



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 10:30 PM EDT

PDB ID : 5ZNM  
Title : Colicin D Central Domain and C-terminal tRNase domain  
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Deposited on : 2018-04-10  
Resolution : 1.85 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

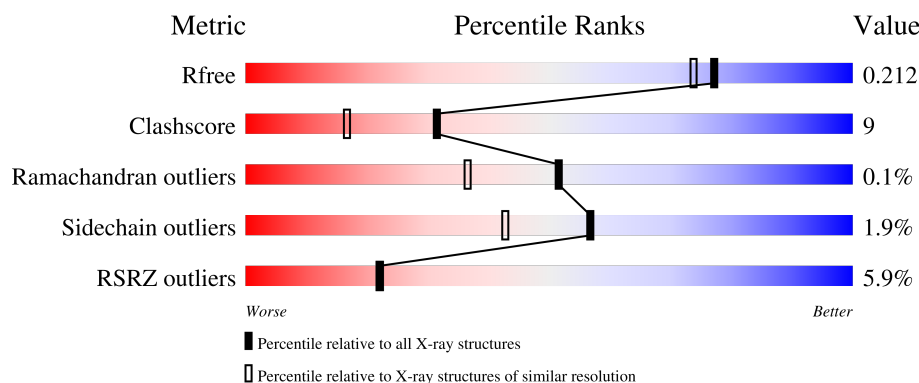
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	387	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>• 7%</div> </div> </div>
1	B	387	<div> <div>6%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>• 8%</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5805 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.

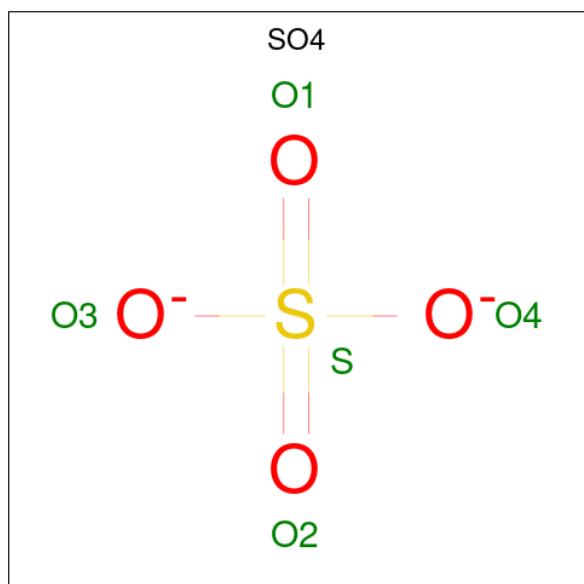
- Molecule 1 is a protein called Colicin-D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2706	1694	471	530	11			
1	B	357	Total	C	N	O	S	0	0	0
			2698	1690	470	527	11			

There are 4 discrepancies between the modelled and reference sequences:

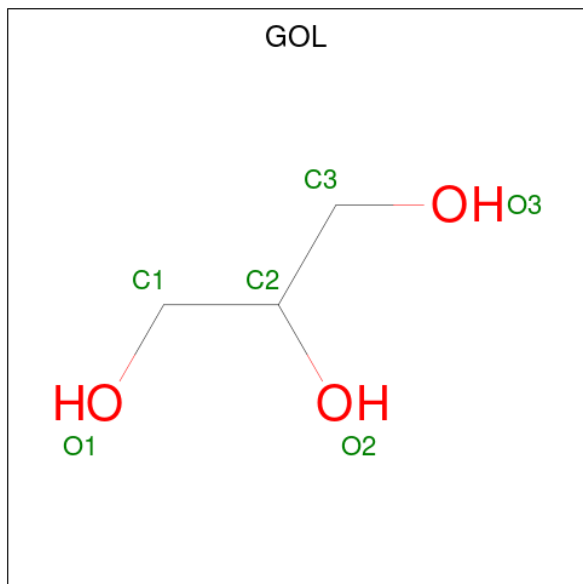
Chain	Residue	Modelled	Actual	Comment	Reference
A	311	MET	-	initiating methionine	UNP P17998
A	312	HIS	-	expression tag	UNP P17998
B	311	MET	-	initiating methionine	UNP P17998
B	312	HIS	-	expression tag	UNP P17998

