



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 02:27 AM EDT

PDB ID : 3NB2  
Title : Crystal structure of E. coli O157:H7 effector protein NleL  
Authors : Lin, D.Y.; Chen, J.  
Deposited on : 2010-06-02  
Resolution : 2.10 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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

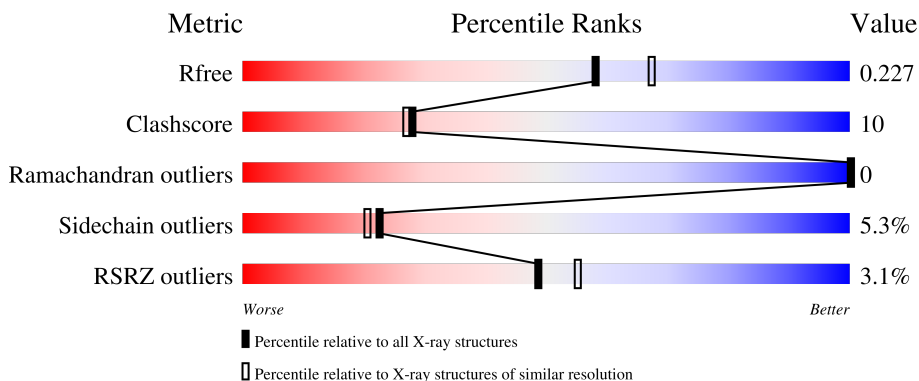
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


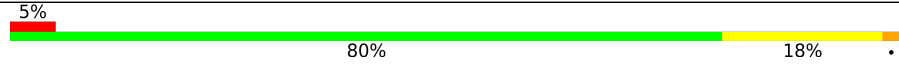
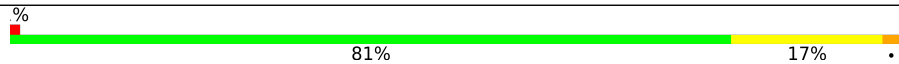

The reported resolution of this entry is 2.10 Å.

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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	613	 3% 80% 18% .
1	B	613	 5% 80% 18% .
1	C	613	 % 81% 17% .
1	D	613	 3% 80% 18% .

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	GOL	A	14	-	-	-	X
2	GOL	A	24	-	-	-	X
2	GOL	C	11	-	-	X	-
2	GOL	C	21	-	-	X	-
4	SO4	D	15	-	-	-	X
5	DTT	A	785	-	-	X	-

## 2 Entry composition [i](#)

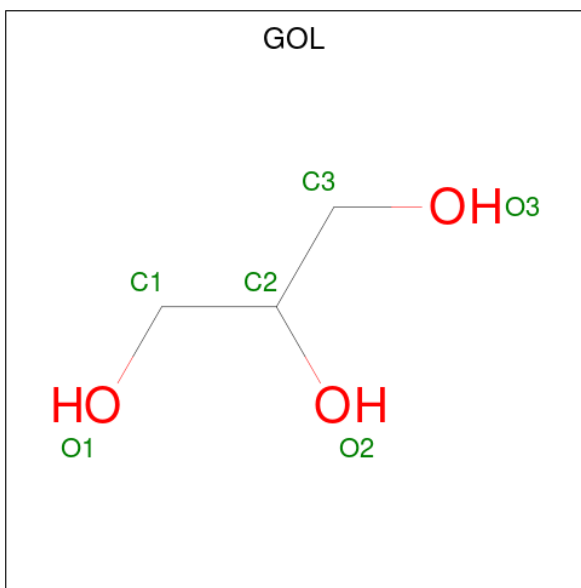
There are 6 unique types of molecules in this entry. The entry contains 20830 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 secreted effector protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	612	Total 4842	C 3066	N 785	O 953	S 38	0	0	0
1	B	612	Total 4850	C 3072	N 788	O 952	S 38	0	2	0
1	C	612	Total 4846	C 3068	N 788	O 952	S 38	0	0	0
1	D	612	Total 4864	C 3082	N 789	O 955	S 38	0	1	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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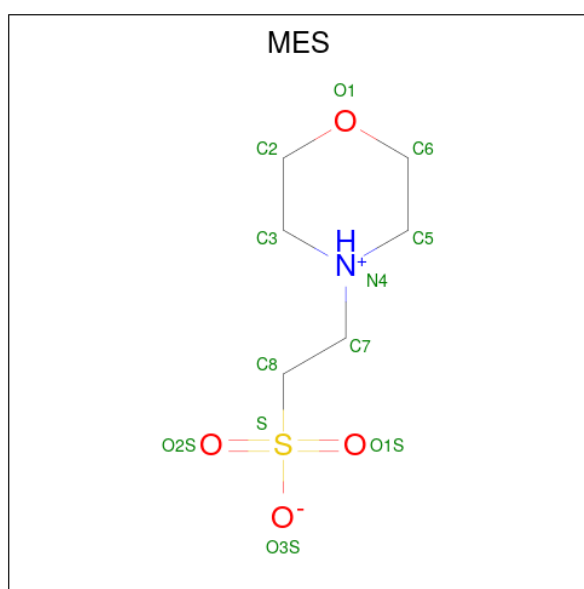
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0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

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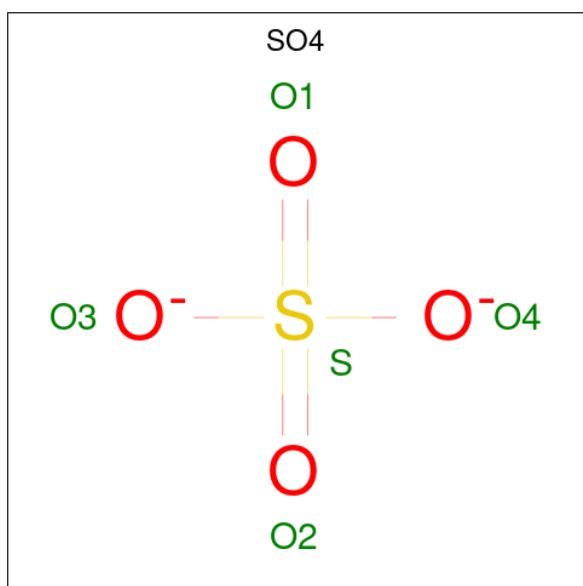
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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



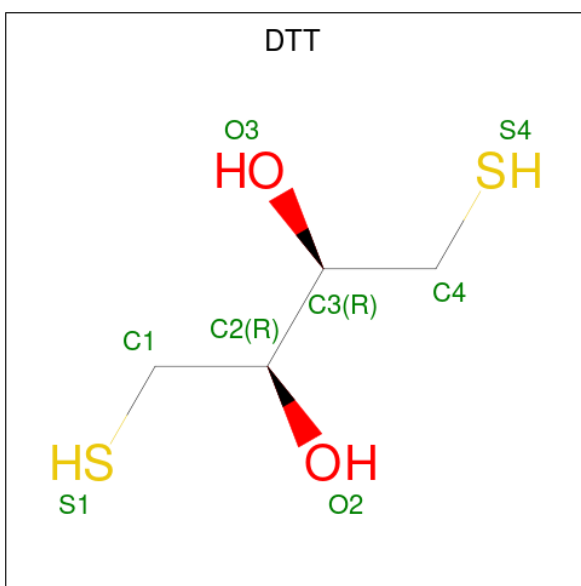
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula:  $C_4H_{10}O_2S_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			8	4	2	2		
5	C	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 6 is water.

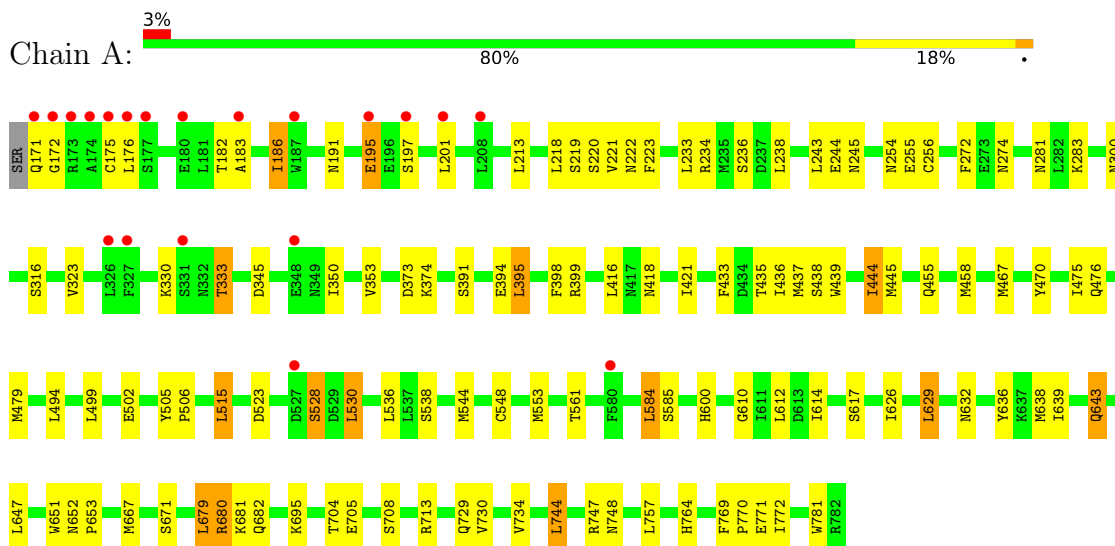
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	328	Total	O	0	0
			328	328		
6	B	273	Total	O	0	0
			273	273		
6	C	270	Total	O	0	0
			270	270		
6	D	227	Total	O	0	0
			227	227		



