



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 03:01 pm BST

PDB ID : 3NAW
Title : Crystal structure of E. coli O157:H7 effector protein NleL
Authors : Lin, D.Y.; Chen, J.
Deposited on : 2010-06-02
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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 : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

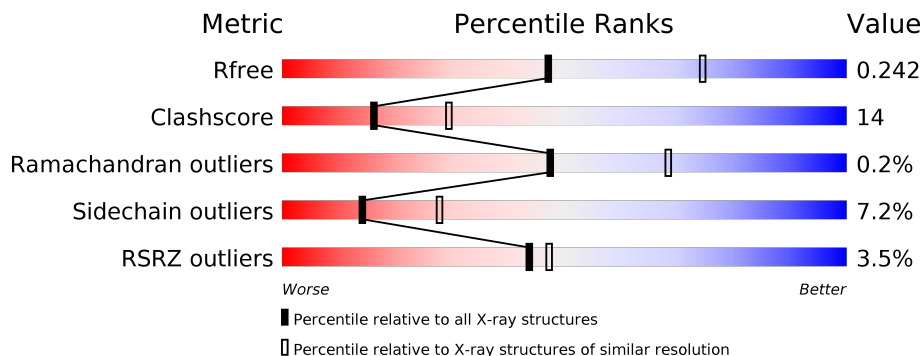
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 2% 72% 23%
1	B	613	 4% 70% 26%

2 Entry composition [i](#)

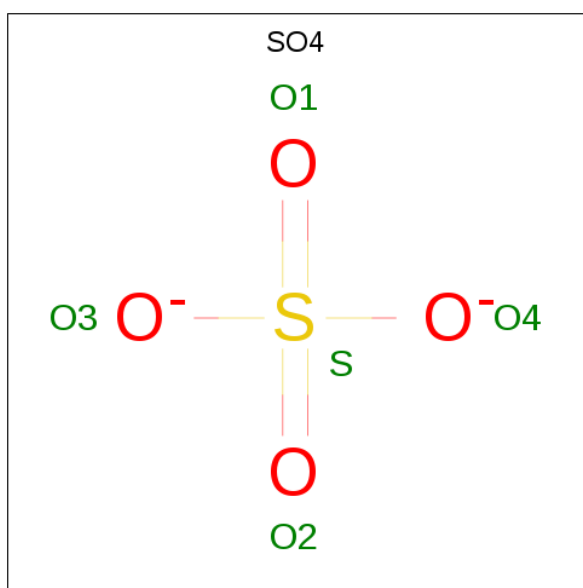
There are 5 unique types of molecules in this entry. The entry contains 10041 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	607	4820	3055	780	948	37	0	0	0
1	B	610	4820	3058	781	944	37	2	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



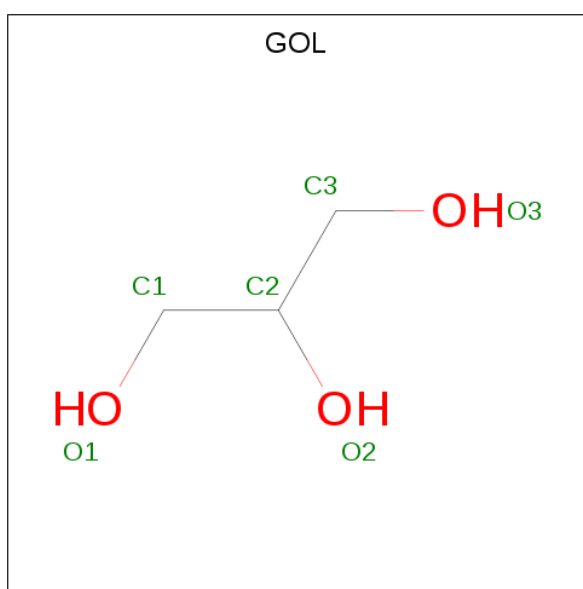
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



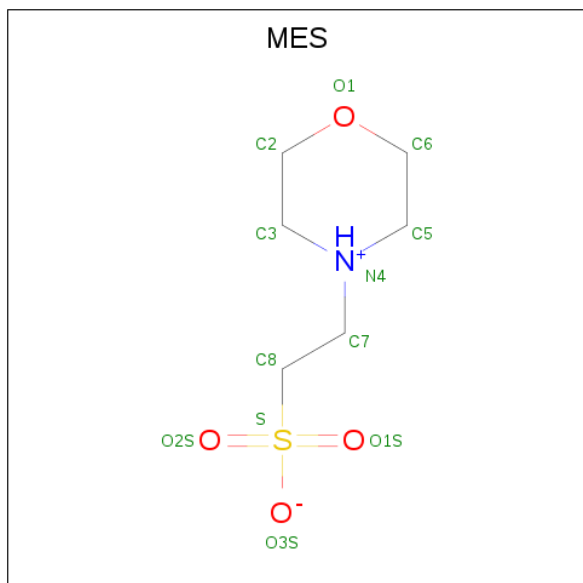
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

