



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 06:11 PM BST

PDB ID : 4HHZ  
Title : Crystal structure of PARP catalytic domain in complex with novel inhibitors  
Authors : Liu, Q.F.; Chen, T.T.; Xu, Y.C.  
Deposited on : 2012-10-10  
Resolution : 2.72 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 : 2.13.1  
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) : 2.13.1

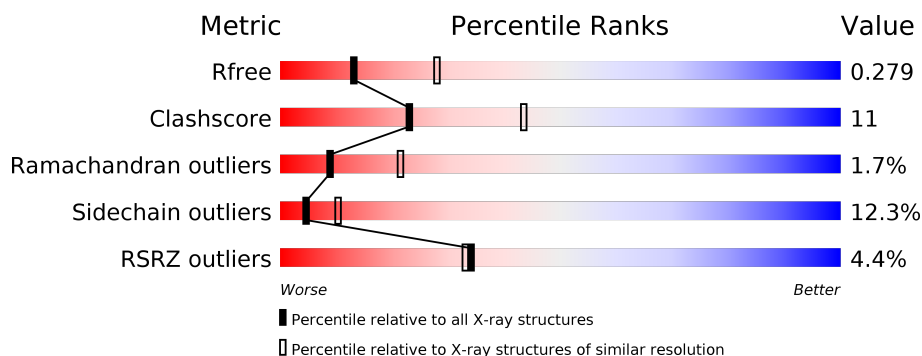
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.72 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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	355	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>28%</div> <div>• •</div> </div> </div>
1	B	355	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>28%</div> <div>• •</div> </div> </div>
1	C	355	<div> <div>5%</div> <div> <div></div> <div>65%</div> <div>29%</div> <div>• •</div> </div> </div>
1	D	355	<div> <div>8%</div> <div> <div></div> <div>51%</div> <div>27%</div> <div>• •</div> <div>17%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10753 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.

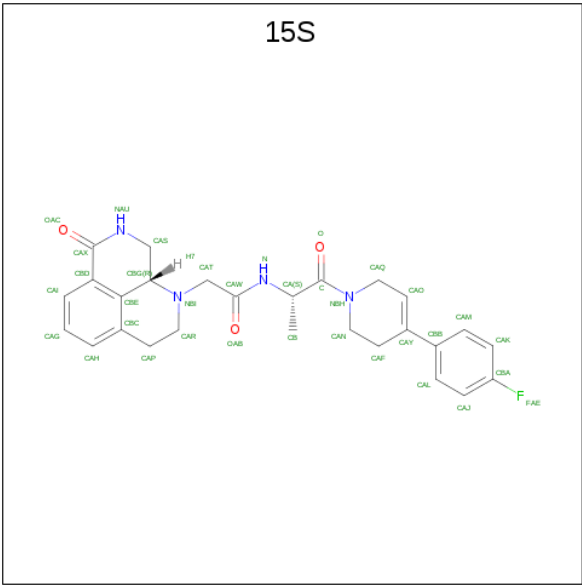
- Molecule 1 is a protein called Poly [ADP-ribose] polymerase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2744	1746	464	523	11			
1	B	350	Total	C	N	O	S	0	0	0
			2748	1749	465	523	11			
1	C	350	Total	C	N	O	S	0	0	0
			2748	1749	465	523	11			
1	D	296	Total	C	N	O	S	0	0	0
			2334	1492	394	439	9			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	EXPRESSION TAG	UNP P09874
A	-3	PRO	-	EXPRESSION TAG	UNP P09874
A	-2	LEU	-	EXPRESSION TAG	UNP P09874
A	0	SER	THR	CONFLICT	UNP P09874
A	101	ALA	VAL	CONFLICT	UNP P09874
B	-4	GLY	-	EXPRESSION TAG	UNP P09874
B	-3	PRO	-	EXPRESSION TAG	UNP P09874
B	-2	LEU	-	EXPRESSION TAG	UNP P09874
B	0	SER	THR	CONFLICT	UNP P09874
B	101	ALA	VAL	CONFLICT	UNP P09874
C	-4	GLY	-	EXPRESSION TAG	UNP P09874
C	-3	PRO	-	EXPRESSION TAG	UNP P09874
C	-2	LEU	-	EXPRESSION TAG	UNP P09874
C	0	SER	THR	CONFLICT	UNP P09874
C	101	ALA	VAL	CONFLICT	UNP P09874
D	-4	GLY	-	EXPRESSION TAG	UNP P09874
D	-3	PRO	-	EXPRESSION TAG	UNP P09874
D	-2	LEU	-	EXPRESSION TAG	UNP P09874
D	0	SER	THR	CONFLICT	UNP P09874
D	101	ALA	VAL	CONFLICT	UNP P09874

- Molecule 2 is N-{(2S)-1-[4-(4-fluorophenyl)-3,6-dihydropyridin-1(2H)-yl]-1-oxopropan-2-yl}-2-[(9aR)-7-oxo-2,3,7,8,9a-hexahydro-1H-benzo[de][1,7]naphthyridin-1-yl]acetamide (three-letter code: 15S) (formula: C<sub>27</sub>H<sub>29</sub>FN<sub>4</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			35	27	1	4	3		
2	B	1	Total	C	F	N	O	0	0
			35	27	1	4	3		
2	C	1	Total	C	F	N	O	0	0
			35	27	1	4	3		
2	D	1	Total	C	F	N	O	0	0
			35	27	1	4	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O	0	0
			6	6		
4	B	9	Total	O	0	0
			9	9		
4	C	7	Total	O	0	0
			7	7		
4	D	2	Total	O	0	0
			2	2		



- Molecule 1: Poly [ADP-ribose] polymerase 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.02Å 107.26Å 142.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.43 – 2.72 48.43 – 2.72	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.43-2.72) 100.0 (48.43-2.72)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.04 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, $R_{free}$	0.205 , 0.275 0.209 , 0.279	Depositor DCC
$R_{free}$ test set	1291 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.7	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.021 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10753	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: 15S, SO4

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	0.52	0/2796	0.67	0/3773
1	B	0.50	0/2800	0.66	0/3779
1	C	0.45	0/2800	0.65	0/3779
1	D	0.44	0/2376	0.62	0/3204
All	All	0.48	0/10772	0.65	0/14535

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	A	2744	0	2787	52	0
1	B	2748	0	2792	57	0
1	C	2748	0	2792	63	0
1	D	2334	0	2352	82	0
2	A	35	0	29	1	0
2	B	35	0	29	4	0
2	C	35	0	29	2	0
2	D	35	0	29	4	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
3	D	5	0	0	1	0
4	A	6	0	0	1	0
4	B	9	0	0	0	0
4	C	7	0	0	0	0
4	D	2	0	0	0	0
All	All	10753	0	10839	245	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 11.

