

# Full wwPDB X-ray Structure Validation Report (i)

#### Aug 24, 2023 – 12:24 PM EDT

PDB ID	:	8TTJ
Title	:	Tryptophan-6-halogenase BorH complexed with 6-chlorotryptophan
Authors	:	Lingkon, K.; Bellizzi, J.J.
Deposited on	:	2023-08-14
Resolution	:	1.98  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
$\mathrm{EDS}$	:	2.35
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)	:	2.35

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 1.98 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.



Motrie	Whole archive	Similar resolution
	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
R <sub>free</sub>	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	А	529	86%	12%	•
1	В	529	4% 88%	11%	
1	С	529	<u>6%</u> 87%	11%	·
1	D	529	87%	11%	·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	А	609	-	-	Х	-
3	SO4	С	602	-	-	Х	-
3	SO4	С	607	-	-	Х	-
3	SO4	D	607	-	-	Х	_

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 18401 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	500	Total	С	Ν	Ο	S	0	0	0
	A	522	4193	2674	737	761	21	0	0	0
1	В	599	Total	С	Ν	Ο	S	0	1	0
1	D	522	4195	2675	737	761	22	0	T	0
1	С	591	Total	С	Ν	0	S	0	2	0
	U	521	4201	2678	740	761	22	0		0
1	П	520	Total	С	Ν	0	S	0	1	0
		520	4182	2668	735	757	22	0		0

• Molecule 1 is a protein called Tryptophan 6-halogenase.

• Molecule 2 is 6-CHLORO-L-TRYPTOPHAN (three-letter code: 6CW) (formula: C<sub>11</sub>H<sub>11</sub>ClN<sub>2</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	
0	٨	1	Total	С	Cl	Ν	Ο	0	0	
	A	1	16	11	1	2	2	0	0	
0	D	1	Total	С	Cl	Ν	Ο	0	0	
	D	1	16	11	1	2	2	0	0	



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Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	
0	C	1	Total	Total C		Ν	Ο	0	0	
	U	L	16	11	1	2	2	0	0	
0	П	1	Total	С	Cl	Ν	0	0	0	
	D	L	16	11	1	2	2	0	0	



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	D	1	$\begin{array}{c cc} \hline \text{Total} & \text{O} & \text{S} \\ \hline 5 & 4 & 1 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 4 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	402	Total O 402 402	0	0
4	В	366	Total O 366 366	0	0
4	С	344	Total O 344 344	0	0
4	D	314	Total         O           314         314	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: Tryptophan 6-halogenase



• Molecule 1: Tryptophan 6-halogenase





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	73.52Å 157.97Å 112.58Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $104.06^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution(Å)	35.47 - 1.98	Depositor
Resolution (A)	35.47 - 1.98	EDS
% Data completeness	98.3 (35.47-1.98)	Depositor
(in resolution range)	98.3 (35.47 - 1.98)	EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.30 (at 1.98 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
B B.	0.199 , $0.236$	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.200 , $0.237$	DCC
$R_{free}$ test set	1997 reflections $(1.18\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	27.4	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33, 45.2	EDS
L-test for $twinning^2$	$ < L >=0.45, < L^2>=0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18401	wwPDB-VP
Average B, all atoms $(Å^2)$	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 11.85% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: SO4,  $6\mathrm{CW}$ 

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).

Mal	Chain	Bond lengths		Bond angles	
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.26	0/4310	0.51	0/5851
1	В	0.25	0/4315	0.51	0/5857
1	С	0.26	0/4322	0.50	0/5867
1	D	0.25	0/4303	0.50	0/5842
All	All	0.26	0/17250	0.51	0/23417

There are no bond length outliers.

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	А	4193	0	4031	44	0
1	В	4195	0	4037	42	0
1	С	4201	0	4042	45	0
1	D	4182	0	4026	41	0
2	А	16	0	9	2	0
2	В	16	0	10	0	0
2	С	16	0	9	2	0
2	D	16	0	10	0	0
3	A	40	0	0	6	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	В	35	0	0	2	0
3	С	30	0	0	5	0
3	D	35	0	0	4	0
4	А	402	0	0	15	0
4	В	366	0	0	13	0
4	С	344	0	0	18	0
4	D	314	0	0	19	0
All	All	18401	0	16174	184	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 6.

