



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:34 am GMT

PDB ID : 4NHO
Title : Structure of the spliceosomal DEAD-box protein Prp28
Authors : Moehlmann, S.; Neumann, P.; Ficner, R.
Deposited on : 2013-11-05
Resolution : 2.00 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

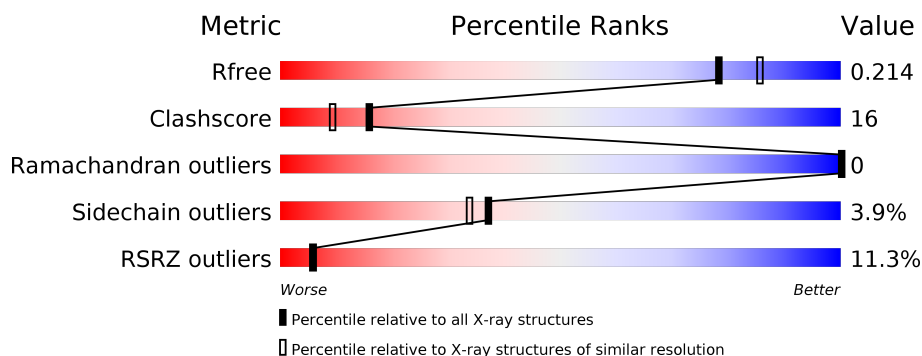
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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. 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	488	<div> <div>10%</div> <div>66%</div> <div>23%</div> <div>9%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	905	-	-	-	X
3	GOL	A	906	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	907	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3833 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.

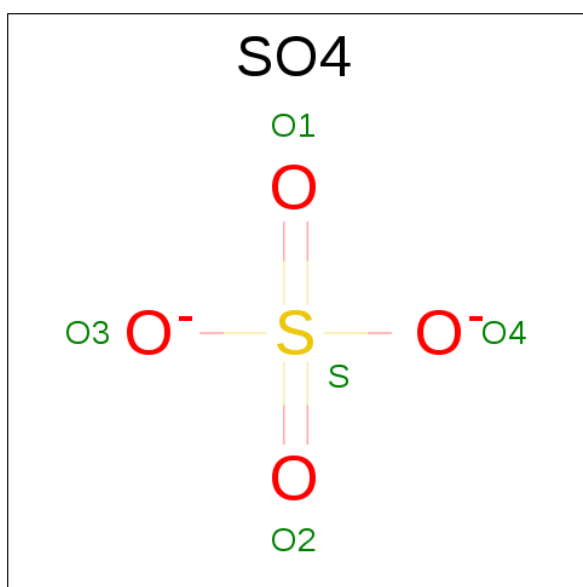
- Molecule 1 is a protein called Probable ATP-dependent RNA helicase DDX23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	443	3560	2254	616	672	18	0	7	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	333	GLY	-	EXPRESSION TAG	UNP Q9BUQ8
A	334	PRO	-	EXPRESSION TAG	UNP Q9BUQ8
A	335	LEU	-	EXPRESSION TAG	UNP Q9BUQ8
A	336	GLY	-	EXPRESSION TAG	UNP Q9BUQ8
A	337	SER	-	EXPRESSION TAG	UNP Q9BUQ8

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



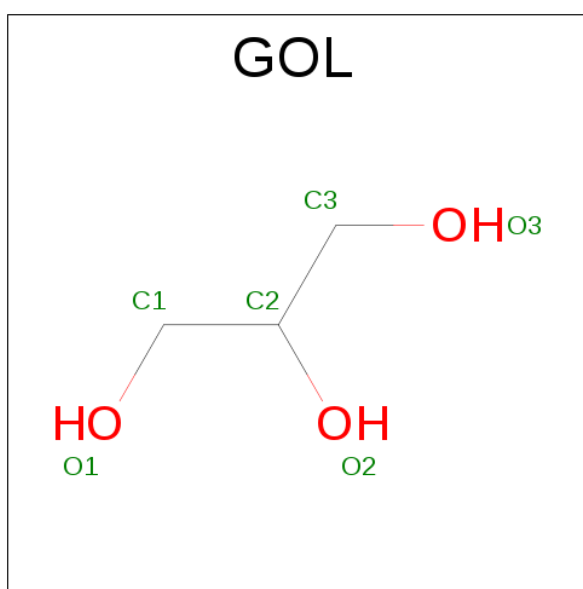
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

