



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:27 am BST

PDB ID : 2Q7W  
Title : Structural Studies Reveals the Inactivation of E. coli L-aspartate aminotransferase (S)-4,5-amino-dihydro-2-thiophenecarboxylic acid (SADTA) via two mechanisms at pH 6.0  
Authors : Liu, D.; Pozharski, E.; Lepore, B.; Fu, M.; Silverman, R.B.; Petsko, G.A.; Ringe, D.  
Deposited on : 2007-06-07  
Resolution : 1.40 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

The 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  
buster-report : 1.1.7 (2018)  
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

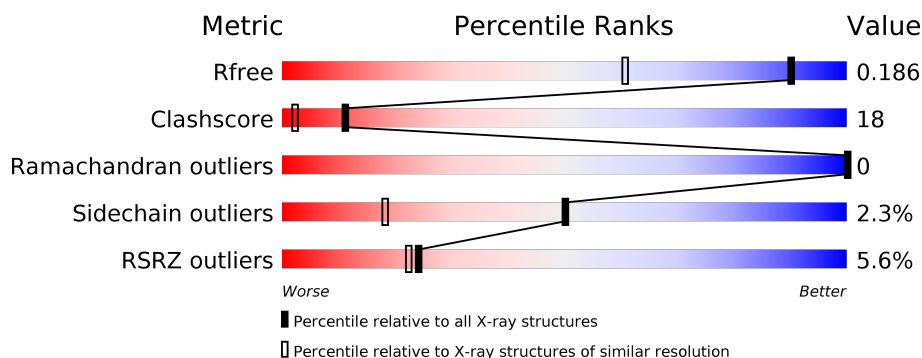
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.40 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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 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	396	<div> <div>5%</div> <div>79%</div> <div>15%</div> <div>..</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
5	GOL	A	801	-	-	X	-
5	GOL	A	804	-	-	X	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	A	805	-	-	X	-
5	GOL	A	806	-	-	X	-
5	GOL	A	807	-	-	X	-
5	GOL	A	809	-	-	X	-
5	GOL	A	810	-	-	X	-
5	GOL	A	811	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3808 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.

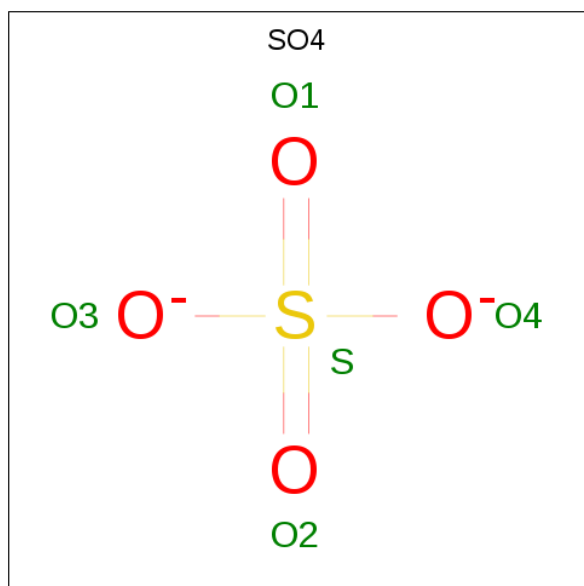
- Molecule 1 is a protein called Aspartate aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	379	3263	2089	556	600	18	0	56	0

There is a discrepancy between the modelled and reference sequences:

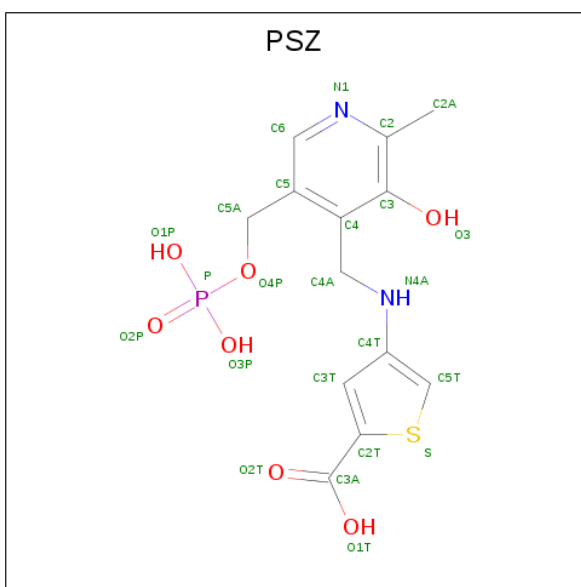
Chain	Residue	Modelled	Actual	Comment	Reference
A	246	KST	LYS	MODIFIED RESIDUE	UNP P00509

