Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 05:37 PM EDT

PDB ID	:	3O0Y
Title	:	The crystal structure of the putative lipoprotein from Colwellia psychrerythraea
Authors	:	Zhang, R.; Chhor, G.; Cobb, G.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2010-07-20
Resolution	:	1.70 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

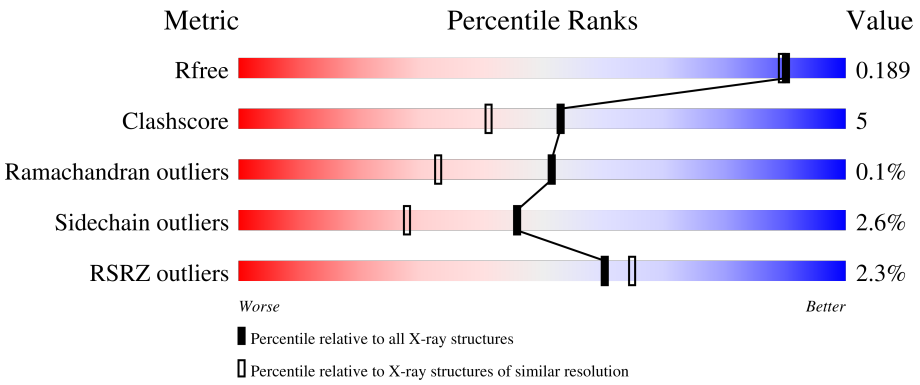
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.70 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 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	609	88% 7% • •
1	B	609	% 86% 9% • •
1	C	609	5% 85% 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	SO4	A	611	-	-	X	-
3	TRS	A	612	-	X	-	-
3	TRS	A	613	-	X	-	-
3	TRS	B	612	-	X	-	-
4	GOL	B	613	-	-	X	-
4	GOL	B	615	-	X	-	-
4	GOL	C	612	-	-	X	-

2 Entry composition (i)

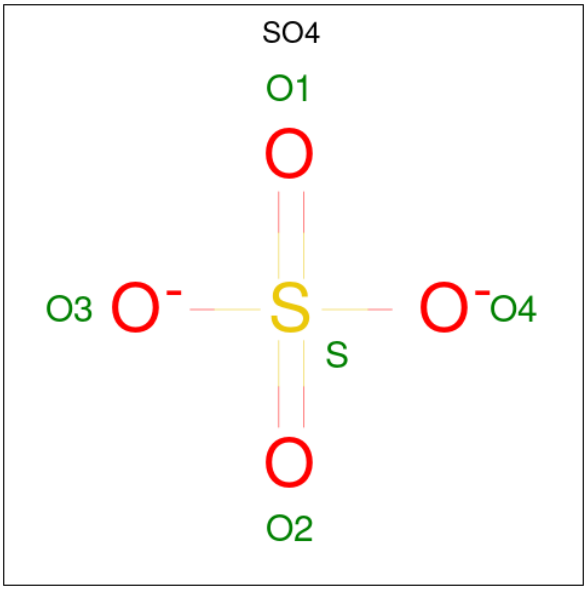
There are 5 unique types of molecules in this entry. The entry contains 16338 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 lipoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	585	4612	2931	780	887	14	0	0	0
1	B	585	4613	2930	780	889	14	0	0	0
1	C	585	4613	2930	780	889	14	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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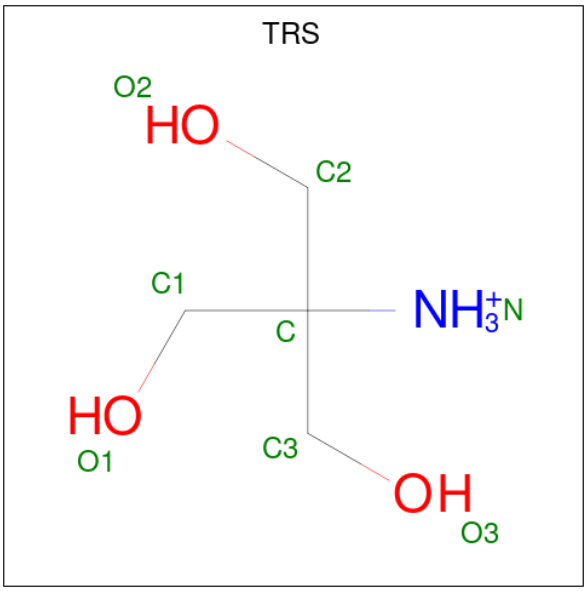
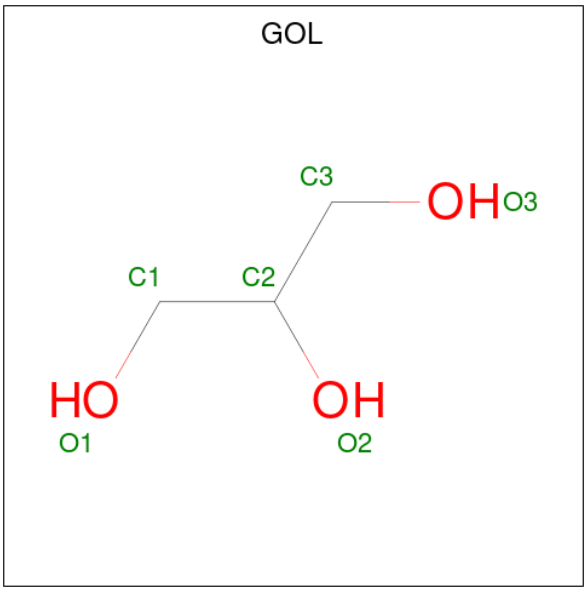
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
2	B	1	5	4	1		0	0
			Total	O	S			
2	C	1	5	4	1		0	0
			Total	O	S			
2	C	1	5	4	1		0	0