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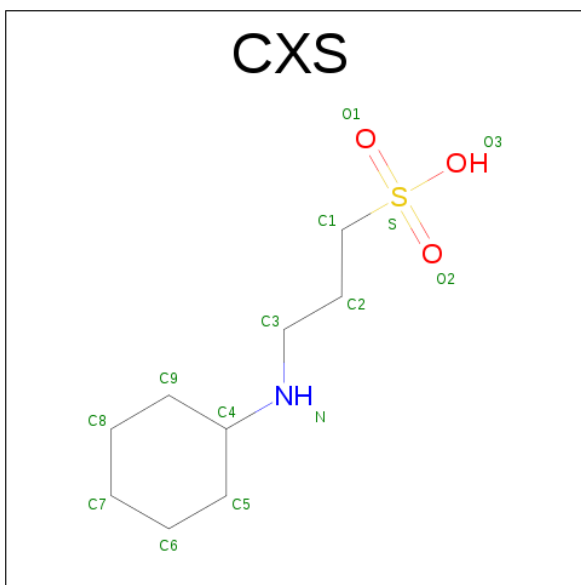
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- 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	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 3-CYCLOHEXYL-1-PROPYLSULFONIC ACID (three-letter code: CXS) (formula: $C_9H_{19}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			14	9	1	3	1		

- Molecule 5 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Hg	0	1
			2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	220	Total	O	0	0
			220	220		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	125.43Å 136.77Å 73.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.82 – 2.00 39.08 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (28.82-2.00) 100.0 (39.08-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.00	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.193 , 0.218 0.189 , 0.214	Depositor DCC
R_{free} test set	2159 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.826	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 67.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3833	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, CSO, CXS, SO4, HG

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	0.57	1/3612 (0.0%)	0.63	0/4879

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	543	CYS	CB-SG	-6.86	1.70	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	3560	0	3596	118	0
2	A	25	0	0	0	0
3	A	12	0	16	14	0
4	A	14	0	19	1	0
5	A	2	0	0	0	0
6	A	220	0	0	6	0
All	All	3833	0	3631	118	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 16.

