Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 03:24 PM EDT

PDB ID	:	6OHO
Title	:	Structure of human Phospholipase D2 catalytic domain
Authors	:	Metrick, C.M.; Chodaparambil, J.V.
Deposited on	:	2019-04-06
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

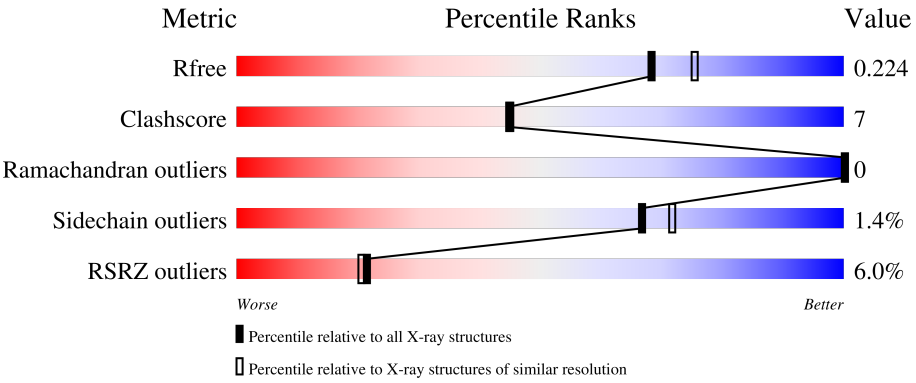
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 of 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 <=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	640	5% 78% 12% 9%
1	B	640	6% 78% 12% • 10%

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	B	1005	-	-	X	-
3	GOL	A	1009	-	-	X	-

2 Entry composition

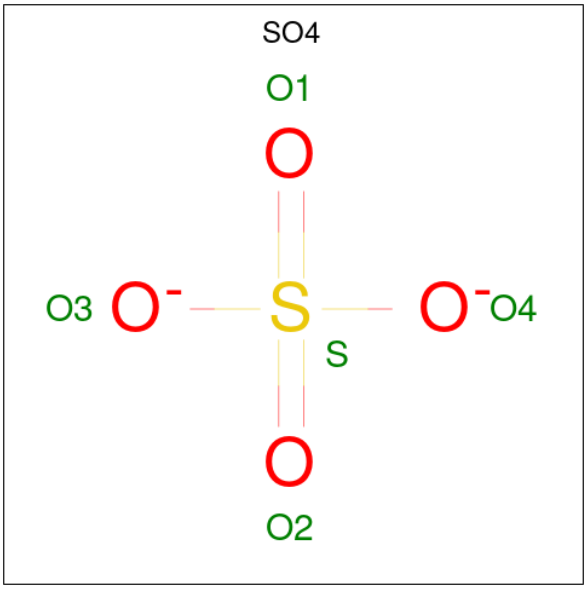
There are 5 unique types of molecules in this entry. The entry contains 9866 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phospholipase D2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	580	Total	C	N	O	S	0	0	0
			4671	2998	817	840	16			
1	B	579	Total	C	N	O	S	0	0	0
			4660	2990	815	840	15			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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		

