Worldwide PDB

Full wwPDB X-ray Structure Validation Report (i)

May 26, 2020 – 12:12 pm BST

PDB ID	:	1ZLP
Title	:	Petal death protein PSR132 with cysteine-linked glutaraldehyde forming a thiohemiacetal adduct
Authors	:	Teplyakov, A.; Liu, S.; Lu, Z.; Howard, A.; Dunaway-Mariano, D.; Herzberg, O.
Deposited on	:	2005-05-08
Resolution	:	2.70 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:

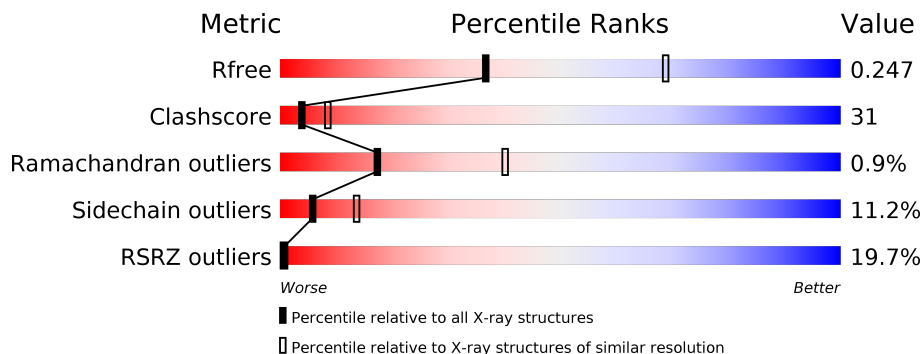|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.247
Clashscore		31
Ramachandran outliers		0.9%
Sidechain outliers		11.2%
RSRZ outliers		19.7%

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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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	318	14% / 49% 35% 5% · 11%
1	B	318	21% / 50% 32% 8% 10%

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
2	MG	B	401	-	-	-	X
3	GAQ	A	402	-	-	X	X
3	GAQ	B	402	-	-	X	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4411 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 petal death protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2159	1364	375	409	11			
1	B	285	Total	C	N	O	S	0	0	0
			2167	1368	377	411	11			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is 5-HYDROXYPENTANAL (three-letter code: GAQ) (formula: $C_5H_{10}O_2$).
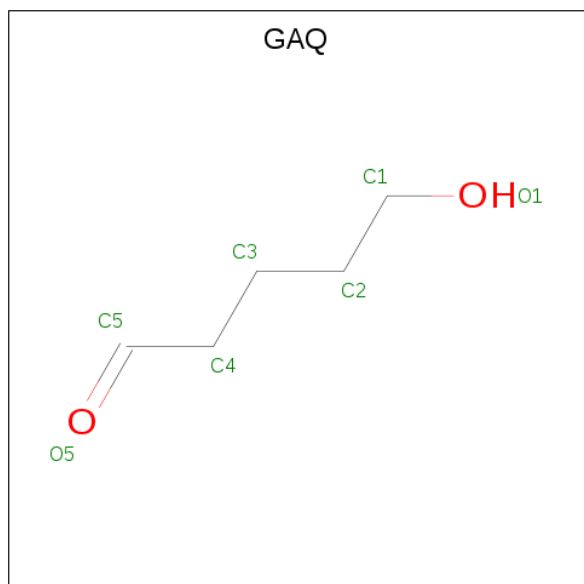
| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 7	C 5	O 2	0	0
3	B	1	Total 7	C 5	O 2	0	0

- Molecule 4 is water.

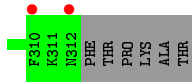| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	38	Total 38	O 38	0	0
4	B	31	Total 31	O 31	0	0