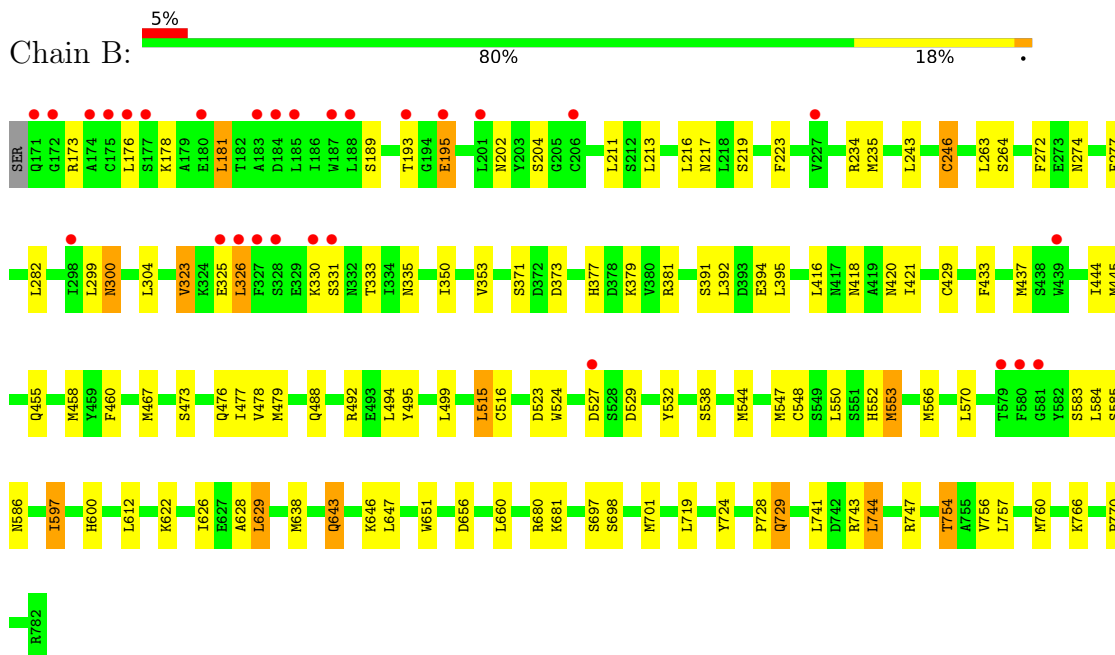
### 3 Residue-property plots [i](#)

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.

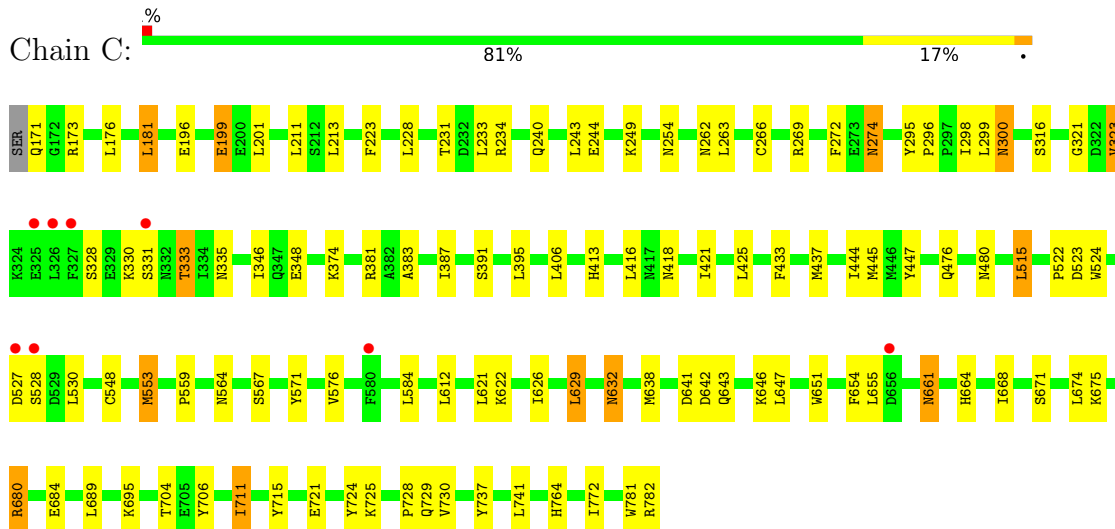
- Molecule 1: secreted effector protein



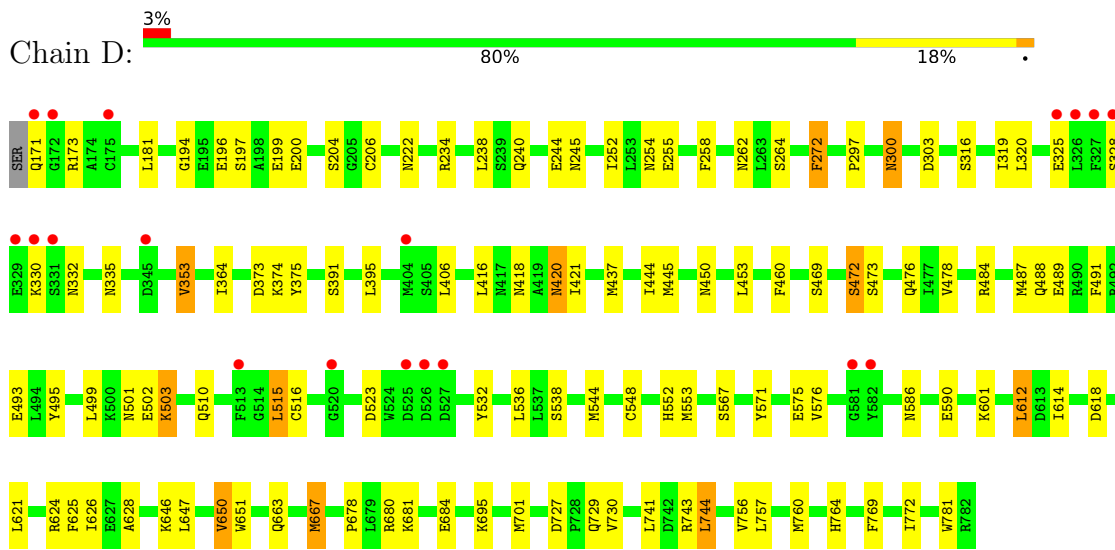
- Molecule 1: secreted effector protein



• Molecule 1: secreted effector protein



• Molecule 1: secreted effector protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	177.01Å 124.20Å 154.90Å 90.00° 107.60° 90.00°	Depositor
Resolution (Å)	44.74 – 2.10 44.74 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.74-2.10) 99.5 (44.74-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.48 (at 2.10Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, $R_{free}$	0.184 , 0.231 0.180 , 0.227	Depositor DCC
$R_{free}$ test set	9326 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.4	Xtrriage
Anisotropy	0.117	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	20830	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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: DTT, SO4, GOL, MES

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	0.44	0/4946	0.54	0/6695
1	B	0.40	1/4960 (0.0%)	0.52	0/6713
1	C	0.42	0/4950	0.52	0/6699
1	D	0.37	0/4972	0.48	0/6727
All	All	0.41	1/19828 (0.0%)	0.52	0/26834

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	429	CYS	CB-SG	-5.12	1.73	1.81

There are no bond angle outliers.

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	4842	0	4638	95	0
1	B	4850	0	4648	99	0
1	C	4846	0	4644	85	0
1	D	4864	0	4673	100	0
2	A	78	0	104	9	0
2	B	24	0	32	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	42	0	56	11	0
2	D	30	0	40	4	0
3	A	12	0	12	1	0
3	C	24	0	24	2	0
3	D	24	0	24	5	0
4	A	20	0	0	0	0
4	B	15	0	0	0	0
4	C	25	0	0	0	0
4	D	20	0	0	0	0
5	A	8	0	10	8	0
5	C	8	0	10	3	0
6	A	328	0	0	2	0
6	B	273	0	0	7	0
6	C	270	0	0	5	0
6	D	227	0	0	4	0
All	All	20830	0	18915	382	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 10.