All (184) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:496:ARG:NH2	4:C:702:HOH:O	1.96	0.98
1:A:447:VAL:O	4:A:701:HOH:O	1.82	0.98
1:C:480:ARG:O	4:C:701:HOH:O	1.83	0.96
3:D:607:SO4:O3	4:D:701:HOH:O	1.86	0.91
1:A:220:GLU:OE2	4:A:702:HOH:O	1.93	0.86
1:D:69:GLU:OE1	4:D:702:HOH:O	1.93	0.84
1:B:231:ARG:O	4:B:701:HOH:O	1.96	0.83
1:D:391:GLU:OE2	4:D:703:HOH:O	1.97	0.83
1:B:304:GLU:OE2	4:B:702:HOH:O	1.97	0.82
1:D:116:GLU:OE2	4:D:704:HOH:O	1.97	0.81
3:C:602:SO4:O1	4:C:703:HOH:O	1.99	0.79
1:C:480:ARG:NH2	3:C:607:SO4:S	2.56	0.79
1:D:66:ARG:HB3	1:D:68:GLU:OE1	1.81	0.78
1:A:423:ASP:OD1	4:A:703:HOH:O	2.02	0.78
3:D:607:SO4:O1	4:D:705:HOH:O	2.01	0.77
1:D:189:ASN:ND2	4:D:711:HOH:O	2.18	0.77
1:D:46:GLY:N	4:D:709:HOH:O	2.16	0.77
1:B:30:ASP:OD2	4:B:704:HOH:O	2.03	0.76
1:D:511:GLU:OE2	4:D:706:HOH:O	2.05	0.74
3:B:607:SO4:O1	4:B:705:HOH:O	2.05	0.73
1:A:480:ARG:NH2	4:A:709:HOH:O	2.22	0.73
1:A:494:GLN:OE1	4:A:704:HOH:O	2.08	0.71
1:C:319:ASP:OD1	4:C:705:HOH:O	2.10	0.70
3:D:602:SO4:O3	4:D:707:HOH:O	2.10	0.69
1:C:136:ASP:OD2	4:C:706:HOH:O	2.10	0.68
1:C:389:ASN:O	1:C:393:GLU:HG3	1.94	0.68



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:187:ARG:NH1	4:A:713:HOH:O	2.26	0.68	
1:A:359:THR:HG21	1:A:399:THR:HG21	1.76	0.68	
1:A:68:GLU:N	3:A:609:SO4:O1	2.28	0.66	
1:D:94:GLU:OE1	4:D:708:HOH:O	2.14	0.66	
1:C:398:ASP:OD1	4:C:707:HOH:O	2.13	0.66	
3:A:609:SO4:O1	4:A:705:HOH:O	2.12	0.65	
3:A:602:SO4:O2	4:A:706:HOH:O	2.13	0.64	
1:D:437:TYR:HB2	1:D:443:ILE:HD11	1.79	0.64	
1:B:449:ASP:OD1	4:B:706:HOH:O	2.14	0.63	
1:C:480:ARG:NH2	3:C:607:SO4:O4	2.32	0.62	
1:C:480:ARG:NH2	3:C:607:SO4:O3	2.18	0.62	
1:D:68:GLU:H	1:D:68:GLU:CD	2.02	0.62	
1:C:245:ASP:OD1	4:C:708:HOH:O	2.16	0.62	
1:C:456:ARG:HD3	4:C:985:HOH:O	2.00	0.62	
1:B:181:ARG:NH2	4:B:720:HOH:O	2.32	0.61	
1:A:433:LYS:HA	1:A:436:MET:HE2	1.83	0.61	
1:A:356:LEU:HB3	1:A:403:ILE:HD12	1.83	0.61	
1:C:437:TYR:HB2	1:C:443:ILE:HD11	1.84	0.60	
1:C:453:TYR:CZ	1:C:460:GLU:HG3	2.36	0.60	
1:C:172:ASP:OD1	4:C:709:HOH:O	2.16	0.59	
2:C:601:6CW:HD1	4:C:777:HOH:O	2.01	0.59	
3:D:605:SO4:O3	4:D:710:HOH:O	2.17	0.59	
1:A:456:ARG:NH1	1:A:458:GLU:H	2.01	0.59	
1:D:187:ARG:NH2	4:D:721:HOH:O	2.35	0.59	
1:A:158:TRP:HB2	1:A:162:ARG:HB2	1.85	0.59	
1:B:230:PHE:CE1	1:B:331:ARG:HB3	2.37	0.59	
1:C:438:LYS:HE2	1:C:479:LEU:HD11	1.85	0.58	
1:C:274:SER:HB2	1:C:285:LYS:HB3	1.85	0.58	
1:D:278:MET:HE3	4:D:922:HOH:O	2.02	0.58	
1:D:334:ARG:CZ	1:D:393:GLU:HG3	2.34	0.58	
1:A:437:TYR:HB2	1:A:443:ILE:HD11	1.84	0.58	
1:C:202[A]:ARG:NH2	4:C:723:HOH:O	2.36	0.58	
1:C:146:GLU:HG3	1:C:165:THR:HG21	1.85	0.58	
1:A:7:ARG:HB2	1:A:221:GLY:HA2	1.86	0.58	
1:A:410:SER:O	1:A:422:LYS:HE3	2.03	0.57	
1:C:66:ARG:HD3	1:C:68:GLU:H	1.69	0.57	
1:C:4:ARG:NE	4:C:717:HOH:O	2.30	0.57	
1:D:7:ARG:HB2	1:D:221:GLY:HA2	1.87	0.56	
1:D:157:LYS:HB3	1:D:163:PRO:HA	1.87	0.56	
1:C:507:ASP:OD1	1:C:510:ARG:NH2	2.38	0.56	
1:A:456:ARG:HH11	1:A:458:GLU:HB2	1.71	0.56	