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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

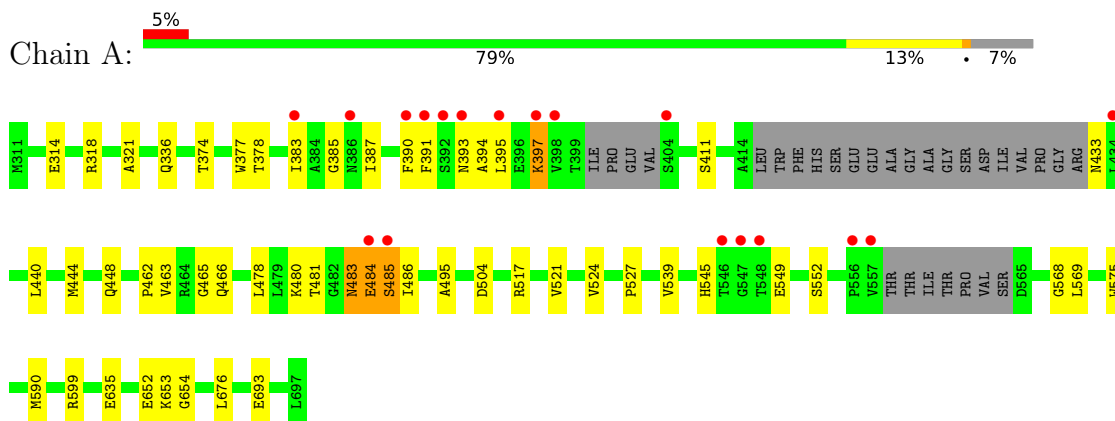
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	170	Total 170	O 170	0	0
4	B	129	Total 129	O 129	0	0

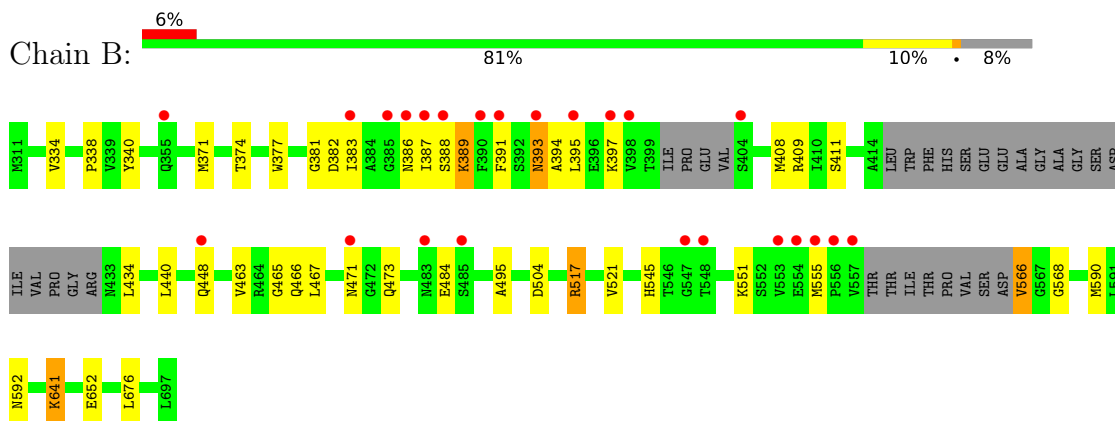
### 3 Residue-property plots

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: Colicin-D



#### • Molecule 1: Colicin-D



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.35Å 146.12Å 45.76Å 90.00° 102.49° 90.00°	Depositor
Resolution (Å)	44.84 – 1.85 44.84 – 1.85	Depositor EDS
% Data completeness (in resolution range)	96.3 (44.84-1.85) 95.6 (44.84-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 1.86Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.172 , 0.212 0.172 , 0.212	Depositor DCC
$R_{free}$ test set	3072 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.1	Xtriage
Anisotropy	0.495	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 55.5	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	5805	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.25% 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: GOL, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.47	1/2751 (0.0%)	0.61	0/3730
1	B	0.42	0/2743	0.60	1/3719 (0.0%)
All	All	0.45	1/5494 (0.0%)	0.60	1/7449 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	397	LYS	CD-CE	-6.54	1.34	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	434	LEU	CA-CB-CG	5.14	127.13	115.30

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	2706	0	2710	57	2
1	B	2698	0	2706	45	1
2	A	15	0	0	0	0
2	B	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	48	0	64	4	0
3	B	24	0	32	4	0
4	A	170	0	0	6	2
4	B	129	0	0	2	1
All	All	5805	0	5512	99	3

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 9.