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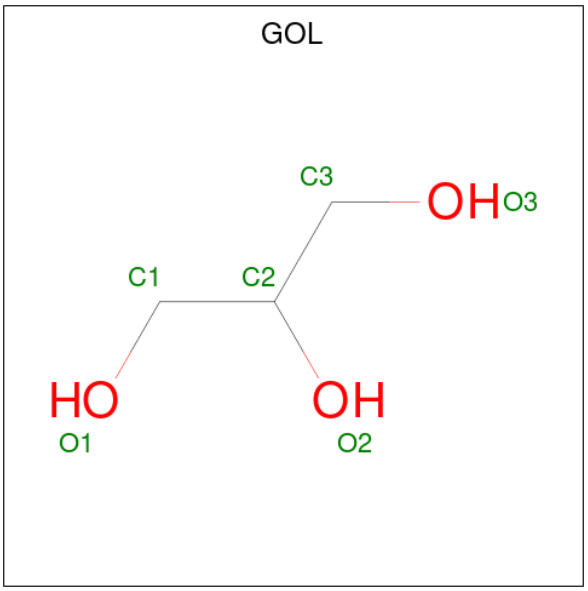
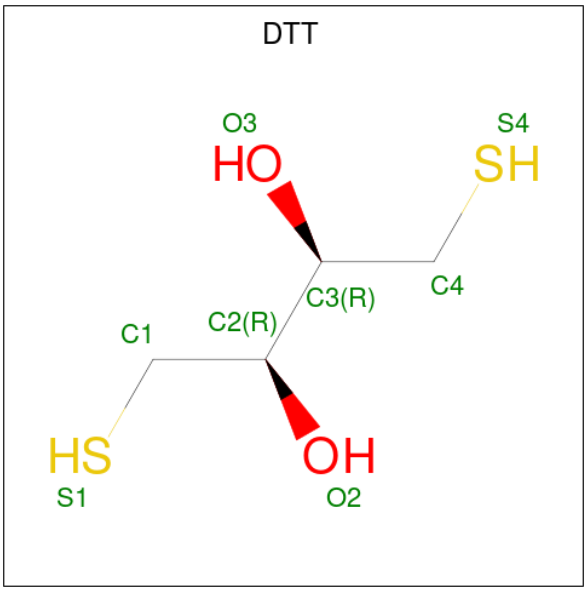
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0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

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



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

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



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

- Molecule 5 is water.

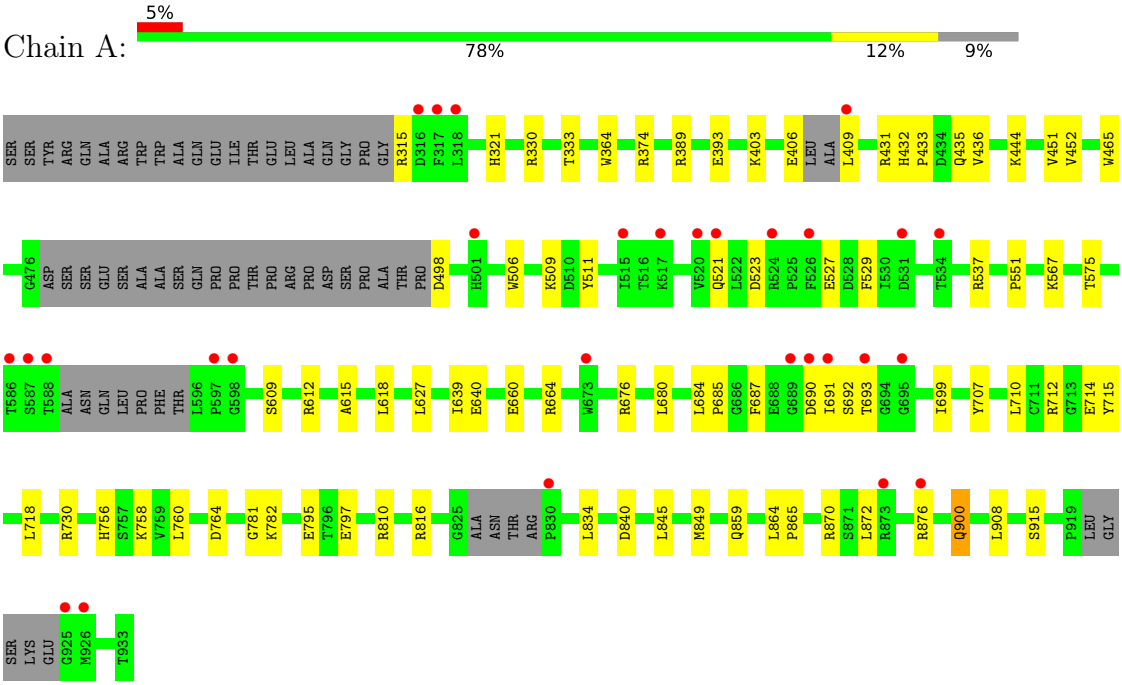
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	217	Total O 217 217	0	0
5	B	177	Total O 177 177	0	0

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.