A + 1	<b>A t</b> and <b>D</b>	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:438:LYS:HE2	1:B:479:LEU:HD11	1.88	0.56
1:B:182:ARG:HD3	4:B:720:HOH:O	2.06	0.55
1:B:346:ILE:HG21	1:B:368:ILE:HD11	1.88	0.55
1:C:205:ARG:O	4:C:710:HOH:O	2.18	0.55
1:D:83:LYS:NZ	4:D:717:HOH:O	2.29	0.55
1:C:209:THR:OG1	4:C:704:HOH:O	2.09	0.54
3:B:606:SO4:O4	4:B:709:HOH:O	2.19	0.54
1:B:71:MET:HE2	1:B:526:LEU:CD2	2.39	0.53
1:A:390:HIS:HB2	4:A:1043:HOH:O	2.08	0.53
1:B:63:LEU:O	4:B:708:HOH:O	2.19	0.53
1:C:66:ARG:NH1	4:C:732:HOH:O	2.41	0.53
1:B:320:PRO:O	4:B:707:HOH:O	2.18	0.53
1:B:13:GLY:HA3	1:B:38:GLU:HG2	1.90	0.52
1:D:274:SER:HB2	1:D:285:LYS:HB3	1.91	0.52
1:D:166:ARG:NH1	4:D:725:HOH:O	2.40	0.51
1:C:410:SER:O	1:C:422:LYS:HE3	2.10	0.51
1:C:447:VAL:HG23	1:C:448:THR:HG23	1.92	0.51
1:A:205:ARG:HG3	1:A:207:PHE:CD1	2.46	0.51
1:A:20:THR:HG21	1:A:225:ILE:HG21	1.92	0.51
1:D:20:THR:HG21	1:D:225:ILE:HG21	1.93	0.51
1:C:247:ASN:ND2	1:C:250:LEU:O	2.42	0.50
1:D:3:ASN:N	4:D:731:HOH:O	2.44	0.50
1:B:20:THR:HG21	1:B:225:ILE:HG21	1.94	0.50
1:B:237:LYS:HG2	4:B:701:HOH:O	2.12	0.50
1:A:154:ARG:NH2	3:A:606:SO4:O3	2.39	0.49
1:B:491:ARG:HH11	1:B:491:ARG:HG2	1.77	0.49
1:B:437:TYR:HB2	1:B:443:ILE:HD11	1.94	0.49
1:B:46:GLY:O	1:B:291:ARG:NH2	2.46	0.49
1:A:243:PHE:CZ	1:A:331:ARG:HG2	2.48	0.49
1:B:438:LYS:HA	1:B:481:PRO:HA	1.93	0.49
1:D:18:TRP:CZ2	1:D:181:ARG:HG3	2.47	0.49
1:A:203:ASP:OD1	1:A:205:ARG:HG2	2.14	0.48
1:C:418:TRP:O	1:C:422:LYS:NZ	2.31	0.48
1:D:258:THR:HB	1:D:325:LEU:HD23	1.95	0.48
1:B:5:ILE:HG23	1:B:222:ASP:HB2	1.95	0.48
1:B:419:LYS:HE3	1:B:419:LYS:HB2	1.54	0.48
1:D:3:ASN:O	1:D:377:ASP:HB2	2.13	0.48
1:C:341:LYS:NZ	3:C:602:SO4:O2	2.46	0.48
1:A:479:LEU:HD12	4:A:1018:HOH:O	2.14	0.48
1:A:493:GLU:HG3	4:A:1070:HOH:O	2.14	0.48
1:A:438:LYS:HA	1:A:481:PRO:HA	1.96	0.47