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



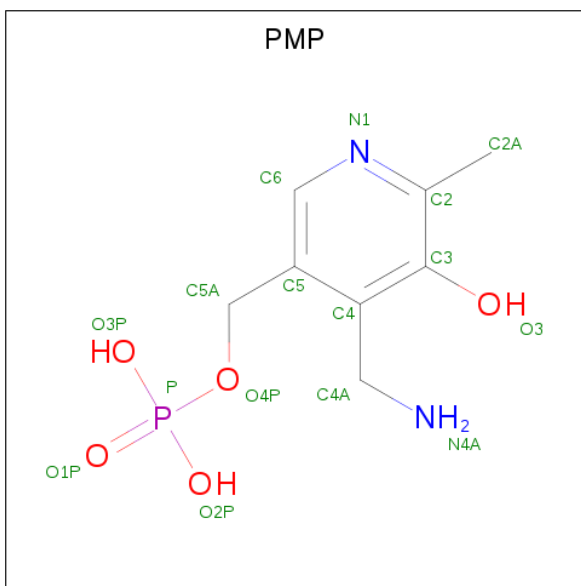
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

- Molecule 3 is 4-[(3-HYDROXY-2-METHYL-5-[(PHOSPHONOOXY)METHYL]PYRIDIN-4-YL)METHYL)AMINO]THIOPHENE-2-CARBOXYLIC ACID (three-letter code: PSZ) (formula: C<sub>13</sub>H<sub>15</sub>N<sub>2</sub>O<sub>7</sub>PS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			24	13	2	7	1		

- Molecule 4 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula:  $C_8H_{13}N_2O_5P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	1
			16	8	2	5	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	1
			12	6	6		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

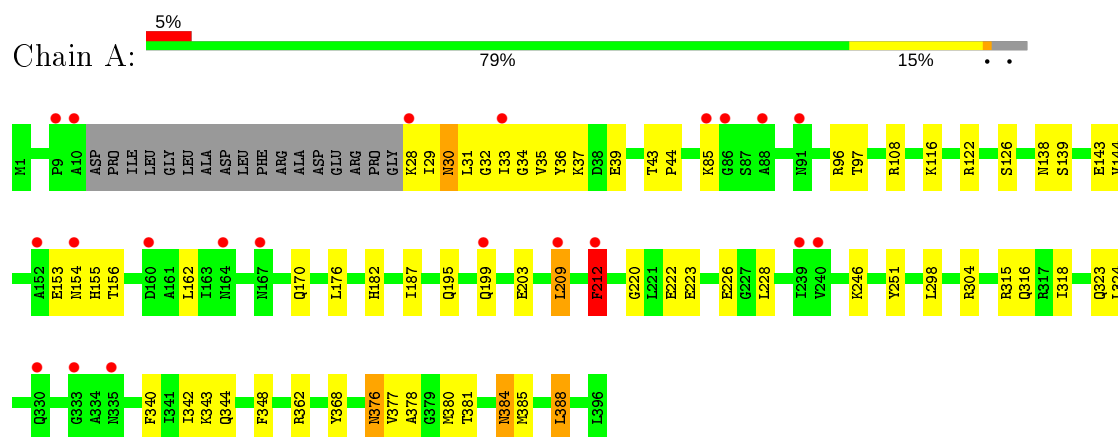
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	428	Total	O	0	0
			428	428		

### 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: Aspartate aminotransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.62Å 85.14Å 78.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.92 – 1.40 28.92 – 1.40	Depositor EDS
% Data completeness (in resolution range)	96.4 (76.92-1.40) 96.4 (28.92-1.40)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.72 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.154 , 0.188 0.152 , 0.186	Depositor DCC
$R_{free}$ test set	4903 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.1	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 67.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.019 for -1/2*h+3/2*k,1/2*h+1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3808	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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: PSZ, KST, PMP, 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	0.80	2/3459 (0.1%)	0.83	2/4668 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	30[A]	ASN	CB-CG	5.25	1.63	1.51
1	A	30[B]	ASN	CB-CG	5.25	1.63	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212[A]	PHE	CB-CG-CD1	-5.34	117.06	120.80
1	A	212[B]	PHE	CB-CG-CD1	-5.34	117.06	120.80

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	3263	0	3379	121	0
2	A	5	0	0	1	0
3	A	24	0	11	0	0
4	A	16	0	10	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	72	0	92	67	1
6	A	428	0	0	15	2
All	All	3808	0	3492	123	2

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 18.

