



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 3, 2017 – 06:00 PM EDT

PDB ID : 5SYT  
Title : Crystal Structure of ZMPSTE24  
Authors : Clark, K.; Jenkins, J.L.; Fedoriw, N.; Dumont, M.E.; Membrane Protein Structural Biology Consortium (MPSBC)  
Deposited on : unknown  
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](mailto: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.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
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) : rb-20029824

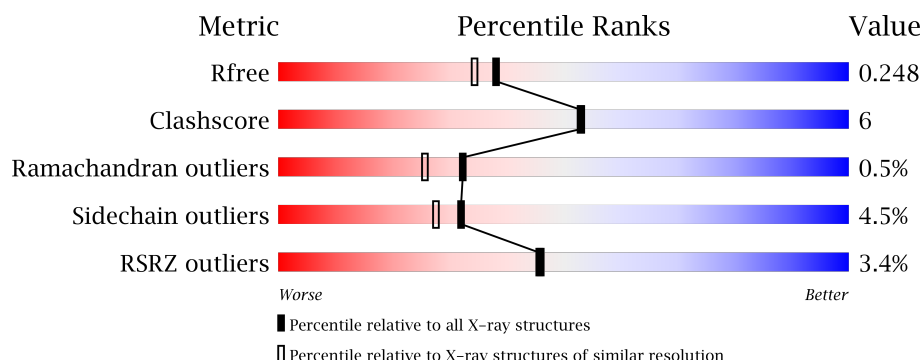
# 1 Overall quality at a glance

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  $\geq 3$ , 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	480	<div> <div>3%</div> <div>79%</div> <div>12%</div> <div>8%</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	501	-	-	-	X
2	SO4	A	502	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	C8E	A	505	-	-	-	X
5	C8E	A	506	-	-	-	X
5	C8E	A	507	-	-	-	X
5	C8E	A	508	-	-	-	X
5	C8E	A	511	-	-	-	X
5	C8E	A	513	-	-	-	X
5	C8E	A	514	-	-	-	X
9	DMS	A	521	-	-	-	X
9	DMS	A	522	-	-	-	X

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 7938 atoms, of which 3932 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.

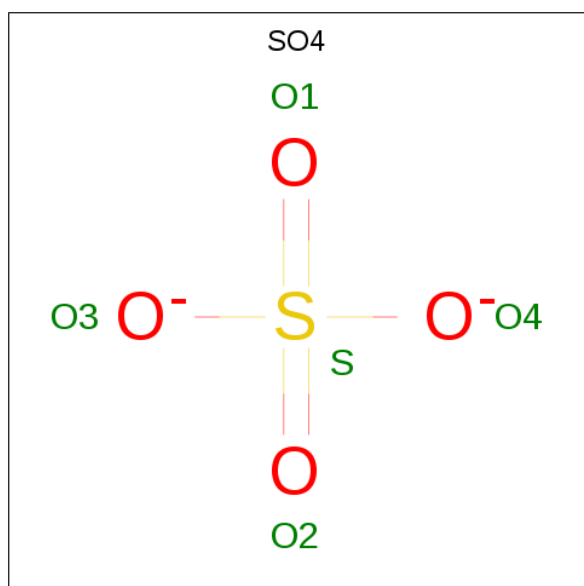
- Molecule 1 is a protein called CAAX prenyl protease 1 homolog.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	444	7123	2380	3554	556	621	12	0	1	0

There are 6 discrepancies between the modelled and reference sequences:

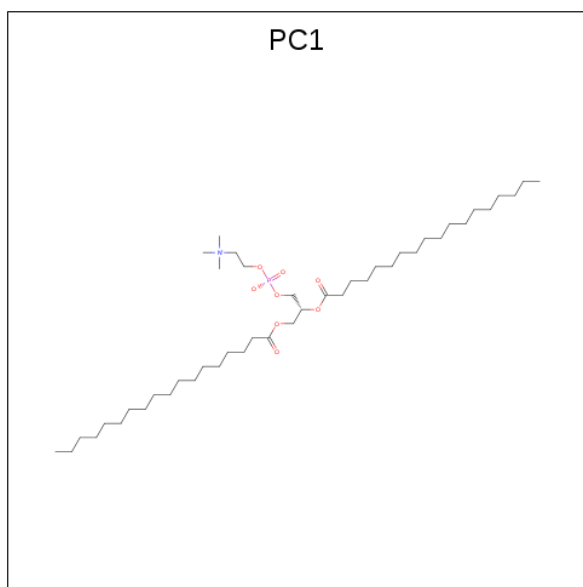
Chain	Residue	Modelled	Actual	Comment	Reference
A	475	SER	-	expression tag	UNP O75844
A	476	GLY	-	expression tag	UNP O75844
A	477	LEU	-	expression tag	UNP O75844
A	478	GLU	-	expression tag	UNP O75844
A	479	VAL	-	expression tag	UNP O75844
A	480	LEU	-	expression tag	UNP O75844

