



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 10:46 pm BST

PDB ID : 5OIZ  
Title : Penicillin-Binding Protein 2X (PBP2X) from *Streptococcus pneumoniae* in complex with oxacillin  
Authors : Bernardo-Garcia, N.; Hermoso, J.A.  
Deposited on : 2017-07-20  
Resolution : 2.70 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.

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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	:	1.8.5 (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

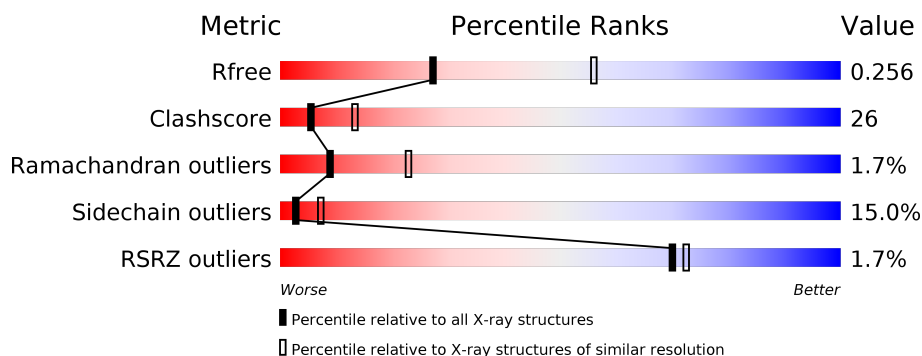
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	702	<div> <div>2%</div> <div> <div></div> <div>49%</div> <div>34%</div> <div>9%</div> <div>7%</div> </div> </div>

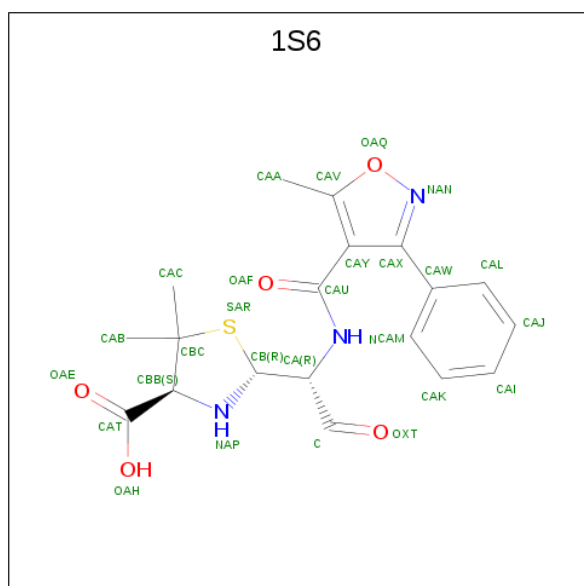


In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Penicillin-binding protein 2X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	651	Total	C	N	O	S	0	0	0
			4994	3131	831	1009	23			

- Molecule 2 is (2R,4S)-5,5-dimethyl-2-[(1R)-1-[(5-methyl-3-phenyl-1,2-oxazol-4-yl)carbon  
yl]amino}-2-oxoethyl]-1,3-thiazolidine-4-carboxylic acid (three-letter code: 1S6) (formula:  
 $\text{C}_{19}\text{H}_{21}\text{N}_3\text{O}_5\text{S}$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			28	19	3	5	1		

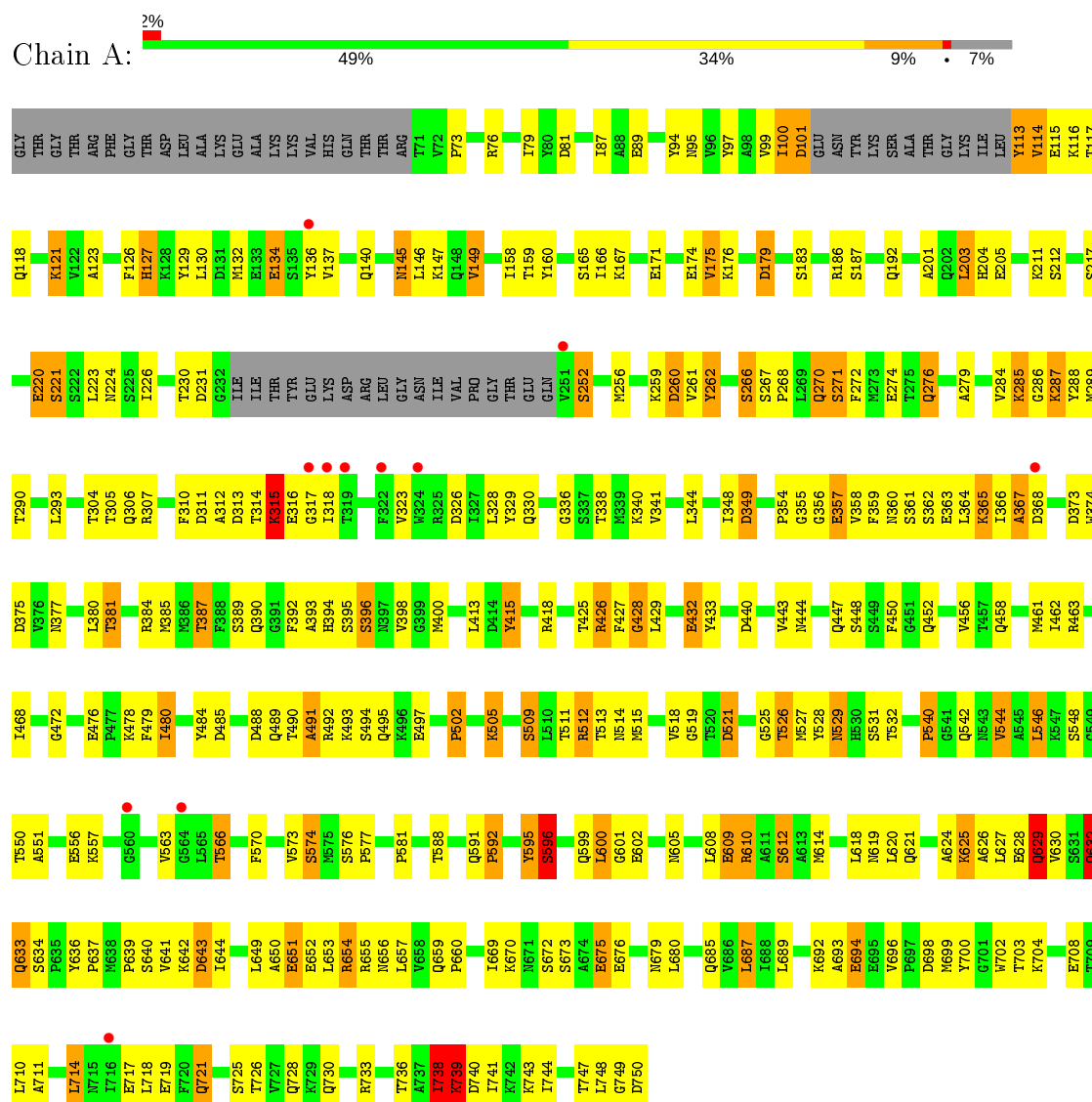
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	100	Total O 100 100	0	0