All (123) 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:35[B]:VAL:CG2	5:A:811:GOL:H12	1.48	1.41
1:A:33[B]:ILE:HD11	5:A:810:GOL:C3	1.60	1.29
1:A:37:LYS:HE3	5:A:811:GOL:O1	1.40	1.20
1:A:315[C]:ARG:NH2	5:A:807:GOL:O3	1.79	1.14
1:A:35[B]:VAL:HG22	5:A:811:GOL:C1	1.82	1.10
1:A:144:VAL:N	5:A:801:GOL:O1	1.85	1.09
1:A:226[B]:GLU:OE2	6:A:1158:HOH:O	1.71	1.08
1:A:33[B]:ILE:CD1	5:A:810:GOL:H32	1.81	1.07
1:A:222:GLU:HB2	5:A:809:GOL:H32	1.36	1.06
1:A:122[A]:ARG:NH2	2:A:500:SO4:O1	1.92	1.01
1:A:187:ILE:HG12	5:A:806:GOL:H31	1.41	1.01
1:A:35[A]:VAL:HG22	5:A:811:GOL:H12	1.44	0.98
1:A:35[B]:VAL:CG2	5:A:811:GOL:C1	2.40	0.95
1:A:220:GLY:HA2	5:A:802[B]:GOL:H12	1.47	0.95
1:A:315[C]:ARG:HH21	5:A:807:GOL:C3	1.79	0.95
1:A:138:ASN:HD21	5:A:801:GOL:H11	1.30	0.94
1:A:362[B]:ARG:HD3	1:A:368:TYR:CE2	2.03	0.93
1:A:44[B]:PRO:HD2	5:A:804:GOL:O3	1.67	0.92
1:A:37:LYS:HE3	5:A:811:GOL:HO1	1.36	0.89
1:A:33[B]:ILE:HD11	5:A:810:GOL:H32	0.90	0.87
1:A:97:THR:H	5:A:805:GOL:H12	1.38	0.87
1:A:35[B]:VAL:HG22	5:A:811:GOL:H12	0.87	0.86
1:A:344:GLN:HG2	5:A:806:GOL:H32	1.55	0.86
1:A:35[B]:VAL:HG21	5:A:811:GOL:H12	1.58	0.86
1:A:34[B]:GLY:CA	1:A:348:PHE:HZ	1.88	0.85
1:A:34[B]:GLY:HA3	1:A:348:PHE:HZ	1.43	0.83
1:A:34[B]:GLY:CA	1:A:348:PHE:CZ	2.61	0.83
1:A:199[B]:GLN:OE1	1:A:203[B]:GLU:OE1	1.98	0.82
1:A:33[B]:ILE:CD1	5:A:810:GOL:C3	2.52	0.81
1:A:343:LYS:HE2	5:A:806:GOL:O3	1.81	0.80
1:A:33[A]:ILE:HB	5:A:811:GOL:H11	1.63	0.80