All (245) 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:33:GLN:HG3	1:B:36:PRO:HB3	1.44	0.98
1:B:35:MET:HE3	1:B:80:PRO:HD2	1.51	0.93
1:D:185:GLN:HB3	1:D:188:LYS:HB2	1.62	0.81
1:B:30:ILE:HD11	1:B:107:LEU:HD11	1.62	0.81
1:B:257:LEU:HD22	1:B:341:LEU:HD21	1.63	0.81
1:D:228:TYR:HE2	2:D:401:15S:H21	1.49	0.77
1:D:260:LEU:HB2	1:D:340:TYR:HB2	1.68	0.74
1:B:109:ASP:OD1	1:B:217:ARG:NH2	2.21	0.73
1:D:144:ASP:HB2	1:D:147:SER:HB3	1.71	0.72
1:D:45:ILE:HA	1:D:222:GLU:HB3	1.73	0.70
1:D:292:LYS:HE2	1:D:319:ASN:HB2	1.74	0.69
2:A:401:15S:H20	2:A:401:15S:H28	1.74	0.68
1:D:217:ARG:O	2:D:401:15S:H25	1.94	0.67
1:C:64:SER:HB3	1:C:67:GLN:HB2	1.76	0.67
1:D:139:ASP:OD1	1:D:141:LYS:NZ	2.26	0.67
1:D:44:GLN:HA	1:D:45:ILE:HG23	1.77	0.67
1:B:180:ARG:HD2	1:B:212:LEU:O	1.96	0.66
1:B:65:ASP:O	1:B:67:GLN:N	2.25	0.66
1:B:14:MET:HE1	1:B:343:LYS:HE3	1.78	0.66
1:A:281:PRO:HG2	1:A:284:LYS:HG3	1.78	0.66
2:B:401:15S:H20	2:B:401:15S:H28	1.76	0.65
1:C:171:GLU:OE2	1:C:347:ASN:ND2	2.31	0.64
1:C:272:LYS:HE3	1:C:318:VAL:HG13	1.81	0.63
1:B:220:PRO:HD3	2:B:401:15S:CBA	2.28	0.63
1:C:220:PRO:HD3	2:C:401:15S:CBA	2.29	0.62
1:C:277:ILE:HD12	1:C:278:SER:H	1.65	0.62
1:C:132:ASN:OD1	1:C:135:LYS:NZ	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:ILE:HG21	1:D:259:LEU:HD11	1.82	0.61
1:D:44:GLN:CB	1:D:45:ILE:HG12	2.30	0.61
1:D:28:TYR:OH	1:D:204:ARG:NH1	2.34	0.61
1:A:65:ASP:C	1:A:67:GLN:H	2.05	0.61
1:B:55:VAL:HG22	1:B:71:LEU:HB3	1.83	0.61
1:D:155:LYS:HB3	1:D:310:LEU:HD22	1.82	0.60
1:A:28:TYR:CG	1:A:103:MET:HG3	2.36	0.60
1:C:28:TYR:CG	1:C:103:MET:HG3	2.37	0.60
1:B:292:LYS:NZ	1:B:321:THR:O	2.36	0.59
1:C:199:LEU:HD12	1:C:263:VAL:HG13	1.84	0.59
1:A:28:TYR:CD1	1:A:103:MET:HG3	2.38	0.59
1:C:170:LEU:HG	1:C:344:LEU:HD13	1.85	0.59
1:C:17:ASP:OD1	1:C:20:SER:N	2.34	0.58
1:D:234:ILE:HD11	1:D:333:ILE:HG22	1.85	0.58
1:A:197:ARG:NH2	4:A:502:HOH:O	2.26	0.57
1:D:129:ILE:HD12	1:D:130:ASP:H	1.68	0.57
1:A:77:THR:HG21	1:C:251:GLN:HB2	1.84	0.57
1:A:255:ILE:HD13	1:A:255:ILE:H	1.69	0.57
1:C:217:ARG:HH11	1:C:217:ARG:HB2	1.69	0.57
1:D:156:TYR:HA	1:D:310:LEU:HB3	1.85	0.57
1:A:196:ARG:HG3	1:A:264:ALA:HA	1.87	0.57
1:C:151:GLU:HG2	1:C:154:ARG:HH12	1.70	0.57
1:C:55:VAL:O	1:C:57:GLN:N	2.38	0.57
1:B:56:GLN:O	1:B:59:VAL:HG12	2.06	0.56
1:C:162:ALA:HB3	1:C:165:HIS:CD2	2.40	0.56
1:C:73:ASN:O	1:C:77:THR:OG1	2.19	0.56
1:C:46:GLN:NE2	1:C:222:GLU:OE1	2.38	0.56
1:B:315:SER:OG	1:B:316:SER:O	2.23	0.56
1:D:150:ALA:O	1:D:154:ARG:HG3	2.06	0.56
1:D:162:ALA:HB1	1:D:325:TYR:CZ	2.41	0.56
1:C:290:LEU:HB3	1:C:318:VAL:HG21	1.86	0.56
1:D:25:MET:HE1	1:D:110:ILE:HG21	1.86	0.56
1:B:273:HIS:CG	1:D:320:ASP:HA	2.40	0.56
1:A:327:GLU:HG2	1:A:329:ILE:HD11	1.87	0.55
1:B:162:ALA:HB3	1:B:165:HIS:ND1	2.21	0.55
1:D:6:LYS:HB3	1:D:7:PRO:HD3	1.88	0.55
1:B:165:HIS:O	1:B:167:ALA:N	2.39	0.55
1:B:170:LEU:HG	1:B:344:LEU:HD13	1.87	0.55
1:C:276:HIS:ND1	1:C:276:HIS:O	2.40	0.55
1:A:180:ARG:HD2	1:A:212:LEU:O	2.07	0.53
1:C:229:MET:HG2	1:C:274:ALA:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:PRO:HD3	2:D:401:15S:CBA	2.38	0.53
1:D:148:GLU:H	1:D:148:GLU:CD	2.12	0.53
1:D:47:ALA:HB2	1:D:224:PRO:HD3	1.91	0.53
1:D:160:THR:HB	1:D:239:MET:HA	1.89	0.53
1:D:28:TYR:CG	1:D:103:MET:HG3	2.44	0.53
1:D:165:HIS:CD2	1:D:245:ASN:HD21	2.27	0.53
1:D:324:LEU:HB2	3:D:402:SO4:O2	2.09	0.53
1:B:40:LEU:O	1:B:111:GLU:HG3	2.09	0.52
1:B:197:ARG:HG2	1:B:307:ASP:HB2	1.90	0.52
1:B:70:ASP:O	1:B:74:ARG:HG3	2.09	0.52
1:B:51:ILE:O	1:B:55:VAL:HG23	2.10	0.52
1:C:257:LEU:HD22	1:C:341:LEU:HD21	1.90	0.52
1:B:173:ILE:HD11	1:B:345:LYS:HB2	1.90	0.51
1:A:66:SER:HA	1:A:69:LEU:HB3	1.91	0.51
1:B:148:GLU:O	1:B:152:ILE:HG12	2.11	0.51
1:C:279:LYS:H	1:C:279:LYS:HD3	1.75	0.51
1:D:228:TYR:CE2	2:D:401:15S:H21	2.39	0.51
1:B:265:LEU:O	1:B:285:HIS:HB2	2.10	0.51
1:C:8:VAL:O	1:C:12:ILE:HG12	2.10	0.51
1:C:277:ILE:O	1:C:279:LYS:HD3	2.11	0.51
1:C:324:LEU:H	1:C:324:LEU:HD23	1.76	0.51
1:D:327:GLU:HG2	1:D:329:ILE:HD11	1.92	0.51
1:D:151:GLU:O	1:D:154:ARG:HD2	2.10	0.51
1:C:55:VAL:HG12	1:C:56:GLN:H	1.77	0.50
1:C:40:LEU:HD22	1:C:45:ILE:HD11	1.93	0.50
1:A:269:TYR:HE2	1:A:277:ILE:HG21	1.77	0.50
1:C:324:LEU:HG	1:C:325:TYR:H	1.76	0.50
1:C:162:ALA:HB1	1:C:325:TYR:CZ	2.47	0.49
1:D:277:ILE:HG21	1:D:280:LEU:HD13	1.94	0.49
1:C:228:TYR:CE1	2:C:401:15S:H22	2.47	0.49
1:D:169:ASP:N	1:D:169:ASP:OD1	2.46	0.49
1:D:186:ARG:O	1:D:189:PRO:HD2	2.13	0.49
1:D:185:GLN:HA	1:D:188:LYS:H	1.78	0.49
1:B:273:HIS:CE1	1:D:320:ASP:HA	2.48	0.48
1:C:281:PRO:HG2	1:C:284:LYS:HG3	1.95	0.48
1:D:44:GLN:HG2	1:D:78:LEU:HD22	1.95	0.48
1:A:180:ARG:HD3	1:A:338:LEU:HD12	1.95	0.48
1:A:320:ASP:N	1:A:320:ASP:OD2	2.43	0.48
1:D:14:MET:HE1	1:D:257:LEU:HD21	1.96	0.48
1:C:114:TYR:CZ	1:C:118:ARG:HG3	2.49	0.48
1:D:228:TYR:CE1	1:D:232:LYS:HG2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:TYR:OH	1:D:118:ARG:NH2	2.47	0.48
1:C:161:HIS:HE1	1:C:165:HIS:O	1.95	0.48
1:C:327:GLU:HG2	1:C:329:ILE:HD11	1.95	0.48
1:A:74:ARG:HE	1:A:74:ARG:HB3	1.49	0.47
1:D:109:ASP:OD1	1:D:217:ARG:NH2	2.47	0.47
1:D:151:GLU:HA	1:D:154:ARG:HH21	1.78	0.47
1:B:37:LEU:HD23	1:B:40:LEU:HD12	1.96	0.47
1:B:322:SER:HA	1:D:322:SER:HA	1.96	0.47
1:B:217:ARG:O	2:B:401:15S:H25	2.14	0.47
1:D:11:LEU:HG	1:D:15:ILE:HD11	1.95	0.47
1:D:251:GLN:HG3	1:D:252:GLY:N	2.29	0.47
1:B:127:ASP:O	1:B:131:VAL:HG23	2.14	0.47
1:C:78:LEU:HD12	1:C:78:LEU:HA	1.61	0.47
1:A:87:LYS:HE2	1:A:87:LYS:HB3	1.68	0.47
1:A:65:ASP:C	1:A:67:GLN:N	2.68	0.47
1:A:31:ASP:OD1	1:A:34:LYS:HG3	2.15	0.47