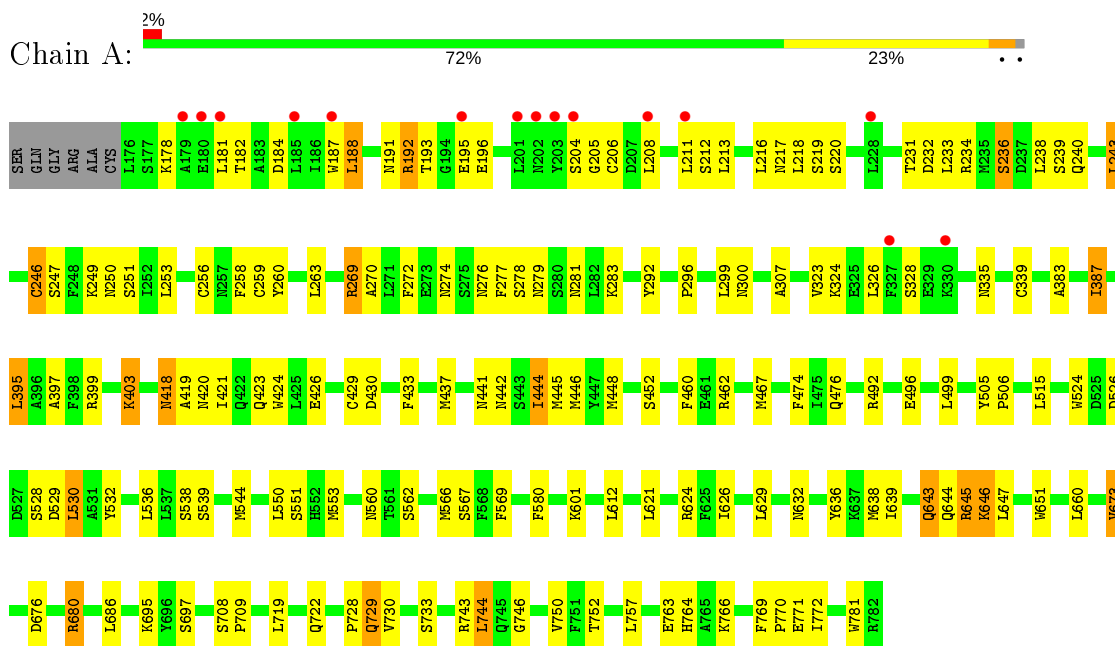
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	173	Total	O	0	0
			173	173		
5	B	122	Total	O	0	0
			122	122		

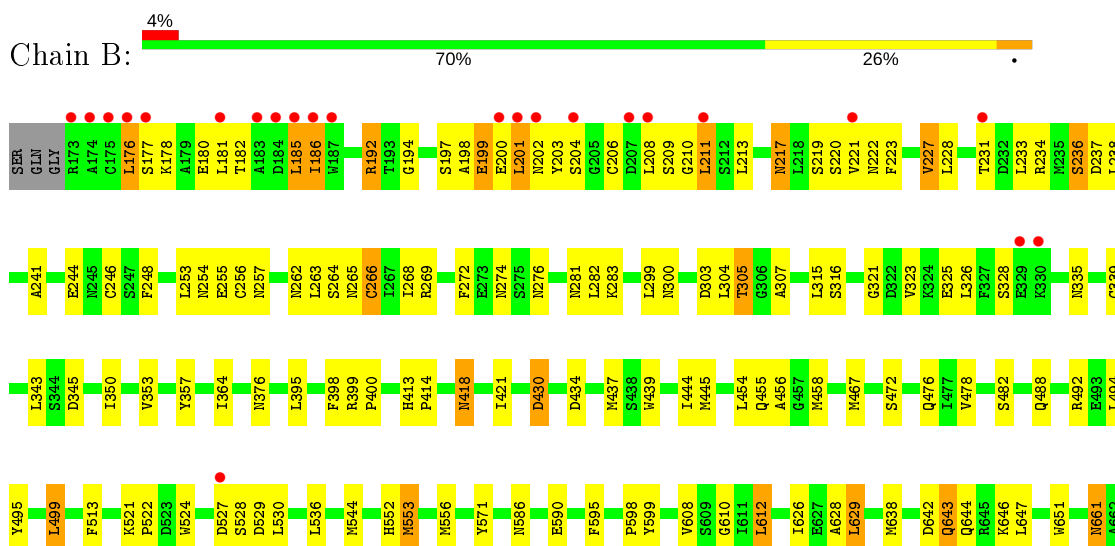
3 Residue-property plots [i](#)

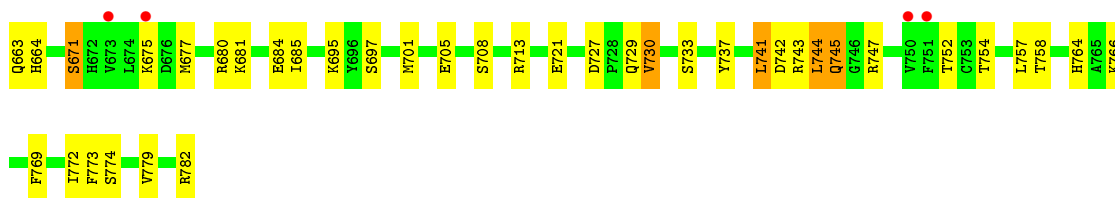
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 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, α , β , γ	313.67Å 77.31Å 61.51Å 90.00° 94.54° 90.00°	Depositor
Resolution (Å)	47.05 – 2.50 47.05 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.5 (47.05-2.50) 90.1 (47.05-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.29Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.184 , 0.246 0.180 , 0.242	Depositor DCC
R_{free} test set	3004 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	47.6	Xtrriage
Anisotropy	0.625	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10041	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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, 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	0.45	1/4925 (0.0%)	0.55	0/6666
1	B	0.42	0/4925	0.53	0/6667
All	All	0.43	1/9850 (0.0%)	0.54	0/13333

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	429	CYS	CB-SG	-7.81	1.69	1.82

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	4820	0	4619	130	0
1	B	4820	0	4609	152	0
2	A	20	0	0	0	0
2	B	20	0	0	0	0
3	A	24	0	32	0	0
3	B	30	0	40	4	0
4	B	12	0	12	3	0
5	A	173	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	122	0	0	4	0
All	All	10041	0	9312	275	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 14.