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:THR:H	5:A:805:GOL:C1	1.95	0.78
1:A:96:ARG:HA	5:A:805:GOL:H11	1.65	0.78
1:A:34[B]:GLY:HA3	1:A:348:PHE:CZ	2.18	0.78
1:A:343:LYS:CE	5:A:806:GOL:O3	2.35	0.75
1:A:344:GLN:CG	5:A:806:GOL:H32	2.17	0.74
1:A:36:TYR:HD1	5:A:804:GOL:H31	1.51	0.74
1:A:343:LYS:HG3	5:A:806:GOL:H2	1.69	0.74
1:A:376[A]:ASN:HD21	1:A:378:ALA:HB3	1.54	0.71
1:A:155[A]:HIS:HD2	6:A:1072:HOH:O	1.72	0.71
5:A:801:GOL:O3	5:A:808:GOL:H12	1.91	0.71
1:A:222:GLU:H	5:A:809:GOL:C1	2.05	0.69
1:A:153[A]:GLU:HG2	6:A:1123:HOH:O	1.92	0.68
1:A:384:ASN:C	1:A:384:ASN:HD22	1.95	0.68
1:A:33[A]:ILE:CB	5:A:811:GOL:H11	2.26	0.66
1:A:220:GLY:HA2	5:A:802[B]:GOL:C1	2.24	0.65
1:A:44[B]:PRO:CD	5:A:804:GOL:O3	2.44	0.65
1:A:222:GLU:HB2	5:A:809:GOL:C3	2.23	0.64
1:A:315[C]:ARG:HH21	5:A:807:GOL:H31	1.61	0.64
1:A:153[A]:GLU:CD	6:A:1123:HOH:O	2.36	0.64
1:A:33[A]:ILE:CG2	5:A:811:GOL:H11	2.29	0.63
1:A:187:ILE:HG12	5:A:806:GOL:C3	2.25	0.63
1:A:376[A]:ASN:HD22	1:A:378:ALA:H	1.47	0.63
1:A:138:ASN:ND2	5:A:801:GOL:H11	2.10	0.63
1:A:30[A]:ASN:OD1	1:A:33[A]:ILE:N	2.33	0.62
1:A:155[A]:HIS:CD2	6:A:1072:HOH:O	2.51	0.61
1:A:220:GLY:CA	5:A:802[B]:GOL:H12	2.28	0.61
1:A:381:THR:H	1:A:384:ASN:ND2	1.98	0.61
1:A:28:LYS:N	6:A:1197:HOH:O	2.33	0.61
1:A:32[B]:GLY:C	6:A:1162:HOH:O	2.39	0.60
1:A:33[A]:ILE:HB	5:A:811:GOL:C1	2.29	0.60
1:A:37:LYS:CE	5:A:811:GOL:O1	2.33	0.60
1:A:298:LEU:O	1:A:304[B]:ARG:HD3	2.02	0.60
1:A:39:GLU:HB2	6:A:1209:HOH:O	2.02	0.60
1:A:222:GLU:H	5:A:809:GOL:H11	1.66	0.59
1:A:176:LEU:HD12	1:A:209[A]:LEU:HD13	1.85	0.59
1:A:35[B]:VAL:HG21	5:A:811:GOL:H2	1.84	0.58
1:A:376[A]:ASN:HD22	1:A:378:ALA:N	2.01	0.58
1:A:34[B]:GLY:HA2	1:A:348:PHE:CZ	2.40	0.57
1:A:138:ASN:HD21	5:A:801:GOL:C1	2.12	0.57
1:A:222:GLU:CB	5:A:809:GOL:H32	2.25	0.57
1:A:376[A]:ASN:ND2	1:A:378:ALA:H	2.02	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35[B]:VAL:HG21	5:A:811:GOL:C1	2.25	0.56
1:A:153[A]:GLU:CG	6:A:1123:HOH:O	2.50	0.56
1:A:222:GLU:H	5:A:809:GOL:H12	1.71	0.56
1:A:381:THR:H	1:A:384:ASN:HD21	1.55	0.55
1:A:226[B]:GLU:HG2	6:A:947:HOH:O	2.07	0.54
1:A:34[B]:GLY:O	1:A:246[B]:KST:N1	2.40	0.54
1:A:343:LYS:HE3	5:A:806:GOL:O3	2.07	0.53
1:A:315[C]:ARG:NH2	5:A:807:GOL:HO3	2.02	0.52
1:A:212[B]:PHE:HE1	1:A:228:LEU:HB2	1.76	0.51
1:A:340:PHE:O	1:A:343:LYS:HG2	2.11	0.51
1:A:36:TYR:CD1	5:A:804:GOL:H31	2.40	0.50
1:A:43:THR:HG23	5:A:804:GOL:H32	1.94	0.50
1:A:35[B]:VAL:HG21	5:A:811:GOL:C2	2.42	0.50
1:A:376[A]:ASN:ND2	1:A:378:ALA:N	2.60	0.49
1:A:384:ASN:C	1:A:384:ASN:ND2	2.65	0.49
1:A:222:GLU:HG2	5:A:809:GOL:H11	1.95	0.49
1:A:223:GLU:HG3	5:A:809:GOL:C3	2.44	0.48
1:A:36:TYR:HB3	5:A:804:GOL:H11	1.94	0.48
1:A:31:LEU:HD11	1:A:388[A]:LEU:HD21	1.96	0.47
1:A:33[B]:ILE:HG13	6:A:987:HOH:O	2.14	0.47
1:A:316:GLN:HG2	5:A:807:GOL:H31	1.97	0.47
1:A:122[A]:ARG:NH1	1:A:170:GLN:NE2	2.62	0.47
1:A:162:LEU:C	1:A:162:LEU:HD23	2.34	0.47
1:A:35[A]:VAL:HB	1:A:251:TYR:CZ	2.50	0.47
1:A:126:SER:OG	1:A:182:HIS:HE1	1.97	0.47
1:A:384:ASN:HD22	1:A:385:MET:N	2.13	0.46
1:A:33[A]:ILE:HG22	5:A:811:GOL:H11	1.98	0.46
1:A:304[A]:ARG:NH2	6:A:932:HOH:O	2.44	0.46
1:A:143[A]:GLU:HA	5:A:801:GOL:O1	2.16	0.45
1:A:33[B]:ILE:HG21	5:A:811:GOL:H32	1.99	0.45
1:A:323:GLN:HA	1:A:342[A]:ILE:CD1	2.46	0.45
1:A:37:LYS:CE	5:A:811:GOL:HO1	2.18	0.45
1:A:154:ASN:O	1:A:156[B]:THR:HG23	2.17	0.44
1:A:195:GLN:NE2	6:A:940:HOH:O	2.51	0.43
1:A:212[B]:PHE:CE1	1:A:228:LEU:HB2	2.51	0.43
1:A:380:MET:HG2	1:A:388[B]:LEU:HD11	2.00	0.43
1:A:28:LYS:C	1:A:29:ILE:HG13	2.39	0.43
1:A:85[B]:LYS:HG2	6:A:1140:HOH:O	2.18	0.43
1:A:212[B]:PHE:CE1	1:A:228:LEU:HD22	2.54	0.43
1:A:85[B]:LYS:NZ	1:A:85[B]:LYS:HB2	2.34	0.42
1:A:108[A]:ARG:CZ	1:A:139[A]:SER:OG	2.68	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:LYS:HG3	5:A:806:GOL:C2	2.45	0.42
1:A:143[B]:GLU:HA	5:A:801:GOL:O1	2.20	0.41
1:A:362[B]:ARG:HD3	1:A:368:TYR:CD2	2.51	0.41
1:A:223:GLU:HG3	5:A:809:GOL:H31	2.02	0.41
1:A:318:ILE:HG23	1:A:377[B]:VAL:CG2	2.51	0.41
1:A:97:THR:H	5:A:805:GOL:H11	1.83	0.41
5:A:811:GOL:H32	6:A:1173:HOH:O	2.19	0.40