All (99) 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:394:ALA:HA	1:A:397:LYS:NZ	1.71	1.06
1:A:394:ALA:HA	1:A:397:LYS:HZ1	1.29	0.96
1:A:397:LYS:HD2	4:A:805:HOH:O	1.67	0.95
1:A:693:GLU:HB3	3:A:706:GOL:H2	1.50	0.93
1:B:394:ALA:HA	1:B:397:LYS:HE2	1.52	0.91
1:A:448:GLN:OE1	4:A:801:HOH:O	1.89	0.90
1:B:397:LYS:HE3	1:B:463:VAL:HG22	1.57	0.86
1:B:397:LYS:CE	1:B:463:VAL:HG22	2.05	0.86
1:A:391:PHE:HD1	1:A:395:LEU:HD12	1.42	0.83
1:B:397:LYS:NZ	1:B:463:VAL:HG22	1.94	0.83
1:A:394:ALA:CA	1:A:397:LYS:HZ1	1.92	0.82
1:A:393:ASN:OD1	1:A:394:ALA:N	2.15	0.79
1:A:480:LYS:NZ	1:A:481:THR:O	2.14	0.78
1:A:599:ARG:NH1	1:A:635:GLU:OE2	2.17	0.76
1:A:397:LYS:HG2	1:A:480:LYS:HD3	1.68	0.75
1:A:394:ALA:HA	1:A:397:LYS:HZ2	1.52	0.74
1:A:397:LYS:HD3	1:A:463:VAL:HG23	1.69	0.74
1:A:378:THR:N	1:B:382:ASP:OD1	2.16	0.73
1:A:391:PHE:CD1	1:A:395:LEU:HD12	2.24	0.72
1:B:397:LYS:HZ1	1:B:463:VAL:HG22	1.55	0.72
1:B:411:SER:OG	1:B:473:GLN:NE2	2.20	0.71
1:B:387:ILE:HB	1:B:391:PHE:CZ	2.26	0.70
1:A:653:LYS:HD2	1:A:654:GLY:N	2.06	0.70
1:A:397:LYS:HD3	1:A:463:VAL:CG2	2.24	0.68
1:B:391:PHE:O	1:B:395:LEU:HD12	1.94	0.68
1:B:504:ASP:HB2	1:B:521:VAL:HB	1.76	0.68
1:A:466:GLN:NE2	1:A:568:GLY:O	2.27	0.67
1:A:393:ASN:HD22	1:A:478:LEU:HD13	1.61	0.65
1:A:484:GLU:HA	1:A:484:GLU:OE1	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:ASN:ND2	1:B:408:MET:SD	2.70	0.64
1:A:374:THR:O	1:A:545:HIS:HA	1.97	0.64
1:A:693:GLU:CB	3:A:706:GOL:H2	2.25	0.64
1:B:466:GLN:NE2	1:B:568:GLY:O	2.30	0.64
1:B:393:ASN:ND2	1:B:408:MET:HB2	2.16	0.60
1:B:397:LYS:HZ1	1:B:463:VAL:CG2	2.14	0.60
1:A:652:GLU:HG3	1:A:676:LEU:HD22	1.83	0.60
1:A:394:ALA:CA	1:A:397:LYS:NZ	2.54	0.59
1:A:504:ASP:HB2	1:A:521:VAL:HB	1.85	0.59
1:B:388:SER:HA	1:B:391:PHE:CD2	2.39	0.58
1:A:394:ALA:C	1:A:397:LYS:HZ1	2.07	0.58
1:A:390:PHE:HA	1:A:393:ASN:ND2	2.18	0.58
1:A:483:ASN:C	1:A:485:SER:H	2.06	0.57
1:A:462:PRO:HB2	4:A:805:HOH:O	2.04	0.57
1:B:389:LYS:O	1:B:393:ASN:OD1	2.24	0.56
1:B:374:THR:O	1:B:545:HIS:HA	2.06	0.56
1:A:377:TRP:HZ2	1:B:383:ILE:HD13	1.72	0.54
1:A:483:ASN:O	1:A:485:SER:N	2.42	0.53
1:B:371:MET:HB2	1:B:374:THR:HG22	1.91	0.53
1:B:387:ILE:HG13	1:B:388:SER:N	2.24	0.53