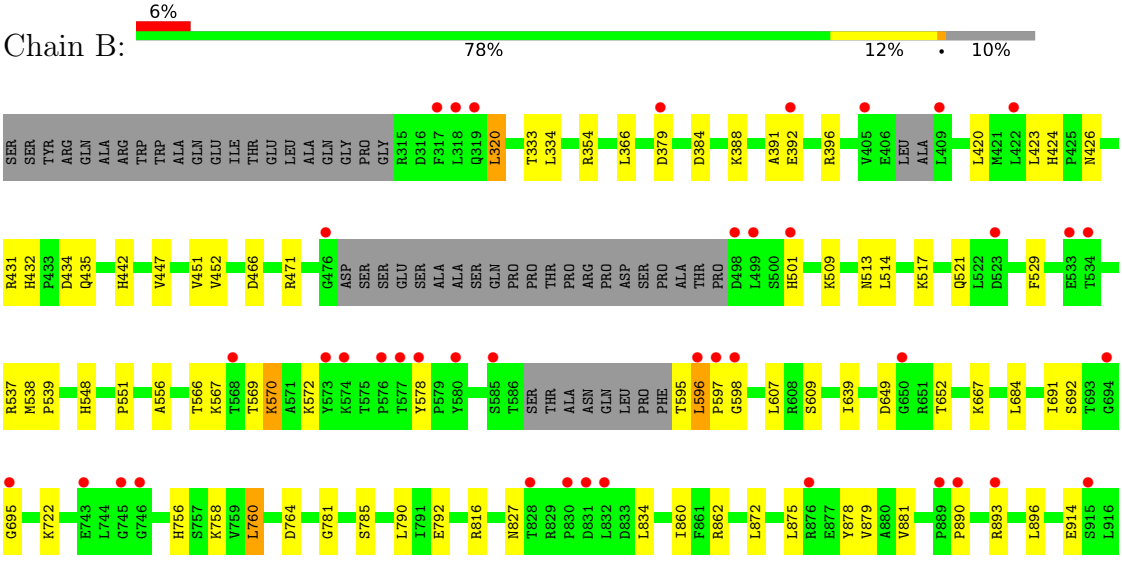
• Molecule 1: Phospholipase D2

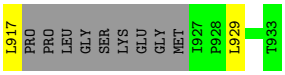
Chain A:



• Molecule 1: Phospholipase D2

Chain B:




L917
PRO
PRO
LEU
GLY
SER
LYS
GLU
GLY
MET
I927
P928
L929
T933

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	91.70Å 131.34Å 107.29Å 90.00° 111.77° 90.00°	Depositor
Resolution (Å)	48.57 – 2.00 48.57 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.57-2.00) 99.7 (48.57-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.181 , 0.224 0.181 , 0.224	Depositor DCC
R_{free} test set	4141 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å^2)	33.9	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9866	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DTT, SO4, GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.33	0/4791	0.55	3/6507 (0.0%)
1	B	0.31	0/4779	0.51	0/6497
All	All	0.32	0/9570	0.53	3/13004 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	612	ARG	NE-CZ-NH2	10.34	125.47	120.30
1	A	612	ARG	NE-CZ-NH1	-6.78	116.91	120.30
1	A	615	ALA	C-N-CA	-5.12	111.56	122.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	596	LEU	Peptide