All (2) 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:A:811:GOL:O3	6:A:1042:HOH:O[4_555]	1.42	0.78
6:A:873:HOH:O	6:A:1036:HOH:O[4_555]	2.06	0.14

## 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	430/396 (109%)	421 (98%)	9 (2%)	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	362/319 (114%)	350 (97%)	12 (3%)	38 9

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	LYS
1	A	209[A]	LEU
1	A	209[B]	LEU
1	A	212[A]	PHE
1	A	212[B]	PHE
1	A	324[A]	LEU
1	A	324[B]	LEU
1	A	376[A]	ASN
1	A	376[B]	ASN
1	A	384	ASN
1	A	388[A]	LEU
1	A	388[B]	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	91	ASN
1	A	170	GLN
1	A	182	HIS
1	A	195	GLN
1	A	235	HIS
1	A	344	GLN
1	A	384	ASN

### 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	KST	A	246[A]	-	12,17,18	1.41	3 (25%)	4,21,23	1.07	0
1	KST	A	246[B]	-	12,8,18	8.05	3 (25%)	4,8,23	10.41	1 (25%)

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	KST	A	246[A]	-	-	1/7/14/16	0/1/1/1
1	KST	A	246[B]	-	-	2/7/7/16	0/1/0/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	246[B]	KST	C5-N1	27.60	2.19	1.38
1	A	246[A]	KST	C5-N1	2.80	1.46	1.38
1	A	246[A]	KST	C6-S	2.12	1.74	1.70
1	A	246[B]	KST	C6-S	2.12	1.74	1.70
1	A	246[A]	KST	C8-S	2.12	1.74	1.72
1	A	246[B]	KST	C8-S	2.12	1.74	1.72

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246[B]	KST	C4-N1-C5	-20.73	77.11	122.94

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	246[A]	KST	C2-C1-CA-C
1	A	246[B]	KST	CA-C1-C2-C3
1	A	246[B]	KST	C2-C1-CA-C

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	246[B]	KST	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