1:D:165:HIS:ND1	1:D:241:SER:HB3	2.29	0.47
1:B:37:LEU:HA	1:B:37:LEU:HD23	1.72	0.47
1:C:324:LEU:HB2	1:C:325:TYR:CD2	2.50	0.47
1:A:14:MET:HE3	1:A:14:MET:HB2	1.56	0.46
1:D:154:ARG:HD3	1:D:155:LYS:N	2.29	0.46
1:A:65:ASP:O	1:A:67:GLN:N	2.45	0.46
1:B:37:LEU:HB3	1:B:114:TYR:CG	2.50	0.46
1:D:239:MET:CE	1:D:295:PRO:HG3	2.46	0.46
1:A:260:LEU:HD23	1:A:260:LEU:HA	1.78	0.46
1:B:15:ILE:HD11	1:B:136:LEU:HD11	1.98	0.46
1:B:165:HIS:CD2	1:B:245:ASN:HD21	2.33	0.46
1:A:277:ILE:O	1:A:279:LYS:HG3	2.15	0.46
1:A:314:ILE:HG13	1:A:315:SER:O	2.15	0.46
1:B:40:LEU:HB3	1:B:111:GLU:HB2	1.98	0.46
1:A:160:THR:HB	1:A:239:MET:HA	1.98	0.45
1:A:211:ILE:HG21	1:A:259:LEU:HD11	1.98	0.45
1:A:252:GLY:HA3	1:B:252:GLY:CA	2.45	0.45
1:A:57:GLN:O	1:A:61:GLN:HB2	2.17	0.45
1:B:28:TYR:CG	1:B:103:MET:HG3	2.52	0.45
1:B:320:ASP:HA	1:D:273:HIS:CG	2.51	0.45
1:D:8:VAL:HG23	1:D:142:VAL:HG23	1.98	0.45
1:C:72:SER:HA	1:C:91:LEU:HD12	1.97	0.45
1:C:116:LEU:HA	1:C:116:LEU:HD23	1.82	0.45
1:A:32:LEU:HA	1:A:32:LEU:HD23	1.72	0.45
1:B:52:LEU:HD11	1:B:100:LYS:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:LEU:HA	1:C:260:LEU:HD23	1.72	0.45
1:D:257:LEU:HD23	1:D:343:LYS:HA	1.98	0.45
1:A:155:LYS:HE3	1:A:310:LEU:HD13	1.99	0.44
1:B:40:LEU:HD22	1:B:45:ILE:HD11	1.99	0.44
1:C:260:LEU:HB2	1:C:340:TYR:HB2	1.99	0.44
1:A:116:LEU:HD23	1:A:116:LEU:HA	1.75	0.44
1:A:190:PHE:CD1	1:A:335:GLN:HG2	2.53	0.44
1:C:122:ASP:HB2	1:C:124:SER:OG	2.17	0.44
1:C:296:ASP:HA	1:C:297:PRO:HD3	1.83	0.44
1:D:187:TYR:CE2	1:D:191:LYS:HA	2.53	0.44
1:A:100:LYS:HD3	1:A:100:LYS:HA	1.80	0.44
1:A:267:ASN:ND2	1:A:284:LYS:HD3	2.32	0.44
1:B:33:GLN:OE1	1:C:19:GLU:HG2	2.18	0.44
1:D:253:ASP:HA	1:D:254:PRO:HD3	1.83	0.44
1:B:273:HIS:CD2	1:D:320:ASP:HA	2.53	0.44
1:D:204:ARG:HG2	1:D:248:HIS:HB2	1.99	0.44
1:D:280:LEU:HD11	1:D:287:VAL:HG23	1.99	0.44
1:A:301:ILE:HA	1:A:301:ILE:HD12	1.60	0.44
2:B:401:15S:H35	2:B:401:15S:H29	1.51	0.44
1:D:28:TYR:CD1	1:D:103:MET:HG3	2.53	0.43
1:C:6:LYS:HB3	1:C:7:PRO:HD3	1.99	0.43
1:D:109:ASP:CG	1:D:217:ARG:HH22	2.22	0.43
1:A:1:LYS:HB3	1:A:2:SER:H	1.57	0.43
1:D:8:VAL:O	1:D:12:ILE:HG12	2.19	0.43
1:B:86:LYS:HG2	1:B:87:LYS:N	2.33	0.43
1:D:101:ALA:HA	1:D:104:LEU:HB2	1.99	0.43
1:D:269:TYR:CA	1:D:284:LYS:HD2	2.49	0.43
1:A:148:GLU:HA	1:A:151:GLU:HB2	2.00	0.43
1:A:164:THR:HG23	1:A:165:HIS:CD2	2.53	0.43
1:C:144:ASP:N	1:C:144:ASP:OD1	2.38	0.43
1:C:267:ASN:HB2	1:C:283:GLY:O	2.19	0.43
1:D:108:LEU:O	1:D:112:VAL:HG23	2.19	0.43
1:A:15:ILE:HD11	1:A:136:LEU:HD11	2.01	0.43
1:A:212:LEU:HA	1:A:212:LEU:HD23	1.76	0.43
1:C:197:ARG:HG3	1:C:307:ASP:HB2	2.01	0.43
1:C:36:PRO:HD2	1:C:39:LYS:HB3	2.01	0.43
1:A:203:SER:O	1:A:247:CYS:HA	2.19	0.42
1:A:295:PRO:HA	1:A:313:GLY:HA2	2.01	0.42
1:A:52:LEU:HD23	1:A:52:LEU:HA	1.90	0.42
1:B:211:ILE:HG21	1:B:259:LEU:HD11	1.99	0.42
1:D:44:GLN:HB2	1:D:45:ILE:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LEU:HD22	1:A:341:LEU:HD21	2.01	0.42
1:B:341:LEU:C	1:B:341:LEU:HD23	2.40	0.42
1:D:14:MET:HE1	1:D:343:LYS:HE2	2.01	0.42
1:C:338:LEU:O	1:C:339:LYS:HD2	2.20	0.42
1:D:11:LEU:O	1:D:15:ILE:HG13	2.18	0.42
1:D:279:LYS:HD3	1:D:280:LEU:O	2.20	0.42
1:D:45:ILE:HG13	1:D:46:GLN:N	2.34	0.42
1:A:275:SER:O	1:A:275:SER:OG	2.32	0.42
1:B:11:LEU:HA	1:B:14:MET:HE3	2.02	0.42
1:A:85:MET:SD	1:B:129:ILE:HD13	2.59	0.42
1:C:204:ARG:HG2	1:C:204:ARG:H	1.53	0.42
1:C:165:HIS:HD2	1:C:241:SER:HB3	1.84	0.42
1:A:180:ARG:HH21	1:A:183:GLU:HG3	1.84	0.42
1:C:41:SER:HB3	1:C:44:GLN:HG2	2.02	0.42
1:D:208:PHE:HE2	1:D:259:LEU:HG	1.83	0.42
1:B:188:LYS:HB3	1:B:189:PRO:HD3	2.01	0.42
1:A:148:GLU:O	1:A:152:ILE:HG12	2.20	0.42
1:B:42:LYS:HD3	1:B:43:ARG:HH12	1.85	0.42
1:C:4:LEU:HA	1:C:5:PRO:HD3	1.95	0.42
1:D:100:LYS:HA	1:D:100:LYS:HD3	1.77	0.42
1:B:260:LEU:HB2	1:B:340:TYR:HB2	2.02	0.41
1:B:296:ASP:HA	1:B:297:PRO:HD3	1.90	0.41
1:D:193:LEU:O	1:D:196:ARG:HD3	2.20	0.41
1:D:204:ARG:HH21	1:D:248:HIS:CG	2.38	0.41
1:A:40:LEU:HD23	1:A:40:LEU:HA	1.75	0.41
1:B:8:VAL:O	1:B:12:ILE:HG12	2.20	0.41
1:C:217:ARG:CB	1:C:217:ARG:HH11	2.32	0.41
1:B:155:LYS:HE3	1:B:155:LYS:HB2	1.93	0.41
1:C:301:ILE:HA	1:C:301:ILE:HD13	1.62	0.41
1:C:319:ASN:OD1	1:C:319:ASN:N	2.51	0.41
1:D:301:ILE:HD13	1:D:301:ILE:HA	1.67	0.41
1:D:308:VAL:HA	1:D:309:PRO:HD3	1.90	0.41
1:D:316:SER:OG	1:D:318:VAL:HG22	2.21	0.41
1:C:56:GLN:NE2	1:C:225:VAL:HG12	2.35	0.41
1:B:1:LYS:HD3	1:B:2:SER:N	2.36	0.41
1:B:42:LYS:HD3	1:B:43:ARG:NH1	2.36	0.41
1:C:71:LEU:HD12	1:C:71:LEU:HA	1.74	0.41
1:D:185:GLN:HA	1:D:187:TYR:N	2.35	0.41
1:D:293:THR:HA	1:D:315:SER:HA	2.02	0.41
1:C:52:LEU:HD23	1:C:52:LEU:HA	1.83	0.41
1:B:119:GLY:O	1:C:85:MET:HE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:GLN:HB2	1:A:56:GLN:HE21	1.69	0.41
1:C:87:LYS:HA	1:C:88:PRO:HD3	1.84	0.41
1:A:199:LEU:HB3	1:A:236:PHE:HB3	2.03	0.41
1:B:204:ARG:HD3	1:B:248:HIS:HB2	2.02	0.41
1:D:230:PHE:HA	1:D:275:SER:O	2.20	0.41
1:D:239:MET:HE3	1:D:295:PRO:HG3	2.02	0.41
1:C:4:LEU:O	1:C:9:GLN:NE2	2.55	0.40
1:C:78:LEU:O	1:C:80:PRO:HD3	2.22	0.40
1:D:194:HIS:NE2	1:D:267:ASN:OD1	2.50	0.40
1:A:8:VAL:O	1:A:12:ILE:HG12	2.22	0.40
1:D:2:SER:HB2	1:D:130:ASP:HB2	2.04	0.40
1:B:273:HIS:ND1	1:D:320:ASP:HA	2.36	0.40
1:D:44:GLN:HB3	1:D:45:ILE:HG12	2.01	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	Percentiles	
1	A	347/355 (98%)	324 (93%)	19 (6%)	4 (1%)	13	30
1	B	348/355 (98%)	316 (91%)	27 (8%)	5 (1%)	11	26
1	C	348/355 (98%)	317 (91%)	22 (6%)	9 (3%)	5	12
1	D	286/355 (81%)	260 (91%)	21 (7%)	5 (2%)	9	21
All	All	1329/1420 (94%)	1217 (92%)	89 (7%)	23 (2%)	9	21