All (382) 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:B:597:ILE:HD12	1:B:597:ILE:H	1.19	1.06
1:A:171:GLN:N	1:A:172:GLY:HA3	1.76	0.99
1:D:374[B]:LYS:H	1:D:374[B]:LYS:HD2	1.31	0.96
1:A:771:GLU:HG2	2:A:16:GOL:O2	1.66	0.95
1:A:638:MET:HA	1:A:643:GLN:HG2	1.52	0.92
1:A:680:ARG:HD3	1:A:729:GLN:HE21	1.35	0.91
1:A:643:GLN:HA	1:A:643:GLN:HE21	1.37	0.89
1:D:437:MET:CE	1:D:473:SER:HB3	2.03	0.89
1:A:617:SER:HB3	2:A:14:GOL:H12	1.55	0.88
1:A:769:PHE:HA	2:A:16:GOL:H2	1.55	0.88
1:B:437:MET:CE	1:B:473:SER:HB3	2.04	0.88
1:B:638:MET:HA	1:B:643:GLN:HG2	1.56	0.87
1:D:437:MET:HE3	1:D:473:SER:HB3	1.54	0.86
1:D:330:LYS:HD3	1:D:332:ASN:H	1.40	0.85
1:C:548:CYS:SG	1:C:553:MET:HG3	2.17	0.84
1:C:299:LEU:H	2:C:11:GOL:H32	1.42	0.84
1:B:437:MET:HE1	1:B:473:SER:HB3	1.60	0.83
1:B:418:ASN:HD22	1:B:421:ILE:H	1.27	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:THR:O	1:A:186:ILE:HG22	1.77	0.82
1:B:323:VAL:HG21	1:B:326:LEU:HD12	1.60	0.81
5:C:785:DTT:HS1	5:C:785:DTT:HS2	1.23	0.81
1:C:480:ASN:OD1	2:C:21:GOL:H31	1.80	0.80
1:A:418:ASN:HD22	1:A:421:ILE:H	1.32	0.78
1:B:330:LYS:O	1:B:331:SER:HB3	1.84	0.77
1:C:418:ASN:HD22	1:C:421:ILE:H	1.30	0.77
1:D:418:ASN:HD22	1:D:421:ILE:H	1.32	0.77
1:B:467:MET:HE3	6:B:1182:HOH:O	1.84	0.76
1:B:757:LEU:HA	1:B:760:MET:HE2	1.66	0.76
1:C:782:ARG:HH22	2:C:23:GOL:H31	1.51	0.76
1:C:196:GLU:HG3	1:C:201:LEU:HD21	1.66	0.75
1:B:680:ARG:CZ	1:B:729:GLN:HG2	2.16	0.75
1:C:664:HIS:CE1	1:C:668:ILE:HD11	2.23	0.74
1:A:502:GLU:HG2	6:A:826:HOH:O	1.87	0.73
1:D:515:LEU:HD13	1:D:523:ASP:HB2	1.70	0.73
1:B:757:LEU:HA	1:B:760:MET:CE	2.19	0.73
1:C:447:TYR:HD1	2:C:21:GOL:H2	1.54	0.72
1:A:614:ILE:O	2:A:14:GOL:H2	1.89	0.72
1:A:680:ARG:CD	1:A:729:GLN:HE21	2.02	0.72
1:D:330:LYS:HE2	1:D:332:ASN:HB2	1.69	0.72
1:C:299:LEU:H	2:C:11:GOL:C3	2.03	0.71
1:C:447:TYR:CD1	2:C:21:GOL:H2	2.25	0.70
1:D:756:VAL:HG12	1:D:760:MET:CE	2.22	0.70
5:A:785:DTT:H41	5:A:785:DTT:S1	2.31	0.70
1:B:643:GLN:HE21	1:B:643:GLN:HA	1.56	0.69
1:D:300:ASN:H	1:D:300:ASN:HD22	1.40	0.69
1:C:559:PRO:HD2	6:C:858:HOH:O	1.93	0.69
1:B:743:ARG:NH1	1:B:760:MET:HE1	2.07	0.68
1:D:453:LEU:HG	1:D:487:MET:HE1	1.74	0.68
1:D:453:LEU:HD23	1:D:487:MET:HE2	1.75	0.68
1:C:480:ASN:CG	2:C:21:GOL:H31	2.14	0.67
1:A:244:GLU:HG2	1:A:245:ASN:OD1	1.95	0.67
1:B:467:MET:HE2	1:B:494:LEU:HD11	1.76	0.67
1:A:747:ARG:O	1:A:748:ASN:HB2	1.95	0.67
5:C:785:DTT:S1	5:C:785:DTT:S4	2.91	0.66
1:B:445:MET:H	1:B:476:GLN:NE2	1.94	0.66
1:D:374[B]:LYS:H	1:D:374[B]:LYS:CD	2.08	0.66
1:B:300:ASN:H	1:B:300:ASN:HD22	1.44	0.65
1:B:437:MET:HE3	1:B:473:SER:HB3	1.76	0.65
1:B:213:LEU:HB3	1:B:216:LEU:HD12	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:743:ARG:HD3	1:D:760:MET:HE3	1.78	0.65
1:D:300:ASN:HD22	1:D:300:ASN:N	1.95	0.65
1:A:680:ARG:HD3	1:A:729:GLN:NE2	2.08	0.65
1:D:536:LEU:HD11	1:D:553:MET:HE1	1.79	0.65
1:B:756:VAL:HG12	1:B:760:MET:CE	2.26	0.64
1:A:515:LEU:HD13	1:A:523:ASP:HA	1.80	0.64
1:C:704:THR:HG23	1:C:706:TYR:H	1.61	0.64
1:A:300:ASN:HD22	1:A:300:ASN:H	1.46	0.64
1:D:437:MET:HE1	1:D:460:PHE:CE2	2.32	0.63
1:C:300:ASN:HD22	1:C:300:ASN:H	1.44	0.63
1:C:643:GLN:HE21	1:C:643:GLN:HA	1.62	0.63
1:D:181:LEU:HD21	1:D:206:CYS:HB3	1.79	0.63
1:A:171:GLN:N	1:A:172:GLY:CA	2.59	0.63
1:B:698:SER:HA	1:B:754:THR:HG22	1.80	0.63
1:C:680:ARG:HD2	1:C:729:GLN:OE1	1.97	0.63
1:D:756:VAL:HG12	1:D:760:MET:HE2	1.81	0.63
1:A:218:LEU:HB2	1:A:238:LEU:HD23	1.80	0.62
1:D:418:ASN:ND2	1:D:421:ILE:H	1.96	0.62
5:A:785:DTT:S1	5:A:785:DTT:C4	2.86	0.62
1:B:680:ARG:NH2	1:B:729:GLN:HG2	2.13	0.62
1:A:643:GLN:HA	1:A:643:GLN:NE2	2.13	0.62
1:D:487:MET:HE3	1:D:491:PHE:CE2	2.35	0.62
1:D:501:ASN:OD1	1:D:503:LYS:HD2	1.99	0.62
1:C:655:LEU:HD12	1:C:711:ILE:HD11	1.82	0.62
1:D:238:LEU:HD22	1:D:258:PHE:CE1	2.35	0.61
1:A:373:ASP:CG	3:C:2:MES:H62	2.21	0.61
1:A:730:VAL:O	1:A:764:HIS:HE1	1.83	0.61
1:D:445:MET:H	1:D:476:GLN:NE2	1.98	0.61
1:C:571:TYR:CE1	1:C:576:VAL:HG22	2.36	0.61
1:D:437:MET:HE1	1:D:460:PHE:HE2	1.64	0.61
1:A:467:MET:CE	1:A:494:LEU:HD11	2.30	0.61
1:D:244:GLU:HG3	1:D:264:SER:HB2	1.81	0.61
1:B:756:VAL:HG12	1:B:760:MET:HE1	1.83	0.61
1:D:646:LYS:O	1:D:650:VAL:HG12	2.01	0.61
1:B:492:ARG:HD2	1:B:524:TRP:CD2	2.36	0.61
1:C:211:LEU:O	1:C:231:THR:HG23	2.01	0.61
1:A:744:LEU:HD13	1:A:757:LEU:CD2	2.31	0.60
1:C:643:GLN:NE2	1:C:646:LYS:HE2	2.16	0.60
1:B:492:ARG:HD2	1:B:524:TRP:CG	2.35	0.60
1:C:298:ILE:HA	2:C:11:GOL:H32	1.84	0.60
1:D:374[B]:LYS:NZ	3:D:783:MES:H21	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:MET:HE2	1:B:460:PHE:CE2	2.36	0.60
1:D:437:MET:HE2	1:D:473:SER:HB3	1.80	0.60
1:D:445:MET:H	1:D:476:GLN:HE22	1.48	0.60
1:B:444:ILE:HA	1:B:476:GLN:HE22	1.66	0.60
1:A:435:THR:HG22	5:A:785:DTT:S1	2.42	0.60
1:C:418:ASN:ND2	1:C:421:ILE:H	1.99	0.60
1:B:445:MET:H	1:B:476:GLN:HE22	1.50	0.60
1:D:234:ARG:HG2	1:D:254:ASN:HB2	1.84	0.60
1:A:744:LEU:HD13	1:A:757:LEU:HD23	1.84	0.59
1:C:651:TRP:HB3	1:C:711:ILE:HD12	1.84	0.59
1:D:680:ARG:O	1:D:684:GLU:HG3	2.03	0.59
1:C:730:VAL:O	1:C:764:HIS:HE1	1.86	0.59
1:D:743:ARG:NH1	1:D:760:MET:HE1	2.18	0.59
1:D:744:LEU:HD13	1:D:757:LEU:CD2	2.33	0.59
1:A:221:VAL:HG11	1:A:223:PHE:CZ	2.38	0.59
1:C:664:HIS:HE1	1:C:715:TYR:OH	1.85	0.58
1:C:300:ASN:HD22	1:C:300:ASN:N	2.02	0.58
1:D:330:LYS:CD	1:D:332:ASN:H	2.13	0.58
1:A:219:SER:O	1:A:220:SER:HB2	2.03	0.57
1:B:418:ASN:ND2	1:B:421:ILE:H	1.99	0.57
1:D:255:GLU:OE2	3:D:4:MES:H31	2.05	0.57
1:D:234:ARG:HG3	1:D:252:ILE:HG22	1.87	0.57
1:D:538:SER:HB2	1:D:544:MET:HB2	1.87	0.57
1:B:597:ILE:HD12	1:B:597:ILE:N	2.05	0.57
1:A:394:GLU:O	1:A:399:ARG:NE	2.38	0.57
1:C:571:TYR:HE1	1:C:576:VAL:HG22	1.68	0.57
1:B:223:PHE:HB2	1:B:243:LEU:HD23	1.86	0.57
1:A:528:SER:OG	1:A:530:LEU:HB2	2.05	0.57
1:D:453:LEU:CD2	1:D:487:MET:HE2	2.34	0.56
1:B:467:MET:CE	1:B:494:LEU:HD11	2.34	0.56
1:B:515:LEU:HD13	1:B:523:ASP:HB2	1.88	0.56
5:C:785:DTT:S4	5:C:785:DTT:C1	2.93	0.56
1:D:238:LEU:HD22	1:D:258:PHE:HE1	1.69	0.56
1:D:453:LEU:HG	1:D:487:MET:CE	2.35	0.56
1:C:632:ASN:H	1:C:632:ASN:HD22	1.51	0.56
1:D:515:LEU:HD13	1:D:523:ASP:CB	2.34	0.56
1:C:445:MET:H	1:C:476:GLN:NE2	2.04	0.56
1:C:173:ARG:HD2	6:C:976:HOH:O	2.04	0.56
1:D:472:SER:HB3	6:D:903:HOH:O	2.06	0.56
1:C:528:SER:HB2	1:C:530:LEU:HD23	1.88	0.55
1:D:756:VAL:HG12	1:D:760:MET:HE1	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:PHE:HB2	1:A:243:LEU:HD23	1.89	0.55
1:B:455:GLN:HA	1:B:458:MET:HE2	1.88	0.55
1:A:213:LEU:HB2	1:A:233:LEU:HD23	1.88	0.55
1:A:467:MET:HE3	1:A:494:LEU:HD11	1.88	0.55
1:A:695:LYS:HG2	1:A:781:TRP:CE3	2.42	0.55
1:B:766:LYS:O	1:B:770:PRO:HG3	2.07	0.55
1:A:708:SER:OG	1:A:713:ARG:HD3	2.06	0.55
1:A:255:GLU:OE2	3:A:3:MES:H31	2.06	0.54
1:B:437:MET:HE2	1:B:460:PHE:HE2	1.72	0.54
1:B:189:SER:HB2	1:B:217:ASN:H	1.72	0.54
1:C:684:GLU:OE1	1:C:772:ILE:HD13	2.07	0.54
1:B:681:LYS:HE2	6:B:896:HOH:O	2.08	0.54
1:D:487:MET:CE	1:D:491:PHE:CE2	2.90	0.54
1:B:274:ASN:HD21	1:D:316:SER:HB3	1.73	0.54
1:B:698:SER:CA	1:B:754:THR:HG22	2.38	0.54
1:B:757:LEU:CA	1:B:760:MET:HE2	2.37	0.54
1:D:373:ASP:CG	3:D:783:MES:H62	2.29	0.54
1:B:193:THR:HG22	1:B:195:GLU:H	1.73	0.53
1:D:628:ALA:HB1	1:D:701:MET:HE1	1.90	0.53
1:D:374[B]:LYS:HZ2	3:D:783:MES:H21	1.73	0.53
1:A:439:TRP:CB	5:A:785:DTT:H11	2.39	0.53
1:C:171:GLN:N	1:C:199:GLU:O	2.42	0.53
1:A:730:VAL:HG22	1:A:769:PHE:CE2	2.43	0.53
1:B:418:ASN:HD21	1:B:420:ASN:HB3	1.74	0.53
1:A:467:MET:CE	1:A:494:LEU:CD1	2.87	0.53
1:A:610:GLY:HA3	2:A:7:GOL:H12	1.91	0.53
1:A:330:LYS:HB2	1:A:333:THR:HG23	1.91	0.52
1:C:444:ILE:HA	1:C:476:GLN:HE22	1.74	0.52
1:D:244:GLU:HG2	1:D:245:ASN:ND2	2.24	0.52
1:D:320:LEU:HB2	1:D:375:TYR:CE1	2.44	0.52
1:D:727:ASP:OD1	1:D:729:GLN:HG2	2.09	0.52
1:B:743:ARG:HD3	1:B:760:MET:HE3	1.91	0.52
1:D:744:LEU:HD13	1:D:757:LEU:HD23	1.92	0.52
1:C:413:HIS:HD2	6:C:841:HOH:O	1.92	0.52
1:D:515:LEU:O	1:D:516:CYS:HB2	2.09	0.52
1:B:585:SER:OG	1:B:600:HIS:HE1	1.93	0.52
1:C:654:PHE:CD2	1:C:664:HIS:CD2	2.98	0.52
1:D:510:GLN:HG3	1:D:571:TYR:CE1	2.44	0.52
1:C:651:TRP:CB	1:C:711:ILE:HD12	2.40	0.51
1:C:173:ARG:HB2	1:C:176:LEU:HD13	1.92	0.51
1:B:529:ASP:HA	6:B:934:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:501:ASN:HD21	1:D:503:LYS:NZ	2.08	0.51
1:D:681:LYS:HD2	1:D:772:ILE:HD11	1.93	0.51
1:B:326:LEU:O	1:B:381[A]:ARG:NH1	2.44	0.51
1:A:391:SER:OG	1:A:394:GLU:HG3	2.11	0.51
1:A:445:MET:H	1:A:476:GLN:NE2	2.09	0.51
1:C:622:LYS:HE2	6:C:1223:HOH:O	2.10	0.51
1:A:183:ALA:HA	1:A:186:ILE:CG2	2.41	0.51
1:D:757:LEU:HA	1:D:760:MET:CE	2.41	0.51
1:A:438:SER:HB3	1:A:470:TYR:CZ	2.46	0.50
1:A:175:CYS:O	1:A:176:LEU:HD12	2.12	0.50
1:A:444:ILE:HA	1:A:476:GLN:HE22	1.76	0.50
1:C:330:LYS:HB2	1:C:333:THR:HG23	1.93	0.50
1:D:173:ARG:HD2	6:D:942:HOH:O	2.12	0.50