### 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: Penicillin-binding protein 2X



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.42Å 100.42Å 189.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.54 – 2.70 48.54 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.54-2.70) 100.0 (48.54-2.70)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.34 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.217 , 0.281 0.207 , 0.256	Depositor DCC
$R_{free}$ test set	1601 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.2	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 59.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.046 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5122	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1S6

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	1.40	21/5081 (0.4%)	1.28	18/6883 (0.3%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	694	GLU	CD-OE1	7.58	1.33	1.25
1	A	596	SER	CB-OG	7.40	1.51	1.42
1	A	595	TYR	CE1-CZ	6.94	1.47	1.38
1	A	367	ALA	CA-C	6.55	1.70	1.52
1	A	415	TYR	CG-CD2	6.33	1.47	1.39
1	A	609	GLU	CD-OE2	6.29	1.32	1.25
1	A	602	GLU	CD-OE2	6.09	1.32	1.25
1	A	700	TYR	CE1-CZ	-5.78	1.31	1.38
1	A	160	TYR	CE1-CZ	5.74	1.46	1.38
1	A	220	GLU	CD-OE1	-5.39	1.19	1.25
1	A	502	PRO	N-CA	-5.35	1.38	1.47
1	A	134	GLU	CD-OE1	5.29	1.31	1.25
1	A	362	SER	CB-OG	-5.28	1.35	1.42
1	A	525	GLY	N-CA	5.28	1.53	1.46
1	A	702	TRP	CB-CG	-5.26	1.40	1.50
1	A	632	GLN	CG-CD	5.22	1.63	1.51
1	A	433	TYR	CB-CG	-5.08	1.44	1.51
1	A	491	ALA	CA-C	5.08	1.66	1.52
1	A	266	SER	C-O	5.06	1.32	1.23
1	A	595	TYR	CG-CD2	5.02	1.45	1.39
1	A	432	GLU	C-O	5.01	1.32	1.23

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	426	ARG	NE-CZ-NH1	9.65	125.13	120.30
1	A	89	GLU	CB-CA-C	-6.86	96.69	110.40
1	A	260	ASP	CB-CG-OD1	-6.72	112.25	118.30
1	A	440	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	A	349	ASP	CB-CG-OD1	6.22	123.90	118.30
1	A	738	ILE	CG1-CB-CG2	-6.16	97.84	111.40
1	A	491	ALA	O-C-N	-6.08	112.97	122.70
1	A	521	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	566	THR	CB-CA-C	-5.85	95.82	111.60
1	A	629	GLN	CA-CB-CG	5.63	125.80	113.40
1	A	512	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	81	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	A	610	ARG	NE-CZ-NH2	5.43	123.01	120.30
1	A	418	ARG	NE-CZ-NH2	5.40	123.00	120.30
1	A	714	LEU	CA-CB-CG	-5.20	103.35	115.30
1	A	433	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	A	463	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	A	262	TYR	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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	4994	0	4907	259	9
2	A	28	0	19	2	0
3	A	100	0	0	6	1
All	All	5122	0	4926	259	10

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 26.