15 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	A	500	-	4,4,4	0.28	0	6,6,6	0.15	0
3	PSZ	A	600[B]	-	21,25,25	2.67	4 (19%)	22,36,36	1.63	2 (9%)
5	GOL	A	807	-	5,5,5	0.28	0	5,5,5	0.62	0
5	GOL	A	808	-	5,5,5	0.39	0	5,5,5	0.15	0
5	GOL	A	811	-	5,5,5	0.73	0	5,5,5	1.06	0
5	GOL	A	806	-	5,5,5	0.74	0	5,5,5	1.58	1 (20%)
5	GOL	A	801	-	5,5,5	0.96	0	5,5,5	0.73	0
4	PMP	A	700[A]	-	16,16,16	2.08	3 (18%)	21,23,23	1.29	2 (9%)
5	GOL	A	805	-	5,5,5	0.57	0	5,5,5	0.81	0
5	GOL	A	802[A]	-	5,5,5	0.21	0	5,5,5	0.84	0
5	GOL	A	809	-	5,5,5	0.48	0	5,5,5	0.69	0
5	GOL	A	810	-	5,5,5	0.85	0	5,5,5	1.44	1 (20%)
5	GOL	A	802[B]	-	5,5,5	0.65	0	5,5,5	0.60	0
5	GOL	A	803	-	5,5,5	0.29	0	5,5,5	0.49	0
5	GOL	A	804	-	5,5,5	1.24	1 (20%)	5,5,5	3.81	2 (40%)

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	PSZ	A	600[B]	-	-	5/9/15/15	0/2/2/2
5	GOL	A	802[A]	-	-	0/4/4/4	-
5	GOL	A	807	-	-	2/4/4/4	-
5	GOL	A	808	-	-	1/4/4/4	-
5	GOL	A	811	-	-	4/4/4/4	-
5	GOL	A	806	-	-	2/4/4/4	-
5	GOL	A	801	-	-	2/4/4/4	-
4	PMP	A	700[A]	-	-	1/8/8/8	0/1/1/1
5	GOL	A	805	-	-	2/4/4/4	-
5	GOL	A	810	-	-	4/4/4/4	-
5	GOL	A	809	-	-	1/4/4/4	-
5	GOL	A	802[B]	-	-	4/4/4/4	-
5	GOL	A	803	-	-	3/4/4/4	-
5	GOL	A	804	-	-	2/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600[B]	PSZ	C3-C2	7.99	1.48	1.40
4	A	700[A]	PMP	C3-C2	-6.50	1.34	1.40
3	A	600[B]	PSZ	C5-C4	5.85	1.48	1.40
3	A	600[B]	PSZ	C3-C4	5.47	1.48	1.40
4	A	700[A]	PMP	P-O2P	-2.84	1.43	1.54
4	A	700[A]	PMP	P-O3P	-2.84	1.43	1.54
3	A	600[B]	PSZ	C4T-N4A	2.50	1.46	1.38
5	A	804	GOL	O3-C3	-2.13	1.33	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	804	GOL	C3-C2-C1	-7.58	82.22	111.70
3	A	600[B]	PSZ	C4A-N4A-C4T	-4.92	109.49	122.15
5	A	810	GOL	O2-C2-C3	-2.71	97.17	109.12
5	A	804	GOL	O1-C1-C2	2.71	123.19	110.20
4	A	700[A]	PMP	C3-C4-C5	2.63	121.25	118.72
5	A	806	GOL	O1-C1-C2	2.57	122.53	110.20
4	A	700[A]	PMP	O4P-C5A-C5	2.35	113.83	109.35
3	A	600[B]	PSZ	C6-N1-C2	2.27	123.37	119.17