1:A:524:VAL:O	4:A:802:HOH:O	2.19	0.52
1:A:549:GLU:H	1:A:549:GLU:CD	2.13	0.52
1:A:321:ALA:HB2	3:B:705:GOL:H11	1.92	0.52
1:A:397:LYS:CG	1:A:480:LYS:HD3	2.39	0.51
1:B:411:SER:HG	1:B:473:GLN:HE21	1.56	0.50
1:A:397:LYS:H	1:A:397:LYS:HZ3	1.59	0.50
1:B:388:SER:HA	1:B:391:PHE:CG	2.47	0.50
1:B:566:VAL:CG1	1:B:568:GLY:H	2.24	0.50
1:A:391:PHE:CD1	1:A:391:PHE:O	2.66	0.49
1:B:566:VAL:HG13	1:B:568:GLY:H	1.76	0.49
1:A:387:ILE:O	1:A:390:PHE:HB2	2.13	0.49
1:B:504:ASP:OD2	3:B:704:GOL:O2	2.26	0.49
1:B:393:ASN:HD21	1:B:408:MET:HB2	1.78	0.48
1:A:383:ILE:HD13	1:B:377:TRP:HZ2	1.77	0.48
1:A:486:ILE:HD12	1:A:569:LEU:HD11	1.95	0.48
1:B:471:ASN:OD1	4:B:801:HOH:O	2.20	0.48
1:A:314:GLU:OE2	1:A:318:ARG:NE	2.47	0.47
1:A:483:ASN:C	1:A:485:SER:N	2.66	0.47
1:A:653:LYS:HD2	1:A:654:GLY:H	1.78	0.47
1:B:495:ALA:HB1	1:B:504:ASP:HB3	1.97	0.47
1:B:397:LYS:HE3	1:B:463:VAL:CG2	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:ASP:OD2	3:A:710:GOL:O2	2.19	0.46
1:A:385:GLY:HA2	1:A:387:ILE:HG12	1.98	0.46
1:B:652:GLU:HG3	1:B:676:LEU:HD22	1.98	0.45
1:A:465:GLY:HA3	1:A:590:MET:SD	2.57	0.45
1:A:495:ALA:HB1	1:A:504:ASP:HB3	1.98	0.45
1:B:334:VAL:HA	3:B:704:GOL:H31	1.99	0.44
1:A:336:GLN:HB2	4:A:883:HOH:O	2.18	0.44
1:B:338:PRO:HG2	1:B:340:TYR:CZ	2.53	0.44
1:A:397:LYS:HE2	1:A:397:LYS:HB2	1.72	0.43
1:B:393:ASN:O	1:B:397:LYS:HG3	2.19	0.43
1:B:409:ARG:HG2	1:B:555:MET:HB2	2.01	0.43
1:A:480:LYS:HD2	1:A:481:THR:N	2.34	0.43
1:B:448:GLN:OE1	1:B:448:GLN:HA	2.19	0.43
1:A:462:PRO:CB	4:A:805:HOH:O	2.63	0.42
1:B:465:GLY:HA3	1:B:590:MET:SD	2.59	0.42
1:A:527:PRO:O	1:B:381:GLY:HA2	2.19	0.42
1:A:397:LYS:HD2	1:A:462:PRO:HB2	2.00	0.42
1:B:517:ARG:HA	1:B:517:ARG:HD3	1.88	0.42
1:A:387:ILE:HG22	1:A:444:MET:SD	2.60	0.42
1:B:386:ASN:O	1:B:389:LYS:HB2	2.18	0.42
1:B:467:LEU:HD23	1:B:467:LEU:HA	1.92	0.42
1:B:484:GLU:O	1:B:484:GLU:HG2	2.20	0.42
1:B:467:LEU:HB2	1:B:592:ASN:HA	2.02	0.41
3:B:707:GOL:H12	4:B:890:HOH:O	2.19	0.41
1:A:575:TRP:O	3:A:710:GOL:O1	2.29	0.41
1:A:411:SER:O	1:A:552:SER:HA	2.20	0.41
1:B:551:LYS:HA	1:B:551:LYS:HD2	1.82	0.41
1:B:391:PHE:N	1:B:391:PHE:CD1	2.86	0.40
1:A:485:SER:HB2	1:A:486:ILE:H	1.77	0.40