All (259) 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:491:ALA:C	1:A:632:GLN:NE2	1.69	1.40
1:A:491:ALA:CB	1:A:632:GLN:OE1	1.78	1.31
1:A:491:ALA:CA	1:A:632:GLN:OE1	1.80	1.27
1:A:491:ALA:HB3	1:A:632:GLN:OE1	1.30	1.25
1:A:175:VAL:N	1:A:176:LYS:HZ2	1.43	1.15
1:A:174:GLU:C	1:A:176:LYS:HZ2	1.49	1.15
1:A:212:SER:O	3:A:901:HOH:O	1.63	1.15
1:A:717:GLU:O	1:A:718:LEU:HD23	1.48	1.14
1:A:491:ALA:H	1:A:632:GLN:CG	1.62	1.12
1:A:174:GLU:C	1:A:176:LYS:NZ	2.03	1.09
1:A:692:LYS:NZ	3:A:902:HOH:O	1.88	1.07
1:A:491:ALA:CA	1:A:632:GLN:CD	2.22	1.06
1:A:491:ALA:H	1:A:632:GLN:CD	1.57	1.06
1:A:491:ALA:O	1:A:632:GLN:CD	1.94	1.06
1:A:276:GLN:HA	1:A:276:GLN:HE21	1.22	1.03
1:A:491:ALA:N	1:A:632:GLN:CD	2.11	1.03
1:A:491:ALA:C	1:A:632:GLN:CD	2.21	0.96
1:A:338:THR:HG23	1:A:461:MET:CE	1.95	0.95
1:A:694:GLU:O	1:A:738:ILE:HG22	1.65	0.95
1:A:204:HIS:N	3:A:901:HOH:O	1.94	0.92
1:A:349:ASP:OD2	1:A:415:TYR:OH	1.87	0.91
1:A:566:THR:HG21	1:A:592:PRO:O	1.70	0.91
1:A:326:ASP:H	1:A:330:GLN:NE2	1.68	0.91
1:A:175:VAL:N	1:A:176:LYS:NZ	2.14	0.90
1:A:497:GLU:OE2	1:A:654:ARG:NH1	2.05	0.89
1:A:326:ASP:N	1:A:330:GLN:HE21	1.70	0.89
1:A:491:ALA:O	1:A:632:GLN:NE2	0.74	0.89
1:A:636:TYR:H	1:A:679:ASN:HD21	1.20	0.89
1:A:636:TYR:H	1:A:679:ASN:ND2	1.71	0.88
1:A:630:VAL:HG22	1:A:632:GLN:HB2	1.53	0.88
1:A:608:LEU:O	1:A:612:SER:OG	1.91	0.87
1:A:270:GLN:O	1:A:270:GLN:NE2	2.08	0.86
1:A:338:THR:HG23	1:A:461:MET:HE2	1.56	0.85
1:A:174:GLU:CA	1:A:176:LYS:NZ	2.39	0.85
1:A:480:ILE:HD11	1:A:657:LEU:HD21	1.58	0.85
1:A:174:GLU:CA	1:A:176:LYS:HZ2	1.92	0.83
1:A:491:ALA:N	1:A:632:GLN:CG	2.39	0.83
1:A:174:GLU:HA	1:A:176:LYS:NZ	1.94	0.82
1:A:566:THR:CG2	1:A:592:PRO:O	2.27	0.81
1:A:480:ILE:CD1	1:A:657:LEU:HD21	2.10	0.81
1:A:491:ALA:N	1:A:632:GLN:OE1	2.10	0.79
1:A:76:ARG:NH1	1:A:220:GLU:OE1	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:VAL:O	1:A:113:TYR:N	2.18	0.76
1:A:628:GLU:O	1:A:629:GLN:HB2	1.83	0.76
1:A:495:GLN:OE1	3:A:904:HOH:O	2.07	0.72
1:A:491:ALA:H	1:A:632:GLN:HG3	1.53	0.72
1:A:100:ILE:HD12	1:A:101:ASP:N	2.04	0.72
1:A:480:ILE:HD11	1:A:657:LEU:CD2	2.19	0.72
1:A:480:ILE:HD11	1:A:657:LEU:HD11	1.71	0.71
1:A:326:ASP:H	1:A:330:GLN:HE21	0.85	0.70
1:A:625:LYS:N	1:A:628:GLU:OE2	2.24	0.70
1:A:518:VAL:O	1:A:526:THR:O	2.09	0.70
1:A:649:LEU:C	1:A:649:LEU:HD23	2.12	0.69
1:A:276:GLN:HA	1:A:276:GLN:NE2	2.02	0.69
1:A:625:LYS:NZ	3:A:903:HOH:O	1.93	0.69
1:A:627:LEU:C	1:A:628:GLU:HG3	2.11	0.68
1:A:628:GLU:O	1:A:629:GLN:CB	2.42	0.67
1:A:717:GLU:C	1:A:718:LEU:HD23	2.15	0.67
1:A:203:LEU:HA	3:A:901:HOH:O	1.94	0.67
1:A:126:PHE:O	1:A:130:LEU:N	2.28	0.66
1:A:673:SER:HB3	1:A:687:LEU:H	1.59	0.66
1:A:627:LEU:O	1:A:628:GLU:HG3	1.96	0.66
1:A:624:ALA:C	1:A:628:GLU:OE2	2.34	0.66
1:A:480:ILE:CG1	1:A:657:LEU:HD21	2.26	0.66
1:A:117:THR:O	1:A:121:LYS:NZ	2.28	0.66
1:A:694:GLU:C	1:A:738:ILE:HG22	2.17	0.65
1:A:338:THR:HG23	1:A:461:MET:HE1	1.78	0.64
1:A:287:LYS:HB2	1:A:591:GLN:HB2	1.79	0.64
1:A:480:ILE:HD11	1:A:657:LEU:CD1	2.29	0.63
1:A:649:LEU:HD23	1:A:650:ALA:N	2.13	0.63
1:A:491:ALA:C	1:A:632:GLN:OE1	2.29	0.63
1:A:360:ASN:ND2	1:A:385:MET:SD	2.70	0.63
1:A:115:GLU:O	1:A:118:GLN:N	2.32	0.63
1:A:529:ASN:O	1:A:532:THR:O	2.17	0.62
1:A:267:SER:O	1:A:271:SER:OG	2.17	0.62
1:A:174:GLU:C	1:A:176:LYS:HZ1	2.00	0.62
1:A:577:PRO:HD2	1:A:581:PRO:HA	1.80	0.61
1:A:696:VAL:HG23	1:A:736:THR:O	2.00	0.61
1:A:311:ASP:O	1:A:313:ASP:N	2.34	0.61
1:A:614:MET:HG3	1:A:618:LEU:CD1	2.31	0.61
1:A:721:GLN:O	1:A:747:THR:HA	2.00	0.60
1:A:728:GLN:HE21	1:A:749:GLY:HA3	1.65	0.60
1:A:217:SER:C	1:A:221:SER:OG	2.39	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:TYR:N	1:A:679:ASN:HD21	1.98	0.60
1:A:488:ASP:O	1:A:489:GLN:HG2	2.02	0.60
1:A:338:THR:CG2	1:A:461:MET:CE	2.75	0.59