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	4671	0	4603	62	0
1	B	4660	0	4586	59	0
2	A	40	0	0	2	0
2	B	45	0	0	3	0
3	A	24	0	32	11	0
3	B	24	0	30	6	0
4	B	8	0	9	1	0
5	A	217	0	0	5	0
5	B	177	0	0	9	1
All	All	9866	0	9260	122	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (122) 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:471:ARG:O	1:B:537:ARG:NH1	1.80	1.15
1:A:693:THR:HA	1:A:876:ARG:HH12	1.20	1.05
1:A:693:THR:HA	1:A:876:ARG:NH1	1.78	0.98
1:B:424:HIS:HD2	1:B:426:ASN:H	1.08	0.95
1:B:466:ASP:OD2	1:B:537:ARG:NH2	2.01	0.93
1:B:442:HIS:NE2	3:B:1010:GOL:O2	2.07	0.88
1:B:388:LYS:O	5:B:1101:HOH:O	1.93	0.87
1:A:908:LEU:HD12	3:A:1010:GOL:H32	1.58	0.85
1:A:730:ARG:HH22	3:A:1010:GOL:H31	1.43	0.82
1:A:693:THR:CA	1:A:876:ARG:HH12	1.91	0.82
1:B:537:ARG:NH2	1:B:539:PRO:HA	1.97	0.79
1:B:424:HIS:CD2	1:B:426:ASN:H	1.96	0.79
1:B:792:GLU:OE1	5:B:1102:HOH:O	2.03	0.75
1:B:756:HIS:NE2	3:B:1010:GOL:H2	2.03	0.72
1:A:498:ASP:O	5:A:1101:HOH:O	2.08	0.72
1:B:639:ILE:HG12	1:B:760:LEU:HD12	1.71	0.72
1:A:756:HIS:CE1	3:A:1009:GOL:H12	2.25	0.71
1:B:692:SER:HB2	1:B:879:VAL:HG21	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:GLU:O	5:A:1102:HOH:O	2.09	0.70
1:B:396:ARG:O	5:B:1103:HOH:O	2.09	0.70
4:B:1014:DTT:S1	4:B:1014:DTT:O3	2.45	0.69
1:A:575:THR:OG1	5:A:1103:HOH:O	2.13	0.67
1:A:409:LEU:O	5:A:1102:HOH:O	2.15	0.65
1:B:860:ILE:HG21	1:B:896:LEU:HD11	1.78	0.65
1:B:435:GLN:HG2	3:B:1013:GOL:O2	1.98	0.64
1:B:695:GLY:O	5:B:1105:HOH:O	2.14	0.64
2:B:1001:SO4:O2	5:B:1104:HOH:O	2.09	0.63
1:B:872:LEU:N	1:B:914:GLU:OE2	2.32	0.62
1:A:915:SER:O	3:A:1011:GOL:O3	2.14	0.62
1:A:764:ASP:OD1	1:A:816:ARG:HD3	2.00	0.62
1:A:364:TRP:CE3	3:A:1009:GOL:H31	2.35	0.62
1:B:434:ASP:N	3:B:1013:GOL:O2	2.33	0.61
1:A:872:LEU:O	1:A:876:ARG:HD3	2.01	0.61
1:B:384:ASP:HB2	1:B:423:LEU:HD11	1.83	0.60
1:A:509:LYS:NZ	1:A:521:GLN:O	2.35	0.59
1:A:693:THR:O	1:A:876:ARG:CZ	2.51	0.59
