



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2025 – 02:29 PM EDT

PDB ID : 3O0Y / pdb\_00003o0y  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

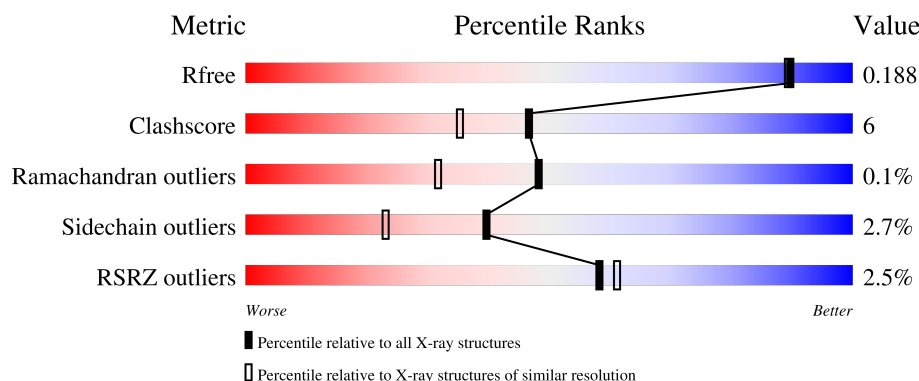
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*




The reported resolution of this entry is 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))
$R_{free}$	164625	5161 (1.70-1.70)
Clashscore	180529	5671 (1.70-1.70)
Ramachandran outliers	177936	5594 (1.70-1.70)
Sidechain outliers	177891	5594 (1.70-1.70)
RSRZ outliers	164620	5159 (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  $\geq 3$ , 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  $\leq 5\%$ . 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	
1	B	609	
1	C	609	

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
1	A	585	Total	C	N	O	S	0	0	0
			4612	2931	780	887	14			
1	B	585	Total	C	N	O	S	0	0	0
			4613	2930	780	889	14			
1	C	585	Total	C	N	O	S	0	0	0
			4613	2930	780	889	14			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



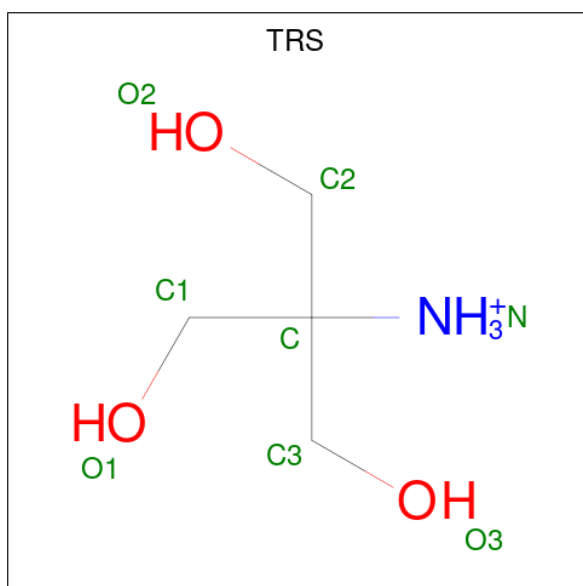
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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

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



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).

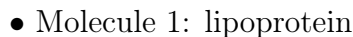
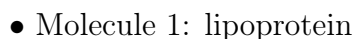


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

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

- Molecule 1: lipoprotein







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.95Å 94.47Å 93.89Å 114.32° 91.11° 100.43°	Depositor
Resolution (Å)	85.13 – 1.70 85.09 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.3 (85.13-1.70) 95.3 (85.09-1.70)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.53 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.146 , 0.185 0.150 , 0.188	Depositor DCC
$R_{free}$ test set	10876 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.8	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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, TRS, GOL

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	1.25	5/4705 (0.1%)	1.07	3/6378 (0.0%)
1	B	1.21	4/4707 (0.1%)	1.05	4/6382 (0.1%)
1	C	1.19	3/4707 (0.1%)	1.09	14/6382 (0.2%)
All	All	1.22	12/14119 (0.1%)	1.07	21/19142 (0.1%)

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 (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	486	MET	SD-CE	-11.09	1.51	1.79
1	C	424	MET	SD-CE	-9.03	1.56	1.79
1	C	486	MET	SD-CE	-7.10	1.61	1.79
1	A	486	MET	SD-CE	-6.94	1.62	1.79
1	A	528	MET	SD-CE	-5.87	1.64	1.79
1	A	91	ALA	CA-CB	5.67	1.62	1.53
1	C	160	THR	CA-CB	5.56	1.62	1.53
1	A	194	LEU	C-O	-5.37	1.18	1.24
1	A	280	ALA	N-CA	5.35	1.53	1.46
1	B	424	MET	SD-CE	-5.33	1.66	1.79
1	B	451	ASN	C-O	5.23	1.30	1.24
1	B	408	ALA	CA-CB	5.14	1.61	1.53