1:A:563:VAL:HG23	1:A:563:VAL:O	2.02	0.59
1:A:601:GLY:O	1:A:605:ASN:HB2	2.02	0.59
1:A:497:GLU:CD	1:A:654:ARG:NH1	2.55	0.59
1:A:94:TYR:O	1:A:158:ILE:HG22	2.03	0.59
1:A:497:GLU:CD	1:A:654:ARG:HH12	2.03	0.59
1:A:725:SER:OG	1:A:726:THR:N	2.33	0.59
1:A:226:ILE:O	1:A:259:LYS:HB2	2.03	0.58
1:A:354:PRO:HB2	1:A:357:GLU:HB3	1.84	0.58
1:A:596:SER:O	1:A:599:GLN:HG2	2.03	0.58
1:A:637:PRO:O	1:A:639:PRO:HD3	2.03	0.58
1:A:286:GLY:HA3	1:A:289:MET:HE3	1.86	0.57
1:A:511:THR:O	1:A:515:MET:HG3	2.04	0.57
1:A:338:THR:CG2	1:A:461:MET:HE2	2.30	0.57
1:A:493:LYS:NZ	1:A:627:LEU:O	2.36	0.57
1:A:428:GLY:HA3	1:A:479:PHE:CE1	2.39	0.57
1:A:340:LYS:HG2	1:A:400:MET:HG3	1.86	0.56
1:A:447:GLN:HA	1:A:450:PHE:CE2	2.40	0.56
1:A:519:GLY:O	1:A:528:TYR:HB2	2.04	0.56
1:A:685:GLN:HE22	1:A:703:THR:H	1.53	0.56
1:A:698:ASP:OD2	1:A:699:MET:N	2.37	0.56
1:A:393:ALA:O	1:A:394:HIS:HB3	2.05	0.56
1:A:336:GLY:HA3	1:A:551:ALA:HB2	1.88	0.56
1:A:492:ARG:NH1	1:A:656:ASN:O	2.38	0.56
1:A:314:THR:HG22	1:A:316:GLU:HB2	1.88	0.56
1:A:614:MET:O	1:A:618:LEU:HD12	2.06	0.55
1:A:625:LYS:HE2	1:A:626:ALA:HA	1.89	0.55
1:A:698:ASP:C	1:A:698:ASP:OD2	2.45	0.55
1:A:484:TYR:HA	1:A:491:ALA:HB2	1.88	0.55
1:A:640:SER:HA	1:A:676:GLU:OE2	2.07	0.54
1:A:100:ILE:HD13	1:A:114:VAL:O	2.08	0.54
1:A:480:ILE:HG12	1:A:657:LEU:HD21	1.90	0.54
1:A:76:ARG:NH2	1:A:224:ASN:OD1	2.40	0.54
1:A:174:GLU:CA	1:A:176:LYS:HZ1	2.17	0.54
1:A:448:SER:HA	1:A:452:GLN:O	2.08	0.54
1:A:174:GLU:HA	1:A:176:LYS:CE	2.38	0.53
1:A:387:THR:HG22	1:A:390:GLN:OE1	2.08	0.53
1:A:305:THR:OG1	1:A:306:GLN:N	2.40	0.53
1:A:348:ILE:O	1:A:348:ILE:HG22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:PRO:HA	1:A:231:ASP:HB2	1.90	0.52
1:A:428:GLY:HA3	1:A:479:PHE:HE1	1.75	0.52
1:A:393:ALA:O	1:A:394:HIS:CB	2.58	0.52
1:A:344:LEU:O	1:A:348:ILE:HG13	2.10	0.52
1:A:373:ASP:OD1	1:A:396:SER:HA	2.10	0.52
1:A:490:THR:HB	1:A:632:GLN:HG2	1.91	0.52
1:A:595:TYR:CG	1:A:596:SER:N	2.78	0.51
1:A:649:LEU:O	1:A:653:LEU:HD23	2.09	0.51
1:A:610:ARG:O	1:A:614:MET:HG2	2.11	0.51
1:A:570:PHE:CE2	1:A:600:LEU:HD21	2.44	0.51
1:A:284:VAL:HG23	1:A:289:MET:CE	2.40	0.51
1:A:632:GLN:CG	1:A:633:GLN:H	2.23	0.51
1:A:179:ASP:C	1:A:179:ASP:OD1	2.49	0.51
1:A:205:GLU:OE2	1:A:211:LYS:NZ	2.44	0.51
1:A:252:SER:OG	1:A:252:SER:O	2.27	0.51
1:A:284:VAL:HG23	1:A:289:MET:HE1	1.91	0.51
1:A:285:LYS:HE3	1:A:285:LYS:O	2.10	0.50
1:A:344:LEU:HD22	1:A:392:PHE:CD1	2.46	0.50
1:A:472:GLY:O	1:A:502:PRO:HD2	2.12	0.50
1:A:145:ASN:O	1:A:146:LEU:HG	2.12	0.50
1:A:117:THR:C	1:A:121:LYS:NZ	2.65	0.50
1:A:728:GLN:HE21	1:A:749:GLY:CA	2.24	0.50
1:A:364:LEU:HD22	1:A:398:VAL:HG23	1.93	0.49
1:A:657:LEU:HD23	1:A:657:LEU:N	2.27	0.49
1:A:341:VAL:HG12	1:A:468:ILE:HD13	1.93	0.49
1:A:284:VAL:CG2	1:A:289:MET:HE1	2.41	0.49
1:A:389:SER:O	1:A:389:SER:OG	2.29	0.49
1:A:344:LEU:CD2	1:A:514:ASN:HD21	2.26	0.49
1:A:123:ALA:HA	1:A:137:VAL:HG11	1.95	0.49
1:A:718:LEU:HD22	1:A:744:ILE:HB	1.93	0.49
1:A:223:LEU:HD23	1:A:655:ARG:HD3	1.95	0.49
1:A:260:ASP:OD1	1:A:484:TYR:HB3	2.12	0.48
1:A:94:TYR:HB2	1:A:158:ILE:HG23	1.95	0.48
1:A:186:ARG:HD3	1:A:201:ALA:HB3	1.94	0.48
1:A:329:TYR:CZ	1:A:429:LEU:HD23	2.47	0.48
1:A:490:THR:HA	1:A:632:GLN:HG3	1.93	0.48
1:A:276:GLN:CA	1:A:276:GLN:HE21	2.07	0.48
1:A:266:SER:O	1:A:270:GLN:N	2.39	0.48
1:A:649:LEU:C	1:A:649:LEU:CD2	2.78	0.48
1:A:217:SER:CA	1:A:221:SER:OG	2.62	0.47
1:A:450:PHE:O	2:A:801:1S6:H6	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:THR:HG22	1:A:476:GLU:OE2	2.13	0.47
1:A:630:VAL:HG13	1:A:630:VAL:O	2.14	0.47
1:A:608:LEU:O	1:A:609:GLU:C	2.50	0.47
1:A:484:TYR:HA	1:A:491:ALA:CB	2.45	0.47
1:A:491:ALA:CA	1:A:632:GLN:NE2	2.62	0.47
1:A:381:THR:HG21	1:A:384:ARG:HD3	1.95	0.47
1:A:127:HIS:HB2	1:A:132:MET:O	2.15	0.47
