Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 10:48 am BST

PDB ID	:	6PM9
Title	:	Crystal structure of the core catalytic domain of human O-GlcNAcase bound to MK-8719
Authors	:	Klein, D.J.; Selnick, H.G.; Duffy, J.L.; McEachern, E.J.
Deposited on	:	2019-07-01
Resolution	:	2.86 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 ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

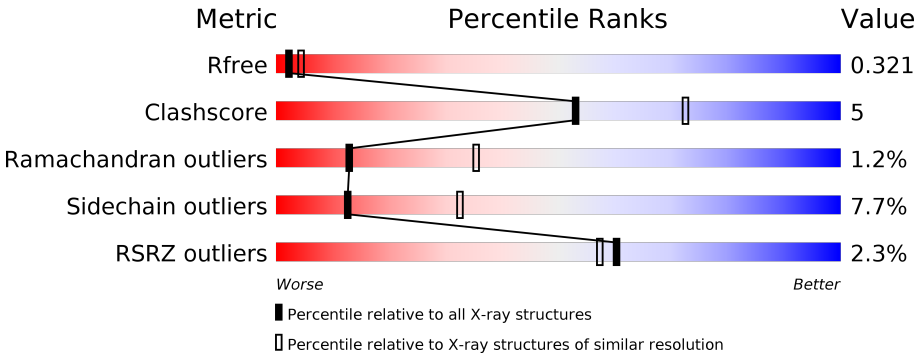
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 >=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	A	388	64% 15% • 20%
1	B	388	67% 11% • 20%
1	C	388	60% 18% • 20%
1	D	388	62% 17% • 20%
2	E	161	4% 53% 16% 30%
2	F	161	2% 53% 12% • 32%

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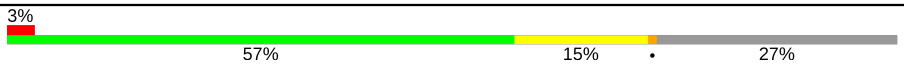
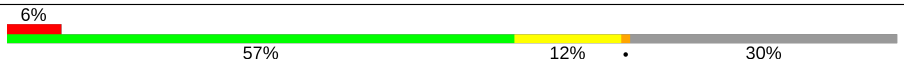
Mol	Chain	Length	Quality of chain
2	G	161	
2	H	161	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13916 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 O-GlcNAcase TIM-barrel domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2540	1644	418	464	14			
1	B	309	Total	C	N	O	S	0	0	0
			2536	1641	417	464	14			
1	C	310	Total	C	N	O	S	0	0	0
			2515	1626	416	459	14			
1	D	310	Total	C	N	O	S	0	0	0
			2512	1624	414	460	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	-	expression tag	UNP O60502
B	13	GLY	-	expression tag	UNP O60502
C	13	GLY	-	expression tag	UNP O60502
D	13	GLY	-	expression tag	UNP O60502

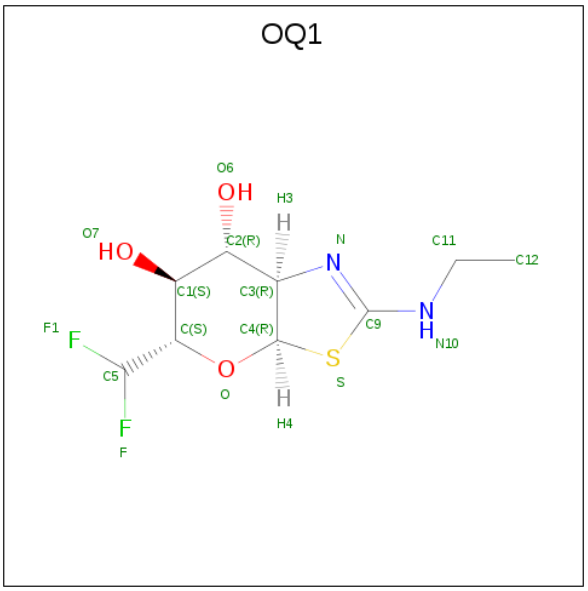
- Molecule 2 is a protein called O-GlcNAcase stalk domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	112	Total	C	N	O	S	0	0	0
			912	588	152	163	9			
2	F	109	Total	C	N	O	S	0	0	0
			896	580	149	158	9			
2	G	117	Total	C	N	O	S	0	0	0
			974	631	163	171	9			
2	H	112	Total	C	N	O	S	0	0	0
			928	600	156	163	9			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	553	MET	-	initiating methionine	UNP O60502
E	706	HIS	-	expression tag	UNP O60502
E	707	HIS	-	expression tag	UNP O60502
E	708	HIS	-	expression tag	UNP O60502
E	709	HIS	-	expression tag	UNP O60502
E	710	HIS	-	expression tag	UNP O60502
E	711	HIS	-	expression tag	UNP O60502
E	712	HIS	-	expression tag	UNP O60502
E	713	HIS	-	expression tag	UNP O60502
F	553	MET	-	initiating methionine	UNP O60502
F	706	HIS	-	expression tag	UNP O60502
F	707	HIS	-	expression tag	UNP O60502
F	708	HIS	-	expression tag	UNP O60502
F	709	HIS	-	expression tag	UNP O60502
F	710	HIS	-	expression tag	UNP O60502
F	711	HIS	-	expression tag	UNP O60502
F	712	HIS	-	expression tag	UNP O60502
F	713	HIS	-	expression tag	UNP O60502
G	553	MET	-	initiating methionine	UNP O60502
G	706	HIS	-	expression tag	UNP O60502
G	707	HIS	-	expression tag	UNP O60502
G	708	HIS	-	expression tag	UNP O60502
G	709	HIS	-	expression tag	UNP O60502
G	710	HIS	-	expression tag	UNP O60502
G	711	HIS	-	expression tag	UNP O60502
G	712	HIS	-	expression tag	UNP O60502
G	713	HIS	-	expression tag	UNP O60502
H	553	MET	-	initiating methionine	UNP O60502
H	706	HIS	-	expression tag	UNP O60502
H	707	HIS	-	expression tag	UNP O60502
H	708	HIS	-	expression tag	UNP O60502
H	709	HIS	-	expression tag	UNP O60502
H	710	HIS	-	expression tag	UNP O60502
H	711	HIS	-	expression tag	UNP O60502
H	712	HIS	-	expression tag	UNP O60502
H	713	HIS	-	expression tag	UNP O60502

- Molecule 3 is (3aR,5S,6S,7R,7aR)-5-(difluoromethyl)-2-(ethylamino)-5,6,7,7a-tetrahydro-3aH-pyrano[3,2-d][1,3]thiazole-6,7-diol (three-letter code: OQ1) (formula: $C_9H_{14}F_2N_2O_3S$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C F N O S 17 9 2 2 3 1	0	0
3	B	1	Total C F N O S 17 9 2 2 3 1	0	0
3	C	1	Total C F N O S 17 9 2 2 3 1	0	0
3	D	1	Total C F N O S 17 9 2 2 3 1	0	0

- Molecule 4 is water.