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	166	ASN
1	D	45	ILE

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Mol	Chain	Res	Type
1	B	17	ASP
1	B	40	LEU
1	B	63	SER
1	C	59	VAL
1	C	63	SER
1	A	64	SER
1	A	65	ASP
1	A	66	SER
1	C	40	LEU
1	C	222	GLU
1	C	318	VAL
1	C	324	LEU
1	D	46	GLN
1	D	228	TYR
1	A	298	SER
1	C	300	ASN
1	C	224	PRO
1	D	44	GLN
1	B	119	GLY
1	D	173	ILE
1	C	87	LYS

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	306/310 (99%)	266 (87%)	40 (13%)	4	9
1	B	306/310 (99%)	269 (88%)	37 (12%)	5	10
1	C	306/310 (99%)	265 (87%)	41 (13%)	4	8
1	D	256/310 (83%)	230 (90%)	26 (10%)	7	16
All	All	1174/1240 (95%)	1030 (88%)	144 (12%)	4	10

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	23	LYS
1	A	29	GLU
1	A	37	LEU
1	A	43	ARG
1	A	49	TYR
1	A	50	SER
1	A	56	GLN
1	A	64	SER
1	A	70	ASP
1	A	71	LEU
1	A	97	VAL
1	A	108	LEU
1	A	122	ASP
1	A	123	ASP
1	A	124	SER
1	A	126	LYS
1	A	156	TYR
1	A	170	LEU
1	A	178	ILE
1	A	188	LYS
1	A	192	GLN
1	A	193	LEU
1	A	226	THR
1	A	243	SER
1	A	255	ILE
1	A	269	TYR
1	A	277	ILE
1	A	278	SER
1	A	279	LYS
1	A	280	LEU
1	A	296	ASP
1	A	301	ILE
1	A	312	THR
1	A	319	ASN
1	A	321	THR
1	A	322	SER
1	A	323	LEU
1	A	343	LYS
1	A	345	LYS
1	B	1	LYS
1	B	3	LYS
1	B	34	LYS

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Mol	Chain	Res	Type
1	B	41	SER
1	B	43	ARG
1	B	49	TYR
1	B	56	GLN
1	B	60	SER
1	B	64	SER
1	B	68	ILE
1	B	71	LEU
1	B	72	SER
1	B	98	GLN
1	B	108	LEU
1	B	118	ARG
1	B	126	LYS
1	B	151	GLU
1	B	156	TYR
1	B	170	LEU
1	B	177	LYS
1	B	185	GLN
1	B	204	ARG
1	B	217	ARG
1	B	226	THR
1	B	255	ILE
1	B	263	VAL
1	B	276	HIS
1	B	277	ILE
1	B	302	SER
1	B	303	LEU
1	B	310	LEU
1	B	312	THR
1	B	323	LEU
1	B	324	LEU
1	B	343	LYS
1	B	345	LYS
1	B	349	LYS
1	C	15	ILE
1	C	22	LYS
1	C	34	LYS
1	C	40	LEU
1	C	43	ARG
1	C	49	TYR
1	C	61	GLN
1	C	71	LEU

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Mol	Chain	Res	Type
1	C	74	ARG
1	C	78	LEU
1	C	90	LEU
1	C	123	ASP
1	C	126	LYS
1	C	144	ASP
1	C	145	ARG
1	C	152	ILE
1	C	156	TYR
1	C	163	THR
1	C	170	LEU
1	C	181	GLU
1	C	204	ARG
1	C	217	ARG
1	C	222	GLU
1	C	229	MET
1	C	239	MET
1	C	241	SER
1	C	242	LYS
1	C	255	ILE
1	C	263	VAL
1	C	277	ILE
1	C	279	LYS
1	C	280	LEU
1	C	301	ILE
1	C	310	LEU
1	C	314	ILE
1	C	319	ASN
1	C	322	SER
1	C	323	LEU
1	C	324	LEU
1	C	343	LYS
1	C	350	THR
1	D	3	LYS
1	D	25	MET
1	D	44	GLN
1	D	45	ILE
1	D	74	ARG
1	D	75	PHE
1	D	97	VAL
1	D	98	GLN
1	D	106	ASN

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Mol	Chain	Res	Type
1	D	108	LEU
1	D	129	ILE
1	D	151	GLU
1	D	154	ARG
1	D	156	TYR
1	D	169	ASP
1	D	170	LEU
1	D	171	GLU
1	D	180	ARG
1	D	241	SER
1	D	272	LYS
1	D	279	LYS
1	D	301	ILE
1	D	310	LEU
1	D	322	SER
1	D	324	LEU
1	D	349	LYS