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	8	4	1	3	0	0
			Total	C	N	O		
3	A	1	8	4	1	3	0	0
			Total	C	N	O		
3	B	1	8	4	1	3	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0
4	B	1	6	3	3	0	0
4	B	1	6	3	3	0	0
4	B	1	6	3	3	0	0
4	C	1	6	3	3	0	0
4	C	1	6	3	3	0	0
4	C	1	6	3	3	0	0
4	C	1	6	3	3	0	0

- Molecule 5 is water.

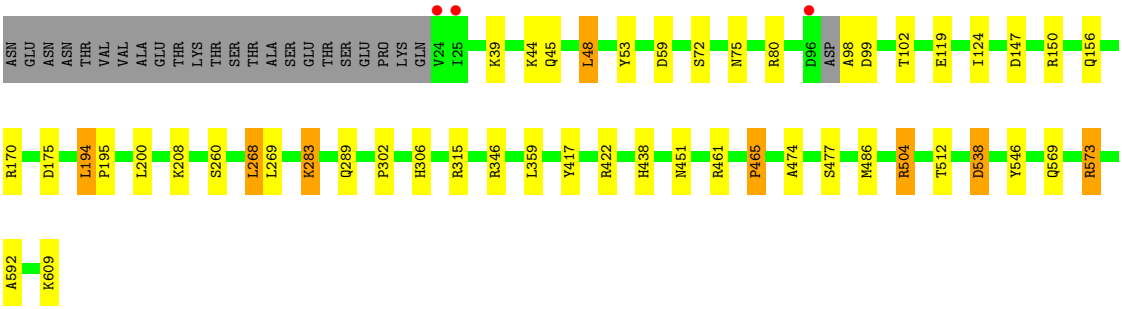
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	829	829	829	0	0
5	B	853	853	853	0	0
5	C	716	716	716	0	0

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.

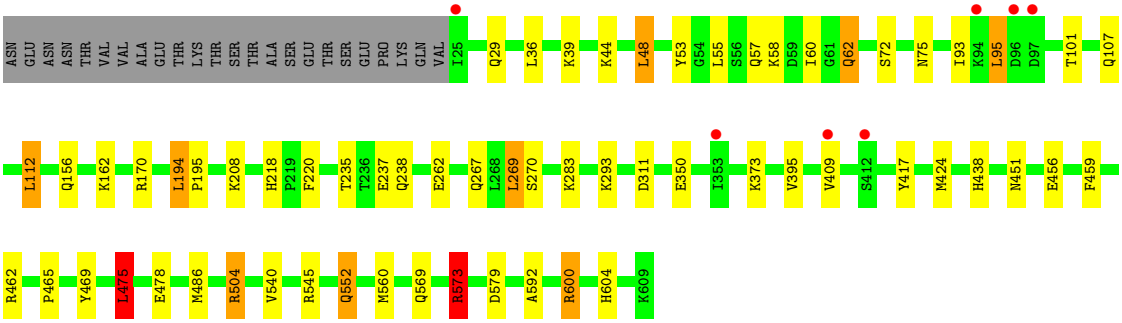
• Molecule 1: lipoprotein

Chain A:



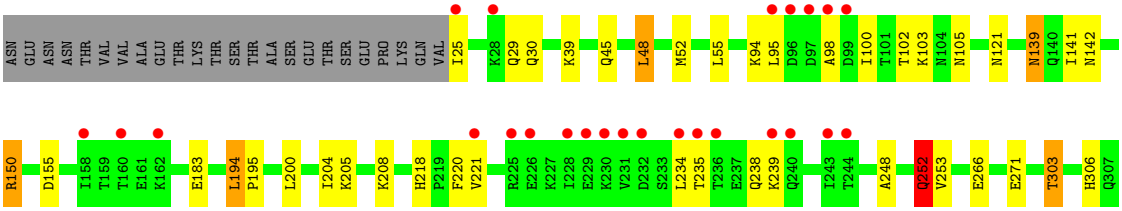
• Molecule 1: lipoprotein

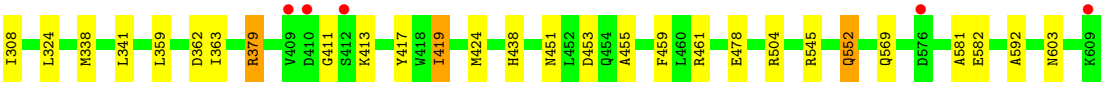
Chain B:



• Molecule 1: lipoprotein

Chain C:




I308
L324
M338
L341
L359
D362
I363
R379
V409
D410
G411
S412
K413
Y417
W418
I419
M424
H438
N451
L452
D453
Q454
A455
F459
L460
R461
E478
R504
R545
Q552
Q569
D576
A581
E582
A592
N603
K609

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	67.95Å 94.47Å 93.89Å 114.32° 91.11° 100.43°	Depositor
Resolution (Å)	85.13 – 1.70 46.31 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.3 (85.13-1.70) 95.4 (46.31-1.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.146 , 0.185 0.150 , 0.189	Depositor DCC
R_{free} test set	10876 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	15.8	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 48.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16338	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL, TRS

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	1.07	2/4705 (0.0%)	0.93	12/6378 (0.2%)
1	B	1.04	3/4707 (0.1%)	0.88	11/6382 (0.2%)
1	C	0.98	1/4707 (0.0%)	0.87	6/6382 (0.1%)
All	All	1.03	6/14119 (0.0%)	0.90	29/19142 (0.2%)

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	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	540	VAL	CB-CG2	5.74	1.64	1.52
1	A	546	TYR	CE2-CZ	-5.73	1.31	1.38
1	C	252	GLN	CB-CG	-5.35	1.38	1.52
1	B	504	ARG	CG-CD	-5.08	1.39	1.51
1	A	53	TYR	CD1-CE1	-5.05	1.31	1.39
1	B	237	GLU	CG-CD	5.02	1.59	1.51

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	486	MET	CG-SD-CE	-9.16	85.55	100.20
1	B	600	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	C	504	ARG	NE-CZ-NH2	-8.19	116.21	120.30
1	A	150	ARG	NE-CZ-NH1	8.00	124.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	362	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	A	150	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	C	424	MET	CG-SD-CE	-7.12	88.81	100.20
1	C	48	LEU	CA-CB-CG	-6.86	99.52	115.30
1	B	48	LEU	CA-CB-CG	-6.78	99.70	115.30
1	A	48	LEU	CA-CB-CG	-6.72	99.84	115.30
1	B	424	MET	CG-SD-CE	-6.66	89.55	100.20
1	B	573	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	A	486	MET	CG-SD-CE	-6.33	90.07	100.20
1	A	80	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	422	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	C	252	GLN	CB-CA-C	-6.04	98.31	110.40
1	A	573	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	315	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	A	346	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	B	48	LEU	CB-CG-CD2	5.42	120.21	111.00
1	B	475	LEU	CB-CG-CD2	5.40	120.19	111.00
1	B	269	LEU	CB-CG-CD1	5.32	120.04	111.00
1	C	453	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	A	538	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	175	ASP	CB-CG-OD1	5.18	122.96	118.30
1	A	461	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	573	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	579	ASP	CB-CG-OD1	5.07	122.86	118.30
1	B	112	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	465	PRO	Mainchain

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	4612	0	4578	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4613	0	4574	48	0
1	C	4613	0	4574	68	0
2	A	10	0	0	2	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
3	A	16	0	24	2	0
3	B	8	0	12	0	0
4	A	6	0	8	0	0
4	B	18	0	22	7	0
4	C	24	0	32	4	1
5	A	829	0	0	18	1
5	B	853	0	0	21	0
5	C	716	0	0	23	0
All	All	16338	0	13824	149	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 5.