All (3) 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)
1:A:483:ASN:OD1	1:B:641:LYS:CB[4_546]	2.07	0.13
1:A:539:VAL:O	4:A:801:HOH:O[1_554]	2.16	0.04
4:A:863:HOH:O	4:B:854:HOH:O[4_545]	2.16	0.04

## 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	350/387 (90%)	337 (96%)	12 (3%)	1 (0%)	41	26
1	B	349/387 (90%)	338 (97%)	11 (3%)	0	100	100
All	All	699/774 (90%)	675 (97%)	23 (3%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	484	GLU

### 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	295/319 (92%)	290 (98%)	5 (2%)	60	47
1	B	294/319 (92%)	288 (98%)	6 (2%)	55	40
All	All	589/638 (92%)	578 (98%)	11 (2%)	57	43

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	433	ASN
1	A	440	LEU
1	A	483	ASN
1	A	485	SER
1	A	517	ARG

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Mol	Chain	Res	Type
1	B	389	LYS
1	B	393	ASN
1	B	440	LEU
1	B	517	ARG
1	B	566	VAL
1	B	641	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	466	GLN
1	B	473	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	GOL	A	711	-	5,5,5	0.45	0	5,5,5	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	A	705	-	5,5,5	0.27	0	5,5,5	0.62	0
3	GOL	B	707	-	5,5,5	0.36	0	5,5,5	0.15	0
3	GOL	A	704	-	5,5,5	0.38	0	5,5,5	0.97	0
2	SO4	A	701	-	4,4,4	0.16	0	6,6,6	0.24	0
3	GOL	A	707	-	5,5,5	0.50	0	5,5,5	0.43	0
3	GOL	B	704	-	5,5,5	0.43	0	5,5,5	0.58	0
3	GOL	A	710	-	5,5,5	0.41	0	5,5,5	0.69	0
3	GOL	B	705	-	5,5,5	0.31	0	5,5,5	0.53	0
3	GOL	B	706	-	5,5,5	0.31	0	5,5,5	0.69	0
2	SO4	A	702	-	4,4,4	0.14	0	6,6,6	0.15	0
2	SO4	B	701	-	4,4,4	0.14	0	6,6,6	0.13	0
3	GOL	A	706	-	5,5,5	0.45	0	5,5,5	1.22	0
3	GOL	A	708	-	5,5,5	0.35	0	5,5,5	0.26	0
3	GOL	A	709	-	5,5,5	0.40	0	5,5,5	0.77	0
2	SO4	B	703	-	4,4,4	0.16	0	6,6,6	0.19	0
2	SO4	B	702	-	4,4,4	0.13	0	6,6,6	0.11	0
2	SO4	A	703	-	4,4,4	0.12	0	6,6,6	0.20	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
3	GOL	A	711	-	-	2/4/4/4	-
3	GOL	A	705	-	-	2/4/4/4	-
3	GOL	B	707	-	-	2/4/4/4	-
3	GOL	A	704	-	-	4/4/4/4	-
3	GOL	A	707	-	-	0/4/4/4	-
3	GOL	B	704	-	-	0/4/4/4	-
3	GOL	B	705	-	-	0/4/4/4	-
3	GOL	A	710	-	-	0/4/4/4	-
3	GOL	B	706	-	-	0/4/4/4	-
3	GOL	A	706	-	-	0/4/4/4	-
3	GOL	A	709	-	-	4/4/4/4	-
3	GOL	A	708	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	705	GOL	O1-C1-C2-C3
3	A	708	GOL	O1-C1-C2-O2
3	A	708	GOL	C1-C2-C3-O3
3	A	709	GOL	O1-C1-C2-C3
3	B	707	GOL	O1-C1-C2-O2