		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:C:7:ARG:HB2	1:C:221:GLY:HA2	1.96	0.47	
1:D:526:LEU:HD12	1:D:527:HIS:CE1	2.49	0.47	
1:A:453:TYR:CZ	1:A:460:GLU:HG3	2.49	0.47	
1:A:94:GLU:HA	1:A:315:MET:HG3	1.96	0.47	
1:B:239:MET:HE1	1:B:341:LYS:HD2	1.97	0.47	
1:D:57:ARG:NH2	4:D:725:HOH:O	2.47	0.47	
1:B:231:ARG:HG3	1:B:231:ARG:HH11	1.77	0.47	
2:A:601:6CW:HD1	4:A:748:HOH:O	2.12	0.47	
1:C:341:LYS:HE2	4:C:854:HOH:O	2.13	0.47	
1:B:96:LYS:HB2	1:B:96:LYS:HE2	1.64	0.47	
3:A:608:SO4:O3	4:A:707:HOH:O	2.17	0.46	
1:D:79:LYS:NZ	1:D:358:SER:OG	2.49	0.46	
1:B:231:ARG:HG3	1:B:231:ARG:NH1	2.31	0.46	
1:C:510:ARG:HG3	4:C:869:HOH:O	2.15	0.46	
1:B:38:GLU:HB3	1:B:39:ALA:H	1.55	0.46	
1:D:519:ASN:O	1:D:523:LEU:HG	2.15	0.45	
1:C:310:LEU:O	1:C:314:ARG:HD3	2.15	0.45	
1:B:274:SER:HB2	1:B:285:LYS:HB3	1.97	0.45	
1:D:146:GLU:O	1:D:150:MET:HG3	2.17	0.45	
1:B:243:PHE:CZ	1:B:331:ARG:HG2	2.52	0.45	
1:A:53:PRO:HD2	2:A:601:6CW:O	2.16	0.45	
1:A:353:LEU:HG	1:A:396:PHE:CE1	2.52	0.45	
1:B:234:LEU:O	1:B:239:MET:HG2	2.17	0.45	
1:C:265:ASP:OD1	1:C:524:ARG:NH2	2.49	0.45	
1:C:243:PHE:CE2	1:C:331:ARG:HG2	2.52	0.45	
1:A:438:LYS:HE2	1:A:479:LEU:HD11	1.99	0.45	
1:B:353:LEU:HG	1:B:396:PHE:CE1	2.51	0.45	
1:C:79:LYS:NZ	1:C:358:SER:OG	2.50	0.45	
1:C:304:GLU:OE2	4:C:712:HOH:O	2.20	0.45	
1:A:274:SER:HB2	1:A:285:LYS:HB3	1.99	0.44	
1:A:243:PHE:CE2	1:A:331:ARG:HG2	2.52	0.44	
1:C:438:LYS:HA	1:C:481:PRO:HA	1.98	0.44	
1:B:230:PHE:CD1	1:B:331:ARG:HB3	2.52	0.44	
1:D:438:LYS:HB2	1:D:438:LYS:HE2	1.71	0.44	
1:B:158:TRP:CE3	1:B:162:ARG:HG3	2.53	0.44	
1:D:353:LEU:HG	1:D:396:PHE:CE1	2.53	0.44	
1:C:157:LYS:HB3	1:C:163:PRO:HA	2.00	0.44	
1:A:512:LEU:O	1:A:516:LEU:HB2	2.18	0.43	
1:B:201:LEU:HD12	1:B:210:ALA:HB3	2.00	0.43	
1:D:237:LYS:HE3	1:D:237:LYS:HB3	1.66	0.43	
1:A:507:ASP:OD1	1:A:510:ARG:NH2	2.50	0.43	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:438:LYS:HA	1:D:481:PRO:HA	2.00	0.43
1:C:20:THR:HG21	1:C:225:ILE:HG21	2.01	0.43
1:B:351:CYS:HB2	1:B:396:PHE:CE1	2.54	0.43
1:A:174:HIS:O	1:A:178:GLU:HG2	2.19	0.42
1:B:7:ARG:HB2	1:B:221:GLY:HA2	1.99	0.42
1:B:157:LYS:HG2	1:B:163:PRO:HA	2.00	0.42
1:B:378:ARG:NH2	4:B:746:HOH:O	2.52	0.42
1:A:67:GLU:HB2	3:A:609:SO4:O1	2.18	0.42
1:A:124:HIS:HE2	1:A:442:PRO:N	2.17	0.42
1:A:215:GLU:HG3	4:A:982:HOH:O	2.18	0.42
1:B:35:THR:HG22	1:B:191:GLU:HB3	2.01	0.42
1:A:255:ALA:HA	1:A:296:TYR:O	2.20	0.42
1:A:255:ALA:HB2	1:A:330:PHE:CZ	2.55	0.42
1:B:306:ASP:OD1	4:B:710:HOH:O	2.21	0.42
1:C:437:TYR:O	1:C:481:PRO:HB3	2.20	0.42
1:B:71:MET:N	1:B:72:PRO:HD2	2.35	0.42
1:D:201:LEU:HA	4:D:850:HOH:O	2.20	0.42
1:C:353:LEU:HG	1:C:396:PHE:CE1	2.55	0.42
1:A:166:ARG:HD3	4:A:1014:HOH:O	2.21	0.41
1:D:89:THR:HG23	1:D:105:ASP:OD2	2.20	0.41
1:B:2:ASP:O	1:B:378:ARG:NH2	2.52	0.41
1:C:53:PRO:HD2	2:C:601:6CW:O	2.19	0.41
1:D:351:CYS:HB2	1:D:396:PHE:CE1	2.56	0.41
1:A:56:GLN:HB2	1:A:169:TRP:CH2	2.56	0.41
1:C:255:ALA:HA	1:C:296:TYR:O	2.20	0.41
1:D:318:LEU:HA	4:D:791:HOH:O	2.20	0.41
1:D:172:ASP:OD2	1:D:175:LEU:HG	2.21	0.41
1:C:250:LEU:HD12	1:C:353:LEU:HD22	2.02	0.41
1:D:88:ARG:HB2	1:D:100:ILE:HD11	2.03	0.41
1:A:3:ASN:O	1:A:377:ASP:HB2	2.21	0.40
1:D:241:GLU:HA	1:D:242:PRO:HD3	1.98	0.40
1:D:57:ARG:HD2	1:D:454:TYR:O	2.21	0.40
1:A:45:ILE:HB	1:A:326:ASN:OD1	2.21	0.40
1:B:447:VAL:HG23	1:B:448:THR:HG23	2.03	0.40
1:D:361:ILE:HD13	1:D:361:ILE:HA	1.90	0.40