1:A:329:TYR:OH	1:A:429:LEU:HD23	2.15	0.47
1:A:641:VAL:O	1:A:644:ILE:HG22	2.15	0.47
1:A:652:GLU:HA	1:A:655:ARG:NH1	2.29	0.47
1:A:714:LEU:HD23	1:A:714:LEU:HA	1.63	0.47
1:A:521:ASP:C	1:A:521:ASP:OD1	2.53	0.46
1:A:619:ASN:O	1:A:621:GLN:N	2.49	0.46
1:A:358:VAL:CG1	1:A:385:MET:HE3	2.45	0.46
1:A:675:GLU:HA	1:A:675:GLU:OE1	2.15	0.46
1:A:497:GLU:OE1	1:A:654:ARG:NH1	2.49	0.46
1:A:654:ARG:NH1	1:A:660:PRO:HD2	2.31	0.46
1:A:739:LYS:N	1:A:739:LYS:HD3	2.31	0.45
1:A:217:SER:C	1:A:221:SER:HG	2.19	0.45
1:A:478:LYS:NZ	1:A:495:GLN:O	2.49	0.45
1:A:304:THR:HG23	1:A:304:THR:O	2.15	0.45
1:A:694:GLU:C	1:A:738:ILE:CG2	2.85	0.45
1:A:694:GLU:O	1:A:738:ILE:CG2	2.52	0.45
1:A:192:GLN:HG2	1:A:274:GLU:OE1	2.17	0.45
1:A:443:VAL:HG13	1:A:444:ASN:N	2.32	0.45
1:A:614:MET:HG3	1:A:618:LEU:HD11	1.97	0.45
1:A:167:LYS:O	1:A:171:GLU:HG3	2.17	0.45
1:A:136:TYR:O	1:A:140:GLN:HG2	2.17	0.45
1:A:344:LEU:HD21	1:A:514:ASN:HD21	1.82	0.45
1:A:290:THR:HG21	1:A:458:GLN:OE1	2.16	0.45
1:A:340:LYS:HE3	1:A:450:PHE:HB2	2.00	0.44
1:A:550:THR:HG22	2:A:801:1S6:N	2.32	0.44
1:A:306:GLN:O	1:A:307:ARG:NH1	2.50	0.44
1:A:267:SER:N	1:A:268:PRO:CD	2.80	0.44
1:A:129:TYR:CE1	1:A:165:SER:HB3	2.53	0.44
1:A:413:LEU:HD23	1:A:413:LEU:HA	1.80	0.44
1:A:492:ARG:NH2	1:A:680:LEU:O	2.50	0.44
1:A:704:LYS:O	1:A:708:GLU:HG3	2.17	0.44
1:A:137:VAL:O	1:A:140:GLN:HB2	2.17	0.44
1:A:166:ILE:O	1:A:167:LYS:C	2.55	0.44
1:A:364:LEU:HD13	1:A:398:VAL:CG2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:TYR:CE1	1:A:627:LEU:HD21	2.54	0.43
1:A:527:MET:HA	1:A:527:MET:HE2	2.00	0.43
1:A:544:VAL:HG22	1:A:546:LEU:HD23	2.00	0.43
1:A:588:THR:O	1:A:588:THR:HG23	2.19	0.43
1:A:591:GLN:N	1:A:592:PRO:HD3	2.33	0.43
1:A:311:ASP:O	1:A:312:ALA:HB3	2.17	0.43
1:A:636:TYR:CZ	1:A:656:ASN:ND2	2.86	0.43
1:A:310:PHE:HB3	1:A:317:GLY:HA3	2.01	0.43
1:A:636:TYR:CE2	1:A:656:ASN:ND2	2.87	0.43
1:A:710:LEU:O	1:A:711:ALA:HB3	2.19	0.42
1:A:741:ILE:HG22	1:A:743:LYS:N	2.34	0.42
1:A:359:PHE:HE2	1:A:398:VAL:HG13	1.84	0.42
1:A:272:PHE:CE1	1:A:610:ARG:HD2	2.54	0.42
1:A:491:ALA:N	1:A:632:GLN:HG2	2.31	0.42
1:A:573:VAL:CG2	1:A:574:SER:N	2.83	0.42
1:A:573:VAL:HG22	1:A:574:SER:N	2.35	0.42
1:A:118:GLN:HE21	1:A:118:GLN:HA	1.85	0.42
1:A:314:THR:O	1:A:314:THR:HG22	2.19	0.42
1:A:394:HIS:CG	1:A:394:HIS:O	2.73	0.42
1:A:272:PHE:CZ	1:A:610:ARG:HD2	2.54	0.42
1:A:747:THR:C	1:A:748:LEU:HD23	2.41	0.41
1:A:287:LYS:HD3	1:A:288:TYR:CE2	2.54	0.41
1:A:480:ILE:C	1:A:480:ILE:HD12	2.40	0.41
1:A:318:ILE:HD12	1:A:318:ILE:N	2.36	0.41
1:A:387:THR:HG23	1:A:390:GLN:CG	2.50	0.41
1:A:505:LYS:O	1:A:509:SER:OG	2.37	0.41
1:A:270:GLN:HE22	1:A:274:GLU:HG2	1.85	0.41
1:A:262:TYR:CZ	1:A:627:LEU:HD21	2.56	0.41
1:A:490:THR:HA	1:A:632:GLN:CG	2.50	0.41
1:A:642:LYS:O	1:A:643:ASP:C	2.58	0.41
1:A:284:VAL:CG2	1:A:289:MET:CE	2.99	0.41
1:A:286:GLY:HA3	1:A:289:MET:CE	2.49	0.41
1:A:485:ASP:HB3	1:A:488:ASP:OD1	2.20	0.41
1:A:488:ASP:O	1:A:490:THR:HG23	2.20	0.41
1:A:217:SER:O	1:A:221:SER:OG	2.38	0.41
1:A:364:LEU:HD13	1:A:398:VAL:HG21	2.02	0.41
1:A:512:ARG:O	1:A:515:MET:HB2	2.20	0.41
1:A:739:LYS:HG2	1:A:740:ASP:N	2.36	0.41
1:A:738:ILE:O	1:A:740:ASP:N	2.54	0.41
1:A:426:ARG:N	1:A:432:GLU:OE1	2.47	0.41
1:A:497:GLU:HG3	1:A:659:GLN:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:VAL:HG13	1:A:669:ILE:CG2	2.50	0.41
1:A:311:ASP:O	1:A:311:ASP:OD1	2.39	0.40
1:A:276:GLN:O	1:A:279:ALA:N	2.55	0.40
1:A:314:THR:O	1:A:315:LYS:C	2.59	0.40
1:A:429:LEU:O	1:A:651:GLU:OE2	2.40	0.40
1:A:79:ILE:O	1:A:87:ILE:HB	2.22	0.40
1:A:374:TRP:CG	1:A:375:ASP:N	2.90	0.40
1:A:653:LEU:N	1:A:653:LEU:CD2	2.84	0.40
1:A:115:GLU:O	1:A:116:LYS:C	2.60	0.40
1:A:355:GLY:O	1:A:387:THR:OG1	2.32	0.40
1:A:356:GLY:O	1:A:387:THR:HB	2.21	0.40
1:A:693:ALA:O	1:A:738:ILE:HG21	2.21	0.40