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



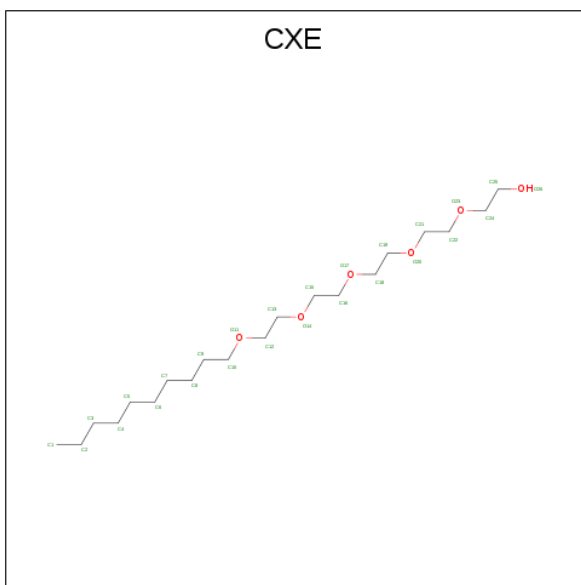
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula:  $C_{44}H_{88}NO_8P$ ).



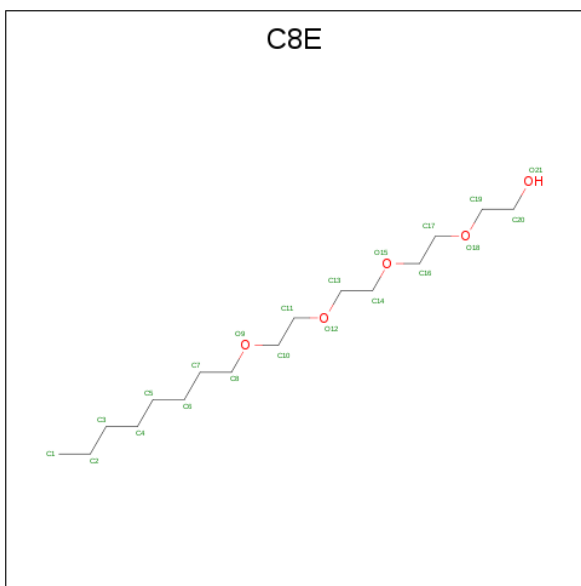
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total	C	H	N	O	P	0	0
			71	21	40	1	8	1		

- Molecule 4 is PENTAETHYLENE GLYCOL MONODECYL ETHER (three-letter code: CXE) (formula:  $C_{20}H_{42}O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			61	18	37	6		

- Molecule 5 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula:  $\text{C}_{16}\text{H}_{34}\text{O}_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 55	C 16	H 34	O 5	0	0
5	A	1	Total 30	C 8	H 17	O 5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			17	7	6	4		
5	A	1	Total	C	H	O	0	0
			55	16	34	5		
5	A	1	Total	C	H	O	0	0
			26	7	15	4		
5	A	1	Total	C	H	O	0	0
			30	8	17	5		
5	A	1	Total	C	H	O	0	0
			39	11	23	5		
5	A	1	Total	C	H	O	0	0
			50	15	31	4		
5	A	1	Total	C	H	O	0	0
			26	7	15	4		
5	A	1	Total	C	H	O	0	0
			29	8	17	4		
5	A	1	Total	C	H	O	0	0
			25	7	14	4		
5	A	1	Total	C	H	O	0	0
			55	16	34	5		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

