1:B:258:ASP:HB3	3:B:374:HOH:O	1.61	0.99
1:C:150:ASN:HA	1:C:155:THR:HG22	1.43	0.98
1:C:9:PRO:HB3	1:C:40:THR:O	1.64	0.98
1:B:163:LYS:HE3	3:B:398:HOH:O	1.63	0.98
1:B:215:THR:HG22	1:B:218:GLU:H	1.25	0.98
1:B:26:ALA:HB1	1:B:28:LEU:N	1.79	0.97
1:A:45:ASN:HB3	3:A:523:HOH:O	1.66	0.96
1:B:26:ALA:CB	1:B:29:ILE:H	1.79	0.95
1:A:45:ASN:HB2	3:A:542:HOH:O	1.64	0.94
1:B:27:ARG:N	3:B:417:HOH:O	2.01	0.92
1:B:98:ASN:CB	3:B:443:HOH:O	2.20	0.90
1:B:98:ASN:HB3	3:B:443:HOH:O	1.70	0.90
1:C:281:MET:SD	3:C:493:HOH:O	2.27	0.89
1:A:210:LEU:HB3	1:A:213:VAL:HG12	1.55	0.88
1:A:226:LEU:C	3:A:521:HOH:O	2.13	0.87
1:C:150:ASN:HD22	1:C:155:THR:HG22	1.37	0.86
1:B:215:THR:HG21	3:B:324:HOH:O	1.74	0.86
1:C:154:LYS:HG2	3:C:489:HOH:O	1.74	0.85
1:B:40:THR:HG23	3:B:370:HOH:O	1.74	0.84
1:C:202:THR:HG23	1:C:226:LEU:O	1.78	0.84
1:B:264:ALA:HB2	3:B:445:HOH:O	1.77	0.83
1:C:206:ARG:HD2	1:C:214:PRO:HA	1.60	0.83
1:B:273:ASP:HB2	3:B:443:HOH:O	1.79	0.83
1:B:26:ALA:HB1	1:B:29:ILE:H	1.40	0.83
1:C:206:ARG:HD3	1:C:218:GLU:OE1	1.78	0.83
1:C:150:ASN:HD22	1:C:155:THR:CG2	1.91	0.82
1:A:135:SER:OG	1:A:159:HIS:HE1	1.62	0.82
1:B:154:LYS:HE3	3:B:439:HOH:O	1.79	0.82
1:B:115:LYS:HD3	3:B:447:HOH:O	1.78	0.82
1:A:225:GLU:O	1:A:288:ARG:NH2	2.13	0.82
1:A:220:GLY:HA3	3:A:553:HOH:O	1.80	0.81
1:B:9:PRO:HB3	3:B:370:HOH:O	1.79	0.80
1:B:29:ILE:HG12	1:B:254:MET:CE	2.12	0.80
1:A:208:ALA:HB2	3:A:452:HOH:O	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:VAL:HG11	1:B:183:THR:HB	1.62	0.79
1:B:209:LEU:HD12	1:B:264:ALA:O	1.82	0.79
1:B:285:ASP:HB2	3:B:383:HOH:O	1.84	0.78
1:B:99:VAL:C	3:B:427:HOH:O	2.22	0.78
1:B:99:VAL:HA	3:B:427:HOH:O	1.82	0.78
1:B:49:ALA:HB2	3:B:437:HOH:O	1.83	0.78
1:C:33:LEU:HA	3:C:416:HOH:O	1.84	0.78
1:B:281:MET:C	3:B:383:HOH:O	2.21	0.77
1:B:25:LEU:HD11	1:B:100:ALA:HB3	1.66	0.77
1:C:148:LEU:HD23	3:C:482:HOH:O	1.83	0.77
1:A:138:ASN:H	1:C:128:ASN:HD21	1.33	0.77
1:A:27:ARG:HH21	1:A:45:ASN:HD21	1.33	0.76
1:C:72:ASN:HD22	1:C:74:SER:H	1.33	0.76
1:C:280:LYS:O	1:C:284:THR:HG23	1.86	0.75
1:A:207:SER:HA	1:A:208:ALA:HB3	1.68	0.75
1:A:46:ARG:O	3:A:441:HOH:O	2.05	0.75
1:B:293:THR:HG23	3:B:367:HOH:O	1.86	0.74
1:B:28:LEU:HB2	3:B:410:HOH:O	1.87	0.74
1:C:226:LEU:CB	3:C:482:HOH:O	2.15	0.73
1:B:25:LEU:HD13	1:B:25:LEU:O	1.88	0.73
1:B:209:LEU:CD1	1:B:264:ALA:O	2.37	0.73
1:B:288:ARG:O	3:B:426:HOH:O	2.06	0.72
1:B:104:SER:H	1:B:202:THR:CG2	2.02	0.72