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: petal death protein
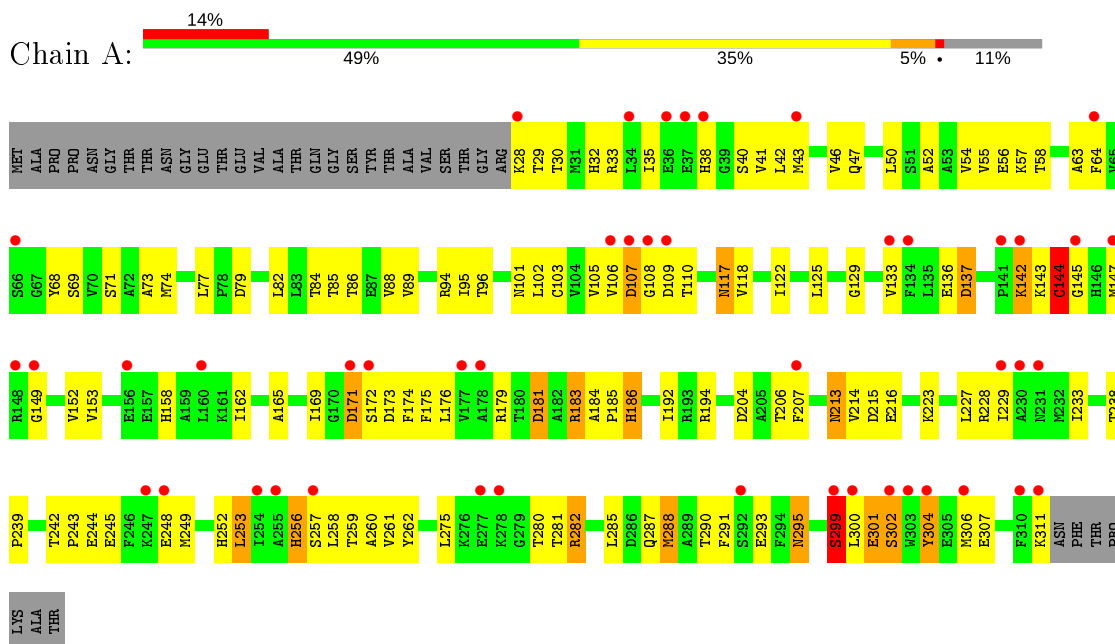
- Molecule 1: petal death protein
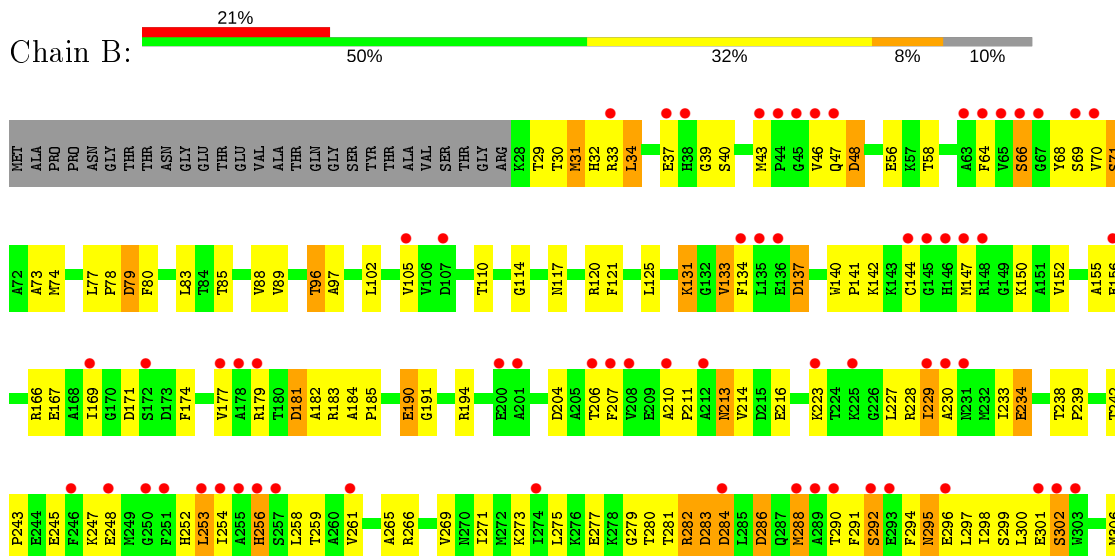
F310 K311 N312 PHE THR PRO LYS ALA THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	156.19Å　　156.19Å　　75.05Å 90.00°　　90.00°　　120.00°	Depositor
Resolution (Å)	10.00　–　2.70 29.52　–　2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (10.00-2.70) 90.2 (29.52-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.88 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.195　,　0.250 0.205　,　0.247	Depositor DCC
R_{free} test set	2045 reflections (7.77%)	wwPDB-VP
Wilson B-factor (Å^2)	57.0	Xtriage
Anisotropy	1.144	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 89.5	EDS
L-test for twinning[2]	$<|L|> = 0.51, <L^2> = 0.35$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4411	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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: MG, GAQ

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	0.62	0/2198	0.89	8/2969 (0.3%)
1	B	0.46	0/2206	0.77	7/2980 (0.2%)
All	All	0.54	0/4404	0.83	15/5949 (0.3%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	ASP	CB-CG-OD2	6.38	124.05	118.30
1	A	181	ASP	CB-CG-OD1	6.26	123.94	118.30
1	A	79	ASP	CB-CG-OD2	6.26	123.93	118.30
1	A	299	SER	N-CA-C	6.14	127.58	111.00
1	A	215	ASP	CB-CG-OD2	5.94	123.65	118.30
1	A	299	SER	N-CA-CB	-5.94	101.59	110.50
1	A	171	ASP	CB-CG-OD2	5.91	123.62	118.30
1	B	137	ASP	CB-CG-OD2	5.63	123.37	118.30
1	B	79	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	283	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	204	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	137	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	181	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	286	ASP	CB-CG-OD2	5.09	122.89	118.30
1	B	171	ASP	CB-CG-OD2	5.04	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2159	0	2164	136	0
1	B	2167	0	2170	132	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	7	0	9	6	0
3	B	7	0	9	5	0
4	A	38	0	0	4	0
4	B	31	0	0	1	0
All	All	4411	0	4352	267	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 31.