There are no symmetry-related clashes.



### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	518/529~(98%)	505~(98%)	13~(2%)	0	100	100
1	В	519/529~(98%)	500~(96%)	19~(4%)	0	100	100
1	С	519/529~(98%)	508~(98%)	11 (2%)	0	100	100
1	D	517/529~(98%)	503~(97%)	14 (3%)	0	100	100
All	All	2073/2116 (98%)	2016 (97%)	57(3%)	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	F	Perce	entiles
1	А	431/436~(99%)	430 (100%)	1 (0%)		93	93
1	В	432/436~(99%)	431 (100%)	1 (0%)		93	93
1	С	433/436~(99%)	431 (100%)	2(0%)		88	87
1	D	431/436~(99%)	429 (100%)	2 (0%)		88	87
All	All	1727/1744 (99%)	1721 (100%)	6 (0%)		92	92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	419	LYS
1	В	96	LYS



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Mol	Chain	Res	Type
1	С	237	LYS
1	С	451	SER
1	D	261	LYS
1	D	301	ARG

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

Mol	Chain	Res	Type
1	А	75	ASN
1	А	198	GLN
1	А	199	GLN
1	В	199	GLN
1	С	119	GLN
1	С	194	GLN
1	D	194	GLN
1	D	527	HIS

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

32 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).