All (275) 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:643:GLN:HE21	1:A:643:GLN:HA	1.04	1.10
1:A:448:MET:HE2	1:A:452:SER:HB3	1.42	1.02
1:B:398:PHE:CD1	1:B:400:PRO:HG3	1.92	1.02
1:A:643:GLN:NE2	1:A:643:GLN:HA	1.85	0.92
1:B:454:LEU:HG	1:B:458:MET:HE2	1.50	0.92
1:A:274:ASN:HD21	1:B:316:SER:HB3	1.34	0.92
1:B:708:SER:OG	1:B:713:ARG:HD3	1.71	0.89
1:B:680:ARG:HE	1:B:729:GLN:HE21	1.21	0.86
1:B:680:ARG:O	1:B:684:GLU:HG3	1.75	0.85
1:B:695:LYS:HD3	1:B:758:THR:HG21	1.56	0.84
1:B:741:LEU:O	1:B:745:GLN:HG3	1.78	0.84
1:A:636:TYR:HE2	1:A:638:MET:HE2	1.43	0.83
1:B:197:SER:HB2	1:B:200:GLU:HB2	1.63	0.81
1:B:263:LEU:O	1:B:266:CYS:HB2	1.81	0.81
1:A:448:MET:CE	1:A:452:SER:HB3	2.11	0.81
1:A:213:LEU:HB3	1:A:216:LEU:HD12	1.65	0.78
1:A:188:LEU:HD22	1:A:192:ARG:HD3	1.66	0.78
1:B:328:SER:HB2	1:B:335:ASN:OD1	1.85	0.77
1:A:233:LEU:O	1:A:236:SER:HB2	1.85	0.76
1:A:281:ASN:HD21	1:A:283:LYS:HD3	1.50	0.76
1:A:560:ASN:HB3	1:A:562:SER:H	1.52	0.75
1:B:211:LEU:HD13	1:B:213:LEU:HG	1.67	0.74
1:A:643:GLN:HE21	1:A:643:GLN:CA	1.93	0.74
1:B:643:GLN:HE21	1:B:643:GLN:N	1.85	0.74
1:A:418:ASN:ND2	1:A:421:ILE:H	1.86	0.72
1:B:325:GLU:HB3	5:B:811:HOH:O	1.89	0.72
1:B:208:LEU:HD12	1:B:211:LEU:HD21	1.70	0.72
1:B:680:ARG:NE	1:B:729:GLN:HE21	1.87	0.72
1:A:279:ASN:HD21	1:B:257:ASN:HD21	1.38	0.71
1:B:178:LYS:NZ	1:B:209:SER:HB3	2.06	0.70
1:A:243:LEU:O	1:A:246:CYS:HB2	1.92	0.70
1:B:398:PHE:CE1	1:B:400:PRO:HG3	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:536:LEU:HD11	1:B:553:MET:HE1	1.75	0.69
1:B:680:ARG:HE	1:B:729:GLN:NE2	1.90	0.68
1:B:697:SER:O	1:B:708:SER:HB2	1.93	0.68
1:B:680:ARG:NH2	1:B:729:GLN:HG3	2.08	0.68
1:B:299:LEU:HD13	1:B:304:LEU:HD11	1.74	0.68
1:B:264:SER:HB3	1:B:281:ASN:OD1	1.93	0.68
1:B:281:ASN:HD21	1:B:283:LYS:HD3	1.59	0.66
1:A:418:ASN:HD22	1:A:421:ILE:H	1.42	0.66
1:B:213:LEU:HB2	1:B:233:LEU:HD23	1.77	0.66
1:B:176:LEU:HD23	1:B:177:SER:H	1.62	0.65
1:A:638:MET:HA	1:A:643:GLN:HG2	1.77	0.65
1:A:274:ASN:ND2	1:B:316:SER:HB3	2.10	0.65
1:B:445:MET:H	1:B:476:GLN:NE2	1.94	0.65
1:A:638:MET:HA	1:A:643:GLN:CG	2.26	0.64
1:B:661:ASN:ND2	1:B:664:HIS:H	1.96	0.63
1:A:528:SER:OG	1:A:530:LEU:HD22	1.98	0.62
1:A:636:TYR:HE2	1:A:638:MET:CE	2.11	0.62
1:A:492:ARG:O	1:A:496:GLU:HG3	1.99	0.62
1:B:766:LYS:HE2	1:B:773:PHE:CE2	2.34	0.62
1:A:253:LEU:HD22	1:A:258:PHE:HZ	1.65	0.62
1:A:292:TYR:CZ	1:A:296:PRO:HB3	2.35	0.61
1:A:251:SER:O	1:A:270:ALA:HB1	1.99	0.61
1:A:448:MET:HE2	1:A:452:SER:CB	2.26	0.61
1:A:184:ASP:O	1:A:188:LEU:HB2	2.00	0.61
1:A:279:ASN:HD21	1:B:257:ASN:ND2	1.97	0.61
1:B:234:ARG:HD3	4:B:1:MES:H21	1.82	0.61
1:B:454:LEU:HG	1:B:458:MET:CE	2.26	0.61
1:A:383:ALA:O	1:A:387:ILE:HG23	2.01	0.61
1:B:231:THR:HG22	1:B:233:LEU:HG	1.83	0.60
1:A:730:VAL:O	1:A:764:HIS:HE1	1.84	0.60
1:A:771:GLU:CD	1:A:771:GLU:H	2.05	0.60
1:A:744:LEU:HD13	1:A:757:LEU:CD2	2.32	0.60
1:A:418:ASN:HD21	1:A:420:ASN:HB3	1.67	0.59
1:A:178:LYS:HG2	5:A:803:HOH:O	2.02	0.59
1:A:529:ASP:HA	5:A:864:HOH:O	2.01	0.59
1:A:526:ASP:OD1	1:A:528:SER:HB3	2.03	0.59
1:B:528:SER:HB2	1:B:530:LEU:HD23	1.84	0.59
1:A:192:ARG:HD2	1:A:196:GLU:OE1	2.02	0.59
1:A:433:PHE:HE1	1:A:448:MET:CE	2.16	0.58
1:A:239:SER:O	1:A:240:GLN:HB2	2.03	0.58
1:A:277:PHE:HB2	1:A:299:LEU:HD23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:VAL:HG11	1:B:223:PHE:CZ	2.39	0.58
1:B:208:LEU:HB3	1:B:211:LEU:HD21	1.86	0.58
1:A:433:PHE:HE1	1:A:448:MET:HE3	1.69	0.58
1:A:208:LEU:O	1:A:211:LEU:HG	2.04	0.57
1:A:528:SER:OG	1:A:530:LEU:HB2	2.04	0.57
1:B:178:LYS:HZ1	1:B:209:SER:HB3	1.67	0.57
1:A:419:ALA:O	1:A:423:GLN:HG3	2.04	0.57
1:B:350:ILE:O	1:B:353:VAL:HG22	2.04	0.57
1:B:628:ALA:HB1	1:B:701:MET:CE	2.35	0.56
1:B:595:PHE:O	1:B:598:PRO:HD2	2.05	0.56
1:A:232:ASP:OD1	1:A:234:ARG:HG3	2.05	0.56
1:A:766:LYS:O	1:A:770:PRO:HG3	2.05	0.56
1:B:185:LEU:HD13	1:B:186:ILE:N	2.21	0.56
1:A:204:SER:C	1:A:206:CYS:H	2.08	0.56
1:A:744:LEU:HD13	1:A:757:LEU:HD21	1.88	0.56
1:B:779:VAL:O	1:B:782:ARG:HG2	2.06	0.56
1:B:528:SER:O	1:B:529:ASP:HB2	2.06	0.56
1:B:186:ILE:O	1:B:186:ILE:HD13	2.06	0.55
1:A:467:MET:HG2	1:A:474:PHE:CE1	2.42	0.55
1:B:455:GLN:HA	1:B:458:MET:HE3	1.88	0.55