1:C:299:LEU:N	2:C:11:GOL:H32	2.18	0.50
1:D:614:ILE:HD13	1:D:667:MET:SD	2.50	0.50
1:A:218:LEU:HB2	1:A:238:LEU:CD2	2.42	0.50
1:A:300:ASN:HD22	1:A:300:ASN:N	2.09	0.50
1:B:515:LEU:HD13	1:B:523:ASP:CB	2.42	0.50
1:C:196:GLU:CG	1:C:201:LEU:HD21	2.37	0.50
1:D:197:SER:OG	1:D:200:GLU:HG3	2.11	0.50
1:C:626:ILE:O	1:C:629:LEU:HB2	2.12	0.50
1:A:445:MET:H	1:A:476:GLN:HE22	1.58	0.50
1:C:695:LYS:HG2	1:C:781:TRP:CE3	2.47	0.50
1:B:455:GLN:HA	1:B:458:MET:CE	2.42	0.49
1:A:734:VAL:CG2	2:A:24:GOL:H11	2.43	0.49
1:A:316:SER:HB3	1:C:274:ASN:HD21	1.77	0.49
1:A:632:ASN:HD21	1:A:695:LYS:NZ	2.11	0.49
1:B:660:LEU:HD11	1:B:719:LEU:HD23	1.95	0.49
1:C:522:PRO:HG2	1:C:524:TRP:NE1	2.28	0.49
1:C:721:GLU:O	1:C:725:LYS:HG3	2.12	0.49
1:A:505:TYR:HB3	1:A:506:PRO:HD3	1.95	0.48
1:B:178:LYS:HG2	1:B:211:LEU:HD21	1.95	0.48
1:D:444:ILE:HA	1:D:476:GLN:HE22	1.77	0.48
1:C:661:ASN:ND2	1:C:664:HIS:H	2.12	0.48
1:D:621:LEU:O	1:D:624:ARG:HB2	2.12	0.48
2:A:7:GOL:H11	6:A:909:HOH:O	2.13	0.48
1:B:243:LEU:O	1:B:246:CYS:HB2	2.12	0.48
1:D:730:VAL:O	1:D:764:HIS:HE1	1.97	0.48
1:A:281:ASN:OD1	1:A:283:LYS:HD3	2.14	0.48
1:B:626:ILE:O	1:B:629:LEU:HB2	2.13	0.48
1:A:538:SER:HB2	1:A:544:MET:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:LEU:HB3	1:B:216:LEU:CD1	2.43	0.47
1:C:621:LEU:HD11	1:C:638:MET:HE1	1.96	0.47
1:C:632:ASN:HD22	1:C:632:ASN:N	2.13	0.47
1:C:643:GLN:HE22	1:C:646:LYS:HE2	1.78	0.47
1:B:756:VAL:HG12	1:B:760:MET:HE2	1.94	0.47
1:C:223:PHE:HB2	1:C:243:LEU:HD23	1.96	0.47
1:D:325:GLU:HG3	1:D:335:ASN:ND2	2.30	0.47
1:C:447:TYR:HA	2:C:21:GOL:H32	1.96	0.47
1:D:450:ASN:OD1	1:D:484:ARG:HD2	2.14	0.47
1:D:532:TYR:CD1	1:D:548:CYS:HA	2.48	0.47
1:B:638:MET:CA	1:B:643:GLN:HG2	2.36	0.47
1:B:724:TYR:CE1	1:B:728:PRO:HB3	2.49	0.47
1:C:234:ARG:HG2	1:C:254:ASN:HB2	1.96	0.47
1:C:651:TRP:HB3	1:C:711:ILE:CD1	2.45	0.47
1:D:756:VAL:C	1:D:760:MET:HE2	2.35	0.47
6:B:815:HOH:O	1:D:601:LYS:HE2	2.14	0.47
1:C:433:PHE:O	1:C:437:MET:HG2	2.15	0.47
1:C:671:SER:O	1:C:675:LYS:HB2	2.14	0.47
1:B:583:SER:HB3	1:B:586:ASN:HB2	1.96	0.46
1:D:624:ARG:HH21	2:D:27:GOL:H12	1.80	0.46
1:A:221:VAL:HG11	1:A:223:PHE:CE2	2.51	0.46
1:C:528:SER:O	1:C:530:LEU:HD22	2.15	0.46
1:A:350:ILE:O	1:A:353:VAL:HG22	2.15	0.46
1:C:330:LYS:O	1:C:331:SER:HB3	2.15	0.46
1:D:536:LEU:N	1:D:536:LEU:HD12	2.31	0.46
1:C:445:MET:H	1:C:476:GLN:HE22	1.64	0.46
1:B:479:MET:HE3	1:B:550:LEU:HG	1.97	0.46
1:C:724:TYR:CE1	1:C:728:PRO:HB3	2.51	0.46
1:A:433:PHE:O	1:A:437:MET:HG2	2.16	0.46
1:A:636:TYR:HE2	1:A:638:MET:HE2	1.81	0.45
1:D:325:GLU:HG3	1:D:335:ASN:HD21	1.80	0.45
1:A:439:TRP:CG	5:A:785:DTT:H11	2.51	0.45
1:B:488:GLN:O	1:B:492:ARG:HG3	2.16	0.45
1:B:478:VAL:HG11	1:B:495:TYR:HB2	1.98	0.45
1:B:597:ILE:H	1:B:597:ILE:CD1	1.97	0.45
1:C:515:LEU:CD1	1:C:523:ASP:HA	2.46	0.45
1:A:548:CYS:SG	1:A:553:MET:HE1	2.56	0.45
1:B:643:GLN:NE2	1:B:646:LYS:HE2	2.31	0.45
1:D:194:GLY:N	1:D:196:GLU:OE1	2.50	0.45
1:C:243:LEU:O	1:C:266:CYS:SG	2.75	0.45
1:C:295:TYR:HA	1:C:296:PRO:HD3	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:GLN:CD	1:A:458:MET:HE3	2.37	0.45
1:A:639:ILE:HG12	1:A:704:THR:HG23	1.99	0.45
1:B:538:SER:HB2	1:B:544:MET:HB2	1.99	0.45
1:D:532:TYR:HD1	1:D:548:CYS:HA	1.80	0.45
2:A:4:GOL:H31	2:A:19:GOL:C1	2.47	0.45
1:B:515:LEU:O	1:B:516:CYS:HB2	2.16	0.45
1:C:244:GLU:HG3	1:C:262:ASN:ND2	2.32	0.45
1:C:661:ASN:C	1:C:661:ASN:HD22	2.20	0.45
1:D:204:SER:HB3	1:D:222:ASN:HD21	1.81	0.45
1:A:398:PHE:CZ	5:A:785:DTT:S1	3.08	0.45
1:A:638:MET:HA	1:A:643:GLN:CG	2.34	0.45
1:B:597:ILE:N	1:B:597:ILE:CD1	2.74	0.45
1:C:323:VAL:HG21	1:C:381:ARG:NH2	2.31	0.45
1:D:678:PRO:HD2	1:D:681:LYS:HB2	1.99	0.45
1:B:202:ASN:ND2	1:B:204:SER:H	2.15	0.44
1:B:766:LYS:HE2	2:D:26:GOL:O3	2.17	0.44
1:D:420:ASN:HB2	6:D:841:HOH:O	2.16	0.44
1:D:484:ARG:O	1:D:488:GLN:HG3	2.18	0.44
1:D:501:ASN:HD21	1:D:503:LYS:HZ2	1.65	0.44
1:D:575:GLU:HB2	6:D:895:HOH:O	2.17	0.44
1:D:695:LYS:HG2	1:D:781:TRP:CE3	2.53	0.44
1:B:330:LYS:O	1:B:331:SER:CB	2.60	0.44
1:C:181:LEU:HD12	1:C:181:LEU:HA	1.86	0.44
1:C:711:ILE:HD13	1:C:711:ILE:O	2.18	0.44
1:C:321:GLY:CA	6:C:1244:HOH:O	2.66	0.44
1:D:272:PHE:CG	1:D:297:PRO:HG3	2.52	0.44
1:D:618:ASP:OD1	1:D:618:ASP:C	2.56	0.44
1:D:628:ALA:HB1	1:D:701:MET:CE	2.48	0.44
1:B:757:LEU:HA	1:B:760:MET:HE3	1.99	0.44
1:D:303:ASP:HA	1:D:319:ILE:HB	1.99	0.44
1:D:489:GLU:O	1:D:493:GLU:HG3	2.17	0.44
1:C:655:LEU:HD12	1:C:711:ILE:CD1	2.46	0.43
1:D:469:SER:HB3	2:D:26:GOL:H31	2.00	0.43
1:A:221:VAL:HG12	1:A:222:ASN:N	2.32	0.43
1:B:628:ALA:HB1	1:B:701:MET:HE1	1.99	0.43
1:C:643:GLN:HA	1:C:643:GLN:NE2	2.31	0.43
1:A:770:PRO:HD2	2:A:16:GOL:H2	1.99	0.43
1:B:350:ILE:O	1:B:353:VAL:HG22	2.18	0.43
1:B:566:MET:HE1	6:B:963:HOH:O	2.18	0.43
1:A:435:THR:CG2	5:A:785:DTT:S1	3.06	0.43
1:A:636:TYR:HE2	1:A:638:MET:CE	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:LEU:HD12	1:B:181:LEU:HA	1.83	0.43
1:D:300:ASN:N	1:D:300:ASN:ND2	2.64	0.43
1:B:282:LEU:HB2	1:B:304:LEU:HD12	2.00	0.43
1:B:544:MET:HE3	1:B:570:LEU:HD11	2.00	0.43
1:C:330:LYS:O	1:C:331:SER:CB	2.67	0.43
1:A:455:GLN:OE1	1:A:458:MET:HE3	2.18	0.43
1:A:730:VAL:CG2	1:A:769:PHE:CE2	3.01	0.43
6:B:1228:HOH:O	2:D:28:GOL:H2	2.19	0.43
1:C:328:SER:N	1:C:335:ASN:HD21	2.16	0.43
1:D:612:LEU:HD21	1:D:625:PHE:HB3	2.00	0.43
1:A:652:ASN:N	1:A:653:PRO:CD	2.82	0.42
1:C:346:ILE:O	1:C:348:GLU:N	2.45	0.42
1:C:383:ALA:O	1:C:387:ILE:HG23	2.19	0.42
1:D:757:LEU:HA	1:D:760:MET:HE2	2.00	0.42
1:B:553:MET:HB2	1:B:553:MET:HE2	1.56	0.42
1:A:374:LYS:HE3	1:A:374:LYS:HB2	1.91	0.42
1:A:548:CYS:SG	1:A:553:MET:CE	3.08	0.42
1:B:330:LYS:HD2	1:B:333:THR:HG21	2.01	0.42
1:B:437:MET:HE3	1:B:460:PHE:HZ	1.85	0.42
1:A:530:LEU:HD12	1:A:530:LEU:HA	1.94	0.42
1:B:277:PHE:HB2	1:B:299:LEU:HD23	2.02	0.42
1:C:249:LYS:HA	1:C:269:ARG:HB3	2.02	0.42
1:D:730:VAL:HG13	1:D:769:PHE:CE2	2.54	0.42
1:A:221:VAL:CG1	1:A:223:PHE:CE2	3.03	0.42
1:B:193:THR:HG22	1:B:195:GLU:N	2.34	0.42
1:B:274:ASN:ND2	1:D:316:SER:HB3	2.34	0.42
1:D:552:HIS:CE1	1:D:567:SER:HB3	2.54	0.42
1:A:584:LEU:HD12	1:A:584:LEU:HA	1.73	0.42
1:B:515:LEU:HD13	1:B:523:ASP:HA	2.01	0.42
1:D:330:LYS:CE	1:D:332:ASN:HB2	2.46	0.42
1:A:233:LEU:O	1:A:236:SER:HB2	2.20	0.42
1:A:626:ILE:O	1:A:629:LEU:HB2	2.20	0.42
1:A:681:LYS:HG3	1:A:772:ILE:HD11	2.02	0.42
1:B:743:ARG:CZ	1:B:760:MET:HE1	2.50	0.42
1:C:196:GLU:HG3	1:C:201:LEU:CD2	2.43	0.42
1:C:564:ASN:OD1	1:C:567:SER:HB2	2.20	0.42
1:C:782:ARG:NH2	2:C:23:GOL:H31	2.28	0.42
1:A:436:ILE:HD13	5:A:785:DTT:H12	2.02	0.42
1:D:478:VAL:HG11	1:D:495:TYR:HB2	2.02	0.42
1:B:437:MET:HE2	1:B:477:ILE:HG13	2.01	0.41
1:B:622:LYS:HG2	1:B:626:ILE:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ARG:O	1:B:235:MET:HB2	2.19	0.41
1:A:373:ASP:OD2	3:C:2:MES:H62	2.21	0.41
1:A:679:LEU:HD12	1:A:682:GLN:NE2	2.35	0.41
1:B:300:ASN:HD22	1:B:300:ASN:N	2.12	0.41
1:B:433:PHE:O	1:B:437:MET:HG2	2.20	0.41
1:A:233:LEU:O	1:A:256:CYS:SG	2.75	0.41
1:A:274:ASN:ND2	1:C:316:SER:HB3	2.36	0.41
1:A:585:SER:OG	1:A:600:HIS:HE1	2.02	0.41
1:B:552:HIS:HD2	6:B:1020:HOH:O	2.03	0.41
1:C:213:LEU:HB2	1:C:233:LEU:HD23	2.01	0.41
1:D:171:GLN:N	1:D:199:GLU:O	2.54	0.41
1:A:175:CYS:C	1:A:176:LEU:HD12	2.41	0.41
1:A:234:ARG:HG2	1:A:254:ASN:HB2	2.02	0.41
1:A:274:ASN:HD21	1:C:316:SER:HB3	1.84	0.41
1:A:395:LEU:HD12	1:A:395:LEU:HA	1.77	0.41
1:A:475:ILE:HG13	1:A:536:LEU:HD23	2.02	0.41
1:B:373:ASP:OD1	3:D:4:MES:H22	2.20	0.41
1:D:586:ASN:O	1:D:590:GLU:HB2	2.20	0.41
1:A:195:GLU:H	1:A:195:GLU:HG3	1.70	0.41
1:B:325:GLU:HG3	1:B:335:ASN:ND2	2.36	0.41
1:B:532:TYR:HB3	1:B:547:MET:HG2	2.03	0.41
1:C:228:LEU:HD22	1:C:233:LEU:HD11	2.03	0.41
1:B:371:SER:OG	1:B:379:LYS:HE2	2.22	0.40
1:C:737:TYR:CZ	1:C:741:LEU:HD11	2.56	0.40
1:D:353:VAL:HG13	1:D:364:ILE:HG22	2.03	0.40
1:A:679:LEU:HD12	1:A:679:LEU:HA	1.84	0.40
1:B:173:ARG:H	1:B:176:LEU:HD13	1.86	0.40
1:B:377:HIS:O	1:B:381[A]:ARG:HG3	2.20	0.40
1:B:532:TYR:CD1	1:B:548:CYS:HA	2.56	0.40
1:A:479:MET:HE3	1:A:553:MET:HE3	2.03	0.40
1:B:391:SER:OG	1:B:394[A]:GLU:HG3	2.21	0.40
1:B:437:MET:CE	1:B:460:PHE:CZ	3.04	0.40
1:B:744:LEU:HD13	1:B:757:LEU:CD2	2.51	0.40
1:D:328:SER:HB2	1:D:335:ASN:OD1	2.22	0.40
1:D:612:LEU:HD23	1:D:626:ILE:HD13	2.04	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	610/613 (100%)	583 (96%)	27 (4%)	0	100	100
1	B	612/613 (100%)	580 (95%)	32 (5%)	0	100	100
1	C	610/613 (100%)	585 (96%)	25 (4%)	0	100	100
1	D	611/613 (100%)	584 (96%)	27 (4%)	0	100	100
All	All	2443/2452 (100%)	2332 (96%)	111 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	541/546 (99%)	512 (95%)	29 (5%)	22	20
1	B	541/546 (99%)	510 (94%)	31 (6%)	20	18
1	C	541/546 (99%)	511 (94%)	30 (6%)	21	19
1	D	545/546 (100%)	521 (96%)	24 (4%)	28	28
All	All	2168/2184 (99%)	2054 (95%)	114 (5%)	22	20