1:A:627:LEU:HD22	1:A:660:GLU:HG3	1.84	0.59
1:B:890:PRO:HA	1:B:893:ARG:HD2	1.84	0.58
1:A:664:ARG:HH22	3:A:1012:GOL:H31	1.70	0.57
1:B:509:LYS:NZ	1:B:521:GLN:O	2.36	0.57
1:A:618:LEU:HD13	1:A:782:LYS:HE3	1.87	0.57
1:B:764:ASP:OD1	1:B:816:ARG:HD3	2.04	0.57
1:A:693:THR:O	1:A:876:ARG:NH2	2.37	0.57
1:A:509:LYS:HE2	1:A:529:PHE:HB3	1.88	0.56
1:A:389:ARG:O	1:A:393:GLU:HG3	2.06	0.56
1:B:609:SER:HB3	1:B:781:GLY:HA2	1.88	0.56
1:B:334:LEU:HD21	1:B:598:GLY:HA2	1.87	0.55
1:B:391:ALA:N	5:B:1101:HOH:O	2.39	0.55
1:A:840:ASP:OD2	5:A:1104:HOH:O	2.19	0.54
1:B:862:ARG:NH1	1:B:881:VAL:HB	2.23	0.54
1:B:392:GLU:N	5:B:1101:HOH:O	2.02	0.54
1:A:511:TYR:CE2	1:A:537:ARG:HG3	2.42	0.54
1:A:690:ASP:OD1	1:A:692:SER:OG	2.26	0.54
1:A:315:ARG:N	1:A:330:ARG:HH12	2.06	0.54
1:A:707:TYR:HB3	1:A:712:ARG:HD2	1.90	0.53
1:A:693:THR:CA	1:A:876:ARG:NH1	2.56	0.53
1:B:756:HIS:CE1	3:B:1010:GOL:H2	2.44	0.52
1:A:432:HIS:CD2	1:A:433:PRO:HA	2.45	0.51
1:A:374:ARG:HG3	1:A:465:TRP:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:ILE:HG23	1:A:864:LEU:HD12	1.94	0.50
1:A:756:HIS:NE2	3:A:1009:GOL:H12	2.26	0.50
1:B:572:LYS:NZ	2:B:1005:SO4:O4	2.35	0.50
1:A:432:HIS:CG	1:A:433:PRO:HA	2.47	0.49
1:A:321:HIS:HB3	2:A:1003:SO4:O1	2.13	0.49
1:A:712:ARG:HD3	3:A:1011:GOL:H12	1.94	0.49
1:B:595:THR:O	1:B:596:LEU:HD13	2.12	0.49
1:B:354:ARG:HH11	1:B:595:THR:HG23	1.77	0.49
1:A:849:MET:SD	1:A:900:GLN:HG3	2.54	0.48
1:B:860:ILE:HG21	1:B:896:LEU:CD1	2.43	0.48
1:B:392:GLU:HA	1:B:424:HIS:CE1	2.49	0.48
1:A:403:LYS:HB2	1:A:431:ARG:HB3	1.96	0.47
1:A:609:SER:HB3	1:A:781:GLY:HA2	1.95	0.47
1:B:517:LYS:HD3	1:B:529:PHE:HD2	1.80	0.47
1:A:451:VAL:HG23	1:A:452:VAL:HG23	1.97	0.46
1:A:693:THR:O	1:A:876:ARG:NH1	2.48	0.46
1:B:513:ASN:HA	1:B:538:MET:HB3	1.97	0.46
1:A:435:GLN:HG3	1:A:436:VAL:N	2.30	0.46
1:B:862:ARG:NH1	1:B:878:TYR:O	2.49	0.46
1:B:862:ARG:NH2	5:B:1125:HOH:O	2.49	0.46
1:A:639:ILE:HG12	1:A:760:LEU:HD12	1.97	0.46