1:B:209:LEU:HB2	1:B:267:GLY:HA2	1.72	0.72
1:A:128:ASN:O	1:A:129:THR:HG23	1.91	0.71
1:C:210:LEU:HB3	1:C:213:VAL:HG13	1.71	0.71
1:B:100:ALA:HB1	1:B:268:TYR:CD1	2.26	0.70
1:B:217:ALA:O	1:B:220:GLY:HA2	1.91	0.70
1:A:207:SER:HA	1:A:208:ALA:CB	2.20	0.70
1:B:218:GLU:CB	3:B:449:HOH:O	2.15	0.70
1:A:277:VAL:O	1:A:281:MET:HG3	1.92	0.69
1:C:235:PRO:O	1:C:238:THR:HG23	1.93	0.69
1:A:72:ASN:HD22	1:A:74:SER:H	1.38	0.69
1:B:297:GLY:HA2	3:B:438:HOH:O	1.91	0.68
1:B:29:ILE:HG12	1:B:254:MET:HE1	1.74	0.68
1:C:277:VAL:O	1:C:281:MET:HG3	1.92	0.68
1:C:104:SER:H	1:C:202:THR:HG22	1.60	0.67
1:B:11:ASP:OD1	1:B:44:GLU:OE2	2.12	0.67
1:B:7:ASN:HB3	3:B:425:HOH:O	1.95	0.67
1:B:248:ASP:O	1:B:252:LYS:HG2	1.96	0.66
1:B:99:VAL:CA	3:B:427:HOH:O	2.41	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:PHE:HA	3:B:426:HOH:O	1.94	0.66
1:C:202:THR:CG2	1:C:226:LEU:O	2.44	0.66
1:B:26:ALA:HB1	1:B:29:ILE:N	2.11	0.66
1:C:281:MET:HE3	3:C:474:HOH:O	1.95	0.65
1:B:100:ALA:HB1	1:B:268:TYR:HD1	1.60	0.65
1:B:206:ARG:NH1	3:B:416:HOH:O	2.29	0.65
1:B:188:ILE:O	1:B:192:LYS:HG2	1.96	0.65
1:A:208:ALA:CB	3:A:452:HOH:O	2.42	0.65
1:B:261:LYS:O	1:B:265:ASP:HB2	1.96	0.65
1:B:277:VAL:HB	3:B:393:HOH:O	1.96	0.65
1:B:16:PHE:C	3:B:406:HOH:O	2.34	0.65
1:C:150:ASN:HD21	1:C:157:MET:H	1.44	0.65
1:C:281:MET:HB3	3:C:474:HOH:O	1.96	0.64
1:B:26:ALA:C	3:B:417:HOH:O	2.34	0.64
1:B:38:GLY:C	3:B:436:HOH:O	2.35	0.64
1:B:259:VAL:O	3:B:400:HOH:O	2.15	0.64
1:B:46:ARG:O	3:B:376:HOH:O	2.14	0.64
1:C:285:ASP:OD1	1:C:288:ARG:HD3	1.96	0.64
1:C:159:HIS:HD2	3:C:358:HOH:O	1.80	0.64
1:B:257:ASP:O	1:B:261:LYS:HB2	1.99	0.63
1:B:135:SER:N	3:B:369:HOH:O	2.24	0.63
1:C:220:GLY:HA3	3:C:439:HOH:O	1.98	0.63
1:B:24:MET:O	1:B:26:ALA:HA	1.99	0.63
1:B:31:ASN:HB2	3:B:409:HOH:O	1.98	0.63
1:C:215:THR:HG22	1:C:218:GLU:H	1.64	0.63
1:C:72:ASN:ND2	1:C:74:SER:H	1.96	0.62
1:B:26:ALA:HB3	1:B:29:ILE:H	1.62	0.62
1:B:115:LYS:HG2	3:B:362:HOH:O	1.98	0.62
1:C:215:THR:CG2	1:C:218:GLU:H	2.12	0.62
1:B:24:MET:SD	1:B:25:LEU:HB2	2.40	0.62
1:B:29:ILE:HG12	1:B:254:MET:HE3	1.81	0.62
1:B:188:ILE:HD13	1:B:209:LEU:HB3	1.81	0.62
1:B:16:PHE:CA	3:B:406:HOH:O	2.48	0.61
1:C:104:SER:H	1:C:202:THR:CG2	2.12	0.61
1:B:164:GLY:O	1:B:165:CYS:HB2	2.01	0.61
1:B:282:VAL:N	3:B:383:HOH:O	2.32	0.61
1:B:132:THR:HA	1:B:158:VAL:O	2.01	0.61
1:C:112:SER:HB2	3:C:484:HOH:O	2.00	0.60