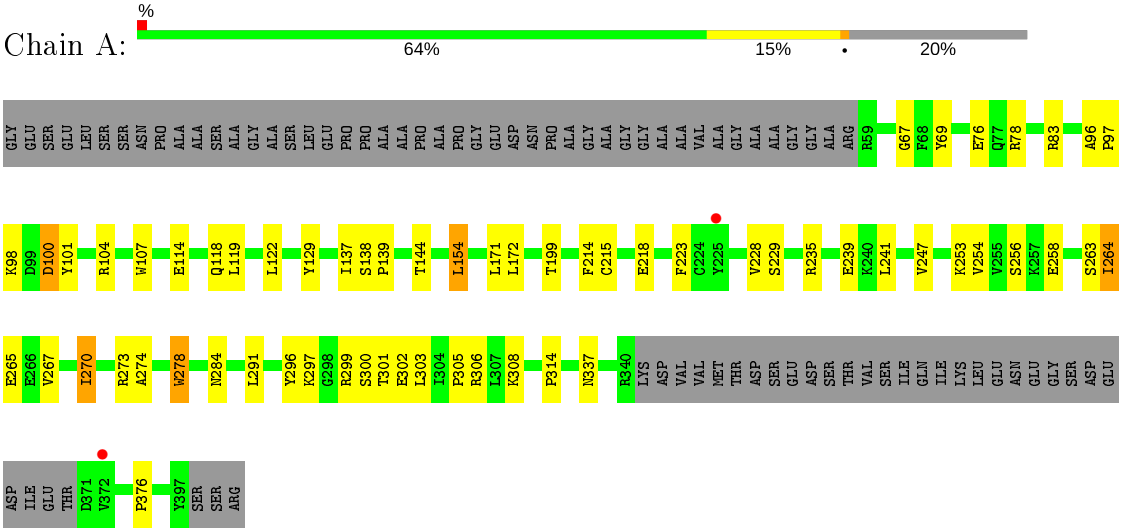
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	6	Total O 6 6	0	0
4	B	9	Total O 9 9	0	0
4	C	8	Total O 8 8	0	0
4	D	3	Total O 3 3	0	0
4	E	2	Total O 2 2	0	0
4	F	3	Total O 3 3	0	0
4	G	1	Total O 1 1	0	0
4	H	3	Total O 3 3	0	0

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.

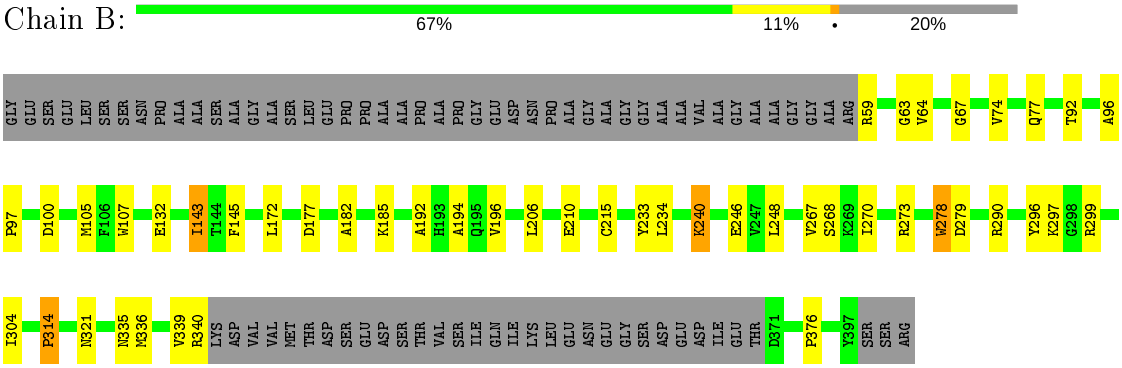
- Molecule 1: O-GlcNAcase TIM-barrel domain

Chain A:



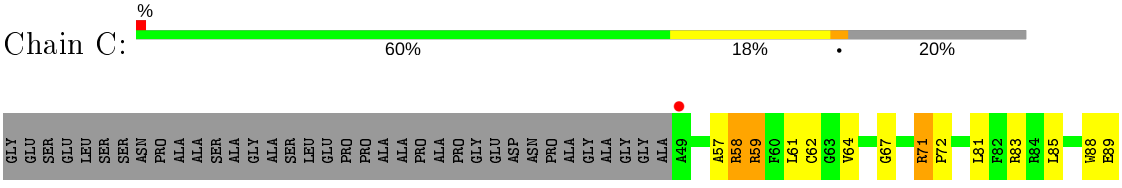
- Molecule 1: O-GlcNAcase TIM-barrel domain

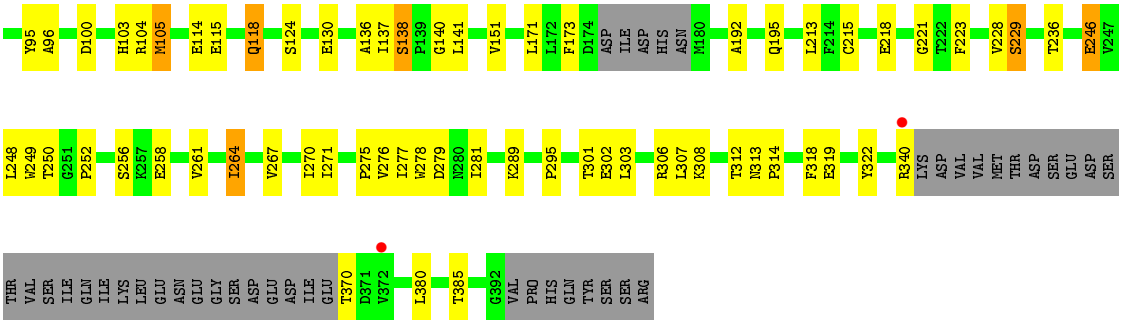
Chain B:



- Molecule 1: O-GlcNAcase TIM-barrel domain

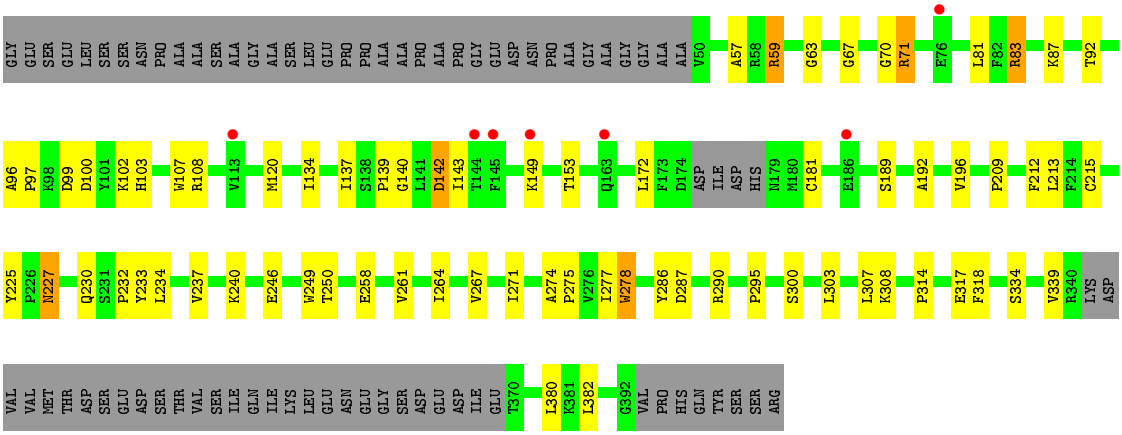
Chain C:





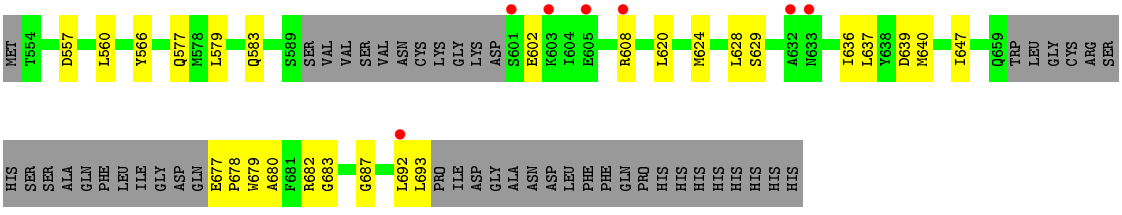
- Molecule 1: O-GlcNAcase TIM-barrel domain