All (10) 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)
3:A:963:HOH:O	3:A:976:HOH:O[6_665]	0.11	2.09
1:A:365:LYS:CE	1:A:367:ALA:C[5_554]	1.25	0.95
1:A:365:LYS:CE	1:A:367:ALA:O[5_554]	1.42	0.78
1:A:365:LYS:CE	1:A:367:ALA:CA[5_554]	1.48	0.72
1:A:365:LYS:CD	1:A:367:ALA:O[5_554]	1.62	0.58
1:A:365:LYS:NZ	1:A:367:ALA:N[5_554]	1.77	0.43
1:A:365:LYS:NZ	1:A:366:ILE:C[5_554]	1.80	0.40
1:A:365:LYS:NZ	1:A:367:ALA:C[5_554]	1.83	0.37
1:A:365:LYS:NZ	1:A:367:ALA:O[5_554]	1.94	0.26
1:A:365:LYS:NZ	1:A:367:ALA:CA[5_554]	2.00	0.20

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	645/702 (92%)	567 (88%)	67 (10%)	11 (2%)	9	23

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	315	LYS
1	A	396	SER
1	A	620	LEU
1	A	633	GLN
1	A	739	LYS
1	A	357	GLU
1	A	380	LEU
1	A	643	ASP
1	A	428	GLY
1	A	540	PRO
1	A	149	VAL