1:B:214:PRO:HB2	3:B:449:HOH:O	2.00	0.60
1:B:26:ALA:HB1	1:B:28:LEU:H	1.62	0.60
1:A:150:ASN:HD21	1:A:157:MET:H	1.47	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:HIS:NE2	3:B:317:HOH:O	2.30	0.60
1:B:50:SER:HB3	1:B:78:ASN:HD21	1.67	0.59
1:B:214:PRO:CB	3:B:449:HOH:O	2.51	0.59
1:B:210:LEU:HB3	1:B:213:VAL:HG13	1.83	0.59
1:B:289:PHE:CA	3:B:426:HOH:O	2.50	0.59
1:A:72:ASN:ND2	1:A:74:SER:H	2.01	0.58
1:C:155:THR:HG21	3:C:410:HOH:O	2.03	0.58
1:A:16:PHE:O	3:A:523:HOH:O	2.16	0.58
1:B:166:GLY:O	1:B:170:ASN:HB2	2.04	0.58
1:B:25:LEU:HD11	1:B:100:ALA:CB	2.34	0.58
1:B:215:THR:HG22	1:B:218:GLU:N	2.08	0.58
1:B:24:MET:C	1:B:26:ALA:HA	2.24	0.58
1:C:95:ALA:H	1:C:279:GLN:HE21	1.51	0.58
1:B:46:ARG:CZ	3:B:340:HOH:O	2.52	0.57
1:C:253:VAL:HG12	1:C:254:MET:HE2	1.84	0.57
1:A:27:ARG:HH21	1:A:45:ASN:ND2	2.02	0.57
1:B:215:THR:CG2	1:B:218:GLU:H	2.11	0.57
1:A:173:LEU:HD11	3:A:554:HOH:O	2.05	0.56
1:A:263:LEU:HD23	1:A:270:THR:HG22	1.87	0.56
1:B:101:TYR:O	1:B:268:TYR:HA	2.05	0.56
1:A:129:THR:HA	3:A:493:HOH:O	2.05	0.56
1:B:247:TYR:OH	1:B:272:SER:HB3	2.06	0.56
1:B:290:SER:HA	1:B:293:THR:HG22	1.88	0.56
1:B:165:CYS:N	3:B:357:HOH:O	2.21	0.56
1:B:289:PHE:C	3:B:426:HOH:O	2.43	0.56
1:B:26:ALA:HB3	1:B:29:ILE:HG13	1.87	0.55
1:A:154:LYS:HE2	3:A:514:HOH:O	2.06	0.55
1:C:120:LEU:C	1:C:120:LEU:HD23	2.27	0.55
1:A:210:LEU:CB	1:A:213:VAL:CG1	2.76	0.55
1:B:13:ILE:HD13	1:B:44:GLU:HG3	1.88	0.54
1:B:202:THR:HG23	1:B:226:LEU:O	2.07	0.54
1:A:245:LYS:HG3	3:A:409:HOH:O	2.06	0.54
1:B:144:LEU:HD11	3:B:430:HOH:O	2.07	0.54
1:C:95:ALA:H	1:C:279:GLN:NE2	2.06	0.54
1:A:135:SER:OG	1:A:159:HIS:CE1	2.53	0.53
1:C:9:PRO:CB	1:C:40:THR:O	2.46	0.53
1:B:265:ASP:HA	3:B:384:HOH:O	2.07	0.53
1:A:138:ASN:H	1:C:128:ASN:ND2	2.03	0.53
1:B:292:LEU:CB	3:B:426:HOH:O	2.32	0.53
1:C:220:GLY:CA	3:C:439:HOH:O	2.54	0.53
1:C:289:PHE:O	1:C:293:THR:HB	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ARG:NH2	3:A:353:HOH:O	2.41	0.53
1:B:212:GLU:CB	3:B:387:HOH:O	2.56	0.53
1:A:206:ARG:HD3	1:A:218:GLU:OE1	2.09	0.53
1:C:135:SER:OG	1:C:159:HIS:HE1	1.92	0.53
1:C:200:ALA:HA	1:C:214:PRO:O	2.08	0.53
1:B:256:ARG:HB3	3:B:374:HOH:O	2.07	0.53
1:B:167:PRO:HA	1:B:170:ASN:HB3	1.90	0.52
1:B:258:ASP:CB	3:B:374:HOH:O	2.35	0.52
1:B:134:GLY:HA2	1:B:160:VAL:O	2.10	0.51
1:B:95:ALA:HB1	1:B:278:PHE:CD2	2.45	0.51
1:B:104:SER:H	1:B:202:THR:HG22	1.73	0.51