All (149) 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:324:LEU:HD21	1:C:338:MET:HE1	1.21	1.14
1:C:324:LEU:HD21	1:C:338:MET:CE	1.94	0.98
1:B:107:GLN:HE22	1:B:600:ARG:HH22	1.12	0.96
1:C:235:THR:HG23	5:C:2237:HOH:O	1.66	0.94
1:C:303:THR:HG23	5:C:675:HOH:O	1.67	0.93
1:A:147:ASP:OD2	5:A:2620:HOH:O	1.87	0.91
1:C:150:ARG:NH2	5:C:2450:HOH:O	2.05	0.89
1:B:235:THR:H	1:B:238:GLN:HE21	1.20	0.87
1:C:545:ARG:HH21	1:C:552:GLN:HE22	1.23	0.86
1:B:57:GLN:HG2	5:B:1515:HOH:O	1.73	0.86
1:C:238:GLN:HB3	5:C:2528:HOH:O	1.74	0.85
1:B:39:LYS:NZ	4:B:613:GOL:O1	2.09	0.83
1:C:569:GLN:HE22	1:C:603:ASN:HD21	1.24	0.82
1:B:218:HIS:HD2	1:B:220:PHE:H	1.28	0.82
1:C:139:ASN:HD21	1:C:142:ASN:H	1.28	0.81
1:C:234:LEU:HA	5:C:2228:HOH:O	1.81	0.81
1:C:235:THR:CG2	5:C:2237:HOH:O	2.24	0.79
1:C:204:ILE:HD12	1:C:266:GLU:HG3	1.66	0.77
1:B:44:LYS:HD3	1:B:62:GLN:HE22	1.50	0.76
1:C:338:MET:HE2	1:C:341:LEU:HD12	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:ASN:HD22	1:C:141:ILE:H	1.32	0.75
2:A:611:SO4:O3	5:A:744:HOH:O	2.05	0.75
1:C:204:ILE:HG22	1:C:208:LYS:HE2	1.69	0.74
1:A:283:LYS:HD2	5:A:1655:HOH:O	1.88	0.73
1:C:306:HIS:HE1	5:C:1010:HOH:O	1.69	0.73
1:A:569:GLN:NE2	5:A:2435:HOH:O	2.22	0.72
1:B:72:SER:H	1:B:75:ASN:HD22	1.39	0.71
1:A:45:GLN:NE2	5:A:1483:HOH:O	2.23	0.70
1:B:107:GLN:HE22	1:B:600:ARG:NH2	1.87	0.70
1:B:459:PHE:H	4:B:613:GOL:H32	1.57	0.70
1:A:208:LYS:HE3	5:A:2300:HOH:O	1.92	0.70
1:C:248:ALA:O	1:C:252:GLN:HB2	1.91	0.69
1:C:105:ASN:HD22	1:C:461:ARG:HH11	1.39	0.69
2:A:611:SO4:O4	5:A:2187:HOH:O	2.08	0.69
1:C:379:ARG:HD2	1:C:581:ALA:HB1	1.75	0.68
1:B:311:ASP:OD2	5:B:1747:HOH:O	2.12	0.68
1:B:604:HIS:HD2	5:B:1507:HOH:O	1.77	0.68
1:B:218:HIS:CD2	1:B:220:PHE:H	2.12	0.67
1:C:303:THR:CG2	5:C:675:HOH:O	2.32	0.67
4:B:615:GOL:H11	5:B:1872:HOH:O	1.96	0.66
1:B:36:LEU:HD13	4:B:613:GOL:H12	1.78	0.66
4:B:613:GOL:H31	5:B:1023:HOH:O	1.94	0.66
1:C:100:ILE:HD13	5:C:1508:HOH:O	1.95	0.65
1:C:39:LYS:NZ	4:C:612:GOL:H31	2.10	0.65
1:B:58:LYS:NZ	5:B:2008:HOH:O	2.29	0.65
1:C:52:MET:HE2	5:C:1690:HOH:O	1.98	0.64
1:B:545:ARG:HH21	1:B:552:GLN:HE22	1.43	0.64
1:A:44:LYS:NZ	5:A:2290:HOH:O	2.20	0.64
1:C:308:ILE:HD13	5:C:784:HOH:O	1.96	0.63
1:C:105:ASN:ND2	1:C:461:ARG:HH11	1.96	0.63
1:C:155:ASP:OD1	1:C:413:LYS:HE3	1.99	0.63
1:B:438:HIS:HD2	1:B:478:GLU:OE2	1.82	0.62
1:B:44:LYS:HD3	1:B:62:GLN:NE2	2.14	0.61
1:C:411:GLY:N	5:C:2226:HOH:O	2.33	0.61
1:B:107:GLN:NE2	1:B:600:ARG:HH12	1.99	0.60
1:C:205:LYS:HA	1:C:208:LYS:HE3	1.83	0.60
1:A:208:LYS:CE	5:A:2300:HOH:O	2.47	0.60
1:A:44:LYS:HE2	5:A:987:HOH:O	2.00	0.60
1:A:72:SER:H	1:A:75:ASN:HD22	1.50	0.59
1:A:438:HIS:HE1	5:A:658:HOH:O	1.85	0.59
1:B:459:PHE:N	4:B:613:GOL:H32	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:ILE:CD1	1:C:266:GLU:HG3	2.33	0.58
1:C:139:ASN:ND2	1:C:141:ILE:H	2.00	0.58
1:C:183:GLU:OE1	5:C:1142:HOH:O	2.17	0.57
1:C:238:GLN:CB	5:C:2528:HOH:O	2.41	0.57
1:B:438:HIS:HE1	5:B:685:HOH:O	1.87	0.56
1:A:504:ARG:CZ	5:A:977:HOH:O	2.52	0.56
1:C:338:MET:CE	1:C:341:LEU:HD12	2.35	0.56
4:B:615:GOL:C1	5:B:1872:HOH:O	2.52	0.55
1:C:569:GLN:HE22	1:C:603:ASN:ND2	2.00	0.55
1:A:44:LYS:CE	5:A:987:HOH:O	2.55	0.55
1:C:139:ASN:ND2	1:C:142:ASN:H	2.03	0.55
1:C:98:ALA:HB1	1:C:102:THR:HB	1.88	0.54
1:C:39:LYS:HZ1	4:C:612:GOL:H31	1.71	0.54
1:C:438:HIS:HD2	1:C:478:GLU:OE2	1.91	0.54