1:B:307:ALA:O	1:B:339:CYS:HB2	2.07	0.55
1:B:727:ASP:OD1	1:B:729:GLN:HG2	2.06	0.55
1:B:742:ASP:HA	1:B:747:ARG:HG3	1.89	0.55
1:B:730:VAL:O	1:B:764:HIS:HE1	1.89	0.55
1:B:305:THR:HG23	1:B:321:GLY:HA3	1.89	0.54
1:A:645:ARG:HB2	1:A:645:ARG:HH11	1.72	0.54
1:B:211:LEU:CD1	1:B:231:THR:HG23	2.37	0.54
1:B:300:ASN:HD22	1:B:300:ASN:H	1.55	0.54
1:A:567:SER:HB3	5:A:817:HOH:O	2.07	0.54
1:B:445:MET:H	1:B:476:GLN:HE22	1.53	0.54
1:B:743:ARG:O	1:B:752:THR:HG23	2.08	0.54
1:B:323:VAL:HG21	1:B:326:LEU:HD23	1.90	0.54
1:B:721:GLU:HG3	1:B:737:TYR:OH	2.08	0.54
1:A:259:CYS:O	1:A:260:TYR:HB2	2.07	0.53
1:B:255:GLU:OE1	4:B:1:MES:H82	2.08	0.53
1:B:181:LEU:HD22	1:B:206:CYS:SG	2.49	0.53
1:B:661:ASN:HD21	1:B:663:GLN:HB3	1.75	0.53
1:B:204:SER:HB3	1:B:222:ASN:HD21	1.74	0.52
1:A:278:SER:O	1:A:279:ASN:HB2	2.09	0.52
1:A:397:ALA:HB3	1:A:399:ARG:CG	2.39	0.52
1:A:445:MET:H	1:A:476:GLN:NE2	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:LEU:HD12	1:A:263:LEU:HD21	1.91	0.52
1:A:673:VAL:HG13	5:A:84:HOH:O	2.09	0.52
1:A:746:GLY:HA2	1:A:750:VAL:O	2.09	0.52
1:B:237:ASP:C	1:B:237:ASP:OD1	2.47	0.52
1:B:325:GLU:OE2	1:B:328:SER:HA	2.09	0.52
1:B:357:TYR:CE1	3:B:783:GOL:H32	2.44	0.51
1:B:219:SER:O	1:B:220:SER:HB2	2.09	0.51
1:A:258:PHE:HB2	1:A:276:ASN:O	2.11	0.51
1:B:178:LYS:HZ3	1:B:209:SER:HB3	1.75	0.51
1:B:744:LEU:HD13	1:B:757:LEU:CD2	2.40	0.51
1:B:467:MET:HE2	1:B:494:LEU:HD11	1.92	0.51
1:B:528:SER:HB2	1:B:530:LEU:CD2	2.39	0.51
1:B:233:LEU:O	1:B:236:SER:HB2	2.10	0.51
1:B:253:LEU:O	1:B:256:CYS:HB2	2.11	0.50
1:B:437:MET:CE	1:B:456:ALA:HB1	2.41	0.50
1:A:399:ARG:O	1:A:403:LYS:HD3	2.12	0.50
1:B:211:LEU:HD12	1:B:231:THR:HG23	1.93	0.50
1:A:323:VAL:HG11	1:A:326:LEU:HD23	1.93	0.50
1:A:445:MET:H	1:A:476:GLN:HE22	1.60	0.50
1:A:566:MET:CE	1:A:580:PHE:CE1	2.94	0.50
1:B:743:ARG:HD2	1:B:757:LEU:HD13	1.92	0.50
1:B:208:LEU:HD12	1:B:211:LEU:CD2	2.41	0.49
1:B:217:ASN:OD1	1:B:217:ASN:N	2.45	0.49
1:B:530:LEU:N	1:B:530:LEU:HD22	2.27	0.49
1:A:528:SER:O	1:A:530:LEU:HD13	2.12	0.49
1:A:660:LEU:HD11	1:A:719:LEU:HD23	1.93	0.49
1:B:208:LEU:O	1:B:211:LEU:HG	2.12	0.49
1:B:221:VAL:CG1	1:B:223:PHE:CZ	2.95	0.49
1:B:528:SER:CB	1:B:530:LEU:HD23	2.42	0.49
1:A:307:ALA:O	1:A:339:CYS:HB2	2.12	0.49
1:A:217:ASN:C	1:A:218:LEU:HD23	2.33	0.49
1:A:697:SER:O	1:A:708:SER:HB2	2.12	0.49
1:A:433:PHE:CE1	1:A:448:MET:CE	2.95	0.49
1:A:253:LEU:HD22	1:A:258:PHE:CZ	2.45	0.49
1:B:644:GLN:NE2	5:B:844:HOH:O	2.46	0.48
1:A:328:SER:HB2	1:A:335:ASN:OD1	2.12	0.48
1:B:684:GLU:HG2	1:B:730:VAL:HG22	1.94	0.48
1:B:628:ALA:HB1	1:B:701:MET:HE1	1.95	0.48
1:A:274:ASN:HD21	1:B:316:SER:CB	2.18	0.48
1:B:208:LEU:HB2	1:B:227:VAL:O	2.13	0.48
1:B:499:LEU:HD21	1:B:522:PRO:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:MET:HA	1:A:643:GLN:HG3	1.94	0.48
1:B:430:ASP:O	1:B:434:ASP:HB2	2.14	0.48
1:A:213:LEU:CB	1:A:216:LEU:HD12	2.40	0.48
1:B:343:LEU:HD21	1:B:364:ILE:HD12	1.96	0.48
1:A:643:GLN:NE2	1:A:646:LYS:HE3	2.29	0.48
1:A:233:LEU:O	1:A:256:CYS:SG	2.72	0.47
1:A:426:GLU:O	1:A:430:ASP:HB2	2.14	0.47
1:A:636:TYR:CE2	1:A:638:MET:CE	2.95	0.47
1:A:680:ARG:HD3	1:A:729:GLN:OE1	2.14	0.47
1:B:246:CYS:HB2	1:B:266:CYS:SG	2.54	0.47
1:B:444:ILE:HA	1:B:476:GLN:HE22	1.78	0.47
1:B:521:LYS:HD3	1:B:521:LYS:HA	1.60	0.47
1:B:680:ARG:HH21	1:B:729:GLN:HG3	1.80	0.47
1:A:187:TRP:NE1	1:A:191:ASN:ND2	2.63	0.47
1:A:213:LEU:HB2	1:A:233:LEU:HD22	1.97	0.47
1:A:188:LEU:O	1:A:192:ARG:HG2	2.15	0.47
1:B:221:VAL:HB	1:B:223:PHE:CE2	2.50	0.47
1:B:238:LEU:O	1:B:241:ALA:HB3	2.15	0.46
1:A:243:LEU:N	1:A:243:LEU:HD23	2.30	0.46
1:B:213:LEU:HB2	1:B:233:LEU:CD2	2.43	0.46
1:A:204:SER:O	1:A:206:CYS:N	2.48	0.46
1:B:203:TYR:O	1:B:206:CYS:HB2	2.16	0.46
1:B:766:LYS:HE3	1:B:766:LYS:HB2	1.60	0.46
1:B:197:SER:HB2	1:B:200:GLU:CB	2.41	0.46
1:A:686:LEU:HD13	1:A:722:GLN:HG3	1.97	0.46
1:B:204:SER:HB3	1:B:222:ASN:ND2	2.30	0.46
1:A:433:PHE:CE1	1:A:448:MET:HE3	2.51	0.45
1:B:608:VAL:HG12	1:B:612:LEU:HD22	1.98	0.45
1:B:178:LYS:HA	1:B:181:LEU:HD21	1.97	0.45
1:A:247:SER:OG	1:A:249:LYS:HE3	2.16	0.45
1:A:444:ILE:HA	1:A:476:GLN:HE22	1.81	0.45
1:B:730:VAL:O	1:B:764:HIS:CE1	2.70	0.45