1:C:195:LYS:HE2	3:C:443:HOH:O	2.09	0.51
1:C:173:LEU:HD22	1:C:195:LYS:HE3	1.93	0.51
1:B:150:ASN:HD21	1:B:157:MET:H	1.59	0.51
1:C:217:ALA:O	1:C:220:GLY:HA2	2.10	0.51
1:B:276:GLU:HB2	3:B:338:HOH:O	2.11	0.51
1:B:282:VAL:CA	3:B:383:HOH:O	2.59	0.51
1:C:148:LEU:CD2	3:C:482:HOH:O	2.49	0.51
1:A:173:LEU:CD1	3:A:554:HOH:O	2.58	0.50
1:B:216:VAL:HG12	1:B:221:VAL:HB	1.94	0.50
1:B:271:ALA:N	3:B:396:HOH:O	2.45	0.50
1:A:128:ASN:CB	3:A:504:HOH:O	2.32	0.49
1:C:82:PHE:HB2	1:C:85:LEU:HD13	1.94	0.49
1:B:105:VAL:HG12	1:B:201:VAL:HG12	1.93	0.49
1:C:79:PRO:HA	1:C:85:LEU:HD22	1.95	0.49
1:B:26:ALA:HB1	1:B:28:LEU:CA	2.41	0.49
1:B:50:SER:CB	1:B:78:ASN:HD21	2.24	0.49
1:A:260:GLN:HG3	3:A:546:HOH:O	2.12	0.49
1:B:282:VAL:HA	3:B:383:HOH:O	2.12	0.49
1:C:98:ASN:HB3	1:C:273:ASP:HB2	1.94	0.49
1:B:259:VAL:HA	3:B:400:HOH:O	2.12	0.49
1:B:293:THR:HG21	3:B:355:HOH:O	2.12	0.49
1:B:209:LEU:HD11	3:B:384:HOH:O	2.12	0.48
1:B:229:TRP:CH2	1:B:282:VAL:HG22	2.47	0.48
1:C:95:ALA:HB1	1:C:278:PHE:CD2	2.48	0.48
1:B:102:VAL:CG1	1:B:183:THR:HB	2.37	0.48
1:A:161:PRO:HB2	1:C:128:ASN:HD22	1.79	0.48
1:B:137:GLY:HA2	1:B:163:LYS:HE2	1.96	0.48
1:B:285:ASP:HA	1:B:288:ARG:HG2	1.95	0.48
1:B:184:ALA:O	1:B:188:ILE:HG13	2.14	0.47
1:C:46:ARG:NH2	3:C:374:HOH:O	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LEU:HB3	1:A:213:VAL:HG11	1.91	0.47
1:B:31:ASN:HA	3:B:452:HOH:O	2.13	0.47
1:C:299:LYS:HE2	3:C:429:HOH:O	2.14	0.47
1:B:145:ALA:HB2	3:B:356:HOH:O	2.14	0.47
1:B:47:PRO:HB3	3:B:406:HOH:O	2.15	0.47
1:C:41:ALA:N	3:C:422:HOH:O	2.47	0.47
1:A:128:ASN:C	3:A:504:HOH:O	2.53	0.46
1:B:104:SER:N	1:B:202:THR:HG22	2.30	0.46
1:B:194:GLY:HA3	3:B:415:HOH:O	2.15	0.46
1:A:242:VAL:HA	1:A:245:LYS:HE3	1.97	0.46
1:B:15:THR:OG1	1:B:71:VAL:HA	2.16	0.46
1:B:102:VAL:HG23	1:B:268:TYR:CE1	2.51	0.46
1:B:164:GLY:O	1:B:165:CYS:CB	2.64	0.46
1:B:133:TYR:HB3	1:B:179:LEU:HD23	1.97	0.46
1:C:126:GLN:HG2	3:C:481:HOH:O	2.16	0.45
1:B:204:LYS:HG3	1:B:225:GLU:OE1	2.17	0.45
1:B:32:TYR:O	1:B:33:LEU:C	2.54	0.45
1:C:195:LYS:HE3	1:C:195:LYS:HB3	1.80	0.45
1:A:33:LEU:O	1:A:36:SER:O	2.34	0.45
1:B:162:TYR:O	1:B:163:LYS:HG3	2.16	0.45
1:B:99:VAL:O	3:B:427:HOH:O	2.21	0.45
1:A:29:ILE:HG13	1:A:254:MET:HE1	1.98	0.45
1:B:98:ASN:HB2	3:B:443:HOH:O	2.01	0.45
1:A:134:GLY:HA2	1:A:160:VAL:O	2.17	0.44
1:C:150:ASN:ND2	1:C:157:MET:H	2.13	0.44
1:C:285:ASP:HA	1:C:288:ARG:HG2	1.99	0.44