All (118) 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:564:GLN:HG2	3:A:906:GOL:H31	1.46	0.96
1:A:564:GLN:HA	3:A:906:GOL:H2	1.48	0.95
1:A:564:GLN:HG2	3:A:906:GOL:C3	1.97	0.94
1:A:445:PHE:CD2	1:A:605:PHE:HE2	1.87	0.93
1:A:567:LEU:HD23	3:A:906:GOL:H11	1.53	0.90
1:A:733[A]:VAL:HG12	1:A:735:MET:H	1.35	0.90
1:A:445:PHE:HD2	1:A:605:PHE:CE2	1.94	0.84
1:A:750:HIS:HB3	6:A:1153:HOH:O	1.78	0.84
1:A:472:ILE:HG13	1:A:540:LEU:HD21	1.62	0.81
1:A:675:LYS:O	1:A:679:VAL:HG12	1.83	0.79
1:A:445:PHE:CD2	1:A:605:PHE:CE2	2.70	0.78
1:A:540:LEU:HD22	1:A:570:MET:SD	2.23	0.78
1:A:692:CYS:SG	1:A:715:LYS:HG3	2.25	0.76
1:A:711:LYS:HA	1:A:731:GLN:HE22	1.52	0.75
1:A:679:VAL:O	1:A:682:LYS:HG2	1.89	0.73
1:A:682:LYS:HG3	1:A:683:SER:N	2.03	0.73
1:A:442:THR:HA	1:A:445:PHE:CE2	2.23	0.72
1:A:690:ASN:HB3	1:A:715:LYS:HD3	1.73	0.71
1:A:560:GLU:O	1:A:564:GLN:HG3	1.92	0.70
1:A:353:ASP:OD2	1:A:355:ARG:HD3	1.92	0.70
1:A:666:PRO:O	1:A:733[A]:VAL:HG13	1.92	0.70
1:A:432:ILE:HG21	1:A:609:MET:HE3	1.74	0.69
1:A:463:GLU:HG3	1:A:467:GLN:OE1	1.92	0.68
1:A:728:ILE:HG23	1:A:729:ASP:H	1.58	0.68
1:A:567:LEU:HD23	3:A:906:GOL:C1	2.21	0.68
1:A:374:ARG:HH21	1:A:420:GLN:HE22	1.42	0.66
1:A:564:GLN:HG2	3:A:906:GOL:H32	1.77	0.66
1:A:366:THR:CG2	1:A:369:ASP:H	2.09	0.65
1:A:746:GLU:OE1	6:A:1174:HOH:O	2.15	0.64
1:A:540:LEU:HD23	1:A:543:CYS:HB2	1.78	0.64
1:A:733[A]:VAL:HG12	1:A:735:MET:N	2.10	0.64
1:A:567:LEU:CD2	3:A:906:GOL:O2	2.45	0.64
1:A:567:LEU:HD23	3:A:906:GOL:O2	1.98	0.63
1:A:768:LEU:HD11	1:A:779:LEU:HD23	1.82	0.62
1:A:536:ARG:O	1:A:536:ARG:HG3	2.01	0.61
1:A:601[B]:GLN:HG2	1:A:602:THR:N	2.16	0.61
1:A:564:GLN:CG	3:A:906:GOL:H31	2.25	0.61
1:A:667:ILE:HA	1:A:733[A]:VAL:HG11	1.83	0.60
1:A:609:MET:HG3	1:A:787:PRO:O	2.03	0.59
1:A:564:GLN:HA	3:A:906:GOL:C2	2.27	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:HIS:CE1	4:A:908:CXS:H61	2.39	0.58
1:A:366:THR:HG22	1:A:369:ASP:H	1.68	0.58
1:A:728:ILE:HG23	1:A:729:ASP:N	2.20	0.57
1:A:675:LYS:H	1:A:675:LYS:HD2	1.71	0.56
1:A:366:THR:HG23	1:A:368:ARG:N	2.21	0.56
1:A:669:ILE:HG12	1:A:737:VAL:CG1	2.37	0.55
1:A:458:LYS:O	1:A:462:ILE:HG13	2.06	0.55
1:A:428:ASN:HD21	1:A:598:LYS:NZ	2.06	0.54
1:A:604:MET:HE3	1:A:621:LEU:HD11	1.90	0.54
1:A:551:ALA:HB3	1:A:606[A]:THR:CG2	2.37	0.54
1:A:744:ASN:OD1	1:A:746:GLU:HG2	2.09	0.53
1:A:728:ILE:HG12	1:A:729:ASP:N	2.23	0.53
1:A:540:LEU:HD13	1:A:570:MET:SD	2.48	0.53
1:A:540:LEU:HD23	1:A:543:CYS:CB	2.39	0.52
1:A:479[B]:GLU:H	1:A:479[B]:GLU:CD	2.12	0.51
1:A:745:ILE:O	1:A:749:ILE:HG12	2.10	0.51
1:A:667:ILE:HA	1:A:733[A]:VAL:CG1	2.40	0.51
1:A:768:LEU:HD22	1:A:776:PHE:CE1	2.46	0.51
1:A:530:ILE:HD11	1:A:565:LYS:HB3	1.93	0.51
1:A:432:ILE:HG21	1:A:609:MET:CE	2.41	0.50
1:A:485:GLU:HA	1:A:523:ILE:HD13	1.93	0.50
1:A:366:THR:HG22	1:A:369:ASP:CG	2.31	0.50
1:A:768:LEU:HD22	1:A:776:PHE:HE1	1.77	0.50
1:A:591:ASN:O	1:A:594[B]:SER:HB3	2.12	0.50
1:A:682:LYS:CG	1:A:683:SER:N	2.74	0.49
1:A:551:ALA:HB3	1:A:606[A]:THR:HG22	1.95	0.49
1:A:567:LEU:HD22	3:A:906:GOL:O2	2.13	0.49
1:A:530:ILE:HD11	1:A:565:LYS:CG	2.44	0.48
1:A:485:GLU:O	1:A:489:ILE:HG12	2.13	0.48
1:A:713:GLY:HA2	6:A:1203:HOH:O	2.14	0.48
1:A:485:GLU:HA	1:A:523:ILE:CD1	2.44	0.47
1:A:673:GLN:HB3	1:A:675:LYS:CD	2.45	0.47
1:A:711:LYS:HA	1:A:731:GLN:NE2	2.26	0.47
1:A:540:LEU:HD23	1:A:543:CYS:SG	2.54	0.47
1:A:675:LYS:HG2	1:A:676:GLY:N	2.30	0.47
1:A:693:THR:O	1:A:694:LEU:HG	2.14	0.47
1:A:366:THR:HG23	1:A:369:ASP:H	1.79	0.47
1:A:457:PRO:HG2	1:A:460:ASP:OD2	2.15	0.47
1:A:798:HIS:HE1	1:A:800:ASP:OD2	1.98	0.46
1:A:540:LEU:CD2	1:A:543:CYS:CB	2.92	0.46
1:A:357:TRP:HB2	1:A:365:MET:SD	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:LYS:HB3	1:A:675:LYS:HE3	1.77	0.46
1:A:511:GLN:OE1	1:A:528:ARG:NE	2.49	0.46
1:A:466:ASP:HB3	6:A:1193:HOH:O	2.16	0.45
1:A:545:TYR:CE1	1:A:601[B]:GLN:OE1	2.69	0.45
1:A:730:ILE:HG13	1:A:730:ILE:O	2.16	0.45
1:A:427:GLN:O	1:A:588:MET:HB3	2.17	0.45
1:A:567:LEU:HD23	3:A:906:GOL:C2	2.46	0.45
1:A:728:ILE:HG12	1:A:729:ASP:H	1.80	0.45
1:A:730:ILE:HD12	1:A:731:GLN:O	2.16	0.45
1:A:670:PHE:CG	1:A:751:ARG:HD3	2.52	0.44
1:A:530:ILE:O	1:A:534:GLU:HG2	2.17	0.44
1:A:673:GLN:HB3	1:A:675:LYS:HD2	1.98	0.44
1:A:404:GLU:O	1:A:408:LYS:HG2	2.17	0.44
1:A:679:VAL:HG23	1:A:682:LYS:HE2	1.99	0.44
1:A:564:GLN:CG	3:A:906:GOL:C3	2.85	0.44
1:A:530:ILE:CD1	1:A:565:LYS:HB3	2.48	0.43
1:A:683:SER:O	1:A:686:LYS:HB2	2.18	0.43
1:A:581[A]:GLU:CD	1:A:587:LYS:HD3	2.38	0.43
1:A:652:ARG:HG2	6:A:1080:HOH:O	2.17	0.43
1:A:733[A]:VAL:CG1	1:A:735:MET:H	2.20	0.43
1:A:576:LYS:HE3	1:A:588:MET:HE1	2.00	0.42
1:A:669:ILE:HG12	1:A:737:VAL:HG13	2.02	0.42
1:A:382:LYS:HB2	1:A:626:VAL:HB	2.02	0.42
1:A:411:TYR:CZ	1:A:491:PHE:HE2	2.37	0.42
1:A:366:THR:HG23	1:A:368:ARG:H	1.85	0.41
1:A:564:GLN:HA	3:A:906:GOL:C3	2.50	0.41
1:A:476:PRO:HD2	1:A:480:LEU:HD23	2.03	0.41
1:A:703:ARG:N	1:A:705:PHE:HD2	2.19	0.41
1:A:647:SER:OG	1:A:650:GLU:HG3	2.21	0.41
1:A:536:ARG:O	1:A:536:ARG:CG	2.68	0.40
1:A:616:LEU:HD23	1:A:616:LEU:HA	1.90	0.40
1:A:589:LEU:HD11	6:A:1058:HOH:O	2.21	0.40
1:A:596:LYS:HD2	1:A:597:HIS:CE1	2.56	0.40
1:A:446:LEU:O	1:A:450:LEU:HG	2.22	0.40
1:A:553:ARG:HD3	1:A:557:MET:HE1	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	442/488 (91%)	432 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	389/416 (94%)	374 (96%)	15 (4%)	37	34