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	252	GLN	CB-CA-C	-7.97	98.31	110.90
1	B	486	MET	CG-SD-CE	-6.98	85.55	100.90
1	C	148	ILE	CA-C-N	-6.74	111.87	119.28
1	C	148	ILE	C-N-CA	-6.74	111.87	119.28
1	C	141	ILE	N-CA-C	6.54	117.20	111.90
1	A	363	ILE	CB-CA-C	-6.41	103.68	111.88
1	A	477	SER	CA-CB-OG	-6.38	98.34	111.10
1	C	415	GLY	N-CA-C	-5.78	104.68	112.14
1	C	427	ASN	CA-C-N	-5.74	113.85	119.76
1	C	427	ASN	C-N-CA	-5.74	113.85	119.76
1	C	424	MET	CG-SD-CE	-5.50	88.81	100.90
1	C	235	THR	N-CA-C	5.41	117.07	110.41
1	A	146	ILE	N-CA-C	-5.38	106.56	111.67
1	C	225	ARG	N-CA-C	-5.38	105.06	111.03
1	B	148	ILE	CA-C-N	-5.17	113.59	119.28
1	B	148	ILE	C-N-CA	-5.17	113.59	119.28
1	B	424	MET	CG-SD-CE	-5.16	89.55	100.90
1	C	375	ALA	CA-C-N	-5.07	114.44	119.56
1	C	375	ALA	C-N-CA	-5.07	114.44	119.56
1	C	363	ILE	CB-CG1-CD1	-5.06	103.17	113.80
1	C	204	ILE	N-CA-C	-5.03	105.59	110.42

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
1	B	4613	0	4574	48	0
1	C	4613	0	4574	73	0
2	A	10	0	0	2	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	5	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	154	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 6.

All (154) 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	1.35	1.05
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:359:LEU:C	1:C:359:LEU:HD23	2.30	0.57
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:C:338:MET:CE	1:C:341:LEU:HD12	2.35	0.57
1:B:438:HIS:HE1	5:B:685:HOH:O	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:ARG:CZ	5:A:977:HOH:O	2.52	0.56
4:B:615:GOL:C1	5:B:1872:HOH:O	2.52	0.55
1:C:324:LEU:HD11	1:C:338:MET:HE3	1.87	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:HZ2	4:C:612:GOL:H31	1.73	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: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:A:359:LEU:C	1:A:359:LEU:HD23	2.36	0.51
1:C:455:ALA:HB2	5:C:1186:HOH:O	2.10	0.51
1:C:52:MET:HE2	5:C:1690:HOH:O	2.11	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:C:52:MET:HE3	1:C:151:VAL:HG22	1.96	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:324:LEU:HD21	1:C:338:MET:HE3	1.89	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:B:569:GLN:NE2	5:B:939:HOH:O	2.51	0.43
1:A:424:MET:HA	1:A:424:MET:HE2	2.01	0.43
1:B:162:LYS:NZ	5:B:1557:HOH:O	2.46	0.43
1:C:232:ASP:C	1:C:234:LEU:H	2.27	0.43
1:C:25:ILE:HG23	1:C:29:GLN:HB3	2.00	0.43
1:C:234:LEU:O	1:C:239:LYS:NZ	2.51	0.43
3:A:612:TRS:H12	5:A:2652:HOH:O	2.19	0.43
1:C:39:LYS:HZ2	4:C:612:GOL:C3	2.32	0.42
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: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:C:124:ILE:C	1:C:124:ILE:HD12	2.45	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
1:B:350:GLU:HG3	5:B:2588:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:39:LYS:HZ1	4:C:612:GOL:H31	1.85	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

### 5.3.1 Protein backbone

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%)	44	29
1	B	583/609 (96%)	570 (98%)	12 (2%)	1 (0%)	44	29
1	C	583/609 (96%)	568 (97%)	15 (3%)	0	100	100
All	All	1747/1827 (96%)	1709 (98%)	36 (2%)	2 (0%)	48	32

All (2) Ramachandran outliers are listed below:

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



### 5.3.2 Protein sidechains ⓘ

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%)	484 (98%)	10 (2%)	50	34
1	B	494/516 (96%)	480 (97%)	14 (3%)	38	21
1	C	494/516 (96%)	478 (97%)	16 (3%)	34	17
All	All	1482/1548 (96%)	1442 (97%)	40 (3%)	40	23

All (40) 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	425	LYS
1	A	573	ARG
1	B	48	LEU
1	B	62	GLN
1	B	95	LEU
1	B	112	LEU
1	B	119	GLU
1	B	194	LEU
1	B	237	GLU
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	573	ARG
1	C	44	LYS
1	C	45	GLN