### 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	548/590 (93%)	466 (85%)	82 (15%)	3	7

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	97	TYR
1	A	100	ILE
1	A	101	ASP
1	A	113	TYR
1	A	114	VAL
1	A	121	LYS
1	A	127	HIS
1	A	134	GLU
1	A	145	ASN

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Mol	Chain	Res	Type
1	A	147	LYS
1	A	149	VAL
1	A	159	THR
1	A	175	VAL
1	A	179	ASP
1	A	183	SER
1	A	187	SER
1	A	203	LEU
1	A	221	SER
1	A	230	THR
1	A	252	SER
1	A	256	MET
1	A	261	VAL
1	A	270	GLN
1	A	271	SER
1	A	276	GLN
1	A	285	LYS
1	A	287	LYS
1	A	293	LEU
1	A	315	LYS
1	A	323	VAL
1	A	328	LEU
1	A	361	SER
1	A	363	GLU
1	A	365	LYS
1	A	368	ASP
1	A	377	ASN
1	A	381	THR
1	A	387	THR
1	A	395	SER
1	A	427	PHE
1	A	456	VAL
1	A	462	ILE
1	A	480	ILE
1	A	494	SER
1	A	505	LYS
1	A	509	SER
1	A	513	THR
1	A	526	THR
1	A	529	ASN
1	A	531	SER
1	A	540	PRO

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Mol	Chain	Res	Type
1	A	542	GLN
1	A	544	VAL
1	A	546	LEU
1	A	548	SER
1	A	556	GLU
1	A	557	LYS
1	A	574	SER
1	A	576	SER
1	A	592	PRO
1	A	596	SER
1	A	600	LEU
1	A	612	SER
1	A	625	LYS
1	A	629	GLN
1	A	632	GLN
1	A	634	SER
1	A	651	GLU
1	A	654	ARG
1	A	670	LYS
1	A	672	SER
1	A	675	GLU
1	A	687	LEU
1	A	689	LEU
1	A	719	GLU
1	A	721	GLN
1	A	730	GLN
1	A	733	ARG
1	A	738	ILE
1	A	739	LYS
1	A	750	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	202	GLN
1	A	276	GLN
1	A	330	GLN
1	A	394	HIS
1	A	397	ASN
1	A	444	ASN
1	A	447	GLN

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Mol	Chain	Res	Type
1	A	656	ASN
1	A	659	GLN
1	A	679	ASN
1	A	685	GLN
1	A	728	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	1S6	A	801	1	20,30,30	2.24	6 (30%)	23,44,44	1.45	5 (21%)

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	1S6	A	801	1	-	0/8/37/37	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	1S6	CAY-CAX	7.72	1.50	1.41
2	A	801	1S6	CAX-NAN	3.23	1.39	1.33
2	A	801	1S6	CBB-NAP	2.66	1.50	1.46
2	A	801	1S6	CBC-SAR	-2.50	1.80	1.85
2	A	801	1S6	OAF-CAU	2.42	1.28	1.23
2	A	801	1S6	OXT-C	2.05	1.28	1.19

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	1S6	OAF-CAU-N	3.05	128.06	122.45
2	A	801	1S6	CA-N-CAU	2.85	126.71	122.26
2	A	801	1S6	OXT-C-CA	-2.78	117.09	124.83
2	A	801	1S6	CB-CA-N	-2.64	104.22	109.98
2	A	801	1S6	CBB-CBC-SAR	2.53	108.81	103.81

There are no chirality outliers.