3	B	707	GOL	O1-C1-C2-C3
3	A	704	GOL	C1-C2-C3-O3
3	A	708	GOL	O1-C1-C2-C3
3	A	709	GOL	C1-C2-C3-O3
3	A	711	GOL	C1-C2-C3-O3
3	A	704	GOL	O1-C1-C2-O2
3	A	705	GOL	O1-C1-C2-O2
3	A	711	GOL	O2-C2-C3-O3
3	A	704	GOL	O2-C2-C3-O3
3	A	709	GOL	O1-C1-C2-O2
3	A	709	GOL	O2-C2-C3-O3
3	A	708	GOL	O2-C2-C3-O3
3	A	704	GOL	O1-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	707	GOL	1	0
3	B	704	GOL	2	0
3	A	710	GOL	2	0
3	B	705	GOL	1	0
3	A	706	GOL	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	358/387 (92%)	-0.22	18 (5%) 28 27	14, 25, 74, 113	0
1	B	357/387 (92%)	-0.07	24 (6%) 17 17	16, 27, 78, 109	0
All	All	715/774 (92%)	-0.14	42 (5%) 22 22	14, 26, 75, 113	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	398	VAL	8.9
1	A	547	GLY	6.3
1	B	557	VAL	5.8
1	B	391	PHE	5.8
1	B	395	LEU	5.3
1	A	485	SER	5.2
1	B	397	LYS	4.9
1	B	556	PRO	4.8
1	A	393	ASN	4.5
1	B	547	GLY	4.2
1	B	485	SER	4.2
1	B	393	ASN	4.1
1	A	391	PHE	3.8
1	A	557	VAL	3.6
1	B	553	VAL	3.4
1	A	395	LEU	3.4
1	B	385	GLY	3.3
1	A	397	LYS	3.3
1	A	556	PRO	3.3
1	A	390	PHE	3.2
1	B	448	GLN	3.2
1	A	404	SER	3.1
1	A	398	VAL	3.1
1	A	484	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	388	SER	2.8
1	B	555	MET	2.7
1	A	383	ILE	2.7
1	A	548	THR	2.7
1	A	434	LEU	2.6
1	A	392	SER	2.5
1	B	548	THR	2.4
1	A	546	THR	2.3
1	A	386	ASN	2.3
1	B	390	PHE	2.2
1	B	554	GLU	2.2
1	B	404	SER	2.2
1	B	471	ASN	2.2
1	B	387	ILE	2.2
1	B	386	ASN	2.1
1	B	355	GLN	2.1
1	B	383	ILE	2.1
1	B	483	ASN	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(Å <sup>2</sup> )	Q<0.9
3	GOL	A	709	6/6	0.55	0.25	52,58,60,67	0
3	GOL	B	707	6/6	0.74	0.16	46,48,52,55	0
3	GOL	A	705	6/6	0.83	0.20	32,55,70,72	0
3	GOL	A	706	6/6	0.83	0.33	33,48,56,57	0
3	GOL	A	710	6/6	0.88	0.14	29,41,44,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	704	6/6	0.90	0.13	25,33,37,39	0
3	GOL	B	704	6/6	0.91	0.16	25,37,42,42	0
3	GOL	B	706	6/6	0.91	0.13	31,44,51,60	0
3	GOL	A	711	6/6	0.91	0.13	33,38,40,45	0
3	GOL	A	708	6/6	0.93	0.12	25,56,59,65	0
3	GOL	B	705	6/6	0.93	0.11	24,32,35,41	0
2	SO4	A	701	5/5	0.95	0.14	50,51,57,57	0
2	SO4	A	703	5/5	0.97	0.15	33,39,48,57	0
2	SO4	B	701	5/5	0.97	0.10	44,47,49,57	0
2	SO4	B	702	5/5	0.97	0.13	53,58,63,68	0
3	GOL	A	707	6/6	0.97	0.07	21,23,25,28	0
2	SO4	A	702	5/5	0.98	0.06	42,43,46,51	0
2	SO4	B	703	5/5	0.99	0.08	40,44,46,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.