All (267) 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:29:THR:HG22	1:A:32:HIS:CD2	1.66	1.28
1:A:43:MET:CE	1:A:105:VAL:HB	1.65	1.26
1:A:43:MET:HE3	1:A:105:VAL:HB	1.33	1.06
1:A:29:THR:CG2	1:A:32:HIS:CD2	2.43	1.01
1:A:295:ASN:HD22	1:A:295:ASN:N	1.58	1.00
1:A:142:LYS:HE3	1:A:143:LYS:O	1.65	0.96
1:B:280:THR:HG22	1:B:282:ARG:H	1.30	0.94
1:A:43:MET:HE1	1:A:105:VAL:HB	1.49	0.93
1:A:213:ASN:HD22	1:A:213:ASN:C	1.72	0.93
1:A:47:GLN:HB3	1:A:69:SER:HB3	1.52	0.88
1:A:29:THR:CG2	1:A:32:HIS:HD2	1.82	0.88
1:B:69:SER:OG	1:B:261:VAL:HG21	1.74	0.88
1:B:254:ILE:HD12	1:B:254:ILE:N	1.89	0.87
1:B:280:THR:CG2	1:B:282:ARG:HB3	2.06	0.86
1:B:281:THR:HG21	1:B:288:MET:SD	2.16	0.86
1:A:295:ASN:H	1:A:295:ASN:HD22	1.19	0.85
1:A:145:GLY:H	3:A:402:GAQ:H31	1.43	0.83
1:A:228:ARG:H	1:A:252:HIS:CD2	1.96	0.83
1:B:133:VAL:HG22	1:B:174:PHE:CE2	2.13	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ASP:HB3	1:A:152:VAL:HG22	1.59	0.83
1:B:40:SER:HB3	1:B:254:ILE:HD11	1.60	0.82
1:B:265:ALA:O	1:B:269:VAL:HG23	1.78	0.81
1:B:295:ASN:HD22	1:B:300:LEU:HD22	1.46	0.80
1:A:227:LEU:HA	1:A:252:HIS:CD2	2.17	0.80
1:B:233:ILE:HD11	3:B:402:GAQ:H32	1.63	0.80
1:B:256:HIS:HD2	1:B:259:THR:OG1	1.65	0.79
1:B:30:THR:O	1:B:34:LEU:HB2	1.82	0.79
1:A:43:MET:HE3	1:A:105:VAL:CB	2.13	0.79
1:A:29:THR:HG22	1:A:32:HIS:HD2	1.06	0.79
1:B:133:VAL:HG22	1:B:174:PHE:HE2	1.49	0.78
1:B:227:LEU:HA	1:B:252:HIS:CD2	2.21	0.76
1:A:295:ASN:ND2	1:A:295:ASN:N	2.31	0.76
1:B:292:SER:O	1:B:296:GLU:CB	2.35	0.75
1:B:280:THR:HG21	1:B:282:ARG:HB3	1.69	0.74
1:B:229:ILE:CG2	1:B:230:ALA:N	2.49	0.73
1:A:144:CYS:SG	1:A:145:GLY:N	2.60	0.73
1:B:133:VAL:CG2	1:B:174:PHE:HE2	2.01	0.73
1:B:280:THR:HG22	1:B:282:ARG:N	2.04	0.73
1:A:295:ASN:H	1:A:295:ASN:ND2	1.82	0.72
1:B:299:SER:HB3	1:B:302:SER:HB3	1.71	0.72
1:B:152:VAL:HB	1:B:194:ARG:NH2	2.06	0.71
1:B:184:ALA:HB3	1:B:185:PRO:HD3	1.73	0.71
1:B:227:LEU:HD23	1:B:252:HIS:CD2	2.26	0.71
1:B:190:GLU:OE1	1:B:190:GLU:HA	1.91	0.71
1:B:190:GLU:OE2	1:B:194:ARG:HD2	1.91	0.71
1:B:280:THR:HG22	1:B:282:ARG:HB3	1.71	0.70
1:B:229:ILE:HG13	1:B:253:LEU:HB3	1.72	0.70
1:B:295:ASN:HB3	1:B:300:LEU:HB2	1.72	0.70
1:A:301:GLU:HA	1:A:301:GLU:OE1	1.90	0.70
1:A:29:THR:HG23	1:A:32:HIS:H	1.57	0.70
1:A:213:ASN:C	1:A:213:ASN:ND2	2.46	0.69
1:A:29:THR:HG22	1:A:32:HIS:CG	2.26	0.69
1:B:47:GLN:HB3	1:B:69:SER:HB3	1.74	0.69
1:B:56:GLU:HB2	1:B:102:LEU:HG	1.75	0.69
1:B:69:SER:OG	1:B:261:VAL:CG2	2.41	0.68
1:A:158:HIS:O	1:A:162:ILE:HG12	1.95	0.67
1:A:145:GLY:N	3:A:402:GAQ:H31	2.10	0.66
1:A:133:VAL:HG13	1:A:174:PHE:CZ	2.30	0.66
1:A:71:SER:HB3	1:A:77:LEU:O	1.95	0.65
1:B:294:PHE:O	1:B:297:LEU:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:SER:O	1:B:296:GLU:HB2	1.95	0.65
1:A:233:ILE:CD1	3:A:402:GAQ:H22	2.27	0.64
1:A:144:CYS:HB3	1:A:147:MET:HG3	1.78	0.64
1:B:179:ARG:HD2	1:B:207:PHE:CE2	2.33	0.64
1:A:106:VAL:HG21	1:A:125:LEU:HD22	1.80	0.64
1:A:281:THR:HG22	1:A:285:LEU:HD23	1.80	0.64