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

Mol	Chain	Res	Type
1	B	44	GLN
1	C	161	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](#)

7 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	$\# Z  > 2$
3	SO4	A	402	-	4,4,4	0.33	0	6,6,6	0.38	0
2	15S	D	401	-	37,39,39	2.72	16 (43%)	47,56,56	2.42	13 (27%)
2	15S	B	401	-	37,39,39	2.59	16 (43%)	47,56,56	2.07	12 (25%)
3	SO4	D	402	-	4,4,4	0.11	0	6,6,6	0.36	0
3	SO4	B	402	-	4,4,4	0.11	0	6,6,6	0.53	0
2	15S	A	401	-	37,39,39	2.65	14 (37%)	47,56,56	2.18	13 (27%)
2	15S	C	401	-	37,39,39	2.78	13 (35%)	47,56,56	2.51	8 (17%)

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	15S	C	401	-	-	3/20/52/52	0/5/5/5
2	15S	D	401	-	-	3/20/52/52	0/5/5/5
2	15S	A	401	-	-	9/20/52/52	0/5/5/5
2	15S	B	401	-	-	4/20/52/52	0/5/5/5

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	15S	C-NBH	9.40	1.48	1.34
2	C	401	15S	C-NBH	8.55	1.47	1.34
2	B	401	15S	C-NBH	7.80	1.46	1.34
2	A	401	15S	C-NBH	7.07	1.45	1.34
2	A	401	15S	OAC-CAX	6.23	1.36	1.23
2	D	401	15S	OAC-CAX	6.18	1.35	1.23
2	C	401	15S	OAC-CAX	5.73	1.34	1.23
2	A	401	15S	CAW-N	5.69	1.46	1.34
2	C	401	15S	CAI-CBD	5.44	1.48	1.39
2	C	401	15S	CAW-N	5.18	1.45	1.34
2	B	401	15S	CAI-CBD	5.15	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	15S	OAC-CAX	5.14	1.33	1.23
2	A	401	15S	CAI-CBD	4.92	1.47	1.39
2	C	401	15S	CAH-CBC	4.89	1.47	1.39
2	B	401	15S	CAH-CBC	4.61	1.47	1.39
2	A	401	15S	CAH-CBC	4.45	1.47	1.39
2	D	401	15S	CAI-CBD	4.32	1.46	1.39
2	B	401	15S	CAW-N	4.10	1.42	1.34
2	D	401	15S	CAW-N	4.06	1.42	1.34
2	C	401	15S	CBB-CAY	4.02	1.55	1.48
2	D	401	15S	CBB-CAY	3.98	1.55	1.48
2	D	401	15S	CAH-CBC	3.51	1.45	1.39
2	D	401	15S	CB-CA	-3.36	1.43	1.52
2	C	401	15S	CB-CA	-3.32	1.43	1.52
2	A	401	15S	CBB-CAY	3.31	1.54	1.48
2	A	401	15S	CB-CA	-3.23	1.44	1.52
2	C	401	15S	CBG-NBI	3.19	1.55	1.47
2	B	401	15S	CB-CA	-3.16	1.44	1.52
2	B	401	15S	CBG-NBI	3.02	1.54	1.47
2	A	401	15S	CBG-NBI	2.91	1.54	1.47
2	A	401	15S	CAO-CAY	2.84	1.49	1.36
2	D	401	15S	CAO-CAY	2.83	1.49	1.36
2	A	401	15S	CBD-CAX	2.77	1.51	1.47
2	B	401	15S	CBB-CAY	2.75	1.53	1.48
2	B	401	15S	CA-N	-2.66	1.40	1.45
2	B	401	15S	CAO-CAY	2.64	1.48	1.36
2	C	401	15S	CAS-CBG	2.63	1.56	1.52
2	C	401	15S	O-C	-2.60	1.17	1.22
2	C	401	15S	FAE-CBA	-2.57	1.30	1.36
2	D	401	15S	FAE-CBA	-2.57	1.30	1.36
2	A	401	15S	O-C	-2.57	1.17	1.22
2	B	401	15S	FAE-CBA	-2.57	1.30	1.36
2	B	401	15S	CAP-CBC	-2.52	1.46	1.51
2	B	401	15S	O-C	-2.43	1.18	1.22
2	C	401	15S	CAO-CAY	2.39	1.47	1.36
2	C	401	15S	CBD-CAX	2.33	1.51	1.47
2	D	401	15S	CAT-NBI	-2.31	1.42	1.47
2	A	401	15S	CAR-CAP	-2.27	1.47	1.51
2	D	401	15S	CAR-CAP	-2.19	1.47	1.51
2	B	401	15S	CAR-CAP	-2.19	1.47	1.51
2	A	401	15S	FAE-CBA	-2.18	1.31	1.36
2	A	401	15S	CAN-NBH	-2.17	1.43	1.47
2	B	401	15S	CAM-CBB	-2.17	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	15S	CA-N	-2.17	1.41	1.45
2	D	401	15S	CBG-NBI	2.16	1.52	1.47
2	D	401	15S	CBD-CAX	2.09	1.50	1.47
2	B	401	15S	CBD-CAX	2.09	1.50	1.47
2	D	401	15S	CA-C	2.05	1.57	1.53
2	D	401	15S	CAT-CAW	-2.02	1.49	1.52

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	15S	CAF-CAY-CAO	-12.62	108.70	120.58
2	D	401	15S	CAF-CAY-CAO	-8.55	112.53	120.58
2	A	401	15S	CBB-CAY-CAO	-8.14	103.76	122.08
2	D	401	15S	OAC-CAX-CBD	-7.14	110.92	123.30
2	B	401	15S	OAC-CAX-CBD	-6.66	111.75	123.30
2	B	401	15S	CBB-CAY-CAO	-6.24	108.03	122.08
2	C	401	15S	OAC-CAX-CBD	-5.55	113.68	123.30
2	A	401	15S	OAC-CAX-CBD	-5.50	113.76	123.30
2	B	401	15S	CAF-CAY-CBB	-4.89	109.20	118.28
2	D	401	15S	CAF-CAY-CBB	-4.76	109.46	118.28
2	A	401	15S	O-C-NBH	-4.51	116.39	121.67
2	C	401	15S	CAQ-CAO-CAY	-4.32	110.00	123.77
2	C	401	15S	CBB-CAY-CAO	-4.16	112.71	122.08
2	D	401	15S	CBD-CBE-CBC	4.04	123.47	119.81
2	D	401	15S	CAR-NBI-CBG	3.86	118.96	111.27
2	B	401	15S	CA-N-CAW	-3.76	115.70	121.34
2	D	401	15S	CAW-CAT-NBI	-3.74	104.83	113.35
2	A	401	15S	CAR-NBI-CBG	3.42	118.08	111.27
2	A	401	15S	CAF-CAY-CBB	-3.28	112.20	118.28
2	C	401	15S	CAR-NBI-CBG	2.92	117.09	111.27
2	D	401	15S	CB-CA-C	2.92	115.04	109.73
2	D	401	15S	CBE-CBD-CAX	2.86	123.12	120.61
2	A	401	15S	CAK-CBA-CAJ	-2.81	119.10	122.83
2	D	401	15S	CBB-CAY-CAO	-2.73	115.93	122.08
2	A	401	15S	CBE-CBD-CAX	2.45	122.76	120.61
2	A	401	15S	CA-C-NBH	2.42	122.69	118.04
2	B	401	15S	CAR-NBI-CBG	2.37	116.00	111.27
2	D	401	15S	CAR-CAP-CBC	-2.31	107.24	111.35
2	B	401	15S	CAM-CBB-CAY	-2.29	118.21	121.23
2	B	401	15S	CAQ-CAO-CAY	-2.28	116.51	123.77
2	D	401	15S	CAS-CBG-NBI	2.28	116.60	112.56
2	B	401	15S	CB-CA-N	-2.27	106.11	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	15S	CB-CA-N	-2.24	106.18	110.38
2	A	401	15S	CAF-CAN-NBH	-2.24	106.76	110.54
2	C	401	15S	CAK-CBA-CAJ	-2.15	119.97	122.83
2	A	401	15S	CAG-CAH-CBC	-2.14	117.70	120.89
2	D	401	15S	CBD-CAX-NAU	-2.13	113.13	116.03
2	D	401	15S	CA-N-CAW	-2.10	118.19	121.34
2	A	401	15S	CBD-CBE-CBC	2.07	121.68	119.81
2	B	401	15S	CBE-CBD-CAX	2.07	122.43	120.61
2	B	401	15S	CAK-CBA-CAJ	-2.06	120.09	122.83
2	B	401	15S	CAG-CAH-CBC	-2.05	117.83	120.89
2	A	401	15S	CAM-CAK-CBA	2.05	120.48	118.36
2	C	401	15S	CA-C-NBH	2.04	121.97	118.04
2	B	401	15S	O-C-NBH	-2.03	119.29	121.67
2	A	401	15S	CAL-CAJ-CBA	2.01	120.44	118.36

There are no chirality outliers.