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	389	PRO
1	A	395	ASP
1	A	472	ILE
1	A	491	PHE
1	A	516	ARG
1	A	532	VAL
1	A	664	ASP
1	A	674	LYS
1	A	675	LYS
1	A	679	VAL
1	A	685	GLU
1	A	703	ARG
1	A	729	ASP

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Mol	Chain	Res	Type
1	A	730	ILE
1	A	746	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	420	GLN
1	A	428	ASN
1	A	535	ASN
1	A	731	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CSO	A	519	1	4,6,7	1.32	1 (25%)	1,6,8	1.37	0
1	CSO	A	791	1	4,6,7	1.75	1 (25%)	1,6,8	1.82	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
1	CSO	A	519	1	-	0/1/5/7	0/0/0/0
1	CSO	A	791	1	-	0/1/5/7	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	519	CSO	CA-C	2.41	1.53	1.50
1	A	791	CSO	CA-C	3.38	1.54	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	901	-	4,4,4	0.12	0	6,6,6	0.36	0
2	SO4	A	902	-	4,4,4	0.15	0	6,6,6	0.43	0
2	SO4	A	903	-	4,4,4	0.17	0	6,6,6	0.08	0
2	SO4	A	904	-	4,4,4	0.17	0	6,6,6	0.25	0
2	SO4	A	905	-	4,4,4	0.18	0	6,6,6	0.17	0
3	GOL	A	906	-	5,5,5	0.46	0	5,5,5	0.87	0
3	GOL	A	907	-	5,5,5	0.35	0	5,5,5	0.47	0
4	CXS	A	908	-	14,14,14	2.37	2 (14%)	16,18,18	1.39	3 (18%)