Chain D:



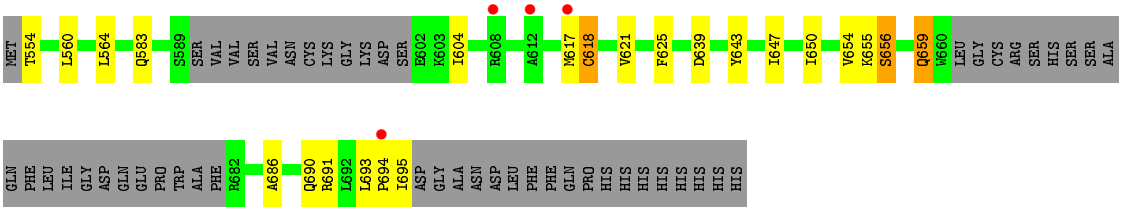
- Molecule 2: O-GlcNAcase stalk domain

Chain E:



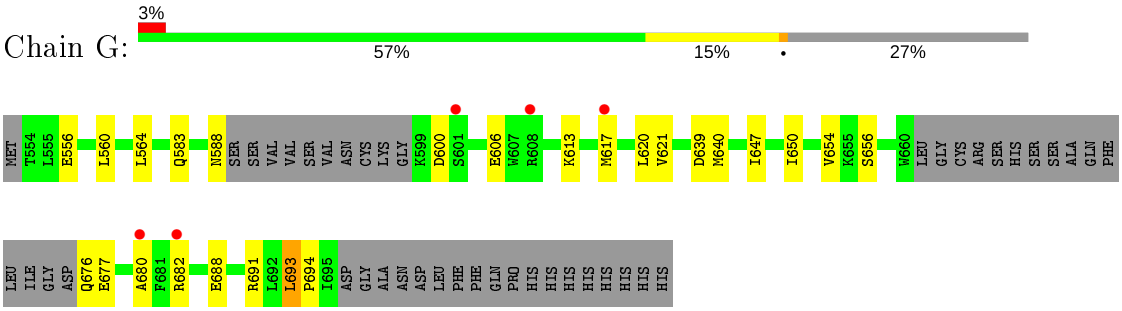
- Molecule 2: O-GlcNAcase stalk domain

Chain F:



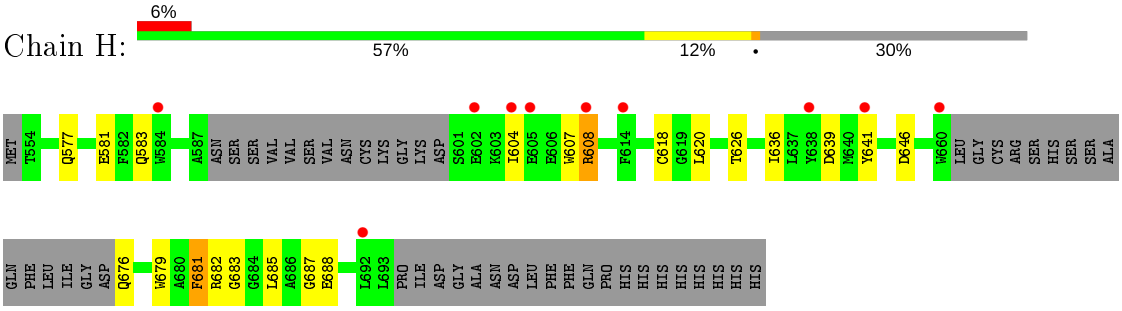
- Molecule 2: O-GlcNAcase stalk domain

Chain G:



- Molecule 2: O-GlcNAcase stalk domain

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	89.92Å 91.46Å 94.61Å 77.27° 62.61° 62.86°	Depositor
Resolution (Å)	40.69 – 2.86 40.69 – 2.86	Depositor EDS
% Data completeness (in resolution range)	95.1 (40.69-2.86) 95.1 (40.69-2.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.239 , 0.309 0.251 , 0.321	Depositor DCC
R_{free} test set	2706 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å^2)	57.5	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 84.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,l,h-k 0.000 for h,h-l,k 0.000 for h,h-k,h-l 0.000 for -h,-h+k,-l 0.000 for -h,-k,-h+l 0.000 for -h,-l,-k 0.000 for -h,-h+l,-h+k	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	13916	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7595e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: OQ1

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	0.51	0/2610	0.74	0/3539
1	B	0.53	0/2606	0.75	0/3535
1	C	0.54	0/2580	0.76	0/3494
1	D	0.51	0/2577	0.73	0/3491
2	E	0.49	0/932	0.69	0/1251
2	F	0.52	0/916	0.70	0/1230
2	G	0.55	0/998	0.77	0/1341
2	H	0.49	0/950	0.69	0/1276
All	All	0.52	0/14169	0.74	0/19157

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

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	2540	0	2484	32	0
1	B	2536	0	2473	18	0
1	C	2515	0	2474	32	0
1	D	2512	0	2464	38	0
2	E	912	0	887	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	896	0	880	10	0
2	G	974	0	953	12	0
2	H	928	0	905	9	0
3	A	17	0	0	1	0
3	B	17	0	0	0	0
3	C	17	0	0	0	0
3	D	17	0	0	1	0
4	A	6	0	0	0	0
4	B	9	0	0	0	0
4	C	8	0	0	0	0
4	D	3	0	0	0	0
4	E	2	0	0	0	0
4	F	3	0	0	0	0
4	G	1	0	0	0	0
4	H	3	0	0	0	0
All	All	13916	0	13520	147	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 5.