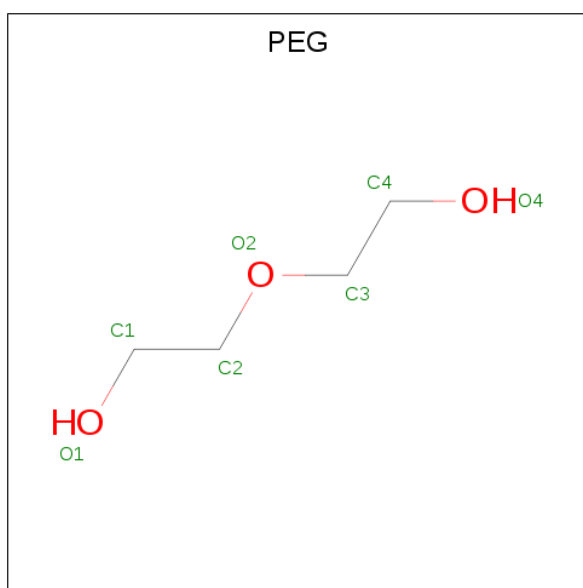
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		

- Molecule 7 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
7	A	1	Total	C	H	O	0	0
			14	3	8	3		
7	A	1	Total	C	H	O	0	0
			14	3	8	3		

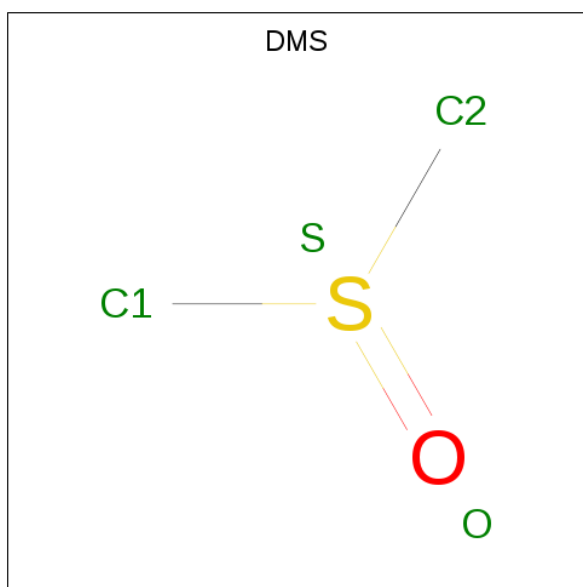
- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 9 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
9	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
9	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

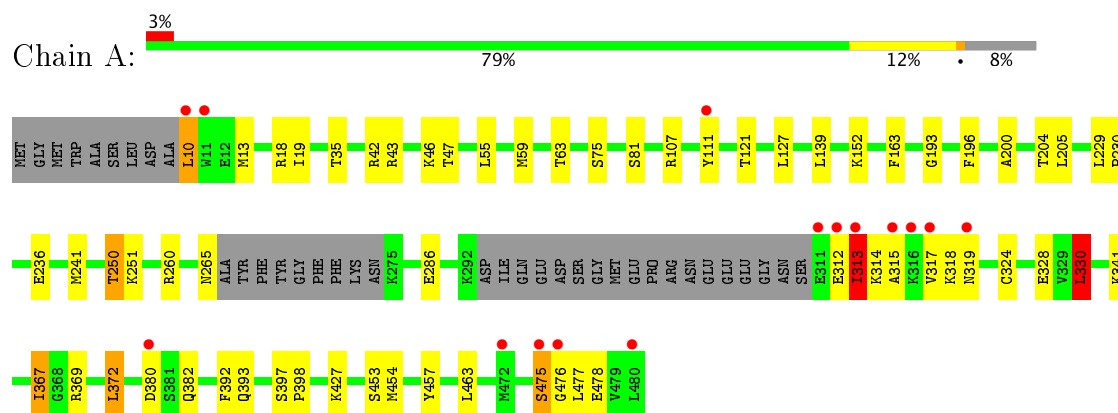
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	158	Total	O	0	2
			160	160		

### 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: CAAX prenyl protease 1 homolog



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.46 Å   84.56 Å   76.89 Å 90.00°   119.07°   90.00°	Depositor
Resolution (Å)	33.60 – 2.00 33.60 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (33.60-2.00) 93.7 (33.60-2.00)	Depositor EDS
$R_{merge}$	0.44	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 2.00 Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.218 , 0.249 0.215 , 0.248	Depositor DCC
$R_{free}$ test set	1870 reflections (3.53%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.3	Xtriage
Anisotropy	0.650	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 62.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.037 for -h-2*k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7938	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, PC1, CXE, DMS, SO4, PEG, C8E