1:A:816:ARG:NH2	1:A:834:LEU:O	2.36	0.46
1:B:431:ARG:NH2	2:B:1005:SO4:O3	2.49	0.46
1:B:424:HIS:HD2	1:B:426:ASN:N	1.92	0.45
1:B:827:ASN:N	1:B:827:ASN:OD1	2.49	0.45
1:A:687:PHE:HB2	1:A:699:ILE:HD11	1.98	0.45
1:A:618:LEU:HD11	1:B:722:LYS:HB3	1.98	0.45
1:B:451:VAL:HG23	1:B:452:VAL:HG23	1.99	0.45
1:B:816:ARG:NH2	1:B:834:LEU:O	2.29	0.45
1:A:567:LYS:HB3	1:A:567:LYS:HE3	1.73	0.45
1:A:664:ARG:HA	1:A:664:ARG:HD2	1.71	0.45
1:A:684:LEU:HG	1:A:865:PRO:HD3	2.00	0.44
1:A:444:LYS:NZ	3:A:1009:GOL:H32	2.32	0.44
1:A:333:THR:HG21	1:A:551:PRO:HG2	1.99	0.44
1:B:567:LYS:NZ	1:B:578:TYR:O	2.43	0.44
1:B:569:THR:HB	3:B:1013:GOL:H31	2.00	0.44
1:B:447:VAL:HG11	1:B:556:ALA:HB2	2.00	0.43
1:A:797:GLU:HG2	1:A:810:ARG:HG2	2.01	0.43
1:B:517:LYS:HD3	1:B:529:PHE:CD2	2.54	0.43
1:B:917:LEU:HD21	1:B:929:LEU:HD11	2.00	0.43
1:B:684:LEU:HD11	1:B:691:ILE:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:GLU:HG3	1:A:715:TYR:CD2	2.53	0.43
1:B:384:ASP:N	1:B:384:ASP:OD1	2.50	0.43
1:A:685:PRO:HD2	1:A:699:ILE:HG23	2.01	0.42
1:B:649:ASP:OD2	1:B:652:THR:HG22	2.19	0.42
1:A:712:ARG:HH11	3:A:1011:GOL:H12	1.84	0.42
1:A:432:HIS:NE2	2:A:1005:SO4:O3	2.42	0.42
1:A:509:LYS:HE3	1:A:527:GLU:O	2.19	0.42
1:B:609:SER:O	1:B:785:SER:HA	2.19	0.42
1:A:795:GLU:OE1	1:A:810:ARG:NH1	2.52	0.42
1:B:548:HIS:NE2	1:B:597:PRO:HD2	2.35	0.42
1:A:506:TRP:CE3	1:A:537:ARG:HD2	2.55	0.41
1:B:320:LEU:HD12	1:B:320:LEU:HA	1.84	0.41
1:B:432:HIS:CD2	1:B:566:THR:HG23	2.55	0.41
1:A:710:LEU:O	1:A:718:LEU:HG	2.21	0.41
1:B:667:LYS:HE2	1:B:667:LYS:HB2	1.79	0.41
1:A:640:GLU:HG3	1:A:680:LEU:HD23	2.03	0.40
1:B:570:LYS:NZ	5:B:1114:HOH:O	2.40	0.40
1:A:676:ARG:NH2	1:A:840:ASP:OD1	2.47	0.40
1:B:333:THR:HG21	1:B:551:PRO:HG3	2.03	0.40
1:A:444:LYS:HZ1	3:A:1009:GOL:H32	1.86	0.40
1:B:366:LEU:HD22	1:B:420:LEU:HD11	2.03	0.40
1:B:607:LEU:HD11	1:B:790:LEU:HB2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1270:HOH:O	5:B:1273:HOH:O[2_556]	2.05	0.15