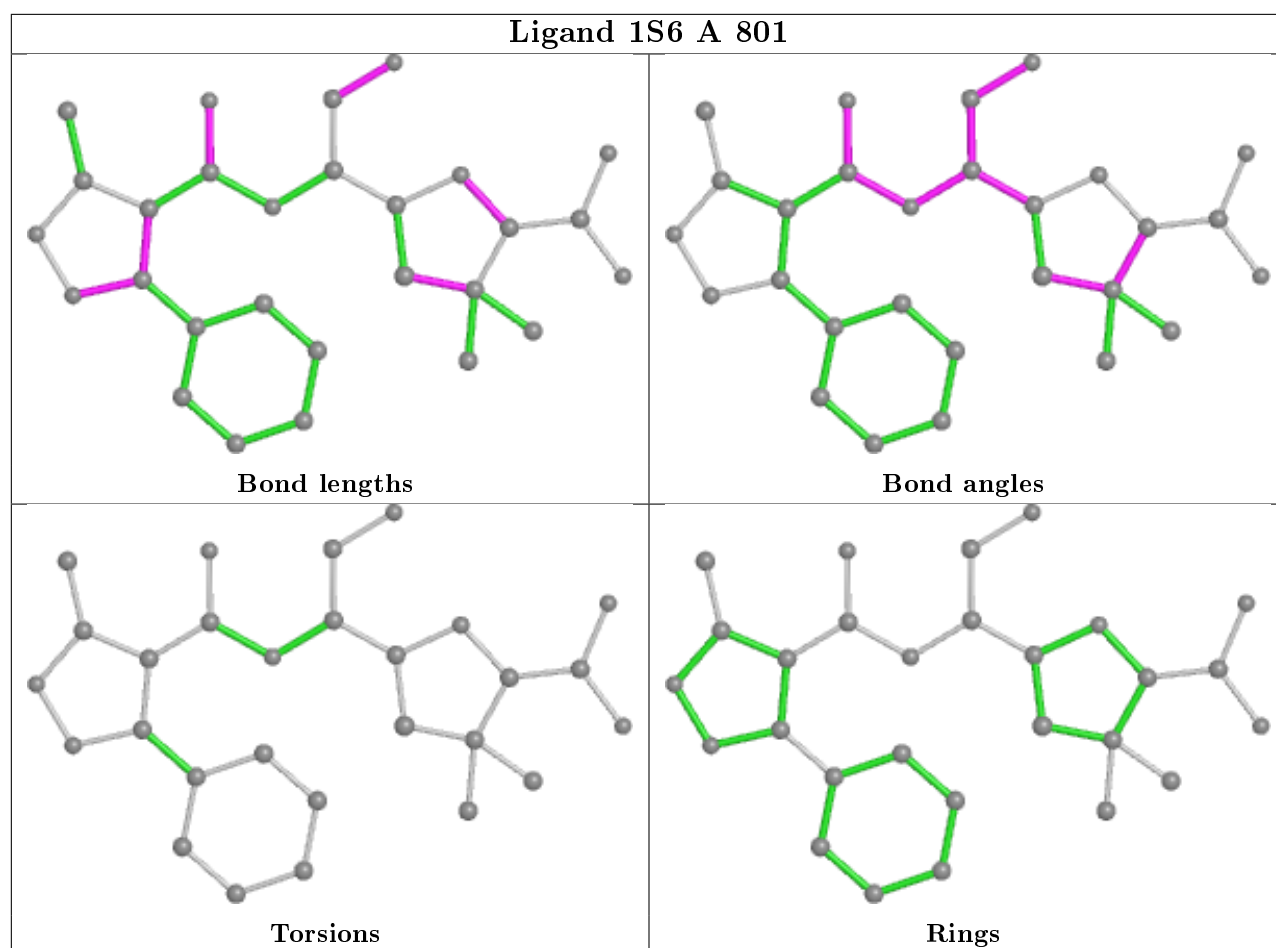
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	1S6	2	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 [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	651/702 (92%)	-0.13	11 (1%) 70 72	52, 62, 74, 84	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	318	ILE	3.3
1	A	716	ILE	2.9
1	A	560	GLY	2.8
1	A	319	THR	2.7
1	A	251	VAL	2.6
1	A	324	TRP	2.6
1	A	317	GLY	2.5
1	A	368	ASP	2.5
1	A	136	TYR	2.3
1	A	564	GLY	2.1
1	A	322	PHE	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 [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,

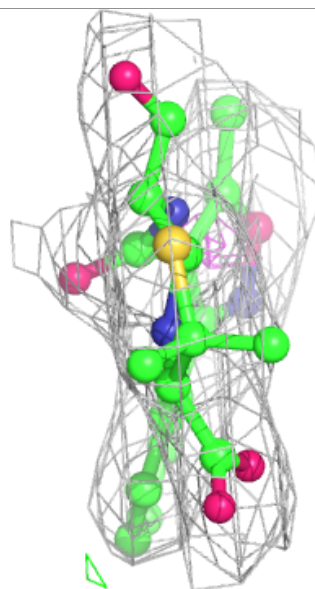
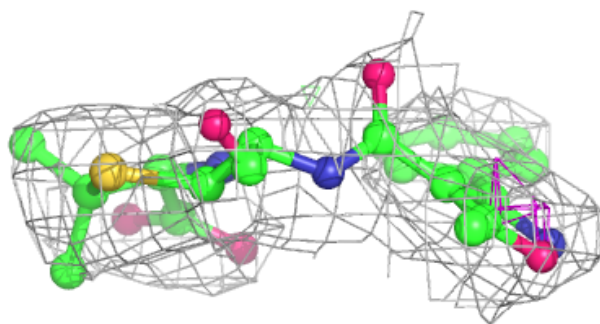
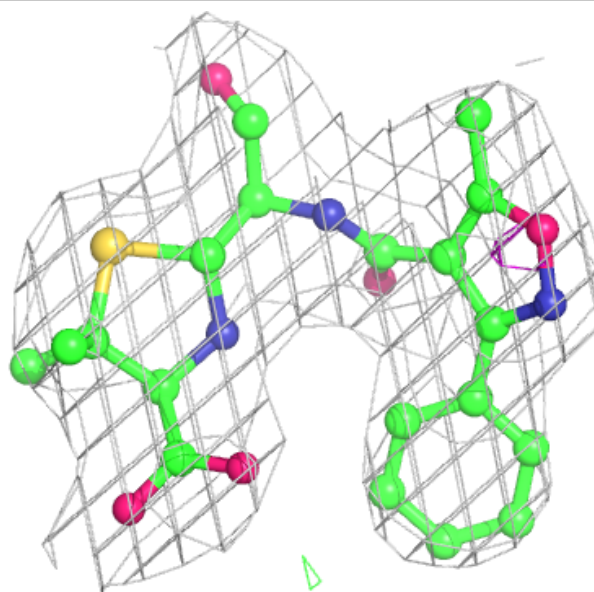
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	1S6	A	801	28/28	0.93	0.20	57,65,69,75	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.

**Electron density around 1S6 A 801:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.