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	0.58	0/3671	0.68	1/4983 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	330	LEU	CA-CB-CG	5.79	128.63	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3569	3554	3549	46	1
2	A	10	0	0	0	0
3	A	31	40	36	4	1
4	A	24	37	35	2	0
5	A	180	257	252	6	0
6	A	1	0	0	0	0
7	A	12	16	16	4	0
8	A	7	10	10	0	0
9	A	12	18	18	0	0
10	A	160	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4006	3932	3916	48	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 6.

All (48) 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:475:SER:OG	1:A:476:GLY:N	2.13	0.81
1:A:265:ASN:ND2	10:A:602:HOH:O	2.20	0.73
1:A:314:LYS:HA	1:A:315:ALA:HB3	1.74	0.68
1:A:43:ARG:NH2	3:A:503:PC1:O12	2.29	0.65
1:A:397:SER:HB2	1:A:398:PRO:HD3	1.84	0.60
1:A:369:ARG:HB2	1:A:372:LEU:HD22	1.82	0.60
1:A:367:ILE:HD12	7:A:518:GOL:H11	1.88	0.54
1:A:13:MET:O	1:A:18:ARG:NH1	2.38	0.54
1:A:19:ILE:HD13	1:A:372:LEU:HD12	1.90	0.54
1:A:241:MET:HE2	1:A:427:LYS:HE3	1.90	0.53
1:A:393:GLN:OE1	4:A:504:CXE:H252	2.09	0.53
1:A:369:ARG:HD2	7:A:519:GOL:H32	1.89	0.53
1:A:454:MET:HE2	10:A:738:HOH:O	2.09	0.52
1:A:369:ARG:CD	7:A:519:GOL:H32	2.40	0.52
1:A:382:GLN:OE1	10:A:601:HOH:O	2.18	0.51
1:A:397:SER:CB	1:A:398:PRO:HD3	2.42	0.49
1:A:250:THR:HG22	1:A:251:LYS:N	2.26	0.49
1:A:312:GLU:O	1:A:313:ILE:HG23	2.13	0.49
1:A:152:LYS:HZ2	5:A:516:C8E:C17	2.25	0.49
1:A:46:LYS:HA	10:A:611:HOH:O	2.14	0.48
1:A:250:THR:HG22	1:A:251:LYS:H	1.77	0.48
1:A:229:LEU:HD12	1:A:230:PRO:HD2	1.95	0.48
1:A:250:THR:CG2	1:A:251:LYS:N	2.76	0.48
1:A:241:MET:HE3	1:A:330:LEU:HD12	1.96	0.47
1:A:286:GLU:H	1:A:286:GLU:CD	2.18	0.47
1:A:193:GLY:N	1:A:196:PHE:HB3	2.30	0.47
1:A:35:THR:HG22	3:A:503:PC1:H232	1.97	0.46
1:A:478:GLU:HG3	1:A:478:GLU:O	2.15	0.46
1:A:260:ARG:HH11	5:A:511:C8E:H72	1.81	0.46
1:A:200:ALA:O	1:A:204:THR:HG23	2.17	0.45
1:A:43:ARG:NH2	3:A:503:PC1:H142	2.31	0.45
5:A:510:C8E:H201	10:A:616:HOH:O	2.16	0.45
1:A:10:LEU:HD22	1:A:10:LEU:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:MET:HE3	1:A:63:THR:HG22	1.98	0.45
1:A:55:LEU:CD2	1:A:463:LEU:HD21	2.47	0.45
1:A:393:GLN:NE2	10:A:607:HOH:O	2.29	0.45
1:A:317:VAL:C	1:A:319:ASN:H	2.21	0.44
1:A:324:CYS:HB3	1:A:328:GLU:HB2	1.98	0.44
1:A:42:ARG:HD2	1:A:75:SER:OG	2.20	0.42
1:A:392:PHE:HE2	4:A:504:CXE:H191	1.85	0.42
1:A:453:SER:HB2	1:A:457:TYR:CD2	2.54	0.42
5:A:510:C8E:C20	10:A:616:HOH:O	2.68	0.41
1:A:314:LYS:CA	1:A:315:ALA:HB3	2.48	0.41
1:A:43:ARG:NH2	3:A:503:PC1:H112	2.36	0.41
1:A:163:PHE:CD2	5:A:511:C8E:H101	2.56	0.40
1:A:367:ILE:CD1	7:A:518:GOL:H11	2.49	0.40
1:A:205:LEU:HD23	1:A:205:LEU:C	2.42	0.40
1:A:397:SER:OG	5:A:510:C8E:H192	2.22	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)
1:A:121:THR:OG1	3:A:503:PC1:O14[4_346]	1.97	0.23