All (19) torsion outliers are listed below:

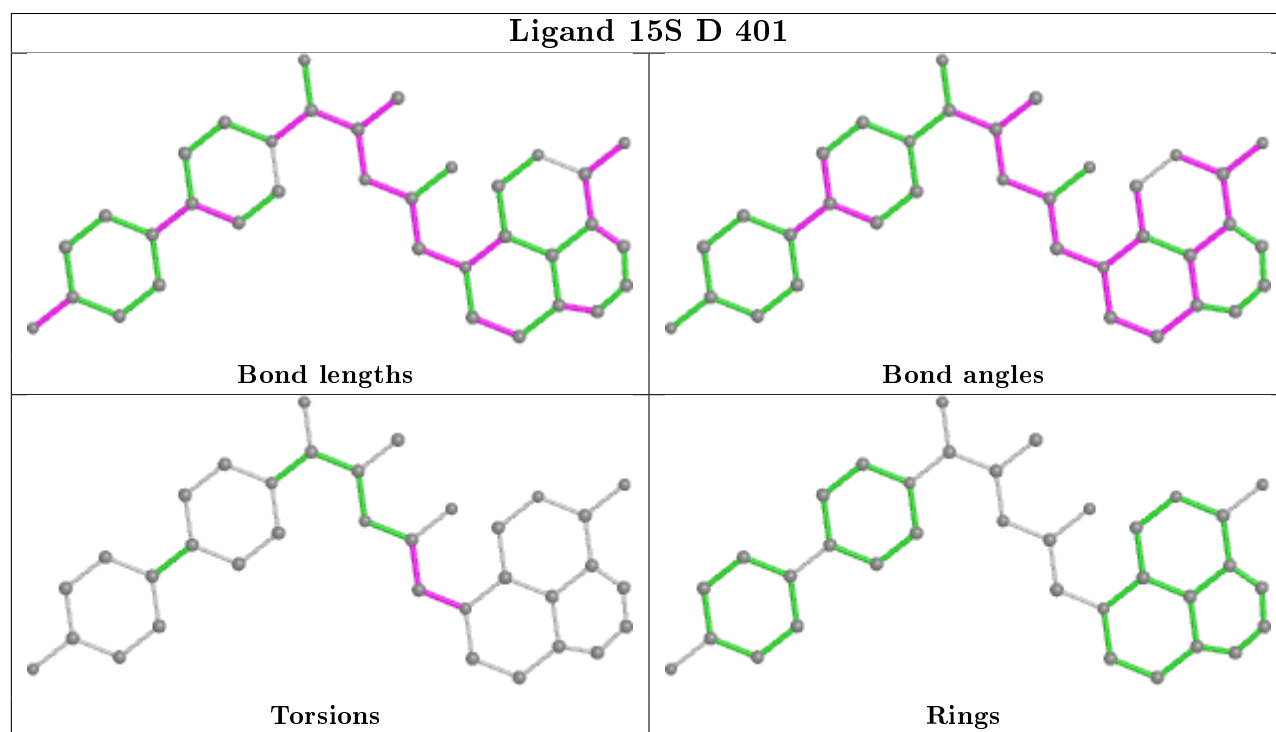
Mol	Chain	Res	Type	Atoms
2	D	401	15S	CAW-CAT-NBI-CAR
2	B	401	15S	CAW-CAT-NBI-CAR
2	A	401	15S	CAF-CAY-CBB-CAL
2	A	401	15S	CAF-CAY-CBB-CAM
2	A	401	15S	CAO-CAY-CBB-CAM
2	A	401	15S	CAO-CAY-CBB-CAL
2	B	401	15S	O-C-CA-CB
2	A	401	15S	O-C-CA-CB
2	D	401	15S	NBI-CAT-CAW-N
2	C	401	15S	O-C-CA-CB
2	B	401	15S	NBH-C-CA-CB
2	A	401	15S	CAW-CAT-NBI-CAR
2	A	401	15S	O-C-CA-N
2	A	401	15S	NBH-C-CA-CB
2	C	401	15S	NBH-C-CA-CB
2	D	401	15S	NBI-CAT-CAW-OAB
2	C	401	15S	CAW-CAT-NBI-CBG
2	B	401	15S	O-C-CA-N
2	A	401	15S	NBH-C-CA-N

There are no ring outliers.

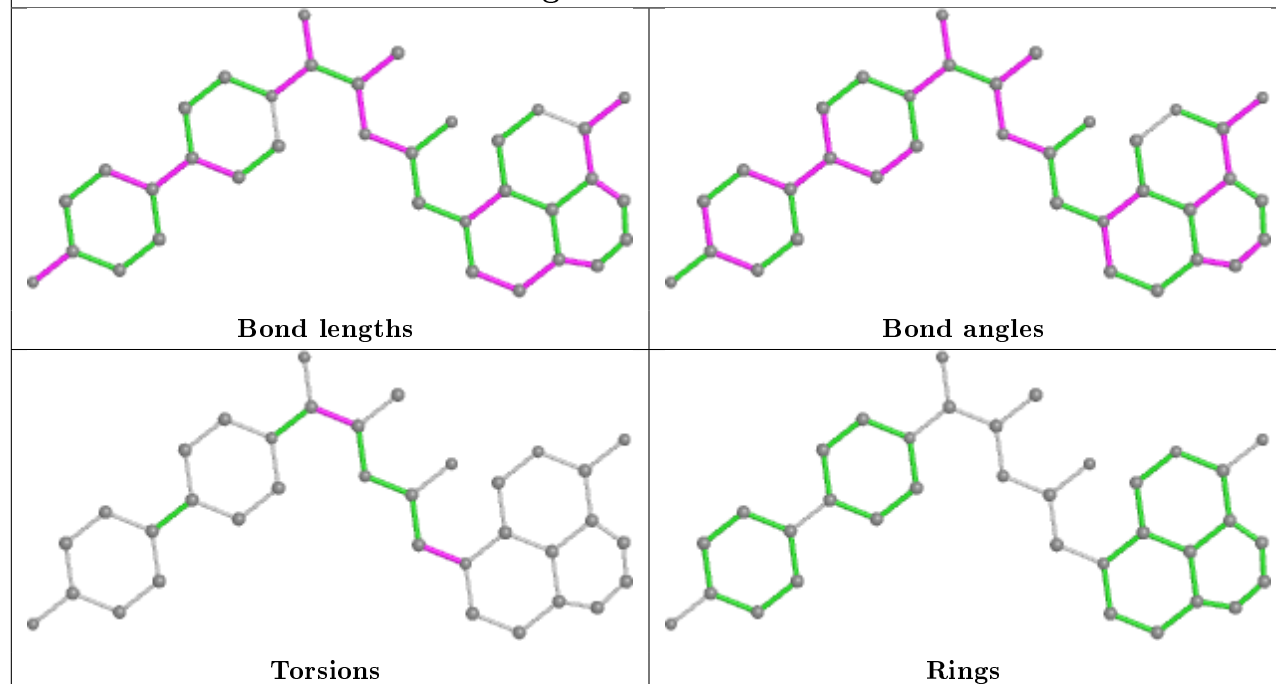
5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	15S	4	0
2	B	401	15S	4	0
3	D	402	SO4	1	0
2	A	401	15S	1	0
2	C	401	15S	2	0