1:B:231:THR:CG2	1:B:233:LEU:HG	2.46	0.45
1:B:228:LEU:HD13	1:B:248:PHE:CZ	2.52	0.45
1:B:413:HIS:HD2	5:B:55:HOH:O	2.00	0.45
1:B:269:ARG:O	1:B:269:ARG:HG2	2.16	0.45
1:A:538:SER:HB2	1:A:544:MET:HB2	1.99	0.45
1:A:769:PHE:N	1:A:770:PRO:HD3	2.31	0.45
1:B:182:THR:HA	1:B:185:LEU:HD12	1.99	0.45
1:B:282:LEU:HB2	1:B:303:ASP:O	2.17	0.45
1:B:399:ARG:N	1:B:400:PRO:HD3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:LEU:HD23	1:A:218:LEU:N	2.32	0.44
1:B:467:MET:CE	1:B:494:LEU:CD1	2.95	0.44
1:A:219:SER:O	1:A:220:SER:HB2	2.17	0.44
1:A:192:ARG:NH2	1:A:219:SER:O	2.51	0.44
1:A:744:LEU:HD13	1:A:757:LEU:HD23	1.99	0.44
1:A:445:MET:HG3	1:A:446:MET:O	2.18	0.44
1:A:279:ASN:ND2	1:B:257:ASN:HD21	2.09	0.44
1:B:586:ASN:HB3	1:B:590:GLU:OE1	2.18	0.44
1:A:433:PHE:CE1	1:A:448:MET:HE1	2.53	0.44
1:B:744:LEU:HD13	1:B:757:LEU:HD23	1.98	0.44
1:B:185:LEU:HD11	1:B:213:LEU:HD22	1.99	0.44
1:B:376:ASN:CG	1:B:414:PRO:HG3	2.39	0.44
1:B:177:SER:HB3	1:B:180:GLU:CB	2.47	0.43
1:B:418:ASN:HD22	1:B:421:ILE:H	1.65	0.43
1:B:599:TYR:OH	3:B:9:GOL:H11	2.18	0.43
1:A:233:LEU:HD13	1:A:238:LEU:HD11	1.99	0.43
1:A:532:TYR:CZ	1:A:569:PHE:HE2	2.36	0.43
1:B:254:ASN:HD22	4:B:1:MES:C6	2.31	0.43
1:A:772:ILE:HA	1:A:772:ILE:HD13	1.80	0.43
1:B:197:SER:O	1:B:198:ALA:C	2.56	0.43
1:A:397:ALA:HB3	1:A:399:ARG:HG2	1.99	0.43
1:B:544:MET:HA	1:B:571:TYR:O	2.18	0.43
1:B:752:THR:HG22	1:B:754:THR:HG23	2.01	0.43
1:A:695:LYS:HG2	1:A:781:TRP:CE3	2.54	0.43
1:A:178:LYS:HD3	1:A:181:LEU:HD21	1.99	0.43
1:A:492:ARG:HG2	1:A:524:TRP:CE2	2.53	0.43
1:B:552:HIS:CE1	1:B:556:MET:SD	3.11	0.43
1:A:231:THR:H	1:A:251:SER:HB3	1.82	0.43
1:B:221:VAL:CG1	1:B:223:PHE:CE2	3.01	0.43
1:B:325:GLU:O	1:B:325:GLU:HG3	2.18	0.43
1:A:448:MET:HE1	1:A:452:SER:O	2.18	0.42
1:B:217:ASN:C	1:B:219:SER:H	2.22	0.42
1:B:300:ASN:HD22	1:B:300:ASN:N	2.16	0.42
1:A:278:SER:CB	1:B:276:ASN:HD21	2.32	0.42
1:B:677:MET:SD	1:B:685:ILE:CD1	3.07	0.42
1:A:233:LEU:O	1:A:234:ARG:C	2.58	0.42
1:A:250:ASN:OD1	1:A:269:ARG:HD2	2.20	0.42
1:B:299:LEU:HD12	1:B:315:LEU:HD23	2.01	0.42
1:B:192:ARG:HA	1:B:192:ARG:HD2	1.88	0.42
1:A:639:ILE:O	1:A:644:GLN:NE2	2.51	0.42
1:B:244:GLU:HB2	1:B:262:ASN:ND2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:SER:C	1:A:206:CYS:N	2.73	0.42
1:A:418:ASN:HD22	1:A:418:ASN:C	2.22	0.42
1:B:350:ILE:HD12	1:B:350:ILE:HA	1.89	0.42
1:A:324:LYS:HG2	5:A:823:HOH:O	2.20	0.42
1:B:192:ARG:HH21	1:B:194:GLY:H	1.66	0.42
1:A:387:ILE:HD12	1:A:424:TRP:CD1	2.54	0.42
1:B:482:SER:O	1:B:488:GLN:HG2	2.20	0.42
1:A:395:LEU:HD12	1:A:395:LEU:HA	1.78	0.41
1:B:626:ILE:O	1:B:629:LEU:HB2	2.20	0.41
1:B:357:TYR:CD1	3:B:783:GOL:H32	2.55	0.41
1:A:260:TYR:CZ	1:A:279:ASN:ND2	2.88	0.41
1:A:730:VAL:HG13	1:A:769:PHE:CE2	2.55	0.41
1:B:199:GLU:HB3	1:B:202:ASN:ND2	2.35	0.41
1:B:499:LEU:HA	1:B:499:LEU:HD12	1.77	0.41
1:A:621:LEU:O	1:A:624:ARG:HB2	2.20	0.41
1:B:492:ARG:HG2	1:B:524:TRP:CE2	2.55	0.41
1:B:671:SER:O	1:B:675:LYS:HB3	2.21	0.41
1:A:326:LEU:HD23	1:A:326:LEU:HA	1.93	0.41
1:B:772:ILE:HD13	1:B:772:ILE:HA	1.93	0.41
1:A:430:ASP:OD1	1:A:462:ARG:NH2	2.29	0.41
1:B:638:MET:SD	1:B:647:LEU:HD11	2.60	0.41
1:B:201:LEU:HA	1:B:203:TYR:CE2	2.56	0.41
1:B:478:VAL:HG11	1:B:495:TYR:HB2	2.03	0.41
1:B:684:GLU:HB3	1:B:769:PHE:CD1	2.56	0.41
1:A:441:ASN:O	1:A:442:ASN:HB2	2.21	0.41
1:B:513:PHE:CD2	1:B:513:PHE:C	2.94	0.41
1:A:300:ASN:H	1:A:300:ASN:HD22	1.69	0.41
1:A:418:ASN:C	1:A:418:ASN:ND2	2.74	0.41
1:A:505:TYR:N	1:A:506:PRO:CD	2.84	0.41
1:A:181:LEU:HD12	1:A:182:THR:N	2.36	0.41
1:A:212:SER:HB2	1:A:232:ASP:HB3	2.03	0.41
1:A:708:SER:HA	1:A:709:PRO:HD3	1.85	0.40
1:A:743:ARG:HH11	1:A:752:THR:HG21	1.86	0.40
1:A:437:MET:HG2	1:A:460:PHE:CZ	2.55	0.40
1:A:530:LEU:HD12	1:A:551:SER:HB3	2.02	0.40
1:B:248:PHE:HB2	1:B:268:ILE:HA	2.03	0.40
1:B:610:GLY:HA3	5:B:819:HOH:O	2.21	0.40
1:B:439:TRP:CH2	3:B:5:GOL:H31	2.56	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	605/613 (99%)	574 (95%)	30 (5%)	1 (0%)	47	68
1	B	608/613 (99%)	550 (90%)	56 (9%)	2 (0%)	41	61
All	All	1213/1226 (99%)	1124 (93%)	86 (7%)	3 (0%)	47	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	210	GLY
1	B	671	SER
1	A	205	GLY