1:B:7:ASN:HD22	1:B:7:ASN:C	2.21	0.44
1:A:127:THR:C	1:A:128:ASN:O	2.51	0.44
1:A:202:THR:C	3:A:521:HOH:O	2.55	0.44
1:A:252:LYS:HG2	3:A:543:HOH:O	2.17	0.44
1:B:225:GLU:O	1:B:288:ARG:NH2	2.50	0.44
1:B:34:THR:OG1	3:B:436:HOH:O	2.21	0.44
1:C:150:ASN:ND2	1:C:155:THR:CG2	2.69	0.44
1:A:150:ASN:ND2	1:A:157:MET:H	2.16	0.44
1:C:169:LEU:HA	1:C:172:VAL:HG12	2.00	0.44
1:A:36:SER:HB3	1:A:37:LEU:HD23	1.98	0.44
1:B:80:GLY:HA3	1:B:293:THR:HG21	2.00	0.44
1:C:34:THR:HG23	1:C:40:THR:HA	2.00	0.44
1:B:193:ALA:C	3:B:415:HOH:O	2.56	0.44
1:A:253:VAL:HG12	1:A:254:MET:HE2	1.99	0.43
1:A:226:LEU:O	3:A:521:HOH:O	2.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:ASN:HD22	1:C:155:THR:HG23	1.78	0.43
1:B:104:SER:H	1:B:202:THR:HG21	1.81	0.43
1:C:201:VAL:HG13	1:C:213:VAL:HG22	2.01	0.43
1:B:115:LYS:HD2	1:B:115:LYS:N	2.33	0.43
1:B:289:PHE:O	1:B:293:THR:HG22	2.19	0.43
1:B:200:ALA:HA	1:B:214:PRO:O	2.19	0.43
1:B:47:PRO:HA	3:B:406:HOH:O	2.18	0.43
1:C:150:ASN:ND2	1:C:155:THR:HG23	2.34	0.43
1:A:36:SER:O	1:A:38:GLY:N	2.49	0.43
1:B:132:THR:HG22	1:B:158:VAL:HB	2.01	0.43
1:B:162:TYR:HD2	3:B:369:HOH:O	2.01	0.42
1:A:77:VAL:HG13	1:A:144:LEU:HD11	2.00	0.42
1:B:281:MET:HB3	1:B:282:VAL:H	1.75	0.42
1:C:104:SER:N	1:C:202:THR:HG22	2.32	0.42
1:A:190:PHE:HB2	1:A:196:LEU:HD12	2.01	0.42
1:B:135:SER:O	3:B:369:HOH:O	2.21	0.42
1:B:26:ALA:CB	1:B:28:LEU:H	2.30	0.42
1:B:72:ASN:HB2	1:B:74:SER:HB3	2.01	0.42
1:B:47:PRO:CA	3:B:406:HOH:O	2.68	0.41
1:C:77:VAL:HG13	1:C:144:LEU:HD11	2.02	0.41
1:B:190:PHE:HD1	1:B:195:LYS:HD3	1.85	0.41
1:B:150:ASN:ND2	1:B:157:MET:H	2.18	0.41
1:A:252:LYS:HD3	3:A:539:HOH:O	2.20	0.41
1:C:120:LEU:HD21	1:C:157:MET:SD	2.60	0.41
1:C:299:LYS:NZ	3:C:342:HOH:O	2.49	0.41
1:C:234:VAL:HB	1:C:238:THR:HG21	2.02	0.41
1:C:72:ASN:C	1:C:72:ASN:HD22	2.24	0.41
1:B:26:ALA:HB2	1:B:28:LEU:HB3	2.02	0.41
1:B:163:LYS:HB3	3:B:390:HOH:O	2.21	0.41
1:B:197:GLN:HB2	3:B:404:HOH:O	2.19	0.41
1:B:290:SER:HA	1:B:293:THR:CG2	2.50	0.41
1:C:215:THR:HG22	1:C:218:GLU:HB3	2.02	0.41
1:C:235:PRO:O	1:C:238:THR:CG2	2.67	0.41
1:B:167:PRO:HD2	3:B:357:HOH:O	2.21	0.40
1:B:210:LEU:HB3	1:B:213:VAL:CG1	2.49	0.40
1:B:169:LEU:HD21	1:B:187:ALA:HA	2.03	0.40
1:B:104:SER:O	1:B:202:THR:HG22	2.21	0.40
1:C:102:VAL:HG12	1:C:230:HIS:HE1	1.86	0.40
1:C:238:THR:HA	1:C:239:PRO:HD3	1.89	0.40
1:B:32:TYR:HB3	3:B:407:HOH:O	2.21	0.40