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	568/640 (89%)	545 (96%)	23 (4%)	0	100	100
1	B	569/640 (89%)	551 (97%)	18 (3%)	0	100	100
All	All	1137/1280 (89%)	1096 (96%)	41 (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	501/554 (90%)	495 (99%)	6 (1%)	71	76
1	B	499/554 (90%)	491 (98%)	8 (2%)	62	67
All	All	1000/1108 (90%)	986 (99%)	14 (1%)	67	72

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	523	ASP
1	A	758	LYS
1	A	845	LEU
1	A	859	GLN
1	A	870	ARG
1	A	900	GLN
1	B	320	LEU
1	B	379	ASP
1	B	501	HIS
1	B	514	LEU
1	B	570	LYS
1	B	758	LYS
1	B	760	LEU
1	B	875	LEU

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

Mol	Chain	Res	Type
1	B	424	HIS
1	B	642	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

26 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	B	1009	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	B	1005	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	A	1006	-	4,4,4	0.13	0	6,6,6	0.06	0
2	SO4	B	1008	-	4,4,4	0.14	0	6,6,6	0.08	0
4	DTT	B	1014	1	7,7,7	0.57	0	4,8,8	0.72	0
2	SO4	A	1004	-	4,4,4	0.13	0	6,6,6	0.06	0
2	SO4	A	1007	-	4,4,4	0.14	0	6,6,6	0.05	0
3	GOL	A	1011	-	5,5,5	0.84	0	5,5,5	1.06	0
3	GOL	A	1010	-	5,5,5	0.79	0	5,5,5	1.06	0
3	GOL	A	1012	-	5,5,5	0.98	0	5,5,5	1.10	0
3	GOL	B	1010	-	5,5,5	1.21	1 (20%)	5,5,5	0.99	0
2	SO4	A	1002	-	4,4,4	0.13	0	6,6,6	0.11	0
2	SO4	A	1001	-	4,4,4	0.14	0	6,6,6	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	B	1004	-	4,4,4	0.15	0	6,6,6	0.11	0
2	SO4	B	1007	-	4,4,4	0.15	0	6,6,6	0.06	0
3	GOL	B	1012	-	5,5,5	0.92	0	5,5,5	0.99	0
2	SO4	A	1005	-	4,4,4	0.14	0	6,6,6	0.08	0
3	GOL	B	1013	-	5,5,5	1.27	1 (20%)	5,5,5	0.68	0
3	GOL	B	1011	-	5,5,5	0.90	0	5,5,5	0.95	0
2	SO4	B	1006	-	4,4,4	0.16	0	6,6,6	0.10	0
2	SO4	A	1003	-	4,4,4	0.14	0	6,6,6	0.10	0
2	SO4	A	1008	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	B	1003	-	4,4,4	0.12	0	6,6,6	0.44	0
2	SO4	B	1001	-	4,4,4	0.14	0	6,6,6	0.12	0
3	GOL	A	1009	-	5,5,5	0.69	0	5,5,5	1.08	0
2	SO4	B	1002	-	4,4,4	0.15	0	6,6,6	0.15	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	1011	-	-	4/4/4/4	-
3	GOL	A	1011	-	-	0/4/4/4	-
3	GOL	A	1010	-	-	4/4/4/4	-
3	GOL	A	1012	-	-	0/4/4/4	-
3	GOL	B	1010	-	-	2/4/4/4	-
3	GOL	A	1009	-	-	0/4/4/4	-
3	GOL	B	1012	-	-	4/4/4/4	-
3	GOL	B	1013	-	-	0/4/4/4	-
4	DTT	B	1014	1	-	7/8/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1010	GOL	O2-C2	-2.55	1.35	1.43
3	B	1013	GOL	O2-C2	-2.48	1.36	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1010	GOL	O1-C1-C2-C3
3	A	1010	GOL	C1-C2-C3-O3
3	B	1011	GOL	O1-C1-C2-C3
3	B	1011	GOL	C1-C2-C3-O3
3	B	1011	GOL	O2-C2-C3-O3
3	B	1012	GOL	O1-C1-C2-C3
3	B	1012	GOL	C1-C2-C3-O3
4	B	1014	DTT	C1-C2-C3-O3
4	B	1014	DTT	C1-C2-C3-C4
4	B	1014	DTT	O2-C2-C3-O3
4	B	1014	DTT	O2-C2-C3-C4
4	B	1014	DTT	C2-C3-C4-S4
4	B	1014	DTT	O3-C3-C4-S4
3	A	1010	GOL	O2-C2-C3-O3
3	B	1011	GOL	O1-C1-C2-O2
3	B	1012	GOL	O2-C2-C3-O3
3	A	1010	GOL	O1-C1-C2-O2
3	B	1010	GOL	O1-C1-C2-O2
3	B	1010	GOL	O1-C1-C2-C3
4	B	1014	DTT	S1-C1-C2-C3
3	B	1012	GOL	O1-C1-C2-O2

There are no ring outliers.