Mal	Trune	Chain	Dec	Tinle	Bo	Bond lengths		Bond angles		
	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	С	602	-	4,4,4	0.15	0	$6,\!6,\!6$	0.09	0
3	SO4	В	603	-	4,4,4	0.15	0	$6,\!6,\!6$	0.08	0
3	SO4	В	606	-	4,4,4	0.13	0	$6,\!6,\!6$	0.10	0
3	SO4	С	607	-	4,4,4	0.13	0	$6,\!6,\!6$	0.13	0
3	SO4	А	605	-	4,4,4	0.14	0	$6,\!6,\!6$	0.06	0
2	6CW	А	601	1	$15,\!17,\!17$	0.97	1 (6%)	18,24,24	2.62	6 (33%)
3	SO4	А	608	-	4,4,4	0.15	0	$6,\!6,\!6$	0.05	0
3	SO4	А	603	-	4,4,4	0.14	0	$6,\!6,\!6$	0.06	0
3	SO4	D	605	-	4,4,4	0.15	0	$6,\!6,\!6$	0.05	0
3	SO4	D	607	-	4,4,4	0.14	0	$6,\!6,\!6$	0.12	0
3	SO4	В	602	-	4,4,4	0.16	0	$6,\!6,\!6$	0.22	0
3	SO4	D	603	-	4,4,4	0.15	0	$6,\!6,\!6$	0.06	0
3	SO4	D	606	-	4,4,4	0.14	0	$6,\!6,\!6$	0.05	0
2	6CW	В	601	-	$15,\!17,\!17$	0.91	0	18,24,24	2.32	5 (27%)
3	SO4	D	608	-	4,4,4	0.13	0	$6,\!6,\!6$	0.10	0
3	SO4	С	603	-	4,4,4	0.14	0	$6,\!6,\!6$	0.06	0
2	6CW	С	601	1	15,17,17	0.99	0	18,24,24	2.65	6 (33%)
3	SO4	С	604	-	4,4,4	0.14	0	$6,\!6,\!6$	0.05	0
3	SO4	С	606	-	4,4,4	0.14	0	$6,\!6,\!6$	0.06	0
3	SO4	А	609	-	4,4,4	0.13	0	$6,\!6,\!6$	0.17	0
3	SO4	В	608	-	4,4,4	0.14	0	$6,\!6,\!6$	0.06	0
3	SO4	В	605	-	4,4,4	0.14	0	$6,\!6,\!6$	0.06	0
3	SO4	А	604	-	4,4,4	0.13	0	$6,\!6,\!6$	0.07	0
3	SO4	А	607	-	4,4,4	0.14	0	$6,\!6,\!6$	0.05	0
3	SO4	А	602	-	4,4,4	0.14	0	$6,\!6,\!6$	0.06	0
3	SO4	D	604	-	4,4,4	0.14	0	$6,\!6,\!6$	0.05	0
3	SO4	D	602	-	4,4,4	0.15	0	$6,\!6,\!6$	0.05	0
2	6CW	D	601	-	$15,\!17,\!17$	0.92	0	18,24,24	2.31	4 (22%)
3	SO4	C	605	-	4,4,4	0.13	0	$6,\!6,\!6$	0.07	0
3	SO4	A	606	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	В	607	-	4,4,4	0.13	0	6,6,6	0.08	0
3	SO4	В	604		4,4,4	0.14	0	6,6,6	0.06	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	6CW	D	601	-	-	2/7/8/8	0/2/2/2
2	6CW	С	601	1	-	2/7/8/8	0/2/2/2



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	6CW	В	601	-	-	2/7/8/8	0/2/2/2
2	6CW	А	601	1	-	2/7/8/8	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	А	601	6CW	CD2-CE2	-2.03	1.37	1.42

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	601	6CW	CZ2-CH2-CLL	6.79	128.14	119.64
2	А	601	6CW	CB-CG-CD1	-6.24	120.26	127.97
2	А	601	6CW	CZ2-CH2-CLL	6.19	127.39	119.64
2	D	601	6CW	CB-CG-CD1	-5.90	120.67	127.97
2	В	601	6CW	CB-CG-CD1	-5.50	121.17	127.97
2	С	601	6CW	CB-CG-CD1	-5.46	121.22	127.97
2	В	601	6CW	CZ2-CH2-CLL	5.07	125.98	119.64
2	D	601	6CW	CZ2-CH2-CLL	4.90	125.77	119.64
2	В	601	6CW	CZ3-CH2-CLL	-4.12	112.91	119.35
2	С	601	6CW	CZ3-CH2-CZ2	-3.80	117.49	121.99
2	D	601	6CW	CZ3-CH2-CLL	-3.71	113.56	119.35
2	А	601	6CW	CZ3-CH2-CZ2	-3.61	117.71	121.99
2	А	601	6CW	CB-CG-CD2	3.50	131.69	126.25
2	С	601	6CW	CZ3-CH2-CLL	-3.19	114.37	119.35
2	С	601	6CW	CB-CG-CD2	3.10	131.08	126.25
2	D	601	6CW	CB-CG-CD2	2.95	130.84	126.25
2	А	601	6CW	CZ3-CH2-CLL	-2.85	114.90	119.35
2	В	601	6CW	CB-CG-CD2	2.69	130.44	126.25
2	С	601	6CW	CE3-CZ3-CH2	2.59	122.22	119.21
2	А	601	6CW	CE3-CZ3-CH2	2.17	121.73	119.21
2	В	601	6CW	OXT-C-CA	2.06	120.40	113.38

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	601	6CW	O-C-CA-N
2	В	601	6CW	O-C-CA-N
2	С	601	6CW	O-C-CA-N
2	D	601	6CW	O-C-CA-N



Mol	Chain	Res	Type	Atoms
2	В	601	6CW	OXT-C-CA-N
2	D	601	6CW	OXT-C-CA-N
2	А	601	6CW	OXT-C-CA-N
2	С	601	6CW	OXT-C-CA-N

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There are no ring outliers.