1:C:238:GLN:NE2	5:C:2228:HOH:O	2.40	0.54
1:B:29:GLN:NE2	5:B:1554:HOH:O	2.40	0.53
1:B:235:THR:H	1:B:238:GLN:NE2	1.97	0.53
1:B:475:LEU:HD13	1:B:560:MET:SD	2.48	0.53
1:C:252:GLN:HB3	1:C:253:VAL:HG23	1.90	0.53
1:C:379:ARG:HH12	1:C:582:GLU:HG3	1.74	0.53
1:C:545:ARG:HH21	1:C:552:GLN:NE2	2.01	0.53
1:C:359:LEU:C	1:C:359:LEU:HD23	2.30	0.52
1:A:156:GLN:NE2	1:A:170:ARG:HH11	2.08	0.52
1:A:289:GLN:HE22	1:A:302:PRO:HD3	1.75	0.51
1:C:455:ALA:HB2	5:C:1186:HOH:O	2.10	0.51
1:C:379:ARG:CD	1:C:581:ALA:HB1	2.40	0.51
1:C:45:GLN:HG3	5:C:1488:HOH:O	2.11	0.50
1:C:235:THR:H	1:C:238:GLN:HE21	1.58	0.50
1:A:438:HIS:CE1	5:A:658:HOH:O	2.60	0.50
1:A:200:LEU:HD21	1:A:268:LEU:HB3	1.93	0.50
1:C:438:HIS:HE1	5:C:651:HOH:O	1.94	0.50
1:C:451:ASN:ND2	1:C:592:ALA:H	2.10	0.49
1:C:238:GLN:NE2	5:C:2237:HOH:O	2.44	0.49
1:C:218:HIS:HD2	1:C:220:PHE:H	1.59	0.49
1:B:438:HIS:CD2	1:B:478:GLU:OE2	2.66	0.48
1:C:205:LYS:HA	1:C:208:LYS:CE	2.44	0.48
1:B:504:ARG:CZ	5:B:1243:HOH:O	2.61	0.48
1:C:194:LEU:HB2	1:C:195:PRO:CD	2.44	0.48
1:B:57:GLN:CG	5:B:1515:HOH:O	2.44	0.47
1:B:283:LYS:HD2	5:B:891:HOH:O	2.14	0.47
1:C:121:ASN:ND2	5:C:2024:HOH:O	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:THR:HG23	5:C:2228:HOH:O	2.15	0.47
1:B:156:GLN:NE2	1:B:170:ARG:HH11	2.13	0.47
1:C:39:LYS:NZ	4:C:612:GOL:C3	2.76	0.46
1:A:359:LEU:C	1:A:359:LEU:HD23	2.36	0.46
1:B:93:ILE:HG22	1:B:95:LEU:HD13	1.97	0.46
1:C:204:ILE:HD12	1:C:266:GLU:CG	2.41	0.46
1:B:55:LEU:HD13	1:B:60:ILE:HD11	1.98	0.46
1:C:39:LYS:HZ1	4:C:612:GOL:C3	2.29	0.45
1:C:45:GLN:CG	5:C:1488:HOH:O	2.63	0.45
1:A:306:HIS:HD2	1:A:512:THR:OG1	1.98	0.45
1:B:72:SER:H	1:B:75:ASN:ND2	2.09	0.45
1:B:573:ARG:HH11	1:B:573:ARG:HG3	1.82	0.45
1:C:55:LEU:HD21	1:C:459:PHE:CZ	2.52	0.45
1:C:363:ILE:HD11	1:C:419:ILE:HD13	1.97	0.45
1:A:39:LYS:HE3	1:A:59:ASP:O	2.16	0.45
1:B:456:GLU:HG2	5:B:2146:HOH:O	2.17	0.44
1:B:53:TYR:O	1:B:409:VAL:HG22	2.16	0.44
1:A:474:ALA:O	1:A:477:SER:HB2	2.18	0.44
1:A:451:ASN:ND2	1:A:592:ALA:H	2.15	0.44
1:B:293:LYS:HD2	5:B:2285:HOH:O	2.17	0.44
1:A:194:LEU:HB2	1:A:195:PRO:CD	2.47	0.44
3:A:612:TRS:N	5:A:2652:HOH:O	1.81	0.44
1:B:451:ASN:ND2	1:B:592:ALA:H	2.15	0.44
1:C:271:GLU:HG3	5:C:958:HOH:O	2.18	0.43
1:A:538:ASP:HB3	5:A:1403:HOH:O	2.18	0.43
1:C:438:HIS:CD2	1:C:478:GLU:OE2	2.71	0.43
1:A:99:ASP:OD2	1:A:99:ASP:N	2.41	0.43
1:B:569:GLN:NE2	5:B:939:HOH:O	2.51	0.43
1:B:162:LYS:NZ	5:B:1557:HOH:O	2.46	0.43
1:C:25:ILE:HG23	1:C:29:GLN:HB3	2.00	0.43
3:A:612:TRS:H12	5:A:2652:HOH:O	2.19	0.43
1:B:208:LYS:HG2	1:B:262:GLU:OE2	2.18	0.42
1:B:604:HIS:CD2	5:B:1507:HOH:O	2.59	0.42
1:C:234:LEU:O	1:C:239:LYS:NZ	2.51	0.42
1:B:36:LEU:HD12	1:B:39:LYS:HE2	2.02	0.42
1:C:25:ILE:HG22	1:C:30:GLN:HG3	2.02	0.41
1:B:462:ARG:HD3	5:B:845:HOH:O	2.21	0.41
1:B:270:SER:OG	5:B:926:HOH:O	2.13	0.41
1:B:573:ARG:HG3	1:B:573:ARG:NH1	2.34	0.41
1:A:39:LYS:NZ	5:A:1839:HOH:O	2.52	0.41
1:C:545:ARG:NH2	1:C:552:GLN:HE22	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:GLU:HG3	5:B:2588:HOH:O	2.21	0.40
1:C:218:HIS:O	1:C:221:VAL:N	2.54	0.40
1:B:101:THR:HG21	5:B:2146:HOH:O	2.21	0.40
1:B:194:LEU:HB2	1:B:195:PRO:CD	2.51	0.40
1:A:98:ALA:HB1	1:A:102:THR:HB	2.04	0.40
1:B:469:TYR:CD2	1:B:592:ALA:HA	2.56	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)
4:C:615:GOL:C1	5:A:837:HOH:O[1_554]	2.19	0.01