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	540/546 (99%)	501 (93%)	39 (7%)	14	28
1	B	535/546 (98%)	497 (93%)	38 (7%)	14	28
All	All	1075/1092 (98%)	998 (93%)	77 (7%)	14	28

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	LEU
1	A	192	ARG
1	A	193	THR

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Mol	Chain	Res	Type
1	A	195	GLU
1	A	236	SER
1	A	243	LEU
1	A	246	CYS
1	A	269	ARG
1	A	272	PHE
1	A	387	ILE
1	A	395	LEU
1	A	403	LYS
1	A	418	ASN
1	A	444	ILE
1	A	499	LEU
1	A	515	LEU
1	A	530	LEU
1	A	536	LEU
1	A	539	SER
1	A	550	LEU
1	A	553	MET
1	A	601	LYS
1	A	612	LEU
1	A	626	ILE
1	A	629	LEU
1	A	632	ASN
1	A	643	GLN
1	A	645	ARG
1	A	646	LYS
1	A	647	LEU
1	A	651	TRP
1	A	673	VAL
1	A	676	ASP
1	A	680	ARG
1	A	728	PRO
1	A	729	GLN
1	A	733	SER
1	A	744	LEU
1	A	763	GLU
1	B	176	LEU
1	B	185	LEU
1	B	186	ILE
1	B	192	ARG
1	B	199	GLU
1	B	201	LEU