## 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	439/480 (92%)	422 (96%)	15 (3%)	2 (0%)	32 26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	313	ILE

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Mol	Chain	Res	Type
1	A	318	LYS

### 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	378/424 (89%)	361 (96%)	17 (4%)	32	27

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	47	THR
1	A	81	SER
1	A	107	ARG
1	A	111	TYR
1	A	127	LEU
1	A	139	LEU
1	A	236	GLU
1	A	250	THR
1	A	313	ILE
1	A	330	LEU
1	A	341	LYS
1	A	367	ILE
1	A	372	LEU
1	A	380	ASP
1	A	475	SER
1	A	477	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 1 is monoatomic - leaving 22 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	501	-	4,4,4	0.24	0	6,6,6	0.39	0
2	SO4	A	502	-	4,4,4	0.26	0	6,6,6	0.37	0
3	PC1	A	503	-	30,30,53	1.25	2 (6%)	35,38,61	1.57	5 (14%)
4	CXE	A	504	-	23,23,25	0.51	0	22,22,24	0.52	0
5	C8E	A	505	-	20,20,20	0.46	0	19,19,19	0.44	0
5	C8E	A	506	-	12,12,20	0.47	0	11,11,19	0.49	0
5	C8E	A	507	-	10,10,20	0.41	0	9,9,19	0.34	0
5	C8E	A	508	-	20,20,20	0.44	0	19,19,19	0.49	0
5	C8E	A	509	-	10,10,20	0.38	0	9,9,19	0.46	0
5	C8E	A	510	-	12,12,20	0.52	0	11,11,19	0.49	0
5	C8E	A	511	-	15,15,20	0.59	0	14,14,19	0.57	0
5	C8E	A	512	-	18,18,20	0.33	0	17,17,19	0.70	0
5	C8E	A	513	-	10,10,20	0.45	0	9,9,19	0.39	0
5	C8E	A	514	-	11,11,20	0.48	0	10,10,19	0.58	0
5	C8E	A	515	-	10,10,20	0.47	0	9,9,19	0.31	0
5	C8E	A	516	-	20,20,20	0.36	0	19,19,19	0.83	1 (5%)
7	GOL	A	518	-	5,5,5	0.36	0	5,5,5	0.85	0
7	GOL	A	519	-	5,5,5	0.43	0	5,5,5	0.48	0
8	PEG	A	520	-	6,6,6	0.58	0	5,5,5	0.79	0
9	DMS	A	521	-	3,3,3	0.60	0	3,3,3	0.67	0
9	DMS	A	522	-	3,3,3	0.74	0	3,3,3	0.95	0
9	DMS	A	523	-	3,3,3	0.67	0	3,3,3	1.00	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	SO4	A	501	-	-	0/0/0/0	0/0/0/0
2	SO4	A	502	-	-	0/0/0/0	0/0/0/0
3	PC1	A	503	-	-	0/34/34/57	0/0/0/0
4	CXE	A	504	-	-	0/21/21/23	0/0/0/0
5	C8E	A	505	-	-	0/18/18/18	0/0/0/0
5	C8E	A	506	-	-	0/10/10/18	0/0/0/0
5	C8E	A	507	-	-	0/8/8/18	0/0/0/0
5	C8E	A	508	-	-	0/18/18/18	0/0/0/0
5	C8E	A	509	-	-	0/8/8/18	0/0/0/0
5	C8E	A	510	-	-	0/10/10/18	0/0/0/0
5	C8E	A	511	-	-	0/13/13/18	0/0/0/0
5	C8E	A	512	-	-	0/16/16/18	0/0/0/0
5	C8E	A	513	-	-	0/8/8/18	0/0/0/0
5	C8E	A	514	-	-	0/9/9/18	0/0/0/0
5	C8E	A	515	-	-	0/8/8/18	0/0/0/0
5	C8E	A	516	-	-	0/18/18/18	0/0/0/0
7	GOL	A	518	-	-	0/4/4/4	0/0/0/0