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	581/609 (95%)	571 (98%)	9 (2%)	1 (0%)	47 30
1	B	583/609 (96%)	570 (98%)	12 (2%)	1 (0%)	47 30
1	C	583/609 (96%)	568 (97%)	15 (3%)	0	100 100
All	All	1747/1827 (96%)	1709 (98%)	36 (2%)	2 (0%)	51 33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	465	PRO
1	A	465	PRO

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	494/516 (96%)	482 (98%)	12 (2%)	49	31
1	B	494/516 (96%)	481 (97%)	13 (3%)	46	28
1	C	494/516 (96%)	480 (97%)	14 (3%)	43	25
All	All	1482/1548 (96%)	1443 (97%)	39 (3%)	46	28

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	119	GLU
1	A	124	ILE
1	A	194	LEU
1	A	260	SER
1	A	268	LEU
1	A	269	LEU
1	A	283	LYS
1	A	417	TYR
1	A	504	ARG
1	A	573	ARG
1	A	609	LYS
1	B	48	LEU
1	B	62	GLN
1	B	95	LEU
1	B	112	LEU
1	B	194	LEU
1	B	267	GLN
1	B	269	LEU
1	B	373	LYS
1	B	395	VAL
1	B	417	TYR
1	B	475	LEU
1	B	552	GLN
1	B	573	ARG
1	C	48	LEU

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Mol	Chain	Res	Type
1	C	94	LYS
1	C	95	LEU
1	C	103	LYS
1	C	139	ASN
1	C	150	ARG
1	C	194	LEU
1	C	200	LEU
1	C	252	GLN
1	C	303	THR
1	C	379	ARG
1	C	417	TYR
1	C	419	ILE
1	C	552	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	156	GLN
1	A	222	ASN
1	A	259	GLN
1	A	289	GLN
1	A	306	HIS
1	A	342	ASN
1	A	427	ASN
1	A	451	ASN
1	A	454	GLN
1	A	569	GLN
1	A	608	ASN
1	B	45	GLN
1	B	62	GLN
1	B	75	ASN
1	B	107	GLN
1	B	156	GLN
1	B	218	HIS
1	B	238	GLN
1	B	267	GLN
1	B	342	ASN
1	B	438	HIS
1	B	451	ASN
1	B	454	GLN
1	B	467	ASN

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Mol	Chain	Res	Type
1	B	552	GLN
1	B	569	GLN
1	B	604	HIS
1	C	45	GLN
1	C	62	GLN
1	C	78	GLN
1	C	105	ASN
1	C	139	ASN
1	C	218	HIS
1	C	238	GLN
1	C	306	HIS
1	C	451	ASN
1	C	454	GLN
1	C	489	ASN
1	C	552	GLN
1	C	603	ASN
1	C	604	HIS
1	C	608	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