1:B:96:THR:HG22	1:B:97:ALA:N	2.13	0.64
1:B:291:PHE:N	1:B:291:PHE:HD1	1.97	0.63
1:B:298:ILE:O	1:B:299:SER:HB2	1.96	0.63
1:A:290:THR:HB	1:A:293:GLU:HB2	1.80	0.63
1:A:133:VAL:HG13	1:A:174:PHE:HZ	1.62	0.62
1:A:213:ASN:ND2	1:A:216:GLU:H	1.97	0.62
1:B:292:SER:O	1:B:296:GLU:HB3	1.98	0.62
1:B:177:VAL:HG13	1:B:229:ILE:HD13	1.82	0.62
1:B:227:LEU:HA	1:B:252:HIS:HD2	1.62	0.61
1:B:291:PHE:N	1:B:291:PHE:CD1	2.65	0.61
1:A:142:LYS:CE	1:A:143:LYS:O	2.46	0.61
1:B:58:THR:HG22	1:B:58:THR:O	2.00	0.61
1:B:256:HIS:CD2	1:B:259:THR:OG1	2.52	0.61
1:A:153:VAL:O	1:A:194:ARG:NH2	2.34	0.61
1:A:84:THR:O	1:A:88:VAL:HG23	2.00	0.60
1:B:69:SER:CB	1:B:261:VAL:HG21	2.32	0.60
1:A:192:ILE:HD13	1:A:223:LYS:HB2	1.83	0.60
1:A:260:ALA:HB3	4:A:405:HOH:O	2.01	0.60
1:A:228:ARG:H	1:A:252:HIS:HD2	1.46	0.59
1:B:152:VAL:HB	1:B:194:ARG:HH21	1.67	0.59
1:B:295:ASN:O	1:B:299:SER:N	2.34	0.59
1:A:144:CYS:HB3	1:A:147:MET:CG	2.33	0.58
1:B:182:ALA:HB3	1:B:191:GLY:HA2	1.85	0.58
1:B:253:LEU:C	1:B:254:ILE:HD12	2.23	0.58
1:B:71:SER:HB3	1:B:77:LEU:O	2.02	0.58
1:A:152:VAL:CG1	1:A:194:ARG:NH2	2.67	0.58
1:B:301:GLU:HA	1:B:301:GLU:OE1	2.04	0.58
1:B:213:ASN:ND2	1:B:216:GLU:H	2.01	0.58
1:B:229:ILE:HG22	1:B:230:ALA:N	2.18	0.58
1:B:43:MET:HE1	1:B:105:VAL:HG21	1.85	0.58
1:A:295:ASN:O	1:A:299:SER:N	2.37	0.58
1:A:280:THR:HG23	1:A:282:ARG:HB3	1.86	0.57
1:B:229:ILE:HG23	1:B:230:ALA:H	1.69	0.57
1:A:184:ALA:HB3	1:A:185:PRO:HD3	1.87	0.57
1:A:64:PHE:CZ	1:A:107:ASP:HB2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:THR:HB	4:B:405:HOH:O	2.03	0.57
1:A:184:ALA:HB3	1:A:185:PRO:CD	2.34	0.57
1:B:238:THR:CG2	1:B:239:PRO:HD2	2.34	0.57
1:B:254:ILE:N	1:B:254:ILE:CD1	2.61	0.57
1:A:259:THR:HB	4:A:404:HOH:O	2.04	0.57
1:B:238:THR:HG23	1:B:239:PRO:HD2	1.87	0.57
1:A:117:ASN:HD22	1:A:117:ASN:H	1.51	0.57
1:B:133:VAL:CG2	1:B:174:PHE:CE2	2.83	0.57
1:A:143:LYS:HD2	1:A:149:GLY:O	2.05	0.56
1:A:58:THR:O	1:A:58:THR:HG22	2.05	0.56
1:B:229:ILE:HG23	1:B:230:ALA:N	2.20	0.56
1:A:281:THR:HG21	1:A:288:MET:HE2	1.87	0.56
1:B:117:ASN:HD22	1:B:117:ASN:H	1.53	0.56
1:B:290:THR:O	1:B:294:PHE:N	2.34	0.56
1:B:66:SER:O	1:B:70:VAL:HG23	2.05	0.56
1:B:295:ASN:HB3	1:B:300:LEU:CB	2.36	0.55
1:B:29:THR:HG22	1:B:30:THR:N	2.20	0.55
1:B:29:THR:HG22	1:B:31:MET:H	1.70	0.55
1:A:125:LEU:HD13	1:A:133:VAL:CG1	2.36	0.55
1:B:284:ASP:OD1	1:B:284:ASP:N	2.33	0.55
1:A:56:GLU:HB2	1:A:102:LEU:HG	1.89	0.55
1:A:142:LYS:C	1:A:142:LYS:HD3	2.27	0.55
1:B:47:GLN:CB	1:B:69:SER:HB3	2.37	0.55
1:B:213:ASN:C	1:B:213:ASN:HD22	2.10	0.54
1:A:179:ARG:HD2	1:A:207:PHE:CE2	2.42	0.54
1:A:213:ASN:HD21	1:A:216:GLU:H	1.54	0.53
1:A:43:MET:CE	1:A:105:VAL:CB	2.60	0.53
1:B:140:TRP:CD2	1:B:141:PRO:HA	2.42	0.53
1:A:69:SER:HA	1:A:261:VAL:HG21	1.89	0.53
1:A:176:LEU:HB3	1:A:204:ASP:OD1	2.09	0.53
1:B:166:ARG:HD3	1:B:166:ARG:O	2.08	0.53
1:A:47:GLN:HG3	1:A:73:ALA:HB2	1.91	0.53
1:B:40:SER:CB	1:B:254:ILE:HD11	2.36	0.53
1:A:183:ARG:NH1	1:A:216:GLU:OE1	2.41	0.52