7	GOL	A	519	-	-	0/4/4/4	0/0/0/0
8	PEG	A	520	-	-	0/4/4/4	0/0/0/0
9	DMS	A	521	-	-	0/0/0/0	0/0/0/0
9	DMS	A	522	-	-	0/0/0/0	0/0/0/0
9	DMS	A	523	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	PC1	O21-C21	3.10	1.43	1.34
3	A	503	PC1	O31-C31	3.40	1.43	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	PC1	C23-C22-C21	-3.37	101.28	113.58
3	A	503	PC1	C15-N-C14	-2.10	103.66	108.98
3	A	503	PC1	C15-N-C13	2.20	114.55	108.98
5	A	516	C8E	O12-C11-C10	2.27	120.82	110.41
3	A	503	PC1	O31-C31-C32	3.71	121.31	111.35
3	A	503	PC1	O21-C21-C22	4.64	121.19	111.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	PC1	4	1
4	A	504	CXE	2	0
5	A	510	C8E	3	0
5	A	511	C8E	2	0
5	A	516	C8E	1	0
7	A	518	GOL	2	0
7	A	519	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	444/480 (92%)	0.05	15 (3%)	46 46	19, 32, 68, 96	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	11	TRP	4.9
1	A	319	ASN	4.4
1	A	317	VAL	4.4
1	A	475	SER	4.0
1	A	480	LEU	3.9
1	A	315	ALA	3.9
1	A	313	ILE	3.4
1	A	476	GLY	3.3
1	A	380	ASP	3.0
1	A	472	MET	2.9
1	A	312	GLU	2.6
1	A	10	LEU	2.5
1	A	316	LYS	2.4
1	A	111	TYR	2.4
1	A	311	GLU	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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	A	501	5/5	0.92	0.30	20.36	62,73,88,92	0
5	C8E	A	511	16/21	0.76	0.33	14.49	28,55,69,79	0
2	SO4	A	502	5/5	0.92	0.24	10.12	47,58,71,83	0
5	C8E	A	507	11/21	0.89	0.17	8.54	41,49,53,62	0
5	C8E	A	514	12/21	0.77	0.22	4.47	44,69,83,85	0
5	C8E	A	513	11/21	0.89	0.21	4.18	43,58,76,79	0
9	DMS	A	521	4/4	0.94	0.25	4.10	46,56,92,92	0
9	DMS	A	522	4/4	0.82	0.20	3.45	32,40,53,82	0
5	C8E	A	506	13/21	0.80	0.16	2.85	41,57,66,69	0
5	C8E	A	505	21/21	0.82	0.15	2.16	32,56,84,84	0
5	C8E	A	508	21/21	0.83	0.18	2.03	42,56,70,72	0
4	CXE	A	504	24/26	0.83	0.15	1.45	33,54,70,85	0
3	PC1	A	503	31/54	0.81	0.18	1.29	30,55,74,78	0
5	C8E	A	516	21/21	0.87	0.12	1.05	30,41,55,63	0
8	PEG	A	520	7/7	0.83	0.17	0.98	46,55,65,67	0
5	C8E	A	510	13/21	0.87	0.14	0.58	34,44,54,56	0
5	C8E	A	509	11/21	0.86	0.14	0.58	36,54,71,74	0
5	C8E	A	515	11/21	0.88	0.12	0.37	41,53,74,80	0
6	ZN	A	517	1/1	0.99	0.11	0.12	30,30,30,30	0
7	GOL	A	518	6/6	0.87	0.14	0.11	35,42,48,50	0
5	C8E	A	512	19/21	0.89	0.11	-0.64	31,44,67,68	0
7	GOL	A	519	6/6	0.77	0.24	-	68,90,105,117	0
9	DMS	A	523	4/4	0.89	0.14	-	47,61,96,96	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.