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	186	ILE
1	A	191	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	195	GLU
1	A	197	SER
1	A	201	LEU
1	A	272	PHE
1	A	323	VAL
1	A	333	THR
1	A	345	ASP
1	A	395	LEU
1	A	416	LEU
1	A	444	ILE
1	A	499	LEU
1	A	515	LEU
1	A	528	SER
1	A	530	LEU
1	A	561	THR
1	A	584	LEU
1	A	612	LEU
1	A	629	LEU
1	A	643	GLN
1	A	647	LEU
1	A	651	TRP
1	A	667	MET
1	A	671	SER
1	A	679	LEU
1	A	680	ARG
1	A	705	GLU
1	A	744	LEU
1	B	181	LEU
1	B	195	GLU
1	B	219	SER
1	B	246	CYS
1	B	263	LEU
1	B	264	SER
1	B	272	PHE
1	B	300	ASN
1	B	323	VAL
1	B	326	LEU
1	B	392	LEU
1	B	395	LEU
1	B	416	LEU
1	B	499	LEU
1	B	515	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	527	ASP
1	B	553	MET
1	B	584	LEU
1	B	597	ILE
1	B	612	LEU
1	B	629	LEU
1	B	643	GLN
1	B	647	LEU
1	B	651	TRP
1	B	656	ASP
1	B	697	SER
1	B	729	GLN
1	B	741	LEU
1	B	744	LEU
1	B	747	ARG
1	B	754	THR
1	C	181	LEU
1	C	199	GLU
1	C	240	GLN
1	C	263	LEU
1	C	272	PHE
1	C	274	ASN
1	C	300	ASN
1	C	323	VAL
1	C	333	THR
1	C	374	LYS
1	C	391	SER
1	C	395	LEU
1	C	406	LEU
1	C	416	LEU
1	C	425	LEU
1	C	515	LEU
1	C	527	ASP
1	C	553	MET
1	C	584	LEU
1	C	612	LEU
1	C	629	LEU
1	C	632	ASN
1	C	641	ASP
1	C	642	ASP
1	C	647	LEU
1	C	661	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	674	LEU
1	C	680	ARG
1	C	689	LEU
1	C	711	ILE
1	D	240	GLN
1	D	262	ASN
1	D	272	PHE
1	D	300	ASN
1	D	353	VAL
1	D	391	SER
1	D	395	LEU
1	D	406	LEU
1	D	416	LEU
1	D	420	ASN
1	D	472	SER
1	D	499	LEU
1	D	502	GLU
1	D	503	LYS
1	D	515	LEU
1	D	576	VAL
1	D	612	LEU
1	D	647	LEU
1	D	650	VAL
1	D	651	TRP
1	D	663	GLN
1	D	667	MET
1	D	741	LEU
1	D	744	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	294	GLN
1	A	300	ASN
1	A	418	ASN
1	A	476	GLN
1	A	480	ASN
1	A	577	GLN
1	A	600	HIS
1	A	632	ASN
1	A	643	GLN
1	A	682	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	717	ASN
1	A	729	GLN
1	A	745	GLN
1	A	764	HIS
1	B	191	ASN
1	B	202	ASN
1	B	300	ASN
1	B	413	HIS
1	B	418	ASN
1	B	476	GLN
1	B	480	ASN
1	B	552	HIS
1	B	600	HIS
1	B	632	ASN
1	B	643	GLN
1	B	663	GLN
1	B	717	ASN
1	B	745	GLN
1	C	300	ASN
1	C	335	ASN
1	C	418	ASN
1	C	476	GLN
1	C	488	GLN
1	C	577	GLN
1	C	632	ASN
1	C	643	GLN
1	C	661	ASN
1	C	664	HIS
1	C	717	ASN
1	C	745	GLN
1	C	764	HIS
1	D	222	ASN
1	D	245	ASN
1	D	300	ASN
1	D	332	ASN
1	D	413	HIS
1	D	418	ASN
1	D	476	GLN
1	D	600	HIS
1	D	632	ASN
1	D	661	ASN
1	D	749	ASN