All (147) 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:D:264:ILE:HD11	1:D:303:LEU:HG	1.61	0.82
1:D:71:ARG:HE	2:H:641:TYR:HD2	1.24	0.82
1:B:97:PRO:HB2	1:B:100:ASP:HB2	1.62	0.80
1:C:64:VAL:HG23	1:C:85:LEU:HD21	1.64	0.78
1:C:218:GLU:HG2	1:C:223:PHE:O	1.94	0.67
1:B:248:LEU:HD22	1:B:278:TRP:HD1	1.62	0.64
1:A:78:ARG:HB3	1:A:122:LEU:HD11	1.80	0.63
1:D:264:ILE:CD1	1:D:303:LEU:HG	2.28	0.63
1:D:70:GLY:H	1:D:99:ASP:HB2	1.64	0.63
1:C:104:ARG:HG3	1:C:138:SER:HB2	1.80	0.62
1:D:71:ARG:NE	2:H:641:TYR:HD2	1.96	0.61
2:E:683:GLY:HA3	2:E:687:GLY:HA3	1.85	0.58
1:B:248:LEU:HD22	1:B:278:TRP:CD1	2.39	0.58
1:C:58:ARG:O	1:C:59:ARG:HG3	2.05	0.57
1:D:108:ARG:HH12	1:D:142:ASP:HB2	1.70	0.56
2:E:557:ASP:HB3	2:E:624:MET:HG2	1.86	0.56
1:D:172:LEU:HD23	1:D:215:CYS:CB	2.34	0.56
1:D:227:ASN:HD21	1:D:230:GLN:HB2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:692:LEU:HD23	2:G:583:GLN:HE21	1.70	0.56
1:D:295:PRO:HD3	1:D:380:LEU:HD22	1.88	0.55
1:C:295:PRO:HD3	1:C:380:LEU:HD22	1.89	0.55
1:A:253:LYS:HE3	1:A:256:SER:HA	1.89	0.55
1:D:250:THR:HG22	1:D:278:TRP:O	2.08	0.54
1:A:83:ARG:HG2	1:A:129:TYR:CZ	2.43	0.54
1:C:81:LEU:HB2	1:C:318:PHE:HE1	1.73	0.54
1:B:192:ALA:HB2	1:B:233:TYR:CD1	2.44	0.53
2:H:577:GLN:O	2:H:581:GLU:HG2	2.09	0.53
2:F:656:SER:HA	2:F:659:GLN:HG3	1.91	0.52
1:B:67:GLY:HA2	1:B:96:ALA:O	2.09	0.52
1:A:241:LEU:HD23	1:A:273:ARG:NH2	2.24	0.52
1:C:295:PRO:HB3	1:C:380:LEU:HB2	1.92	0.52
1:D:209:PRO:HG2	1:D:212:PHE:HB2	1.93	0.51
1:D:192:ALA:HB2	1:D:233:TYR:CD1	2.45	0.51
1:B:296:TYR:CZ	1:B:299:ARG:HD3	2.45	0.51
2:F:617:MET:O	2:F:621:VAL:HG23	2.10	0.51
1:C:95:TYR:O	1:C:136:ALA:HB3	2.11	0.51
2:F:690:GLN:HA	2:F:693:LEU:HD12	1.93	0.51
1:C:173:PHE:HB3	1:C:195:GLN:HE21	1.75	0.51
1:D:172:LEU:HD23	1:D:215:CYS:HB2	1.92	0.51
1:D:267:VAL:O	1:D:271:ILE:HG12	2.11	0.51
1:A:263:SER:O	1:A:267:VAL:HG23	2.12	0.50
1:C:115:GLU:O	1:C:118:GLN:HG2	2.11	0.50
1:D:317:GLU:HB2	2:E:639:ASP:HB3	1.93	0.49
1:B:297:LYS:HG3	1:B:376:PRO:HG3	1.94	0.49
1:D:300:SER:O	1:D:303:LEU:HB2	2.12	0.49
1:D:249:TRP:O	1:D:277:ILE:HA	2.12	0.49
2:G:617:MET:SD	2:G:620:LEU:HD23	2.52	0.49
1:C:267:VAL:O	1:C:271:ILE:HG12	2.12	0.49
1:A:97:PRO:HB2	1:A:100:ASP:HB3	1.93	0.49
1:C:312:THR:O	1:C:314:PRO:HD3	2.13	0.49
2:G:650:ILE:O	2:G:654:VAL:HG23	2.13	0.49
1:B:339:VAL:HG23	1:B:340:ARG:H	1.78	0.49
1:A:104:ARG:HG3	1:A:138:SER:HB2	1.95	0.49
1:B:234:LEU:HB3	1:B:270:ILE:HG12	1.95	0.49
1:C:301:THR:C	1:C:303:LEU:H	2.16	0.48
2:G:560:LEU:HD21	2:G:621:VAL:HA	1.95	0.48
1:C:252:PRO:HD2	1:C:256:SER:OG	2.14	0.48
1:C:276:VAL:HG22	1:C:308:LYS:HB2	1.96	0.48
1:D:107:TRP:CE2	1:D:139:PRO:HB3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:PHE:CG	1:B:194:ALA:HB1	2.49	0.48
1:C:264:ILE:HD11	1:C:306:ARG:HB3	1.95	0.48
1:D:196:VAL:HG11	1:D:240:LYS:HB2	1.95	0.48
1:A:264:ILE:HD11	1:A:306:ARG:HB3	1.95	0.47
1:D:59:ARG:HG2	1:D:59:ARG:O	2.12	0.47
1:D:274:ALA:HB3	1:D:308:LYS:HG2	1.96	0.47
1:A:284:ASN:HD22	1:A:291:LEU:HA	1.80	0.47
1:A:296:TYR:CZ	1:A:299:ARG:HD3	2.50	0.47
1:D:287:ASP:HB3	1:D:290:ARG:HB2	1.96	0.47
2:F:560:LEU:O	2:F:564:LEU:HG	2.15	0.47
1:B:196:VAL:HG11	1:B:240:LYS:HB2	1.97	0.47
1:C:250:THR:HG22	1:C:278:TRP:O	2.15	0.47
1:A:172:LEU:HA	1:A:215:CYS:HB3	1.97	0.47
1:D:277:ILE:HG12	1:D:307:LEU:HD22	1.96	0.47
1:C:319:GLU:HB3	2:H:636:ILE:HG23	1.97	0.47
1:C:215:CYS:HB2	1:C:248:LEU:HD12	1.96	0.47
1:A:67:GLY:HA3	1:A:278:TRP:CZ2	2.50	0.46
1:C:278:TRP:HE1	1:C:313:ASN:ND2	2.13	0.46
1:A:254:VAL:H	2:G:676:GLN:N	2.12	0.46
1:A:291:LEU:HD13	2:F:643:TYR:CE2	2.49	0.46
1:B:304:ILE:HD12	1:B:335:ASN:HB3	1.98	0.46
2:F:618:CYS:HB3	2:F:655:LYS:HD2	1.97	0.46
2:G:688:GLU:HA	2:G:691:ARG:HD2	1.95	0.46
1:C:229:SER:O	1:C:270:ILE:HD12	2.15	0.46
1:A:218:GLU:HA	1:A:223:PHE:HB3	1.98	0.46
1:D:83:ARG:O	1:D:87:LYS:HB2	2.17	0.46
1:A:297:LYS:HG3	1:A:376:PRO:HG3	1.97	0.45
2:G:693:LEU:HG	2:G:694:PRO:HD2	1.98	0.45
1:A:302:GLU:O	1:A:305:PRO:HD2	2.15	0.45
1:A:274:ALA:HB3	1:A:308:LYS:HG3	1.99	0.45
1:C:249:TRP:O	1:C:277:ILE:HA	2.17	0.45
1:D:63:GLY:HA3	1:D:92:THR:O	2.16	0.45
1:A:300:SER:O	1:A:303:LEU:HB2	2.16	0.44
1:C:213:LEU:HD12	1:C:246:GLU:HB2	2.00	0.44
2:E:636:ILE:HD12	2:E:637:LEU:H	1.83	0.44
1:B:314:PRO:HB2	1:B:321:ASN:OD1	2.17	0.44
2:H:604:ILE:O	2:H:608:ARG:HB2	2.18	0.44
1:D:225:TYR:O	1:D:232:PRO:HD2	2.18	0.43
1:D:81:LEU:HB2	1:D:318:PHE:HE1	1.82	0.43
1:A:214:PHE:HD2	1:A:247:VAL:HG13	1.84	0.43
2:E:579:LEU:HD21	2:H:688:GLU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LEU:HA	1:B:215:CYS:HB3	2.01	0.43
2:F:694:PRO:C	2:F:695:ILE:HG13	2.38	0.43
1:A:139:PRO:HG3	1:A:154:LEU:HD11	1.99	0.43
1:D:67:GLY:HA2	1:D:96:ALA:O	2.17	0.43
1:A:78:ARG:CB	1:A:122:LEU:HD11	2.48	0.43
1:A:107:TRP:HB2	1:A:137:ILE:HD11	2.00	0.42
1:C:261:VAL:HG22	1:C:303:LEU:HD13	2.01	0.42
2:E:560:LEU:HD23	2:E:624:MET:HG3	2.00	0.42
1:B:107:TRP:CZ2	1:B:143:ILE:HD12	2.54	0.42
1:B:63:GLY:HA3	1:B:92:THR:O	2.18	0.42
1:C:100:ASP:HB3	1:C:103:HIS:HB3	2.02	0.42
1:C:192:ALA:HB1	1:C:236:THR:HB	2.01	0.42
2:G:682:ARG:HG3	2:G:682:ARG:H	1.67	0.42
1:A:215:CYS:SG	3:A:501:OQ1:C12	3.08	0.42
1:A:67:GLY:HA2	1:A:96:ALA:O	2.20	0.42
2:G:560:LEU:HD11	2:G:621:VAL:HG22	2.02	0.42
1:D:172:LEU:HD23	1:D:215:CYS:HB3	2.00	0.41
2:F:650:ILE:O	2:F:654:VAL:HG23	2.19	0.41
2:F:686:ALA:HB1	2:G:650:ILE:HD13	2.01	0.41
1:C:104:ARG:HB3	1:C:105:MET:H	1.72	0.41
2:G:560:LEU:O	2:G:564:LEU:HG	2.21	0.41
1:C:71:ARG:HA	1:C:72:PRO:HD3	1.90	0.41
1:D:261:VAL:HA	1:D:264:ILE:HD12	2.01	0.41
1:D:286:TYR:CD1	2:H:679:TRP:HB3	2.55	0.41
2:H:683:GLY:HA3	2:H:687:GLY:HA3	2.01	0.41
1:B:268:SER:HA	1:B:273:ARG:O	2.21	0.41
2:F:625:PHE:CZ	2:F:647:ILE:HG23	2.55	0.41
1:D:134:ILE:HG21	1:D:213:LEU:HD13	2.02	0.41
2:G:556:GLU:H	2:G:556:GLU:CD	2.24	0.41
1:A:69:TYR:CZ	1:A:98:LYS:HD2	2.56	0.41
1:B:74:VAL:HG22	1:B:77:GLN:OE1	2.21	0.41
1:D:234:LEU:HA	1:D:237:VAL:HB	2.03	0.41
1:C:221:GLY:HA2	1:C:228:VAL:CG2	2.51	0.41
1:A:235:ARG:O	1:A:239:GLU:HB2	2.21	0.41
1:C:88:TRP:HZ2	1:C:322:TYR:CZ	2.39	0.41
1:C:67:GLY:HA2	1:C:96:ALA:O	2.21	0.41
1:A:101:TYR:N	1:A:101:TYR:CD1	2.89	0.40
1:D:97:PRO:HB2	1:D:100:ASP:HB2	2.03	0.40
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.99	0.40
1:A:270:ILE:HG13	1:A:270:ILE:H	1.71	0.40
1:D:103:HIS:HD2	1:D:137:ILE:HA	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ALA:N	1:A:97:PRO:HD3	2.36	0.40
1:C:275:PRO:HD2	1:C:307:LEU:HD23	2.02	0.40
1:D:71:ARG:NE	2:H:641:TYR:CD2	2.79	0.40
1:D:215:CYS:SG	3:D:501:OQ1:C12	3.09	0.40
1:A:171:LEU:HD12	1:A:199:THR:HA	2.03	0.40
1:D:275:PRO:HD2	1:D:307:LEU:HD23	2.04	0.40