13 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	С	602	SO4	2	0
3	В	606	SO4	1	0
3	С	607	SO4	3	0
2	А	601	6CW	2	0
3	А	608	SO4	1	0
3	D	605	SO4	1	0
3	D	607	SO4	2	0
2	С	601	6CW	2	0
3	А	609	SO4	3	0
3	А	602	SO4	1	0
3	D	602	SO4	1	0
3	А	606	SO4	1	0
3	В	607	SO4	1	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 then 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 (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,  $95^{th}$  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	< <b>RSRZ</b> >	# RSRZ > 2	$OWAB(Å^2)$	Q < 0.9
1	А	522/529~(98%)	0.23	14 (2%) 54 56	16, 29, 49, 60	0
1	В	522/529~(98%)	0.33	23 (4%) 34 36	15, 34, 60, 81	0
1	С	521/529~(98%)	0.34	32 (6%) 21 23	20, 36, 58, 81	0
1	D	520/529~(98%)	0.65	67 (12%) 3 3	21, 42, 67, 91	0
All	All	2085/2116~(98%)	0.38	136 (6%) 18 20	15, 35, 61, 91	0

All (136) RSRZ outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	RSRZ
1	D	100	ILE	8.2
1	С	322	ASN	6.3
1	D	322	ASN	6.3
1	D	101	ASP	5.6
1	D	159	LEU	5.2
1	С	101	ASP	5.1
1	С	324	PRO	4.7
1	D	356	LEU	4.3
1	D	50	ALA	4.1
1	D	102	GLY	4.1
1	D	162	ARG	4.0
1	В	45	ILE	3.9
1	D	318	LEU	3.9
1	D	306	ASP	3.9
1	С	100	ILE	3.9
1	С	321	GLU	3.9
1	В	266	ALA	3.8
1	А	101	ASP	3.8
1	В	204	GLU	3.7
1	В	356	LEU	3.7
1	D	323	THR	3.6



Mol	Chain	Res	Type	RSRZ
1	D	324	PRO	3.6
1	В	186	GLU	3.6
1	С	162	ARG	3.6
1	В	39	ALA	3.5
1	С	361	ILE	3.4
1	С	319	ASP	3.4
1	С	356	LEU	3.4
1	В	324	PRO	3.3
1	D	196	GLU	3.3
1	D	319	ASP	3.2
1	D	160	ASP	3.2
1	D	358	SER	3.2
1	D	526	LEU	3.2
1	А	267	HIS	3.1
1	D	52	VAL	3.1
1	С	40	PRO	3.1
1	D	525	SER	3.0
1	В	185	THR	3.0
1	D	230	PHE	3.0
1	С	159	LEU	3.0
1	D	303	ALA	3.0
1	С	360	GLY	2.9
1	D	320	PRO	2.9
1	D	413	THR	2.9
1	D	361	ILE	2.8
1	D	304	GLU	2.8
1	В	267	HIS	2.8
1	D	266	ALA	2.8
1	D	321	GLU	2.8
1	В	321	GLU	2.8
1	D	359	THR	2.8
1	D	216	GLY	2.7
1	А	45	ILE	2.7
1	С	525	SER	2.7
1	D	522	PHE	2.7
1	D	51	THR	2.7
1	D	521	GLU	2.7
1	D	353	LEU	2.6
1	В	275	ALA	2.6
1	С	323	THR	2.6
1	В	101	ASP	2.6
1	В	263	ASP	2.6