17 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	$\#\|Z\| > 2$
4	GOL	C	614	-	5,5,5	0.36	0	5,5,5	1.45	1 (20%)
3	TRS	A	613	-	7,7,7	0.93	0	9,9,9	1.79	3 (33%)
4	GOL	A	614	-	5,5,5	0.35	0	5,5,5	1.25	1 (20%)
4	GOL	B	615	-	5,5,5	0.51	0	5,5,5	2.68	4 (80%)
4	GOL	B	613	-	5,5,5	1.12	0	5,5,5	2.43	3 (60%)
2	SO4	A	610	-	4,4,4	0.47	0	6,6,6	0.78	0
2	SO4	B	610	-	4,4,4	0.32	0	6,6,6	0.54	0
4	GOL	B	614	-	5,5,5	1.14	0	5,5,5	0.93	0
4	GOL	C	612	-	5,5,5	0.80	0	5,5,5	1.93	3 (60%)
2	SO4	C	611	-	4,4,4	0.29	0	6,6,6	0.34	0
4	GOL	C	615	-	5,5,5	0.58	0	5,5,5	0.70	0
2	SO4	B	611	-	4,4,4	0.83	0	6,6,6	0.53	0
3	TRS	B	612	-	7,7,7	0.88	0	9,9,9	2.10	3 (33%)
2	SO4	A	611	-	4,4,4	0.51	0	6,6,6	0.21	0
2	SO4	C	610	-	4,4,4	0.63	0	6,6,6	0.74	0
4	GOL	C	613	-	5,5,5	0.49	0	5,5,5	1.03	0
3	TRS	A	612	-	7,7,7	1.31	1 (14%)	9,9,9	3.21	5 (55%)

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
4	GOL	C	614	-	-	1/4/4/4	-
3	TRS	A	613	-	-	8/9/9/9	-
4	GOL	A	614	-	-	2/4/4/4	-
4	GOL	B	615	-	-	2/4/4/4	-
4	GOL	B	613	-	-	2/4/4/4	-
4	GOL	C	612	-	-	2/4/4/4	-
4	GOL	B	614	-	-	1/4/4/4	-
4	GOL	C	615	-	-	4/4/4/4	-
3	TRS	B	612	-	-	8/9/9/9	-
4	GOL	C	613	-	-	2/4/4/4	-
3	TRS	A	612	-	-	8/9/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	612	TRS	O2-C2	2.92	1.51	1.42

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	612	TRS	C3-C-N	-6.22	92.32	108.17
3	A	612	TRS	C2-C-N	4.42	119.44	108.17
3	B	612	TRS	C3-C-C2	-3.93	100.18	110.66
3	A	613	TRS	C3-C-C1	-3.54	101.22	110.66
4	B	615	GOL	O2-C2-C1	-3.50	94.70	109.18
4	B	613	GOL	O2-C2-C3	3.44	123.43	109.18
3	A	612	TRS	C3-C-C1	3.44	119.82	110.66
4	B	613	GOL	C3-C2-C1	-3.27	99.80	111.80
3	A	612	TRS	O1-C1-C	3.14	119.63	110.88
3	B	612	TRS	C3-C-C1	3.06	118.80	110.66
3	A	612	TRS	O2-C2-C	2.91	118.97	110.88
4	B	615	GOL	O1-C1-C2	-2.85	97.57	110.38
4	C	612	GOL	O2-C2-C3	-2.69	98.03	109.18
3	B	612	TRS	O3-C3-C	2.61	118.16	110.88
4	B	613	GOL	O2-C2-C1	2.60	119.96	109.18
4	B	615	GOL	O2-C2-C3	2.60	119.93	109.18
4	C	612	GOL	O3-C3-C2	-2.39	99.61	110.38
4	A	614	GOL	O1-C1-C2	-2.39	99.61	110.38
3	A	613	TRS	C2-C-C1	2.33	116.86	110.66
4	B	615	GOL	C3-C2-C1	-2.32	103.29	111.80
3	A	613	TRS	C1-C-N	2.28	113.98	108.17
4	C	614	GOL	O3-C3-C2	2.10	119.85	110.38
4	C	612	GOL	O2-C2-C1	2.01	117.50	109.18