1:B:70:VAL:O	1:B:74:MET:HB3	2.09	0.52
1:B:295:ASN:N	1:B:295:ASN:OD1	2.42	0.52
1:A:306:MET:HE3	1:B:167:GLU:OE1	2.10	0.52
1:B:179:ARG:NH1	3:B:402:GAQ:O5	2.43	0.52
1:B:258:LEU:HD11	3:B:402:GAQ:O1	2.10	0.51
1:A:162:ILE:O	1:A:165:ALA:HB3	2.11	0.51
1:B:85:THR:O	1:B:89:VAL:HG23	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:THR:HG21	1:A:175:PHE:HD1	1.76	0.51
1:B:210:ALA:N	1:B:211:PRO:HD3	2.26	0.51
1:B:83:LEU:HD21	1:B:88:VAL:HG12	1.92	0.51
1:B:227:LEU:CD2	1:B:252:HIS:CD2	2.93	0.51
1:A:299:SER:HB3	1:A:302:SER:HB3	1.93	0.50
1:A:136:GLU:HG3	4:A:412:HOH:O	2.11	0.50
1:A:228:ARG:N	1:A:252:HIS:CD2	2.75	0.50
1:A:96:THR:HG21	1:A:129:GLY:HA3	1.93	0.50
1:B:78:PRO:O	1:B:80:PHE:N	2.43	0.50
1:A:106:VAL:HG21	1:A:125:LEU:CD2	2.41	0.50
1:A:227:LEU:HA	1:A:252:HIS:HD2	1.73	0.50
1:A:229:ILE:HG13	1:A:253:LEU:HB3	1.93	0.50
1:A:43:MET:HE1	1:A:105:VAL:CB	2.33	0.50
1:B:117:ASN:ND2	1:B:117:ASN:H	2.09	0.50
1:A:47:GLN:HB3	1:A:69:SER:CB	2.35	0.50
1:B:242:THR:N	1:B:245:GLU:OE1	2.38	0.50
1:B:177:VAL:CG1	1:B:229:ILE:HD13	2.42	0.49
1:B:43:MET:SD	1:B:64:PHE:HB2	2.52	0.49
1:A:30:THR:HA	1:A:33:ARG:NH1	2.27	0.49
1:B:152:VAL:CG2	1:B:194:ARG:NH2	2.75	0.49
1:B:228:ARG:H	1:B:252:HIS:CD2	2.30	0.49
1:A:238:THR:HG23	1:A:239:PRO:HD2	1.95	0.49
1:B:282:ARG:HG2	1:B:283:ASP:N	2.25	0.49
1:A:85:THR:O	1:A:89:VAL:HG23	2.13	0.49
1:A:68:TYR:CD1	1:A:258:LEU:HD22	2.47	0.49
1:A:47:GLN:CB	1:A:69:SER:HB3	2.34	0.49
1:B:288:MET:CE	1:B:288:MET:N	2.76	0.48
1:B:33:ARG:O	1:B:37:GLU:HG3	2.13	0.48
1:B:179:ARG:HH12	3:B:402:GAQ:H42	1.78	0.48
1:B:43:MET:CE	1:B:105:VAL:HG21	2.43	0.48
1:B:227:LEU:CA	1:B:252:HIS:HD2	2.26	0.48
1:A:290:THR:CG2	1:A:291:PHE:N	2.77	0.48
1:B:47:GLN:O	1:B:48:ASP:HB3	2.13	0.48
1:A:244:GLU:CD	1:A:244:GLU:H	2.17	0.48
1:B:290:THR:HG22	1:B:291:PHE:H	1.78	0.48
1:A:233:ILE:CD1	3:A:402:GAQ:C2	2.92	0.48
1:B:68:TYR:CD2	1:B:79:ASP:HB2	2.49	0.48
1:B:144:CYS:HB3	1:B:147:MET:SD	2.53	0.47
1:B:288:MET:H	1:B:288:MET:HE3	1.78	0.47
1:B:295:ASN:ND2	1:B:300:LEU:HD22	2.23	0.47
1:B:297:LEU:HD23	1:B:297:LEU:HA	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:PHE:CE1	1:B:125:LEU:HD21	2.50	0.47
1:A:256:HIS:HD2	1:A:259:THR:OG1	1.98	0.47
1:A:280:THR:CG2	1:A:282:ARG:HB3	2.44	0.46
1:A:46:VAL:HG23	1:A:55:VAL:HG21	1.97	0.46
1:A:307:GLU:OE1	1:A:311:LYS:HE3	2.15	0.46
1:A:110:THR:CG2	1:A:110:THR:O	2.63	0.46
1:B:131:LYS:O	1:B:174:PHE:HA	2.15	0.46
1:B:279:GLY:O	1:B:280:THR:OG1	2.31	0.46
1:A:101:ASN:O	1:A:102:LEU:C	2.52	0.46
1:A:233:ILE:HD13	3:A:402:GAQ:H22	1.97	0.46
1:A:29:THR:HG21	1:A:32:HIS:CD2	2.45	0.46
1:B:156:GLU:H	1:B:156:GLU:CD	2.18	0.46
1:A:290:THR:HG22	1:A:291:PHE:N	2.31	0.46
1:B:39:GLY:HA3	1:B:247:LYS:HD2	1.96	0.46
1:A:227:LEU:CA	1:A:252:HIS:HD2	2.29	0.46
1:A:125:LEU:HD13	1:A:133:VAL:HG12	1.98	0.46
1:A:43:MET:HE2	1:A:63:ALA:O	2.15	0.45
1:A:117:ASN:ND2	1:A:117:ASN:H	2.15	0.45
1:B:47:GLN:HG3	1:B:73:ALA:CB	2.46	0.45
1:A:57:LYS:HD3	1:A:57:LYS:C	2.37	0.45
1:A:118:VAL:O	1:A:122:ILE:HG12	2.17	0.45