There are no symmetry-related clashes.

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	305/388 (79%)	287 (94%)	17 (6%)	1 (0%)	41 68
1	B	305/388 (79%)	286 (94%)	16 (5%)	3 (1%)	15 40
1	C	304/388 (78%)	275 (90%)	24 (8%)	5 (2%)	9 28
1	D	304/388 (78%)	279 (92%)	21 (7%)	4 (1%)	12 33
2	E	106/161 (66%)	97 (92%)	6 (6%)	3 (3%)	5 16
2	F	103/161 (64%)	98 (95%)	5 (5%)	0	100 100
2	G	111/161 (69%)	105 (95%)	4 (4%)	2 (2%)	8 25
2	H	106/161 (66%)	99 (93%)	6 (6%)	1 (1%)	17 43
All	All	1644/2196 (75%)	1526 (93%)	99 (6%)	19 (1%)	13 35

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	677	GLU
2	G	680	ALA
1	C	57	ALA
1	D	140	GLY

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Mol	Chain	Res	Type
1	D	181	CYS
1	C	140	GLY
1	C	141	LEU
2	E	566	TYR
2	H	681	PHE
1	B	105	MET
1	B	182	ALA
1	C	58	ARG
2	E	678	PRO
2	E	680	ALA
1	A	314	PRO
1	C	105	MET
1	D	57	ALA
1	D	314	PRO
1	B	314	PRO

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	277/331 (84%)	262 (95%)	15 (5%)	22 49
1	B	276/331 (83%)	261 (95%)	15 (5%)	22 49
1	C	270/331 (82%)	245 (91%)	25 (9%)	9 24
1	D	270/331 (82%)	253 (94%)	17 (6%)	18 42
2	E	95/140 (68%)	82 (86%)	13 (14%)	3 9
2	F	94/140 (67%)	86 (92%)	8 (8%)	10 28
2	G	102/140 (73%)	93 (91%)	9 (9%)	10 26
2	H	96/140 (69%)	84 (88%)	12 (12%)	4 12
All	All	1480/1884 (79%)	1366 (92%)	114 (8%)	13 32

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	GLU
1	A	100	ASP
1	A	114	GLU
1	A	118	GLN
1	A	144	THR
1	A	154	LEU
1	A	228	VAL
1	A	229	SER
1	A	258	GLU
1	A	264	ILE
1	A	265	GLU
1	A	270	ILE
1	A	278	TRP
1	A	301	THR
1	A	337	ASN
1	B	59	ARG
1	B	64	VAL
1	B	132	GLU
1	B	143	ILE
1	B	177	ASP
1	B	185	LYS
1	B	206	LEU
1	B	210	GLU
1	B	240	LYS
1	B	246	GLU
1	B	267	VAL
1	B	278	TRP
1	B	279	ASP
1	B	290	ARG
1	B	336	MET
1	C	59	ARG
1	C	61	LEU
1	C	62	CYS
1	C	71	ARG
1	C	83	ARG
1	C	89	GLU
1	C	114	GLU
1	C	118	GLN
1	C	124	SER
1	C	130	GLU
1	C	137	ILE
1	C	138	SER
1	C	151	VAL

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Mol	Chain	Res	Type
1	C	171	LEU
1	C	229	SER
1	C	246	GLU
1	C	258	GLU
1	C	264	ILE
1	C	279	ASP
1	C	281	ILE
1	C	289	LYS
1	C	302	GLU
1	C	340	ARG
1	C	370	THR
1	C	385	THR
1	D	59	ARG
1	D	71	ARG
1	D	83	ARG
1	D	102	LYS
1	D	120	MET
1	D	142	ASP
1	D	143	ILE
1	D	149	LYS
1	D	153	THR
1	D	189	SER
1	D	227	ASN
1	D	246	GLU
1	D	258	GLU
1	D	278	TRP
1	D	334	SER
1	D	339	VAL
1	D	382	LEU
2	E	577	GLN
2	E	583	GLN
2	E	602	GLU
2	E	608	ARG
2	E	620	LEU
2	E	628	LEU
2	E	629	SER
2	E	640	MET
2	E	647	ILE
2	E	677	GLU
2	E	679	TRP
2	E	682	ARG
2	E	693	LEU