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	612	TRS	C2-C-C1-O1
3	A	612	TRS	C3-C-C1-O1
3	A	612	TRS	N-C-C1-O1
3	A	612	TRS	C1-C-C3-O3
3	A	612	TRS	C2-C-C3-O3
3	A	613	TRS	C1-C-C2-O2
3	A	613	TRS	C3-C-C2-O2
3	A	613	TRS	N-C-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	613	TRS	N-C-C3-O3
3	B	612	TRS	C2-C-C1-O1
3	B	612	TRS	C3-C-C1-O1
3	B	612	TRS	N-C-C1-O1
3	B	612	TRS	C3-C-C2-O2
4	A	614	GOL	O1-C1-C2-C3
4	B	613	GOL	C1-C2-C3-O3
4	B	615	GOL	O2-C2-C3-O3
4	C	612	GOL	C1-C2-C3-O3
4	C	615	GOL	O1-C1-C2-C3
4	C	615	GOL	C1-C2-C3-O3
4	C	613	GOL	C1-C2-C3-O3
4	A	614	GOL	O1-C1-C2-O2
4	B	613	GOL	O2-C2-C3-O3
4	C	612	GOL	O2-C2-C3-O3
4	C	615	GOL	O1-C1-C2-O2
4	C	615	GOL	O2-C2-C3-O3
3	A	612	TRS	N-C-C3-O3
3	B	612	TRS	C1-C-C2-O2
3	B	612	TRS	N-C-C2-O2
4	C	613	GOL	O2-C2-C3-O3
3	A	612	TRS	C3-C-C2-O2
3	A	613	TRS	C2-C-C1-O1
3	A	613	TRS	C1-C-C3-O3
3	A	613	TRS	C2-C-C3-O3
3	B	612	TRS	C1-C-C3-O3
4	C	614	GOL	O1-C1-C2-O2
3	A	612	TRS	C1-C-C2-O2
3	A	613	TRS	C3-C-C1-O1
4	B	615	GOL	C1-C2-C3-O3
3	B	612	TRS	C2-C-C3-O3
4	B	614	GOL	O2-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	615	GOL	2	0
4	B	613	GOL	5	0
4	C	612	GOL	4	0
4	C	615	GOL	0	1
2	A	611	SO4	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	612	TRS	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 (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	585/609 (96%)	-0.33	3 (0%)	91	92	4, 11, 25, 42	0
1	B	585/609 (96%)	-0.35	7 (1%)	79	82	5, 12, 26, 47	0
1	C	585/609 (96%)	-0.05	30 (5%)	28	31	5, 13, 35, 52	0
All	All	1755/1827 (96%)	-0.25	40 (2%)	60	65	4, 12, 29, 52	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	24	VAL	7.3
1	C	96	ASP	7.2
1	C	97	ASP	7.0
1	C	234	LEU	4.8
1	C	25	ILE	4.8
1	C	236	THR	4.4
1	C	412	SER	4.1
1	C	232	ASP	3.9
1	A	25	ILE	3.6
1	A	96	ASP	3.6
1	C	240	GLN	3.6
1	B	25	ILE	3.5
1	C	95	LEU	3.5
1	B	96	ASP	3.4
1	C	229	GLU	3.3
1	C	231	VAL	3.2
1	C	239	LYS	3.2
1	C	98	ALA	3.2
1	C	409	VAL	3.2
1	B	412	SER	2.9
1	C	243	ILE	2.8
1	B	94	LYS	2.7
1	C	230	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	160	THR	2.5
1	B	97	ASP	2.4
1	C	226	GLU	2.4
1	C	228	ILE	2.3
1	C	162	LYS	2.3
1	C	244	THR	2.3
1	C	235	THR	2.3
1	C	221	VAL	2.2
1	B	409	VAL	2.2
1	C	410	ASP	2.2
1	C	158	ILE	2.2
1	C	99	ASP	2.2
1	B	353	ILE	2.1
1	C	576	ASP	2.1
1	C	225	ARG	2.1
1	C	609	LYS	2.1
1	C	28	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 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, 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
4	GOL	B	615	6/6	0.73	0.18	39,42,45,48	0
3	TRS	A	612	8/8	0.81	0.15	25,30,35,36	0
4	GOL	C	615	6/6	0.81	0.21	27,31,34,34	0
4	GOL	B	613	6/6	0.82	0.15	21,28,30,30	0
3	TRS	B	612	8/8	0.85	0.14	24,32,32,35	0
4	GOL	C	614	6/6	0.86	0.23	27,35,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	TRS	A	613	8/8	0.87	0.13	28,31,33,35	0
4	GOL	A	614	6/6	0.90	0.12	16,24,27,35	0
4	GOL	C	612	6/6	0.91	0.09	23,29,32,33	0
2	SO4	A	611	5/5	0.91	0.28	54,55,57,58	0
2	SO4	C	611	5/5	0.91	0.23	57,59,61,62	0
4	GOL	B	614	6/6	0.93	0.10	18,25,27,34	0
4	GOL	C	613	6/6	0.95	0.11	16,19,21,29	0
2	SO4	A	610	5/5	0.98	0.09	20,22,25,29	0
2	SO4	B	610	5/5	0.98	0.11	33,40,41,44	0
2	SO4	B	611	5/5	0.98	0.09	17,21,26,27	0
2	SO4	C	610	5/5	0.98	0.09	18,20,26,28	0

6.5 Other polymers (i)

There are no such residues in this entry.