1:B:288:MET:N	1:B:288:MET:HE2	2.31	0.45
1:A:300:LEU:O	1:A:304:TYR:HD2	1.99	0.45
1:A:301:GLU:CA	1:A:301:GLU:OE1	2.58	0.45
1:B:31:MET:CE	1:B:253:LEU:HD21	2.47	0.45
1:A:281:THR:HG21	1:A:288:MET:CE	2.46	0.45
1:A:108:GLY:O	1:A:109:ASP:C	2.54	0.45
1:A:137:ASP:HB2	1:A:181:ASP:H	1.81	0.45
1:A:152:VAL:HG13	1:A:194:ARG:NH2	2.31	0.45
1:A:242:THR:HB	1:A:243:PRO:HD2	1.99	0.45
1:A:245:GLU:O	1:A:248:GLU:HB2	2.17	0.44
1:B:134:PHE:CE1	1:B:177:VAL:HG21	2.52	0.44
1:A:291:PHE:O	1:A:295:ASN:ND2	2.51	0.44
1:B:299:SER:O	1:B:300:LEU:C	2.55	0.44
1:B:137:ASP:HB2	1:B:181:ASP:H	1.82	0.44
1:B:234:GLU:HG2	1:B:234:GLU:H	1.44	0.44
1:A:171:ASP:O	1:A:172:SER:C	2.56	0.44
1:A:253:LEU:HA	1:A:253:LEU:HD23	1.85	0.44
1:A:109:ASP:HB3	1:A:142:LYS:HG2	2.00	0.44
1:A:43:MET:HE3	1:A:105:VAL:CG2	2.48	0.44
1:A:228:ARG:N	1:A:252:HIS:HD2	2.12	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:GLY:H	1:B:117:ASN:ND2	2.16	0.43
1:B:31:MET:HE1	1:B:253:LEU:HD21	2.00	0.43
1:A:214:VAL:HG22	1:A:249:MET:HE1	2.00	0.43
1:A:82:LEU:HA	1:A:82:LEU:HD23	1.74	0.43
1:B:152:VAL:CB	1:B:194:ARG:NH2	2.78	0.43
1:B:245:GLU:O	1:B:248:GLU:HB2	2.18	0.43
1:A:258:LEU:CB	1:A:262:TYR:CE2	3.01	0.43
1:A:137:ASP:HB3	1:A:152:VAL:CG2	2.39	0.43
1:A:52:ALA:HB2	1:A:95:ILE:HG23	2.00	0.43
1:A:74:MET:HE2	1:A:94:ARG:HH12	1.83	0.43
1:B:169:ILE:CD1	1:B:174:PHE:HD2	2.31	0.43
1:B:253:LEU:HA	1:B:253:LEU:HD23	1.80	0.43
1:A:69:SER:OG	1:A:261:VAL:CG2	2.67	0.43
1:A:50:LEU:O	1:A:54:VAL:HG23	2.19	0.43
1:A:184:ALA:N	1:A:185:PRO:HD2	2.34	0.43
1:A:47:GLN:NE2	4:A:407:HOH:O	2.51	0.43
1:B:271:ILE:HD11	1:B:288:MET:CE	2.48	0.43
1:B:290:THR:HG22	1:B:291:PHE:N	2.34	0.43
1:B:47:GLN:HG3	1:B:73:ALA:HB2	2.01	0.43
1:B:242:THR:HB	1:B:243:PRO:HD2	2.01	0.42
1:A:233:ILE:HD11	3:A:402:GAQ:C2	2.49	0.42
1:B:134:PHE:CD1	1:B:177:VAL:HB	2.55	0.42
1:B:179:ARG:HH12	3:B:402:GAQ:C4	2.32	0.42
1:A:185:PRO:C	1:A:186:HIS:ND1	2.73	0.42
1:A:227:LEU:HA	1:A:252:HIS:NE2	2.34	0.42
1:A:69:SER:CB	1:A:261:VAL:HG21	2.50	0.42
1:A:85:THR:CG2	1:A:86:THR:N	2.82	0.42
1:B:213:ASN:HA	1:B:239:PRO:HD3	2.02	0.42
1:A:173:ASP:C	1:A:173:ASP:OD1	2.58	0.41
1:B:69:SER:CB	1:B:261:VAL:CG2	2.98	0.41
1:A:183:ARG:NH1	1:A:216:GLU:OE2	2.53	0.41
1:A:242:THR:HB	1:A:244:GLU:OE1	2.20	0.41
1:A:35:ILE:O	1:A:38:HIS:O	2.38	0.41
1:B:155:ALA:O	1:B:156:GLU:C	2.59	0.41
1:A:42:LEU:HB2	1:A:243:PRO:HG3	2.03	0.40
1:B:117:ASN:ND2	1:B:117:ASN:N	2.69	0.40
1:A:258:LEU:HB3	1:A:262:TYR:CE2	2.57	0.40
1:A:47:GLN:HG3	1:A:73:ALA:CB	2.51	0.40
1:B:150:LYS:HE3	1:B:150:LYS:HB2	1.75	0.40
1:A:169:ILE:O	1:A:172:SER:HB2	2.21	0.40
1:A:41:VAL:HB	1:A:253:LEU:HD23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:TRP:CG	1:B:141:PRO:HA	2.57	0.40
1:B:273:LYS:CD	1:B:277:GLU:OE2	2.69	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	282/318 (89%)	251 (89%)	27 (10%)	4 (1%)	11	28
1	B	283/318 (89%)	259 (92%)	23 (8%)	1 (0%)	34	60
All	All	565/636 (89%)	510 (90%)	50 (9%)	5 (1%)	17	40