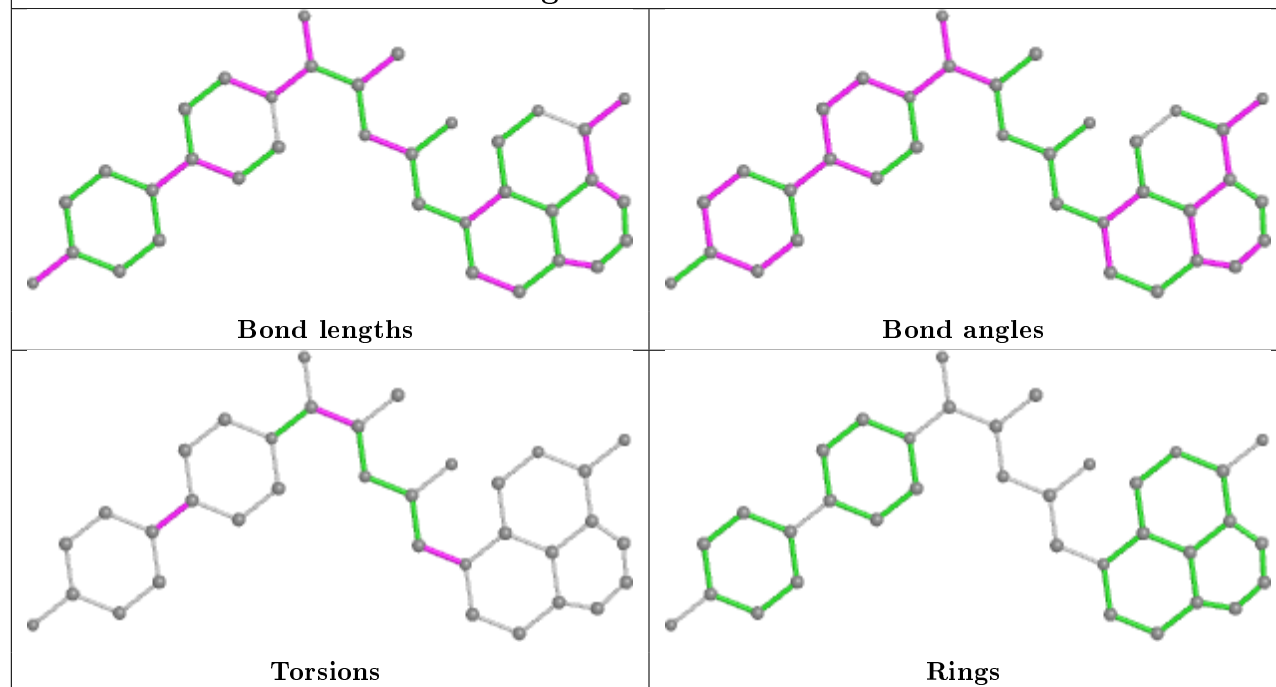
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

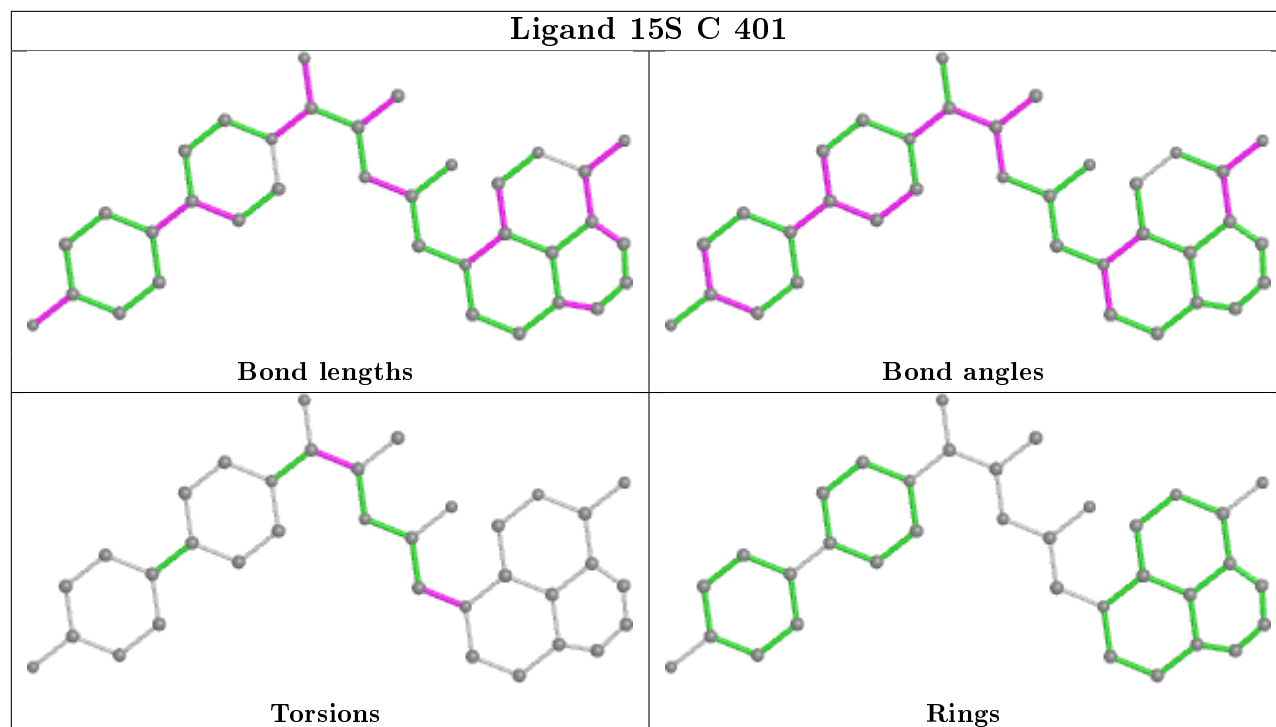


## Ligand 15S B 401



## Ligand 15S A 401





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	349/355 (98%)	-0.07	6 (1%) 70 72	1, 14, 41, 82	0
1	B	350/355 (98%)	-0.06	5 (1%) 75 77	1, 15, 55, 87	0
1	C	350/355 (98%)	0.20	19 (5%) 25 25	3, 25, 61, 85	0
1	D	296/355 (83%)	0.42	29 (9%) 7 6	7, 38, 64, 70	0
All	All	1345/1420 (94%)	0.11	59 (4%) 34 33	1, 19, 59, 87	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	40	LEU	6.7
1	C	226	THR	6.2
1	D	75	PHE	5.2
1	B	64	SER	4.8
1	C	38	GLY	4.1
1	D	116	LEU	3.9
1	D	114	TYR	3.7
1	D	222	GLU	3.4
1	D	45	ILE	3.2
1	A	122	ASP	3.1
1	C	228	TYR	3.0
1	D	132	ASN	2.9
1	D	113	ALA	2.9
1	C	63	SER	2.9
1	A	124	SER	2.9
1	C	77	THR	2.9
1	C	278	SER	2.8
1	C	39	LYS	2.8
1	C	86	LYS	2.8
1	C	126	LYS	2.7
1	D	76	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	83	PHE	2.6
1	C	60	SER	2.6
1	D	77	THR	2.6
1	D	47	ALA	2.6
1	C	124	SER	2.6
1	C	85	MET	2.5
1	C	276	HIS	2.5
1	D	118	ARG	2.5
1	B	122	ASP	2.5
1	D	117	LEU	2.5
1	D	80	PRO	2.4
1	D	2	SER	2.4
1	D	220	PRO	2.4
1	D	166	ASN	2.3
1	C	125	SER	2.3
1	D	164	THR	2.3
1	C	61	GLN	2.3
1	C	166	ASN	2.3
1	D	13	LYS	2.3
1	B	45	ILE	2.3
1	D	15	ILE	2.2
1	D	142	VAL	2.2
1	D	4	LEU	2.2
1	D	226	THR	2.2
1	D	110	ILE	2.2
1	D	136	LEU	2.2
1	A	121	SER	2.2
1	D	46	GLN	2.2
1	C	78	LEU	2.1
1	A	3	LYS	2.1
1	D	30	ILE	2.1
1	B	350	THR	2.1
1	C	121	SER	2.1
1	C	122	ASP	2.1
1	B	68	ILE	2.0
1	D	9	GLN	2.0
1	A	166	ASN	2.0
1	D	228	TYR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