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Mol	Chain	Res	Type
1	D	764	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

52 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	GOL	A	15	-	5,5,5	0.39	0	5,5,5	0.47	0
2	GOL	C	20	-	5,5,5	0.39	0	5,5,5	0.24	0
2	GOL	C	23	-	5,5,5	0.35	0	5,5,5	0.29	0
4	SO4	D	16	-	4,4,4	0.14	0	6,6,6	0.10	0
2	GOL	C	29	-	5,5,5	0.42	0	5,5,5	0.43	0
5	DTT	A	785	-	7,7,7	0.74	0	4,8,8	1.06	0
2	GOL	A	1	-	5,5,5	0.44	0	5,5,5	0.58	0
2	GOL	B	8	-	5,5,5	0.38	0	5,5,5	0.49	0
3	MES	A	3	-	12,12,12	2.18	1 (8%)	14,16,16	2.51	8 (57%)
4	SO4	D	15	-	4,4,4	0.13	0	6,6,6	0.09	0
2	GOL	A	7	-	5,5,5	0.39	0	5,5,5	0.49	0
2	GOL	B	10	-	5,5,5	0.39	0	5,5,5	0.31	0
2	GOL	A	25	-	5,5,5	0.39	0	5,5,5	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	C	17	-	5,5,5	0.35	0	5,5,5	0.36	0
4	SO4	B	784	-	4,4,4	0.14	0	6,6,6	0.13	0
3	MES	D	783	-	12,12,12	2.17	1 (8%)	14,16,16	2.57	7 (50%)
2	GOL	A	16	-	5,5,5	0.39	0	5,5,5	0.36	0
4	SO4	B	12	-	4,4,4	0.15	0	6,6,6	0.09	0
2	GOL	D	26	-	5,5,5	0.32	0	5,5,5	0.42	0
2	GOL	A	19	-	5,5,5	0.40	0	5,5,5	0.26	0
4	SO4	C	10	-	4,4,4	0.13	0	6,6,6	0.09	0
4	SO4	A	783	-	4,4,4	0.14	0	6,6,6	0.08	0
2	GOL	C	21	-	5,5,5	0.31	0	5,5,5	0.61	0
2	GOL	B	3	-	5,5,5	0.37	0	5,5,5	0.29	0
2	GOL	A	4	-	5,5,5	0.43	0	5,5,5	0.29	0
2	GOL	A	13	-	5,5,5	0.37	0	5,5,5	0.40	0
2	GOL	D	5	-	5,5,5	0.40	0	5,5,5	0.38	0
4	SO4	D	785	-	4,4,4	0.15	0	6,6,6	0.17	0
2	GOL	A	12	-	5,5,5	0.33	0	5,5,5	0.28	0
2	GOL	D	27	-	5,5,5	0.37	0	5,5,5	0.31	0
4	SO4	A	784	-	4,4,4	0.15	0	6,6,6	0.10	0
4	SO4	C	783	-	4,4,4	0.19	0	6,6,6	0.09	0
2	GOL	A	24	-	5,5,5	0.34	0	5,5,5	0.28	0
4	SO4	A	5	-	4,4,4	0.13	0	6,6,6	0.16	0
3	MES	C	2	-	12,12,12	2.32	1 (8%)	14,16,16	2.51	6 (42%)
2	GOL	C	22	-	5,5,5	0.38	0	5,5,5	0.48	0
4	SO4	C	784	-	4,4,4	0.15	0	6,6,6	0.22	0
4	SO4	D	784	-	4,4,4	0.14	0	6,6,6	0.18	0
2	GOL	B	6	-	5,5,5	0.37	0	5,5,5	0.21	0
3	MES	C	1	-	12,12,12	2.21	1 (8%)	14,16,16	2.36	6 (42%)
2	GOL	D	28	-	5,5,5	0.35	0	5,5,5	0.30	0
5	DTT	C	785	-	7,7,7	0.93	0	4,8,8	0.90	0
4	SO4	A	17	-	4,4,4	0.22	0	6,6,6	0.23	0
2	GOL	D	9	-	5,5,5	0.34	0	5,5,5	0.27	0
4	SO4	B	783	-	4,4,4	0.16	0	6,6,6	0.24	0
2	GOL	A	14	-	5,5,5	0.35	0	5,5,5	0.45	0
2	GOL	C	11	-	5,5,5	0.28	0	5,5,5	0.78	0
4	SO4	C	3	-	4,4,4	0.14	0	6,6,6	0.08	0
2	GOL	A	18	-	5,5,5	0.38	0	5,5,5	0.38	0
3	MES	D	4	-	12,12,12	2.04	1 (8%)	14,16,16	2.49	5 (35%)
2	GOL	A	2	-	5,5,5	0.30	0	5,5,5	0.39	0
4	SO4	C	7	-	4,4,4	0.14	0	6,6,6	0.19	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
2	GOL	A	15	-	-	2/4/4/4	-
2	GOL	C	20	-	-	2/4/4/4	-
2	GOL	C	23	-	-	2/4/4/4	-
2	GOL	C	29	-	-	4/4/4/4	-
5	DTT	A	785	-	-	5/8/8/8	-
2	GOL	A	1	-	-	2/4/4/4	-
2	GOL	B	8	-	-	2/4/4/4	-
3	MES	A	3	-	-	4/6/14/14	0/1/1/1
2	GOL	A	7	-	-	0/4/4/4	-
2	GOL	B	10	-	-	2/4/4/4	-
2	GOL	A	25	-	-	4/4/4/4	-
2	GOL	C	17	-	-	2/4/4/4	-
3	MES	D	783	-	-	1/6/14/14	0/1/1/1
2	GOL	A	16	-	-	2/4/4/4	-
2	GOL	D	26	-	-	2/4/4/4	-
2	GOL	A	19	-	-	2/4/4/4	-
2	GOL	C	21	-	-	1/4/4/4	-
2	GOL	B	3	-	-	0/4/4/4	-
2	GOL	A	4	-	-	2/4/4/4	-
2	GOL	A	13	-	-	4/4/4/4	-
2	GOL	D	5	-	-	2/4/4/4	-
2	GOL	A	12	-	-	2/4/4/4	-
2	GOL	D	27	-	-	3/4/4/4	-
2	GOL	A	24	-	-	3/4/4/4	-
3	MES	C	2	-	-	1/6/14/14	0/1/1/1
2	GOL	C	22	-	-	3/4/4/4	-
2	GOL	B	6	-	-	2/4/4/4	-
3	MES	C	1	-	-	1/6/14/14	0/1/1/1
2	GOL	D	28	-	-	2/4/4/4	-
5	DTT	C	785	-	-	4/8/8/8	-
2	GOL	D	9	-	-	4/4/4/4	-
2	GOL	A	14	-	-	4/4/4/4	-
2	GOL	C	11	-	-	0/4/4/4	-
2	GOL	A	18	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MES	D	4	-	-	4/6/14/14	0/1/1/1
2	GOL	A	2	-	-	4/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	MES	C8-S	-7.73	1.66	1.77
3	C	1	MES	C8-S	-7.27	1.67	1.77
3	A	3	MES	C8-S	-7.23	1.67	1.77
3	D	783	MES	C8-S	-7.22	1.67	1.77
3	D	4	MES	C8-S	-6.80	1.67	1.77