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	ARG
1	A	103	CYS
1	A	144	CYS
1	A	304	TYR
1	B	48	ASP

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	223/249 (90%)	204 (92%)	19 (8%)	10	24
1	B	224/249 (90%)	193 (86%)	31 (14%)	3	8
All	All	447/498 (90%)	397 (89%)	50 (11%)	6	13

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	40	SER
1	A	117	ASN
1	A	142	LYS
1	A	144	CYS
1	A	183	ARG
1	A	186	HIS
1	A	206	THR
1	A	213	ASN
1	A	253	LEU
1	A	256	HIS
1	A	257	SER
1	A	275	LEU
1	A	287	GLN
1	A	288	MET
1	A	295	ASN
1	A	299	SER
1	A	301	GLU
1	A	302	SER
1	B	31	MET
1	B	32	HIS
1	B	34	LEU
1	B	46	VAL
1	B	66	SER
1	B	71	SER
1	B	96	THR
1	B	120	ARG
1	B	131	LYS
1	B	133	VAL
1	B	142	LYS
1	B	183	ARG
1	B	190	GLU
1	B	206	THR
1	B	213	ASN
1	B	214	VAL

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Mol	Chain	Res	Type
1	B	223	LYS
1	B	229	ILE
1	B	234	GLU
1	B	253	LEU
1	B	256	HIS
1	B	266	ARG
1	B	275	LEU
1	B	282	ARG
1	B	284	ASP
1	B	286	ASP
1	B	288	MET
1	B	292	SER
1	B	295	ASN
1	B	302	SER
1	B	306	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	117	ASN
1	A	158	HIS
1	A	213	ASN
1	A	252	HIS
1	A	256	HIS
1	A	287	GLN
1	A	295	ASN
1	B	117	ASN
1	B	119	GLN
1	B	213	ASN
1	B	252	HIS
1	B	256	HIS

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)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	GAQ	A	402	1	6,6,6	1.80	1 (16%)	5,5,5	1.73	2 (40%)
3	GAQ	B	402	1	6,6,6	1.80	1 (16%)	5,5,5	1.74	2 (40%)

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
3	GAQ	A	402	1	-	1/3/4/4	-
3	GAQ	B	402	1	-	1/3/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	GAQ	O5-C5	4.32	1.44	1.19
3	A	402	GAQ	O5-C5	4.31	1.44	1.19