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	600[B]	PSZ	C5A-O4P-P-O3P
3	A	600[B]	PSZ	C5A-O4P-P-O1P
5	A	807	GOL	O1-C1-C2-C3
5	A	811	GOL	O1-C1-C2-C3
5	A	806	GOL	O1-C1-C2-C3
4	A	700[A]	PMP	C5A-O4P-P-O2P
5	A	810	GOL	O1-C1-C2-C3
5	A	810	GOL	C1-C2-C3-O3
5	A	804	GOL	O1-C1-C2-O2
5	A	804	GOL	O1-C1-C2-C3
5	A	802[B]	GOL	O2-C2-C3-O3
5	A	803	GOL	O2-C2-C3-O3
3	A	600[B]	PSZ	C4-C4A-N4A-C4T
5	A	811	GOL	C1-C2-C3-O3
5	A	801	GOL	C1-C2-C3-O3
5	A	805	GOL	O1-C1-C2-C3
5	A	802[B]	GOL	C1-C2-C3-O3
5	A	803	GOL	C1-C2-C3-O3
5	A	807	GOL	O1-C1-C2-O2
5	A	811	GOL	O2-C2-C3-O3
5	A	806	GOL	O1-C1-C2-O2
5	A	810	GOL	O1-C1-C2-O2
5	A	810	GOL	O2-C2-C3-O3
5	A	811	GOL	O1-C1-C2-O2
5	A	801	GOL	O2-C2-C3-O3
3	A	600[B]	PSZ	C5A-O4P-P-O2P
3	A	600[B]	PSZ	C5-C4-C4A-N4A
5	A	805	GOL	O1-C1-C2-O2
5	A	802[B]	GOL	O1-C1-C2-O2
5	A	803	GOL	O1-C1-C2-C3
5	A	802[B]	GOL	O1-C1-C2-C3
5	A	808	GOL	O1-C1-C2-C3
5	A	809	GOL	O1-C1-C2-O2

There are no ring outliers.

11 monomers are involved in 69 short contacts:

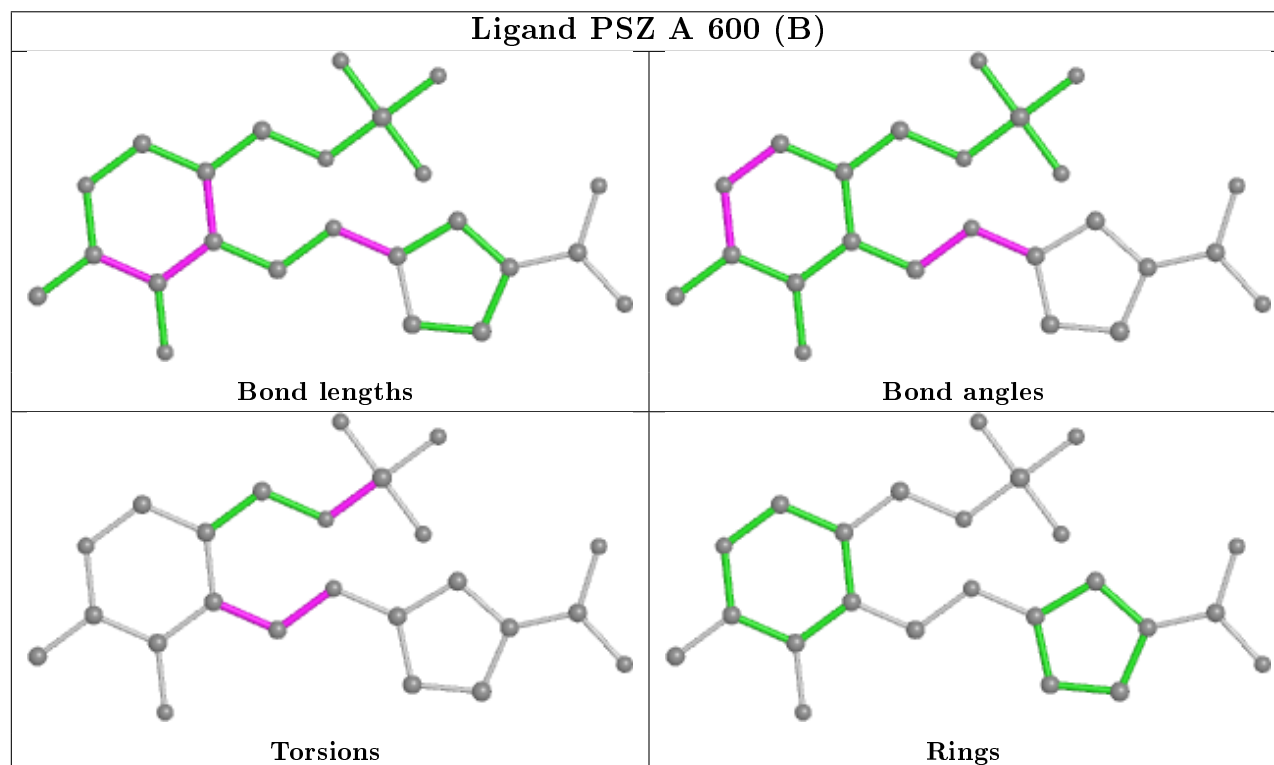
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	SO4	1	0
5	A	807	GOL	5	0
5	A	808	GOL	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	811	GOL	20	1
5	A	806	GOL	9	0
5	A	801	GOL	7	0
5	A	805	GOL	4	0
5	A	809	GOL	9	0
5	A	810	GOL	4	0
5	A	802[B]	GOL	3	0
5	A	804	GOL	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [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	378/396 (95%)	0.15	21 (5%) 24 22	12, 19, 33, 46	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	10	ALA	8.2
1	A	335	ASN	5.0
1	A	85[A]	LYS	4.3
1	A	9	PRO	3.7
1	A	330	GLN	3.3
1	A	164[A]	ASN	3.3
1	A	88	ALA	3.2
1	A	33[A]	ILE	2.9
1	A	86	GLY	2.8
1	A	154	ASN	2.7
1	A	152	ALA	2.7
1	A	212[A]	PHE	2.6
1	A	28	LYS	2.6
1	A	199[A]	GLN	2.6
1	A	239	ILE	2.3
1	A	333	GLY	2.3
1	A	91	ASN	2.3
1	A	167	ASN	2.3
1	A	209[A]	LEU	2.3
1	A	240	VAL	2.2
1	A	160	ASP	2.1