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Mol	Chain	Res	Type
1	B	211	LEU
1	B	217	ASN
1	B	227	VAL
1	B	236	SER
1	B	265	ASN
1	B	266	CYS
1	B	272	PHE
1	B	274	ASN
1	B	305	THR
1	B	345	ASP
1	B	395	LEU
1	B	418	ASN
1	B	430	ASP
1	B	472	SER
1	B	499	LEU
1	B	527	ASP
1	B	553	MET
1	B	612	LEU
1	B	629	LEU
1	B	642	ASP
1	B	643	GLN
1	B	646	LYS
1	B	651	TRP
1	B	661	ASN
1	B	681	LYS
1	B	705	GLU
1	B	730	VAL
1	B	733	SER
1	B	741	LEU
1	B	744	LEU
1	B	745	GLN
1	B	774	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	ASN
1	A	279	ASN
1	A	281	ASN
1	A	294	GLN
1	A	300	ASN
1	A	418	ASN

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Mol	Chain	Res	Type
1	A	476	GLN
1	A	480	ASN
1	A	552	HIS
1	A	577	GLN
1	A	632	ASN
1	A	643	GLN
1	A	717	ASN
1	A	722	GLN
1	A	745	GLN
1	A	764	HIS
1	B	240	GLN
1	B	245	ASN
1	B	281	ASN
1	B	300	ASN
1	B	418	ASN
1	B	476	GLN
1	B	480	ASN
1	B	600	HIS
1	B	606	ASN
1	B	643	GLN
1	B	661	ASN
1	B	682	GLN
1	B	717	ASN
1	B	729	GLN
1	B	745	GLN
1	B	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 carbohydrates 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	784	-	5,5,5	0.44	0	5,5,5	0.31	0
2	SO4	B	10	-	4,4,4	0.13	0	6,6,6	0.18	0
2	SO4	A	4	-	4,4,4	0.16	0	6,6,6	0.12	0
2	SO4	B	2	-	4,4,4	0.13	0	6,6,6	0.14	0
2	SO4	A	3	-	4,4,4	0.13	0	6,6,6	0.16	0
3	GOL	A	8	-	5,5,5	0.33	0	5,5,5	0.29	0
4	MES	B	1	-	12,12,12	2.25	1 (8%)	14,16,16	2.66	7 (50%)
3	GOL	B	5	-	5,5,5	0.35	0	5,5,5	0.28	0
3	GOL	B	9	-	5,5,5	0.36	0	5,5,5	0.66	0
2	SO4	B	7	-	4,4,4	0.10	0	6,6,6	0.20	0
3	GOL	B	6	-	5,5,5	0.35	0	5,5,5	0.41	0
3	GOL	A	783	-	5,5,5	0.35	0	5,5,5	0.20	0
2	SO4	A	5	-	4,4,4	0.13	0	6,6,6	0.09	0
3	GOL	B	783	-	5,5,5	0.40	0	5,5,5	0.47	0
2	SO4	B	8	-	4,4,4	0.16	0	6,6,6	0.10	0
3	GOL	B	3	-	5,5,5	0.37	0	5,5,5	0.21	0
2	SO4	A	1	-	4,4,4	0.09	0	6,6,6	0.24	0
3	GOL	A	7	-	5,5,5	0.37	0	5,5,5	0.39	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	MES	B	1	-	-	1/6/14/14	0/1/1/1
3	GOL	B	783	-	-	2/4/4/4	-
3	GOL	A	8	-	-	2/4/4/4	-
3	GOL	B	5	-	-	3/4/4/4	-
3	GOL	B	9	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	6	-	-	4/4/4/4	-
3	GOL	A	783	-	-	2/4/4/4	-
3	GOL	A	784	-	-	4/4/4/4	-
3	GOL	A	7	-	-	0/4/4/4	-
3	GOL	B	3	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1	MES	C8-S	-7.54	1.66	1.77