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Mol	Chain	Res	Type
2	F	554	THR
2	F	583	GLN
2	F	604	ILE
2	F	618	CYS
2	F	639	ASP
2	F	656	SER
2	F	659	GLN
2	F	691	ARG
2	G	588	ASN
2	G	600	ASP
2	G	606	GLU
2	G	613	LYS
2	G	639	ASP
2	G	640	MET
2	G	647	ILE
2	G	656	SER
2	G	693	LEU
2	H	583	GLN
2	H	607	TRP
2	H	608	ARG
2	H	618	CYS
2	H	620	LEU
2	H	626	THR
2	H	639	ASP
2	H	646	ASP
2	H	676	GLN
2	H	681	PHE
2	H	682	ARG
2	H	685	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	118	GLN
1	C	195	GLN
1	D	86	GLN
1	D	118	GLN
1	D	227	ASN
1	D	230	GLN
2	E	630	ASN
2	E	690	GLN
2	G	583	GLN

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Mol	Chain	Res	Type
2	G	690	GLN
2	H	630	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 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	OQ1	B	501	-	15,18,18	0.59	0	15,26,26	0.94	0
3	OQ1	A	501	-	15,18,18	0.61	0	15,26,26	1.50	3 (20%)
3	OQ1	D	501	-	15,18,18	0.68	0	15,26,26	1.47	2 (13%)
3	OQ1	C	501	-	15,18,18	0.72	0	15,26,26	2.54	6 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OQ1	B	501	-	-	1/7/35/35	0/2/2/2
3	OQ1	A	501	-	-	4/7/35/35	0/2/2/2
3	OQ1	D	501	-	-	4/7/35/35	0/2/2/2
3	OQ1	C	501	-	-	3/7/35/35	0/2/2/2

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	501	OQ1	C4-O-C	6.22	122.56	114.12
3	C	501	OQ1	O-C-C1	4.95	114.82	107.87
3	D	501	OQ1	C4-O-C	3.83	119.32	114.12
3	A	501	OQ1	F1-C5-F	3.27	112.92	105.51
3	A	501	OQ1	F1-C5-C	3.12	113.56	109.77
3	C	501	OQ1	O-C4-C3	2.70	121.20	115.27
3	C	501	OQ1	O7-C1-C2	-2.49	104.59	110.35
3	C	501	OQ1	N10-C9-N	2.39	127.39	124.26
3	A	501	OQ1	C5-C-C1	2.26	117.79	113.41
3	C	501	OQ1	F1-C5-F	-2.17	100.59	105.51
3	D	501	OQ1	O-C4-C3	2.12	119.94	115.27

There are no chirality outliers.

All (12) torsion outliers are listed below:

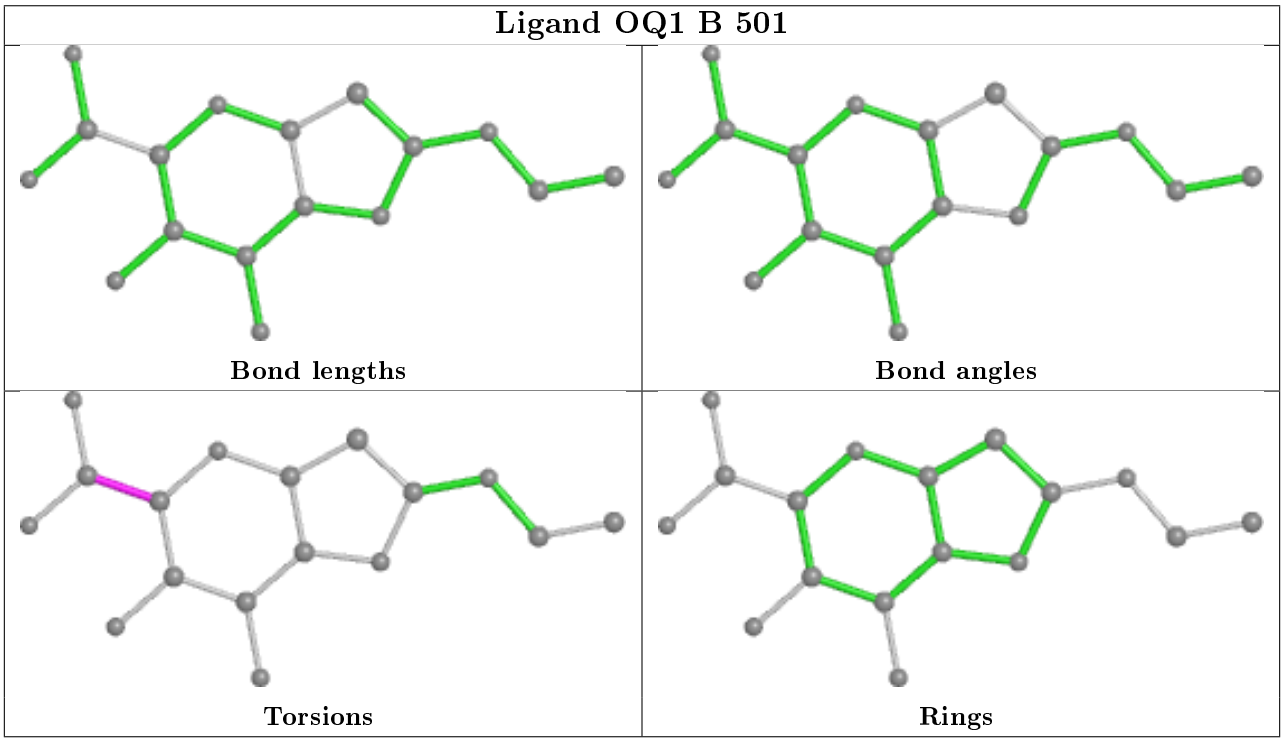
Mol	Chain	Res	Type	Atoms
3	B	501	OQ1	O-C-C5-F1
3	A	501	OQ1	C1-C-C5-F
3	A	501	OQ1	O-C-C5-F
3	A	501	OQ1	C1-C-C5-F1
3	A	501	OQ1	O-C-C5-F1
3	D	501	OQ1	C1-C-C5-F
3	D	501	OQ1	O-C-C5-F
3	D	501	OQ1	C1-C-C5-F1
3	D	501	OQ1	O-C-C5-F1
3	C	501	OQ1	O-C-C5-F
3	C	501	OQ1	C1-C-C5-F1
3	C	501	OQ1	O-C-C5-F1

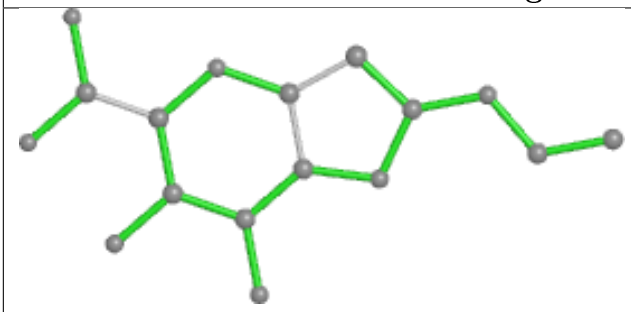
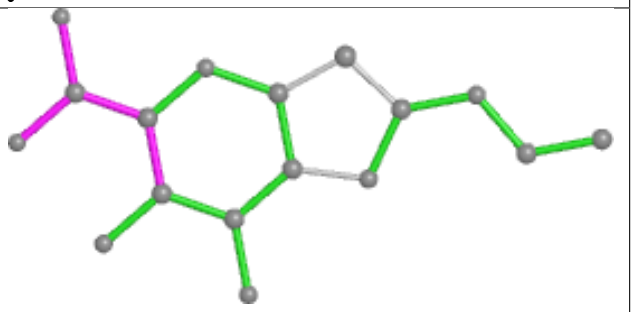
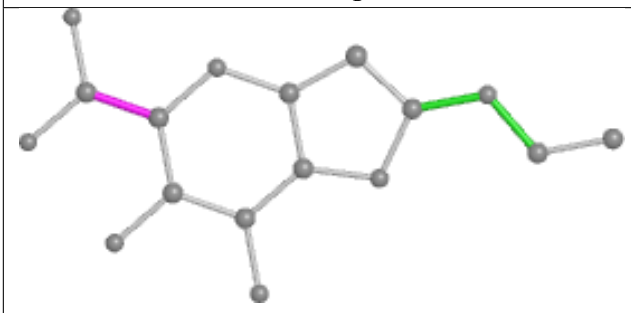
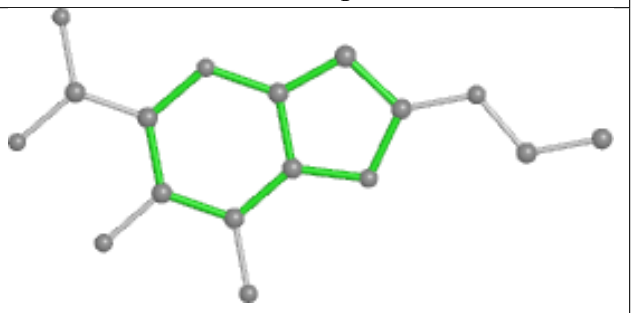
There are no ring outliers.