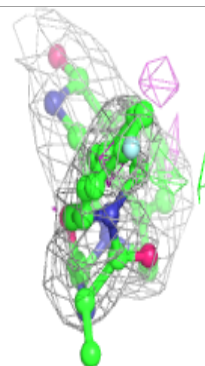
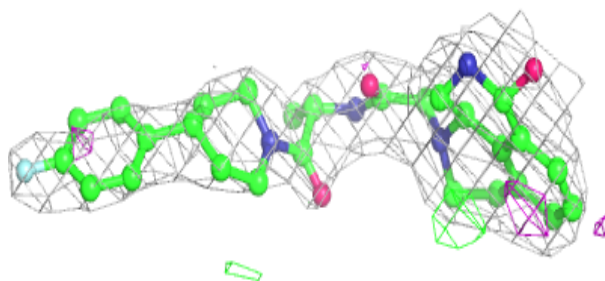
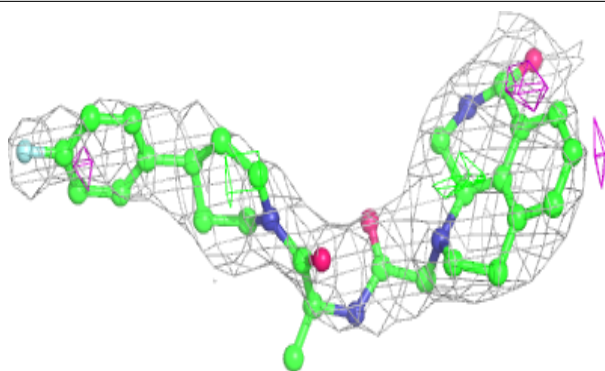
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	15S	D	401	35/35	0.88	0.29	11,38,54,63	0
3	SO4	A	402	5/5	0.92	0.17	11,16,31,36	0
2	15S	B	401	35/35	0.92	0.22	1,12,30,33	0
2	15S	A	401	35/35	0.92	0.20	2,10,25,36	0
2	15S	C	401	35/35	0.93	0.23	5,31,48,49	0
3	SO4	B	402	5/5	0.94	0.14	7,10,24,34	0
3	SO4	D	402	5/5	0.96	0.13	19,25,34,34	0

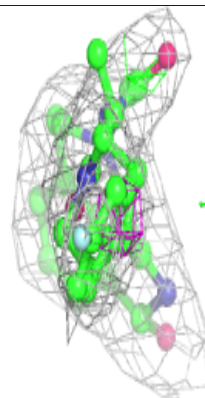
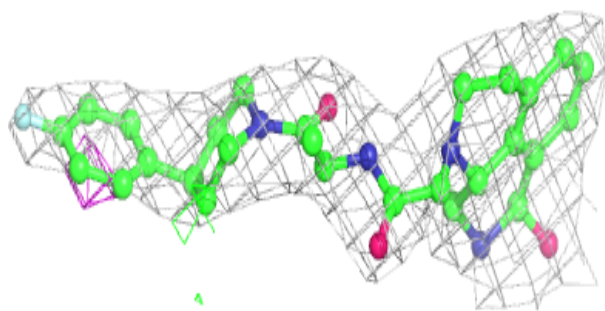
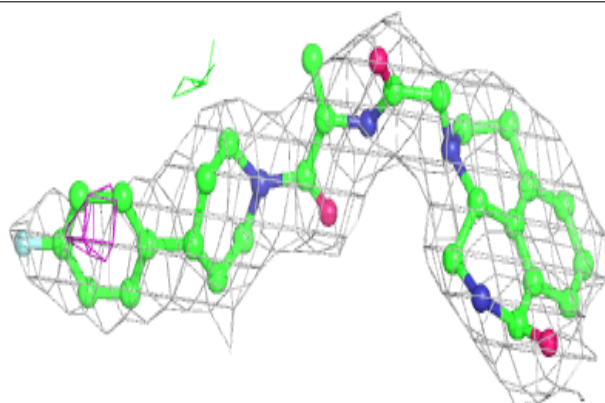
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 15S D 401:**

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

**Electron density around 15S B 401:**

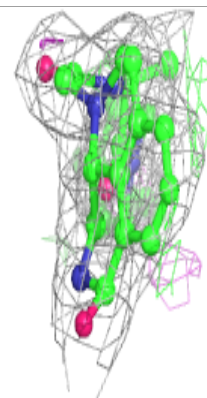
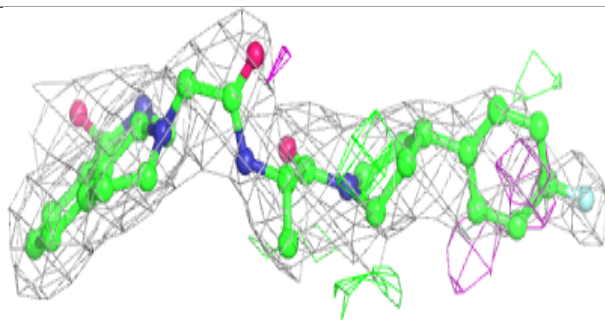
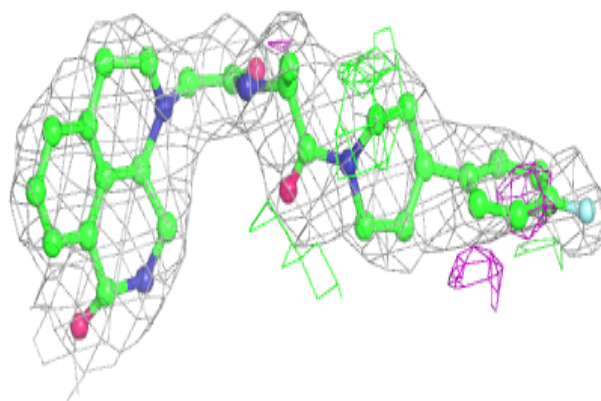
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



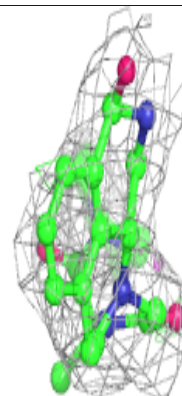
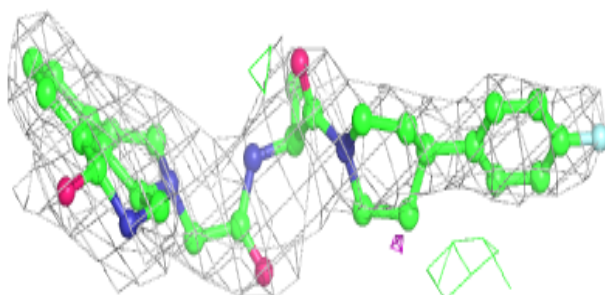
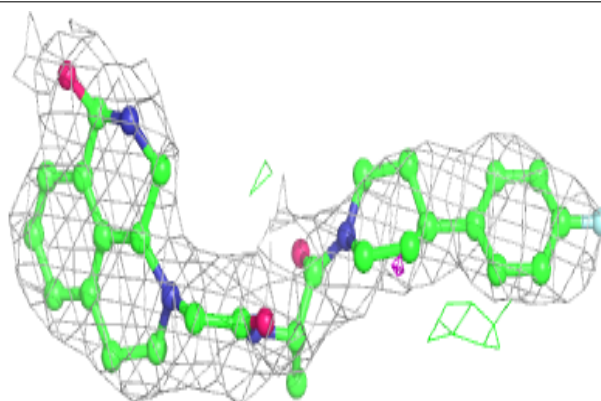


**Electron density around 15S A 401:**

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

**Electron density around 15S C 401:**

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



## 6.5 Other polymers

There are no such residues in this entry.