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Mol	Chain	Res	Type
1	C	48	LEU
1	C	94	LYS
1	C	95	LEU
1	C	103	LYS
1	C	105	ASN
1	C	150	ARG
1	C	194	LEU
1	C	200	LEU
1	C	204	ILE
1	C	244	THR
1	C	252	GLN
1	C	303	THR
1	C	379	ARG
1	C	419	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	156	GLN
1	A	173	GLN
1	A	191	GLN
1	A	222	ASN
1	A	289	GLN
1	A	306	HIS
1	A	342	ASN
1	A	427	ASN
1	A	451	ASN
1	A	531	GLN
1	A	569	GLN
1	A	590	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	245	GLN
1	B	294	GLN
1	B	342	ASN
1	B	438	HIS

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Mol	Chain	Res	Type
1	B	447	GLN
1	B	451	ASN
1	B	467	ASN
1	B	552	GLN
1	B	569	GLN
1	B	604	HIS
1	C	62	GLN
1	C	78	GLN
1	C	105	ASN
1	C	121	ASN
1	C	139	ASN
1	C	218	HIS
1	C	238	GLN
1	C	306	HIS
1	C	342	ASN
1	C	451	ASN
1	C	552	GLN
1	C	569	GLN
1	C	603	ASN
1	C	604	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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

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

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(°)	Ideal(°)
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 17 short contacts:

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	615	GOL	0	1

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	585/609 (96%)	-0.43	2 (0%) 90 91	4, 11, 25, 42	0
1	B	585/609 (96%)	-0.32	5 (0%) 81 83	5, 12, 26, 47	0
1	C	585/609 (96%)	-0.00	37 (6%) 27 28	5, 13, 35, 52	0
All	All	1755/1827 (96%)	-0.25	44 (2%) 58 61	4, 12, 29, 52	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	234	LEU	4.9
1	A	24	VAL	4.8
1	C	231	VAL	4.2
1	C	96	ASP	3.9
1	C	409	VAL	3.6
1	C	97	ASP	3.6
1	C	233	SER	3.5
1	C	228	ILE	3.4
1	C	232	ASP	3.4
1	C	235	THR	3.3
1	C	236	THR	3.2
1	C	244	THR	3.1
1	C	243	ILE	2.9
1	C	239	LYS	2.9
1	C	168	ILE	2.8
1	C	98	ALA	2.8
1	C	95	LEU	2.7
1	C	221	VAL	2.7
1	C	412	SER	2.6
1	C	224	PHE	2.6
1	C	25	ILE	2.6
1	A	96	ASP	2.6
1	B	414	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	165	LEU	2.5
1	C	242	LEU	2.5
1	C	237	GLU	2.4
1	C	398	GLY	2.4
1	B	96	ASP	2.4
1	C	240	GLN	2.4
1	C	214	SER	2.4
1	C	241	SER	2.3
1	C	222	ASN	2.3
1	B	409	VAL	2.3
1	C	164	ALA	2.2
1	C	212	SER	2.2
1	B	97	ASP	2.2
1	C	100	ILE	2.1
1	C	226	GLU	2.1
1	C	160	THR	2.1
1	C	223	VAL	2.1
1	C	213	GLY	2.1
1	C	216	GLU	2.0
1	B	94	LYS	2.0
1	C	158	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	GOL	B	615	6/6	0.77	0.15	39,42,45,48	0
3	TRS	A	612	8/8	0.81	0.15	25,30,35,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	TRS	A	613	8/8	0.81	0.14	28,31,33,35	0
2	SO4	C	611	5/5	0.81	0.12	57,59,61,62	0
4	GOL	B	613	6/6	0.82	0.17	21,28,30,30	0
3	TRS	B	612	8/8	0.82	0.15	24,32,32,35	0
4	GOL	C	615	6/6	0.85	0.14	27,31,34,34	0
4	GOL	A	614	6/6	0.86	0.12	16,24,27,35	0
4	GOL	C	614	6/6	0.87	0.10	27,35,39,39	0
2	SO4	A	611	5/5	0.90	0.11	54,55,57,58	0
4	GOL	B	614	6/6	0.92	0.11	18,25,27,34	0
4	GOL	C	612	6/6	0.92	0.10	23,29,32,33	0
4	GOL	C	613	6/6	0.94	0.09	16,19,21,29	0
2	SO4	B	610	5/5	0.95	0.06	33,40,41,44	0
2	SO4	A	610	5/5	0.98	0.06	20,22,25,29	0
2	SO4	B	611	5/5	0.98	0.06	17,21,26,27	0
2	SO4	C	610	5/5	0.98	0.07	18,20,26,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.