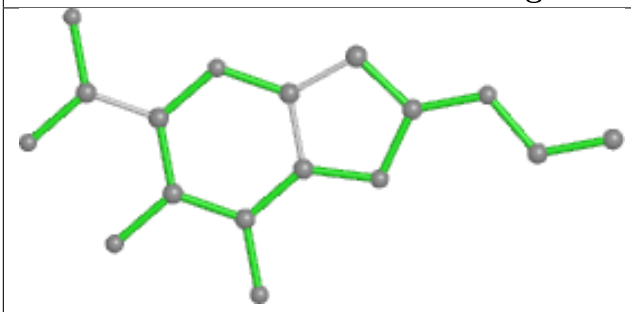
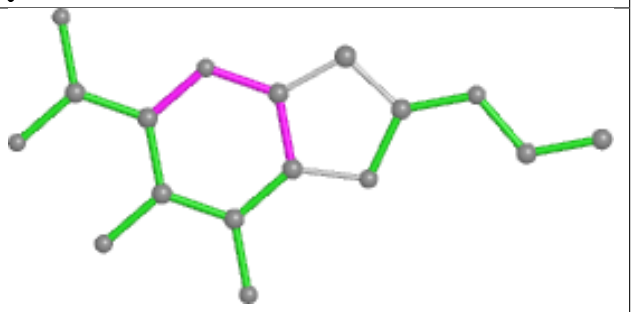
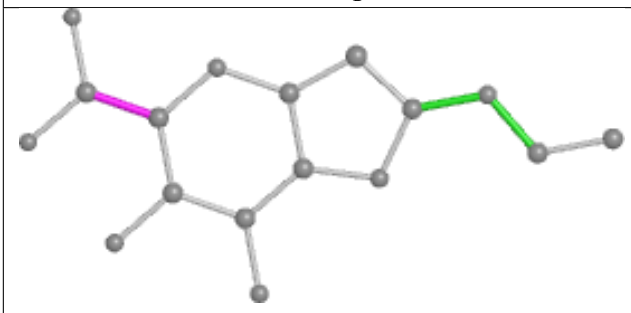
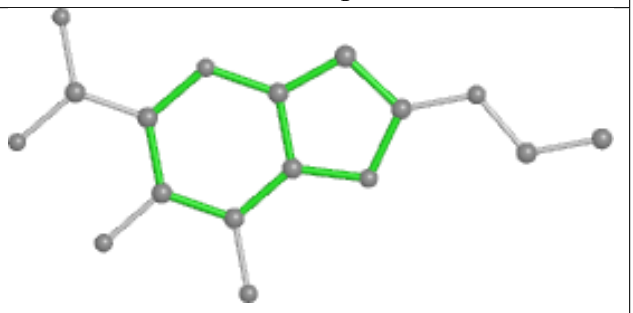
2 monomers are involved in 2 short contacts:

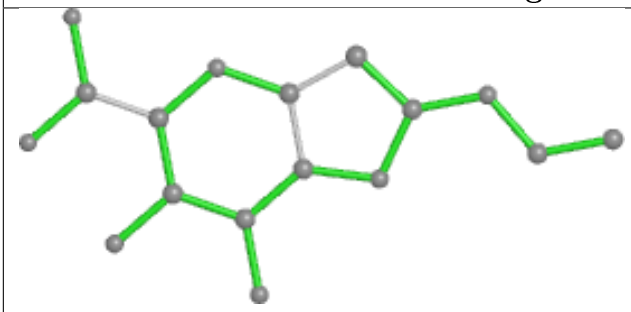
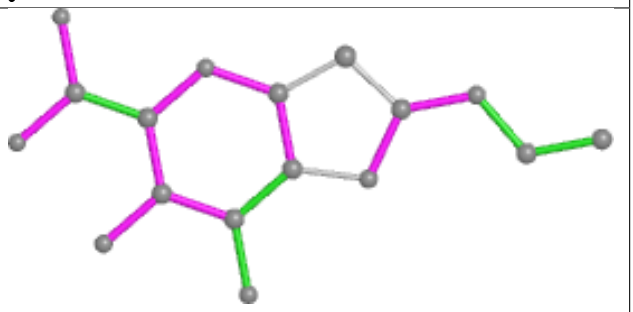
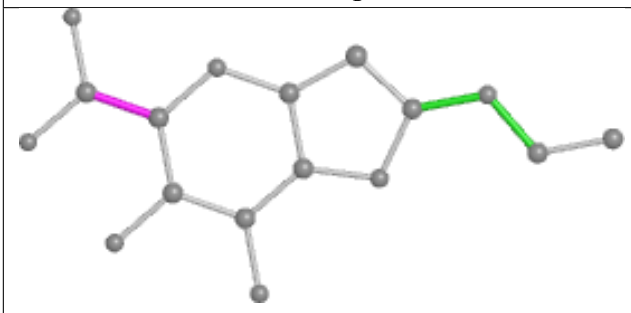
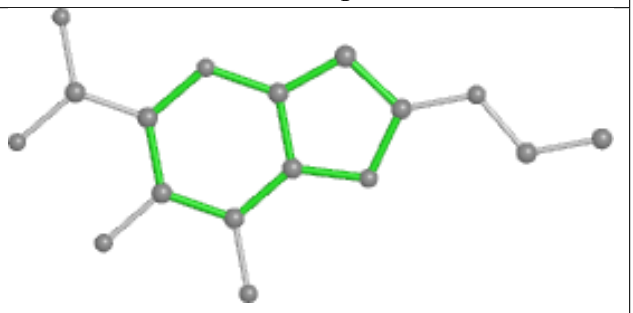
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	OQ1	1	0
3	D	501	OQ1	1	0

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.