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	MES	C5-N4-C3	5.28	120.72	108.83
3	C	2	MES	C5-N4-C3	5.22	120.57	108.83
3	A	3	MES	C5-N4-C3	4.79	119.61	108.83
3	D	4	MES	C5-N4-C3	4.76	119.55	108.83
3	D	783	MES	C5-N4-C3	4.42	118.78	108.83
3	D	783	MES	C2-C3-N4	-4.06	103.94	110.10
3	D	4	MES	O1S-S-C8	3.91	111.62	106.92
3	A	3	MES	C7-N4-C3	3.77	120.87	111.23
3	C	2	MES	C7-N4-C3	3.73	120.77	111.23
3	D	4	MES	C7-N4-C3	3.72	120.74	111.23
3	D	783	MES	C7-N4-C3	3.71	120.72	111.23
3	D	783	MES	C7-N4-C5	3.60	120.43	111.23
3	C	1	MES	C7-N4-C3	3.46	120.09	111.23
3	C	2	MES	C2-C3-N4	-3.37	104.99	110.10
3	D	4	MES	C7-N4-C5	3.31	119.70	111.23
3	D	4	MES	C6-C5-N4	-3.24	105.19	110.10
3	A	3	MES	C7-N4-C5	3.24	119.51	111.23
3	A	3	MES	C6-C5-N4	-3.24	105.20	110.10
3	C	1	MES	C7-N4-C5	3.11	119.18	111.23
3	C	1	MES	C6-C5-N4	-2.96	105.62	110.10
3	D	783	MES	O1S-S-C8	2.95	110.47	106.92
3	D	783	MES	C6-C5-N4	-2.91	105.70	110.10
3	C	2	MES	C7-N4-C5	2.88	118.61	111.23
3	C	1	MES	C2-C3-N4	-2.81	105.84	110.10
3	C	2	MES	C6-C5-N4	-2.76	105.92	110.10
3	C	2	MES	O2S-S-C8	2.62	110.08	106.92
3	A	3	MES	O1S-S-C8	2.52	109.95	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3	MES	O3S-S-C8	2.43	109.70	105.77
3	A	3	MES	C2-C3-N4	-2.33	106.56	110.10
3	C	1	MES	O2S-S-C8	2.26	109.63	106.92
3	D	783	MES	O3S-S-C8	2.21	109.34	105.77
3	A	3	MES	O2S-S-C8	2.18	109.54	106.92

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	GOL	O1-C1-C2-C3
2	A	2	GOL	C1-C2-C3-O3
2	A	2	GOL	O2-C2-C3-O3
2	A	13	GOL	O1-C1-C2-C3
2	A	14	GOL	O1-C1-C2-O2
2	A	14	GOL	O1-C1-C2-C3
2	A	18	GOL	O1-C1-C2-C3
2	A	19	GOL	O1-C1-C2-C3
2	A	24	GOL	O1-C1-C2-C3
2	A	25	GOL	O1-C1-C2-O2
2	A	25	GOL	O1-C1-C2-C3
2	B	6	GOL	C1-C2-C3-O3
2	C	17	GOL	O1-C1-C2-C3
2	C	20	GOL	O1-C1-C2-C3
2	C	22	GOL	O1-C1-C2-C3
2	C	23	GOL	O1-C1-C2-C3
2	C	29	GOL	O1-C1-C2-C3
2	C	29	GOL	C1-C2-C3-O3
2	C	29	GOL	O2-C2-C3-O3
2	D	9	GOL	O1-C1-C2-O2
2	D	9	GOL	O1-C1-C2-C3
2	D	9	GOL	C1-C2-C3-O3
2	D	26	GOL	O1-C1-C2-C3
2	D	27	GOL	O1-C1-C2-C3
2	D	28	GOL	O1-C1-C2-C3
3	A	3	MES	C8-C7-N4-C5
3	A	3	MES	C7-C8-S-O3S
3	D	4	MES	C8-C7-N4-C5
3	D	4	MES	C7-C8-S-O2S
3	D	4	MES	C7-C8-S-O3S
5	A	785	DTT	S1-C1-C2-O2
5	A	785	DTT	S1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	A	785	DTT	C1-C2-C3-C4
5	C	785	DTT	S1-C1-C2-O2
5	C	785	DTT	S1-C1-C2-C3
5	C	785	DTT	C2-C3-C4-S4
2	A	24	GOL	O1-C1-C2-O2
2	B	8	GOL	O1-C1-C2-O2
2	A	2	GOL	O1-C1-C2-C3
2	A	4	GOL	C1-C2-C3-O3
2	A	12	GOL	C1-C2-C3-O3
2	A	13	GOL	C1-C2-C3-O3
2	A	14	GOL	C1-C2-C3-O3
2	A	15	GOL	O1-C1-C2-C3
2	A	25	GOL	C1-C2-C3-O3
2	B	8	GOL	O1-C1-C2-C3
2	D	5	GOL	O1-C1-C2-C3
2	A	1	GOL	O1-C1-C2-O2
2	A	13	GOL	O1-C1-C2-O2
2	A	15	GOL	O1-C1-C2-O2
2	A	19	GOL	O1-C1-C2-O2
2	B	6	GOL	O2-C2-C3-O3
2	C	17	GOL	O1-C1-C2-O2
2	C	22	GOL	O1-C1-C2-O2
2	C	29	GOL	O1-C1-C2-O2
2	D	5	GOL	O1-C1-C2-O2
2	D	9	GOL	O2-C2-C3-O3
2	D	27	GOL	O1-C1-C2-O2
2	A	12	GOL	O2-C2-C3-O3
2	A	13	GOL	O2-C2-C3-O3
2	C	20	GOL	O1-C1-C2-O2
2	C	23	GOL	O1-C1-C2-O2
2	D	26	GOL	O1-C1-C2-O2
2	D	28	GOL	O1-C1-C2-O2
3	C	1	MES	C8-C7-N4-C3
2	A	4	GOL	O2-C2-C3-O3
2	A	18	GOL	O1-C1-C2-O2
2	A	25	GOL	O2-C2-C3-O3
2	A	16	GOL	O1-C1-C2-O2
2	B	10	GOL	O2-C2-C3-O3
2	A	16	GOL	O1-C1-C2-C3
2	B	10	GOL	C1-C2-C3-O3
3	A	3	MES	C7-C8-S-O1S
3	A	3	MES	C7-C8-S-O2S