1:C:33:LEU:O	1:C:35:GLU:O	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ILE:CD1	1:B:209:LEU:HB3	2.48	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:537:HOH:O	3:C:325:HOH:O[2_657]	2.02	0.18

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	294/301 (98%)	283 (96%)	6 (2%)	5 (2%)	9	2
1	B	287/301 (95%)	262 (91%)	17 (6%)	8 (3%)	5	0
1	C	294/301 (98%)	286 (97%)	8 (3%)	0	100	100
All	All	875/903 (97%)	831 (95%)	31 (4%)	13 (2%)	10	3

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	129	THR
1	B	165	CYS
1	B	209	LEU
1	B	281	MET
1	A	127	THR
1	A	208	ALA
1	B	208	ALA
1	B	282	VAL
1	A	207	SER
1	B	249	GLY

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Mol	Chain	Res	Type
1	B	275	PRO
1	B	177	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	234/238 (98%)	224 (96%)	10 (4%)	29	18
1	B	232/238 (98%)	203 (88%)	29 (12%)	4	1
1	C	233/238 (98%)	215 (92%)	18 (8%)	13	5
All	All	699/714 (98%)	642 (92%)	57 (8%)	11	4

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	37	LEU
1	A	72	ASN
1	A	125	LYS
1	A	127	THR
1	A	176	GLN
1	A	206	ARG
1	A	207	SER
1	A	213	VAL
1	A	226	LEU
1	B	7	ASN
1	B	25	LEU
1	B	27	ARG
1	B	33	LEU
1	B	34	THR
1	B	36	SER
1	B	37	LEU
1	B	46	ARG
1	B	56	ARG
1	B	73	SER

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Mol	Chain	Res	Type
1	B	112	SER
1	B	120	LEU
1	B	130	GLN
1	B	131	VAL
1	B	144	LEU
1	B	171	ASP
1	B	176	GLN
1	B	185	SER
1	B	197	GLN
1	B	206	ARG
1	B	209	LEU
1	B	213	VAL
1	B	215	THR
1	B	226	LEU
1	B	245	LYS
1	B	250	ILE
1	B	263	LEU
1	B	265	ASP
1	B	266	LEU
1	C	7	ASN
1	C	10	LEU
1	C	36	SER
1	C	39	GLN
1	C	72	ASN
1	C	120	LEU
1	C	132	THR
1	C	155	THR
1	C	202	THR
1	C	213	VAL
1	C	215	THR
1	C	226	LEU
1	C	238	THR
1	C	245	LYS
1	C	260	GLN
1	C	263	LEU
1	C	284	THR
1	C	293	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN

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Mol	Chain	Res	Type
1	A	72	ASN
1	A	78	ASN
1	A	150	ASN
1	A	159	HIS
1	A	176	GLN
1	A	197	GLN
1	B	7	ASN
1	B	45	ASN
1	B	78	ASN
1	B	150	ASN
1	B	170	ASN
1	B	176	GLN
1	B	197	GLN
1	B	219	GLN
1	C	31	ASN
1	C	45	ASN
1	C	72	ASN
1	C	78	ASN
1	C	98	ASN
1	C	128	ASN
1	C	138	ASN
1	C	150	ASN
1	C	159	HIS
1	C	170	ASN
1	C	197	GLN
1	C	219	GLN
1	C	260	GLN
1	C	279	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

2 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	#$|Z| > 2$
2	CIT	C	302	-	3,12,12	1.40	0	3,17,17	1.43	1 (33%)