11 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1005	SO4	2	0
4	B	1014	DTT	1	0
3	A	1011	GOL	3	0
3	A	1010	GOL	2	0
3	A	1012	GOL	1	0
3	B	1010	GOL	3	0
2	A	1005	SO4	1	0
3	B	1013	GOL	3	0
2	A	1003	SO4	1	0
2	B	1001	SO4	1	0
3	A	1009	GOL	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	580/640 (90%)	-0.00	29 (5%)	28	28	23, 37, 78, 95	0
1	B	579/640 (90%)	0.18	41 (7%)	16	15	23, 46, 85, 104	0
All	All	1159/1280 (90%)	0.09	70 (6%)	21	20	23, 41, 83, 104	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	830	PRO	5.8
1	A	691	ILE	5.2
1	A	693	THR	4.7
1	A	587	SER	4.6
1	B	576	PRO	4.5
1	A	598	GLY	4.5
1	A	318	LEU	4.1
1	A	690	ASP	4.0
1	B	318	LEU	4.0
1	B	501	HIS	3.9
1	B	578	TYR	3.8
1	A	501	HIS	3.7
1	B	828	THR	3.6
1	A	534	THR	3.6
1	B	476	GLY	3.5
1	B	405	VAL	3.4
1	A	586	THR	3.4
1	B	573	TYR	3.3
1	B	498	ASP	3.3
1	B	319	GLN	3.3
1	A	876	ARG	3.3
1	B	746	GLY	3.2
1	B	534	THR	3.2
1	B	831	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	317	PHE	3.1
1	B	915	SER	3.1
1	B	523	ASP	3.1
1	B	409	LEU	3.1
1	A	524	ARG	3.0
1	B	379	ASP	2.9
1	B	422	LEU	2.9
1	A	588	THR	2.9
1	A	316	ASP	2.9
1	A	597	PRO	2.8
1	B	585	SER	2.8
1	B	832	LEU	2.7
1	B	533	GLU	2.6
1	A	689	GLY	2.6
1	B	743	GLU	2.6
1	B	694	GLY	2.6
1	A	515	ILE	2.6
1	B	574	LYS	2.6
1	B	577	THR	2.6
1	A	695	GLY	2.6
1	A	521	GLN	2.6
1	B	889	PRO	2.5
1	B	597	PRO	2.5
1	A	526	PHE	2.5
1	B	745	GLY	2.5
1	B	499	LEU	2.4
1	B	568	THR	2.4
1	B	890	PRO	2.4
1	A	520	VAL	2.4
1	A	926	MET	2.4
1	B	598	GLY	2.4
1	B	893	ARG	2.4
1	B	876	ARG	2.4
1	A	409	LEU	2.4
1	A	517	LYS	2.3
1	A	673	TRP	2.3
1	A	873	ARG	2.3
1	B	650	GLY	2.3
1	B	580	TYR	2.2
1	B	392	GLU	2.2
1	B	596	LEU	2.2
1	A	531	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	830	PRO	2.1
1	A	925	GLY	2.1
1	B	317	PHE	2.1
1	B	695	GLY	2.1

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^{th} 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	1011	6/6	0.72	0.33	87,94,95,96	0
2	SO4	A	1006	5/5	0.78	0.31	117,119,120,123	0
3	GOL	B	1013	6/6	0.80	0.30	76,79,87,92	0
2	SO4	B	1007	5/5	0.83	0.27	127,128,130,131	0
3	GOL	B	1012	6/6	0.83	0.16	73,80,83,85	0
3	GOL	A	1010	6/6	0.83	0.21	72,73,78,78	0
2	SO4	B	1003	5/5	0.84	0.20	71,71,88,88	0
3	GOL	B	1011	6/6	0.84	0.15	65,67,69,71	0
3	GOL	B	1010	6/6	0.85	0.27	56,70,76,77	0
2	SO4	B	1008	5/5	0.85	0.39	170,172,173,174	0
4	DTT	B	1014	8/8	0.86	0.18	53,114,136,140	0
2	SO4	B	1006	5/5	0.88	0.15	89,91,93,93	0
2	SO4	A	1007	5/5	0.88	0.25	135,135,137,138	0
3	GOL	A	1012	6/6	0.89	0.24	94,99,105,109	0
3	GOL	A	1009	6/6	0.89	0.20	47,53,55,60	0
2	SO4	B	1009	5/5	0.90	0.20	161,161,162,162	0
2	SO4	A	1005	5/5	0.92	0.21	108,109,112,113	0
2	SO4	A	1004	5/5	0.93	0.10	83,84,90,92	0
2	SO4	B	1005	5/5	0.93	0.12	95,96,97,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	1008	5/5	0.93	0.21	123,125,126,129	0
2	SO4	B	1004	5/5	0.94	0.12	83,84,85,88	0
2	SO4	A	1001	5/5	0.95	0.15	60,60,68,69	0
2	SO4	A	1003	5/5	0.96	0.17	65,68,79,81	0
2	SO4	B	1001	5/5	0.98	0.10	54,55,60,61	0
2	SO4	B	1002	5/5	0.98	0.09	56,60,64,66	0
2	SO4	A	1002	5/5	0.98	0.12	59,67,67,72	0

6.5 Other polymers

There are no such residues in this entry.