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	SO4	A	901	-	-	0/0/0/0	0/0/0/0
2	SO4	A	902	-	-	0/0/0/0	0/0/0/0
2	SO4	A	903	-	-	0/0/0/0	0/0/0/0
2	SO4	A	904	-	-	0/0/0/0	0/0/0/0
2	SO4	A	905	-	-	0/0/0/0	0/0/0/0
3	GOL	A	906	-	-	0/4/4/4	0/0/0/0
3	GOL	A	907	-	-	0/4/4/4	0/0/0/0
4	CXS	A	908	-	-	0/8/16/16	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	908	CXS	C1-S	-7.22	1.66	1.77
4	A	908	CXS	O3-S	4.86	1.63	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	908	CXS	O3-S-C1	2.79	109.49	106.06
4	A	908	CXS	O2-S-C1	3.06	109.42	106.79
4	A	908	CXS	O1-S-C1	3.08	109.44	106.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	906	GOL	14	0
4	A	908	CXS	1	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	441/488 (90%)	0.50	50 (11%) 6 6	29, 50, 113, 181	9 (2%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	352	TRP	10.7
1	A	705	PHE	8.9
1	A	712	ALA	8.7
1	A	464	GLU	8.2
1	A	713	GLY	7.9
1	A	709	ASN	5.9
1	A	714	ALA	5.6
1	A	710	LEU	5.1
1	A	806	GLY	4.6
1	A	706	ALA	4.2
1	A	707	LEU	4.1
1	A	805	PRO	4.0
1	A	682	LYS	4.0
1	A	688	GLY	3.9
1	A	803	HIS	3.7
1	A	537	TYR	3.7
1	A	708	SER	3.7
1	A	694	LEU	3.6
1	A	619	SER	3.4
1	A	704	GLU	3.4
1	A	686	LYS	3.3
1	A	685	GLU	3.2
1	A	715	LYS	3.1
1	A	687	MET	3.1
1	A	678	ASP	3.1
1	A	703	ARG	2.9
1	A	689	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	546	VAL	2.7
1	A	804	LYS	2.7
1	A	617	ALA	2.7
1	A	621	LEU	2.6
1	A	411	TYR	2.6
1	A	690	ASN	2.6
1	A	513	PHE	2.4
1	A	362	LEU	2.4
1	A	603	VAL	2.4
1	A	545	TYR	2.4
1	A	466	ASP	2.4
1	A	547	VAL	2.3
1	A	728	ILE	2.3
1	A	620	TYR	2.3
1	A	800	ASP	2.3
1	A	516	ARG	2.3
1	A	679	VAL	2.2
1	A	543	CYS	2.2
1	A	684	LEU	2.2
1	A	602	THR	2.2
1	A	471	ALA	2.1
1	A	711	LYS	2.1
1	A	618	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
1	CSO	A	519	7/8	0.93	0.12	-	57,59,62,65	0
1	CSO	A	791	7/8	0.91	0.12	-	44,47,64,73	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	A	905	5/5	0.78	1.27	28.52	51,56,57,58	5
3	GOL	A	907	6/6	0.77	0.26	2.49	82,83,83,84	0
4	CXS	A	908	14/14	0.91	0.17	1.73	61,66,110,138	0
3	GOL	A	906	6/6	0.79	0.29	1.58	59,64,67,69	0
2	SO4	A	901	5/5	0.97	0.11	-0.32	64,65,67,68	0
2	SO4	A	902	5/5	0.98	0.11	-0.51	54,56,58,62	0
5	HG	A	909[B]	1/1	0.99	0.09	-2.64	60,60,60,60	1
5	HG	A	909[A]	1/1	0.99	0.09	-3.13	48,48,48,48	1
2	SO4	A	903	5/5	0.95	0.13	-	59,62,64,66	5
2	SO4	A	904	5/5	0.88	0.13	-	72,73,74,74	5

6.5 Other polymers [i](#)

There are no such residues in this entry.