2	CIT	A	302	-	3,12,12	1.31	0	3,17,17	3.38	1 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIT	C	302	-	-	1/6/16/16	-
2	CIT	A	302	-	-	0/6/16/16	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	302	CIT	C3-C2-C1	-5.29	106.51	114.98
2	C	302	CIT	C3-C2-C1	-2.08	111.65	114.98

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	302	CIT	C1-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

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(Å²)	Q<0.9
1	A	296/301 (98%)	-0.23	11 (3%)	41	44	14, 23, 39, 52	0
1	B	291/301 (96%)	1.02	57 (19%)	1	1	19, 39, 55, 64	0
1	C	296/301 (98%)	-0.23	11 (3%)	41	44	15, 24, 37, 53	0
All	All	883/903 (97%)	0.18	79 (8%)	9	11	14, 27, 52, 64	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	267	GLY	5.9
1	B	130	GLN	5.7
1	B	128	ASN	5.5
1	B	266	LEU	4.7
1	C	7	ASN	4.6
1	A	208	ALA	4.6
1	B	209	LEU	4.4
1	B	265	ASP	4.4
1	B	174	GLY	4.4
1	B	264	ALA	4.2
1	B	129	THR	4.0
1	B	300	VAL	3.9
1	B	164	GLY	3.7
1	B	126	GLN	3.7
1	B	261	LYS	3.7
1	C	84	ASN	3.6
1	B	257	ASP	3.6
1	B	84	ASN	3.5
1	C	36	SER	3.5
1	C	38	GLY	3.5
1	B	137	GLY	3.4
1	A	129	THR	3.4
1	B	35	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	40	THR	3.3
1	B	193	ALA	3.2
1	B	259	VAL	3.2
1	B	127	THR	3.2
1	B	31	ASN	3.1
1	B	136	CYS	3.1
1	B	165	CYS	3.0
1	B	32	TYR	3.0
1	A	7	ASN	3.0
1	C	35	GLU	2.9
1	A	37	LEU	2.9
1	C	9	PRO	2.9
1	B	140	THR	2.9
1	B	263	LEU	2.8
1	B	83	ARG	2.8
1	B	262	LYS	2.8
1	B	295	GLN	2.8
1	B	73	SER	2.7
1	A	38	GLY	2.7
1	B	99	VAL	2.7
1	A	127	THR	2.7
1	B	301	ASP	2.7
1	A	207	SER	2.6
1	B	176	GLN	2.6
1	C	39	GLN	2.6
1	A	36	SER	2.6
1	A	35	GLU	2.5
1	B	138	ASN	2.5
1	B	26	ALA	2.5
1	B	249	GLY	2.5
1	B	170	ASN	2.5
1	B	36	SER	2.4
1	B	197	GLN	2.4
1	B	34	THR	2.4
1	B	258	ASP	2.4
1	B	25	LEU	2.4
1	B	171	ASP	2.4
1	B	270	THR	2.4
1	C	34	THR	2.4
1	B	16	PHE	2.3
1	B	167	PRO	2.3
1	B	110	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	289	PHE	2.2
1	B	166	GLY	2.2
1	B	208	ALA	2.2
1	B	277	VAL	2.2
1	B	49	ALA	2.1
1	B	5	PHE	2.1
1	C	37	LEU	2.1
1	C	6	PRO	2.1
1	C	40	THR	2.1
1	B	40	THR	2.1
1	A	128	ASN	2.1
1	B	195	LYS	2.0
1	B	111	GLY	2.0
1	B	269	SER	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 carbohydrates 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CIT	C	302	13/13	0.88	0.15	37,40,41,42	0
2	CIT	A	302	13/13	0.92	0.14	29,34,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.