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1	MES	C5-N4-C3	4.59	119.16	108.83
4	B	1	MES	C2-C3-N4	-4.05	103.96	110.10
4	B	1	MES	C7-N4-C3	3.94	121.30	111.23
4	B	1	MES	C6-C5-N4	-3.72	104.47	110.10
4	B	1	MES	C7-N4-C5	3.24	119.53	111.23
4	B	1	MES	O3S-S-C8	2.57	109.93	105.77
4	B	1	MES	O1S-S-C8	2.51	109.93	106.92

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	8	GOL	O1-C1-C2-C3
3	B	9	GOL	O1-C1-C2-C3
3	A	784	GOL	O1-C1-C2-C3
3	B	6	GOL	C1-C2-C3-O3
3	B	783	GOL	O1-C1-C2-C3
3	A	784	GOL	O1-C1-C2-O2
3	B	6	GOL	O1-C1-C2-O2
3	B	5	GOL	O1-C1-C2-C3
3	A	784	GOL	C1-C2-C3-O3
3	B	6	GOL	O1-C1-C2-C3
3	B	3	GOL	C1-C2-C3-O3
3	A	8	GOL	O1-C1-C2-O2
3	B	9	GOL	O1-C1-C2-O2
3	B	6	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	B	783	GOL	O1-C1-C2-O2
3	A	784	GOL	O2-C2-C3-O3
3	B	3	GOL	O2-C2-C3-O3
3	A	783	GOL	O1-C1-C2-O2
3	B	5	GOL	C1-C2-C3-O3
3	B	5	GOL	O2-C2-C3-O3
4	B	1	MES	C8-C7-N4-C3
3	A	783	GOL	O1-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	MES	3	0
3	B	5	GOL	1	0
3	B	9	GOL	1	0
3	B	783	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	607/613 (99%)	-0.26	15 (2%) 57 61	26, 52, 112, 177	2 (0%)
1	B	610/613 (99%)	-0.18	27 (4%) 34 37	30, 58, 118, 159	3 (0%)
All	All	1217/1226 (99%)	-0.22	42 (3%) 44 47	26, 56, 114, 177	5 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	185	LEU	6.9
1	B	187	TRP	5.9
1	B	184	ASP	5.1
1	A	211	LEU	5.0
1	B	202	ASN	4.7
1	A	201	LEU	4.6
1	B	181	LEU	4.4
1	A	180	GLU	4.3
1	B	211	LEU	3.8
1	B	208	LEU	3.7
1	B	527	ASP	3.6
1	B	175	CYS	3.5
1	A	208	LEU	3.3
1	B	183	ALA	3.3
1	A	187	TRP	3.2
1	B	751	PHE	3.2
1	A	181	LEU	3.2
1	B	174	ALA	2.9
1	A	327	PHE	2.8
1	B	231	THR	2.8
1	B	204	SER	2.8
1	B	176	LEU	2.8
1	A	330	LYS	2.7
1	B	177	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	185	LEU	2.6
1	B	750	VAL	2.6
1	B	673	VAL	2.6
1	B	201	LEU	2.6
1	B	200	GLU	2.5
1	A	195	GLU	2.5
1	A	179	ALA	2.4
1	B	186	ILE	2.3
1	B	330	LYS	2.3
1	A	228	LEU	2.3
1	B	329	GLU	2.3
1	A	203	TYR	2.2
1	A	202	ASN	2.1
1	B	221	VAL	2.0
1	B	675	LYS	2.0
1	B	173	ARG	2.0
1	A	204	SER	2.0
1	B	207	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	A	783	6/6	0.72	0.23	87,98,100,102	0
2	SO4	A	5	5/5	0.75	0.27	144,144,146,146	0
3	GOL	A	7	6/6	0.77	0.18	87,89,92,93	0
3	GOL	A	8	6/6	0.83	0.11	84,89,91,92	0
3	GOL	B	783	6/6	0.85	0.19	59,73,77,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	B	6	6/6	0.85	0.26	49,84,91,94	0
2	SO4	B	10	5/5	0.86	0.24	95,103,107,114	0
2	SO4	B	8	5/5	0.87	0.16	118,119,120,121	0
4	MES	B	1	12/12	0.89	0.15	85,91,159,161	0
3	GOL	B	9	6/6	0.89	0.20	77,91,97,104	0
2	SO4	A	3	5/5	0.93	0.16	106,107,110,115	0
3	GOL	B	5	6/6	0.94	0.29	41,50,51,55	0
3	GOL	B	3	6/6	0.94	0.12	43,62,68,72	0
3	GOL	A	784	6/6	0.94	0.26	46,51,56,61	0
2	SO4	A	4	5/5	0.95	0.15	116,119,121,122	0
2	SO4	B	7	5/5	0.96	0.07	81,82,93,94	0
2	SO4	B	2	5/5	0.98	0.10	64,65,72,81	0
2	SO4	A	1	5/5	0.99	0.14	61,62,67,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.