### 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. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	KST	A	246[A]	17/18	0.96	0.12	9,14,18,21	13
1	KST	A	246[B]	9/18	0.96	0.12	13,14,25,27	5

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

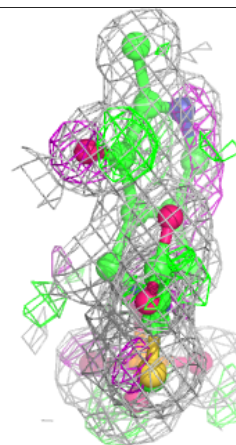
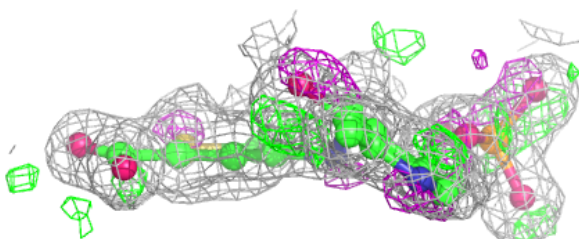
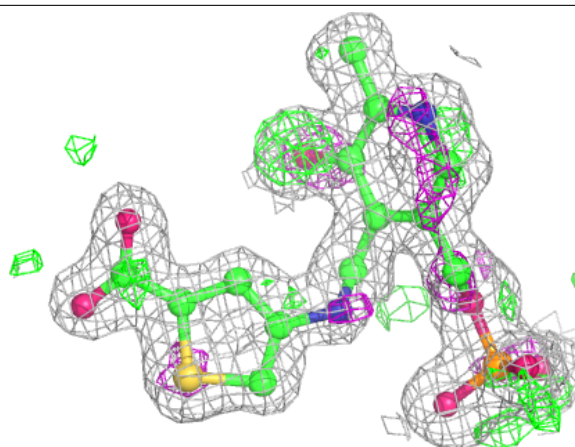
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	A	811	6/6	0.78	0.29	26,30,32,32	6
5	GOL	A	803	6/6	0.78	0.30	44,52,54,58	0
5	GOL	A	810	6/6	0.82	0.17	25,28,30,31	6
5	GOL	A	808	6/6	0.82	0.30	58,59,61,63	0
5	GOL	A	806	6/6	0.86	0.16	34,44,45,46	0
5	GOL	A	807	6/6	0.88	0.23	43,54,57,57	0
5	GOL	A	805	6/6	0.88	0.14	11,21,29,30	6
5	GOL	A	809	6/6	0.89	0.30	24,38,44,45	0
2	SO4	A	500	5/5	0.93	0.12	47,47,47,47	5
5	GOL	A	801	6/6	0.93	0.28	20,32,40,44	0
5	GOL	A	804	6/6	0.93	0.28	12,21,25,28	6
5	GOL	A	802[A]	6/6	0.94	0.13	19,20,22,23	6
5	GOL	A	802[B]	6/6	0.94	0.13	19,20,23,24	6
4	PMP	A	700[A]	16/16	0.97	0.10	10,12,19,22	16
3	PSZ	A	600[B]	24/24	0.97	0.09	14,16,19,20	24

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around PSZ A 600 (B):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.