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Mol	Chain	Res	Type	Atoms
3	D	4	MES	C7-C8-S-O1S
5	A	785	DTT	O3-C3-C4-S4
5	C	785	DTT	O3-C3-C4-S4
2	D	27	GOL	O2-C2-C3-O3
2	A	2	GOL	O1-C1-C2-O2
2	A	14	GOL	O2-C2-C3-O3
3	C	2	MES	C8-C7-N4-C5
3	D	783	MES	C8-C7-N4-C3
5	A	785	DTT	C2-C3-C4-S4
2	A	24	GOL	C1-C2-C3-O3
2	C	22	GOL	C1-C2-C3-O3
2	C	21	GOL	O1-C1-C2-C3

There are no ring outliers.

18 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	23	GOL	2	0
5	A	785	DTT	8	0
3	A	3	MES	1	0
2	A	7	GOL	2	0
3	D	783	MES	3	0
2	A	16	GOL	3	0
2	D	26	GOL	2	0
2	A	19	GOL	1	0
2	C	21	GOL	5	0
2	A	4	GOL	1	0
2	D	27	GOL	1	0
2	A	24	GOL	1	0
3	C	2	MES	2	0
2	D	28	GOL	1	0
5	C	785	DTT	3	0
2	A	14	GOL	2	0
2	C	11	GOL	4	0
3	D	4	MES	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	612/613 (99%)	-0.05	20 (3%) 46 53	21, 36, 78, 128	0
1	B	612/613 (99%)	0.01	29 (4%) 31 37	24, 40, 80, 139	0
1	C	612/613 (99%)	-0.12	8 (1%) 77 80	22, 40, 74, 145	0
1	D	612/613 (99%)	0.04	19 (3%) 49 55	26, 48, 80, 122	0
All	All	2448/2452 (99%)	-0.03	76 (3%) 49 55	21, 41, 79, 145	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	ALA	6.6
1	B	175	CYS	6.4
1	A	580	PHE	6.0
1	C	327	PHE	5.8
1	D	327	PHE	5.8
1	B	176	LEU	5.2
1	B	327	PHE	5.2
1	C	326	LEU	5.1
1	B	174	ALA	5.1
1	B	187	TRP	5.0
1	A	175	CYS	4.9
1	D	326	LEU	4.8
1	D	582	TYR	4.2
1	C	325	GLU	4.2
1	B	171	GLN	4.1
1	C	331	SER	4.1
1	D	328	SER	4.0
1	B	326	LEU	3.7
1	A	527	ASP	3.7
1	D	329	GLU	3.7
1	B	188	LEU	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	581	GLY	3.6
1	A	172	GLY	3.5
1	A	326	LEU	3.5
1	D	527	ASP	3.4
1	D	325	GLU	3.3
1	D	513	PHE	3.2
1	C	527	ASP	3.2
1	B	193	THR	3.1
1	A	195	GLU	3.0
1	A	187	TRP	3.0
1	A	183	ALA	3.0
1	D	331	SER	3.0
1	D	525	ASP	3.0
1	A	173	ARG	2.9
1	C	580	PHE	2.9
1	B	206	CYS	2.9
1	B	527	ASP	2.9
1	D	526	ASP	2.8
1	A	177	SER	2.8
1	D	171	GLN	2.8
1	B	331	SER	2.7
1	B	184	ASP	2.7
1	D	172	GLY	2.7
1	B	579	THR	2.7
1	D	175	CYS	2.6
1	A	327	PHE	2.6
1	A	331	SER	2.6
1	B	580	PHE	2.6
1	A	176	LEU	2.6
1	A	208	LEU	2.6
1	B	201	LEU	2.6
1	B	172	GLY	2.5
1	B	185	LEU	2.4
1	B	177	SER	2.4
1	D	520	GLY	2.4
1	A	180	GLU	2.3
1	A	171	GLN	2.3
1	B	180	GLU	2.3
1	B	581	GLY	2.3
1	A	197	SER	2.3
1	B	328	SER	2.3
1	D	345	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	325	GLU	2.2
1	B	330	LYS	2.2
1	D	330	LYS	2.2
1	B	439	TRP	2.2
1	B	227	VAL	2.1
1	B	183	ALA	2.1
1	C	528	SER	2.1
1	A	348	GLU	2.1
1	D	404	MET	2.1
1	C	656	ASP	2.1
1	A	201	LEU	2.0
1	B	195	GLU	2.0
1	B	298	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(Å <sup>2</sup> )	Q<0.9
4	SO4	D	15	5/5	0.44	0.48	160,161,162,162	0
2	GOL	A	14	6/6	0.69	0.43	43,65,73,78	0
2	GOL	D	28	6/6	0.72	0.39	78,81,87,89	0
2	GOL	D	27	6/6	0.73	0.19	72,79,85,89	0
2	GOL	C	22	6/6	0.76	0.20	51,68,74,79	0
2	GOL	A	24	6/6	0.76	0.41	56,59,62,62	0
4	SO4	A	783	5/5	0.78	0.20	143,146,148,148	0
2	GOL	C	11	6/6	0.80	0.30	41,51,59,67	0
2	GOL	C	21	6/6	0.81	0.24	25,54,61,64	0
2	GOL	C	20	6/6	0.82	0.24	82,89,91,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	D	26	6/6	0.82	0.21	76,79,83,85	0
4	SO4	B	12	5/5	0.83	0.29	138,140,141,142	0
2	GOL	A	18	6/6	0.84	0.29	49,71,77,79	0
4	SO4	C	783	5/5	0.84	0.18	91,99,102,105	0
2	GOL	A	25	6/6	0.84	0.21	76,81,84,87	0
4	SO4	A	784	5/5	0.85	0.21	116,120,121,121	0
2	GOL	C	23	6/6	0.85	0.21	61,83,85,91	0
2	GOL	B	3	6/6	0.87	0.38	45,70,78,81	0
2	GOL	A	1	6/6	0.87	0.34	27,35,44,44	0
2	GOL	C	29	6/6	0.88	0.37	61,75,83,87	0
2	GOL	D	5	6/6	0.88	0.42	50,58,60,69	0
4	SO4	C	3	5/5	0.89	0.15	109,109,113,114	0
2	GOL	A	7	6/6	0.89	0.18	43,54,62,67	0
5	DTT	C	785	8/8	0.89	0.17	42,53,75,85	0
2	GOL	C	17	6/6	0.90	0.36	46,59,76,81	0
2	GOL	D	9	6/6	0.90	0.15	55,66,68,68	0
2	GOL	A	16	6/6	0.90	0.11	47,58,68,71	0
2	GOL	A	2	6/6	0.91	0.33	34,40,47,50	0
4	SO4	D	785	5/5	0.91	0.22	88,94,96,107	0
2	GOL	B	6	6/6	0.91	0.31	39,56,60,62	0
2	GOL	A	15	6/6	0.91	0.19	52,62,67,74	0
2	GOL	B	8	6/6	0.92	0.15	49,57,65,70	0
2	GOL	A	13	6/6	0.92	0.12	42,51,56,58	0
2	GOL	A	19	6/6	0.92	0.24	47,51,56,62	0
4	SO4	D	16	5/5	0.93	0.21	112,115,118,121	0
5	DTT	A	785	8/8	0.93	0.24	26,50,85,114	0
4	SO4	C	10	5/5	0.93	0.16	107,110,111,114	0
3	MES	D	783	12/12	0.94	0.14	59,62,90,94	0
2	GOL	A	12	6/6	0.94	0.21	50,55,69,72	0
2	GOL	A	4	6/6	0.94	0.25	41,54,59,64	0
4	SO4	B	784	5/5	0.94	0.20	77,83,88,100	0
4	SO4	C	784	5/5	0.94	0.24	27,76,88,95	0
2	GOL	B	10	6/6	0.95	0.27	55,60,62,64	0
3	MES	C	2	12/12	0.97	0.10	48,50,68,74	0
3	MES	D	4	12/12	0.97	0.09	50,62,67,69	0
3	MES	A	3	12/12	0.97	0.10	50,57,62,64	0
3	MES	C	1	12/12	0.97	0.10	35,56,61,63	0
4	SO4	D	784	5/5	0.98	0.12	62,63,67,72	0
4	SO4	C	7	5/5	0.98	0.11	47,54,59,63	0
4	SO4	B	783	5/5	0.99	0.11	45,47,58,65	0
4	SO4	A	17	5/5	0.99	0.08	51,51,58,63	0
4	SO4	A	5	5/5	1.00	0.10	28,38,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.