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	GAQ	O5-C5-C4	-2.96	107.45	126.89
3	A	402	GAQ	O5-C5-C4	-2.79	108.55	126.89
3	A	402	GAQ	C2-C3-C4	-2.50	102.91	113.79
3	B	402	GAQ	C2-C3-C4	-2.33	103.64	113.79

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	GAQ	C1-C2-C3-C4
3	A	402	GAQ	C2-C3-C4-C5

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	GAQ	6	0
3	B	402	GAQ	5	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	284/318 (89%)	0.97	46 (16%)	1	1	64, 79, 101, 130	0
1	B	285/318 (89%)	1.07	66 (23%)	0	0	68, 80, 100, 125	0
All	All	569/636 (89%)	1.02	112 (19%)	1	0	64, 80, 101, 130	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	141	PRO	7.9
1	B	312	ASN	7.7
1	B	290	THR	7.1
1	B	293	GLU	6.0
1	A	149	GLY	6.0
1	A	310	PHE	5.6
1	A	300	LEU	5.1
1	A	148	ARG	5.0
1	A	28	LYS	4.9
1	B	248	GLU	4.4
1	A	230	ALA	4.4
1	A	37	GLU	4.4
1	A	231	ASN	4.4
1	B	200	GLU	4.4
1	B	169	ILE	4.1
1	B	301	GLU	4.0
1	B	177	VAL	4.0
1	B	64	PHE	3.9
1	A	304	TYR	3.8
1	A	134	PHE	3.6
1	B	45	GLY	3.6
1	A	107	ASP	3.6
1	A	147	MET	3.5
1	B	289	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	43	MET	3.4
1	A	292	SER	3.4
1	B	107	ASP	3.4
1	B	225	LYS	3.4
1	B	66	SER	3.3
1	A	172	SER	3.3
1	B	229	ILE	3.3
1	A	38	HIS	3.3
1	A	302	SER	3.2
1	B	146	HIS	3.2
1	B	230	ALA	3.2
1	B	255	ALA	3.2
1	B	207	PHE	3.1
1	B	250	GLY	3.1
1	A	257	SER	3.1
1	B	147	MET	3.1
1	A	133	VAL	3.1
1	B	303	TRP	3.1
1	B	310	PHE	3.1
1	B	292	SER	3.0
1	B	212	ALA	3.0
1	B	231	ASN	3.0
1	B	70	VAL	3.0
1	B	46	VAL	3.0
1	B	65	VAL	3.0
1	B	145	GLY	3.0
1	B	201	ALA	3.0
1	B	254	ILE	2.9
1	A	66	SER	2.9
1	B	37	GLU	2.9
1	A	207	PHE	2.9
1	B	223	LYS	2.9
1	B	288	MET	2.9
1	A	109	ASP	2.9
1	B	69	SER	2.9
1	B	251	PHE	2.8
1	A	255	ALA	2.8
1	B	274	ILE	2.8
1	A	142	LYS	2.8
1	B	206	THR	2.8
1	A	229	ILE	2.8
1	B	296	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	261	VAL	2.7
1	B	178	ALA	2.7
1	B	256	HIS	2.7
1	B	38	HIS	2.6
1	A	43	MET	2.6
1	B	134	PHE	2.6
1	A	178	ALA	2.6
1	B	47	GLN	2.6
1	B	253	LEU	2.5
1	A	64	PHE	2.5
1	A	277	GLU	2.5
1	A	108	GLY	2.5
1	A	160	LEU	2.5
1	A	34	LEU	2.4
1	B	44	PRO	2.4
1	A	299	SER	2.4
1	A	254	ILE	2.4
1	B	208	VAL	2.3
1	A	303	TRP	2.3
1	B	135	LEU	2.3
1	B	156	GLU	2.3
1	A	311	LYS	2.3
1	B	33	ARG	2.3
1	B	284	ASP	2.3
1	B	63	ALA	2.2
1	A	171	ASP	2.2
1	A	306	MET	2.2
1	A	177	VAL	2.2
1	B	144	CYS	2.2
1	B	136	GLU	2.2
1	B	257	SER	2.2
1	B	67	GLY	2.2
1	B	148	ARG	2.2
1	B	246	PHE	2.2
1	B	210	ALA	2.1
1	B	172	SER	2.1
1	A	36	GLU	2.1
1	A	106	VAL	2.1
1	B	179	ARG	2.1
1	B	105	VAL	2.1
1	A	156	GLU	2.1
1	B	302	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	145	GLY	2.0
1	A	278	LYS	2.0
1	A	248	GLU	2.0
1	A	247	LYS	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
3	GAQ	B	402	7/7	0.36	0.58	68,74,81,84	0
3	GAQ	A	402	7/7	0.67	0.43	66,75,80,83	0
2	MG	B	401	1/1	0.73	0.62	98,98,98,98	0
2	MG	A	401	1/1	0.93	0.47	94,94,94,94	0

6.5 Other polymers (i)

There are no such residues in this entry.