Mol	Chain	Res	Type	RSRZ
1	D	198	GLN	2.6
1	C	267	HIS	2.6
1	D	515	THR	2.6
1	C	526	LEU	2.6
1	B	194	GLN	2.6
1	A	321	GLU	2.6
1	A	360	GLY	2.5
1	D	47	VAL	2.5
1	B	189	ASN	2.5
1	D	46	GLY	2.5
1	C	318	LEU	2.5
1	A	356	LEU	2.5
1	D	520	LEU	2.5
1	C	355	PRO	2.4
1	D	40	PRO	2.4
1	D	74[A]	CYS	2.4
1	B	276	ILE	2.4
1	D	514	GLU	2.4
1	D	161	GLY	2.4
1	B	2	ASP	2.4
1	D	267	HIS	2.4
1	D	363	PHE	2.4
1	D	275	ALA	2.4
1	D	368	ILE	2.4
1	A	472	CYS	2.3
1	C	403	ILE	2.3
1	D	301	ARG	2.3
1	D	194	GLN	2.3
1	D	289	LEU	2.3
1	D	364	ILE	2.3
1	B	84	PHE	2.3
1	B	33	THR	2.2
1	D	163	PRO	2.2
1	C	194	GLN	2.2
1	D	39	ALA	2.2
1	C	317	GLY	2.2
1	Ā	265	ASP	2.2
1	C	320	PRO	2.2
1	C	359	THR	2.2
1	D	313	CYS	2.2
1	D	330	PHE	2.2
1	B	187	ARG	2.2
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Mol	Chain	Res	Type	RSRZ
1	А	364	ILE	2.2
1	D	82	VAL	2.2
1	D	110	PRO	2.1
1	А	361	ILE	2.1
1	В	6	ASN	2.1
1	С	363	PHE	2.1
1	С	68	GLU	2.1
1	D	297	VAL	2.1
1	С	160	ASP	2.1
1	D	273	THR	2.1
1	D	362	TYR	2.1
1	D	214	VAL	2.1
1	D	346	ILE	2.1
1	А	201	LEU	2.1
1	D	325	LEU	2.1
1	В	282	TRP	2.1
1	D	261	LYS	2.1
1	С	39	ALA	2.1
1	D	366	ALA	2.1
1	С	282	TRP	2.1
1	D	84	PHE	2.1
1	А	266	ALA	2.1
1	А	346	ILE	2.1
1	D	493	GLU	2.0
1	А	275	ALA	2.0
1	С	353	LEU	2.0
1	С	358	SER	2.0
1	С	50	ALA	2.0
1	С	465	TRP	2.0
1	В	323	THR 2.0	
1	D	288	MET	2.0

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### 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	SO4	D	607	5/5	0.79	0.24	$66,\!69,\!80,\!85$	5
3	SO4	С	607	5/5	0.81	0.25	53,57,65,68	5
3	SO4	А	608	5/5	0.84	0.27	27,31,50,52	5
3	SO4	С	606	5/5	0.84	0.21	42,46,57,60	5
2	6CW	С	601	16/16	0.86	0.17	22,31,42,44	0
3	SO4	С	605	5/5	0.87	0.20	56,63,74,81	0
3	SO4	А	609	5/5	0.87	0.34	53,57,61,63	0
3	SO4	А	605	5/5	0.88	0.44	61,61,64,72	5
3	SO4	D	605	5/5	0.89	0.15	40,44,51,52	5
3	SO4	В	606	5/5	0.89	0.14	34,44,54,55	5
3	SO4	В	608	5/5	0.90	0.16	50,54,62,67	5
2	6CW	А	601	16/16	0.90	0.17	19,23,35,47	0
3	SO4	А	604	5/5	0.91	0.12	34,37,48,55	5
3	SO4	А	606	5/5	0.91	0.19	46,49,54,59	5
3	SO4	А	607	5/5	0.91	0.30	34,64,86,125	5
2	6CW	D	601	16/16	0.92	0.14	$29,\!34,\!40,\!57$	0
3	SO4	В	607	5/5	0.92	0.12	51,54,58,62	5
2	6CW	В	601	16/16	0.93	0.13	21,25,33,44	0
3	SO4	D	604	5/5	0.94	0.20	$43,\!54,\!55,\!62$	5
3	SO4	С	604	5/5	0.94	0.17	52,57,65,70	0
3	SO4	В	605	5/5	0.94	0.26	33,38,43,49	5
3	SO4	D	603	5/5	0.95	0.18	32,46,53,54	5
3	SO4	D	608	5/5	0.95	0.21	$50,\!53,\!63,\!63$	0
3	SO4	D	606	5/5	0.96	0.17	57,59,64,64	5
3	SO4	А	603	5/5	0.97	0.18	54,62,68,70	0
3	SO4	В	604	5/5	0.97	0.20	$56,\!57,\!60,\!61$	0
3	SO4	В	603	5/5	0.98	0.16	43,43,44,49	0
3	SO4	А	602	5/5	0.98	0.17	31,34,38,43	5
3	SO4	В	602	5/5	0.98	0.34	50,62,67,70	0
3	SO4	С	602	5/5	0.98	0.13	42,46,52,54	0
3	SO4	С	603	5/5	0.98	0.20	49,57,62,62	0
3	SO4	D	602	5/5	0.99	0.12	47,47,56,56	0

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.











## 6.5 Other polymers (i)

There are no such residues in this entry.