Ligand OQ1 A 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand OQ1 D 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand OQ1 C 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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^{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	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	309/388 (79%)	-0.22	2 (0%) 89 89	35, 51, 70, 88	0
1	B	309/388 (79%)	-0.29	0 100 100	33, 47, 63, 76	0
1	C	310/388 (79%)	-0.20	3 (0%) 82 81	35, 53, 75, 99	0
1	D	310/388 (79%)	0.07	7 (2%) 60 57	37, 67, 96, 116	0
2	E	112/161 (69%)	0.37	7 (6%) 20 15	55, 84, 117, 129	0
2	F	109/161 (67%)	0.08	4 (3%) 41 36	41, 60, 82, 96	0
2	G	117/161 (72%)	0.22	5 (4%) 35 30	34, 59, 88, 106	0
2	H	112/161 (69%)	0.54	10 (8%) 9 6	47, 78, 113, 134	0
All	All	1688/2196 (76%)	-0.04	38 (2%) 60 57	33, 56, 95, 134	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	601	SER	6.9
2	G	680	ALA	6.2
2	E	632	ALA	5.0
1	A	372	VAL	4.4
1	D	145	PHE	3.8
2	E	608	ARG	3.7
1	D	163	GLN	3.6
2	E	633	ASN	3.3
2	G	682	ARG	3.1
2	G	617	MET	3.1
2	H	660	TRP	3.0
1	D	186	GLU	3.0
2	E	603	LYS	2.9
1	D	76	GLU	2.9
1	C	340	ARG	2.8
2	F	612	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
2	H	641	TYR	2.7
2	H	604	ILE	2.6
2	F	608	ARG	2.6
1	C	49	ALA	2.6
2	E	692	LEU	2.6
1	D	149	LYS	2.5
2	H	605	GLU	2.5
1	A	225	TYR	2.5
2	H	614	PHE	2.4
2	G	608	ARG	2.3
2	F	617	MET	2.3
1	D	113	VAL	2.3
2	F	694	PRO	2.2
1	C	372	VAL	2.2
2	H	608	ARG	2.2
2	H	584	TRP	2.2
2	E	601	SER	2.2
2	H	602	GLU	2.2
2	E	605	GLU	2.2
1	D	144	THR	2.1
2	H	638	TYR	2.1
2	H	692	LEU	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^{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	OQ1	A	501	17/17	0.94	0.17	29,54,59,59	0

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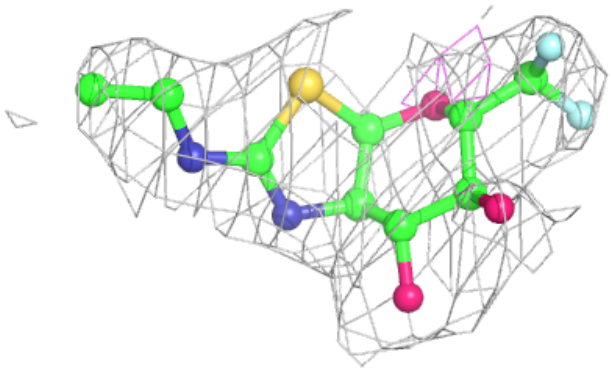
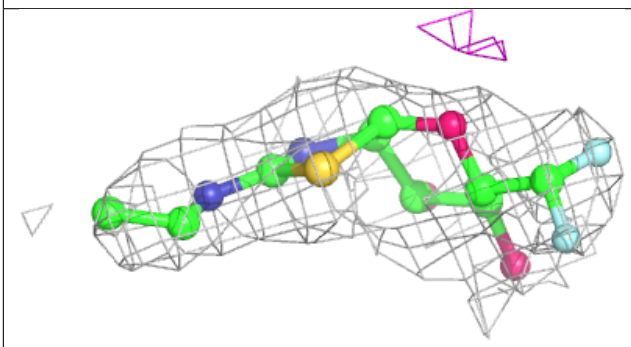
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	OQ1	B	501	17/17	0.96	0.17	25,45,55,57	0
3	OQ1	D	501	17/17	0.96	0.14	49,52,58,58	0
3	OQ1	C	501	17/17	0.96	0.15	44,52,57,57	0

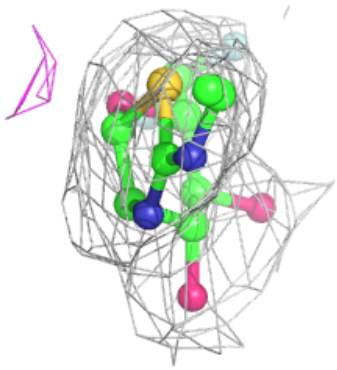
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OQ1 A 501:

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

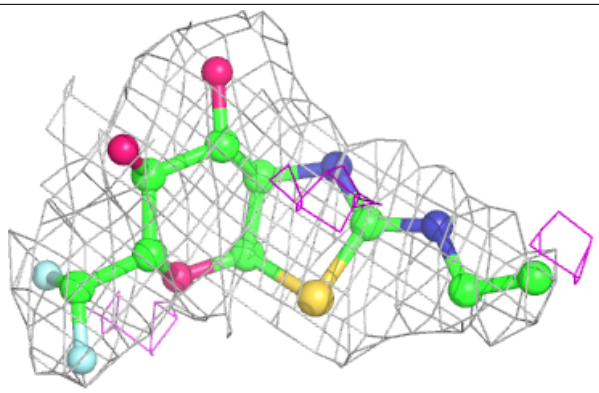


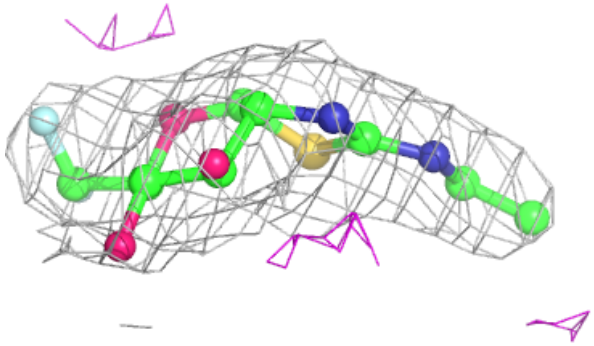


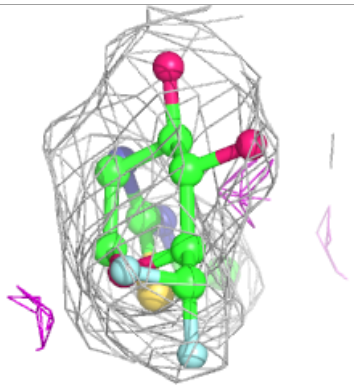


Electron density around OQ1 B 501:

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

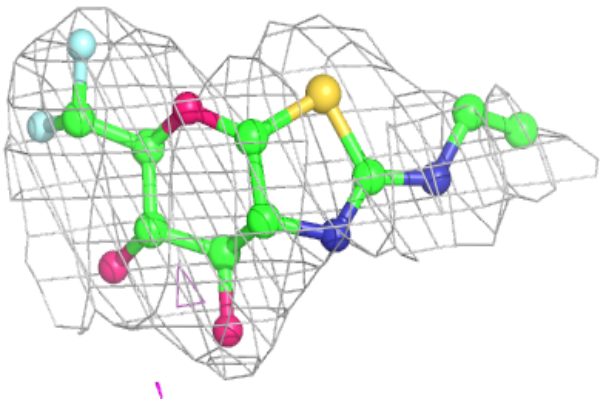


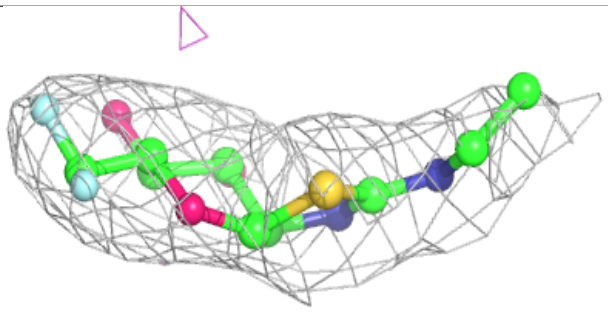


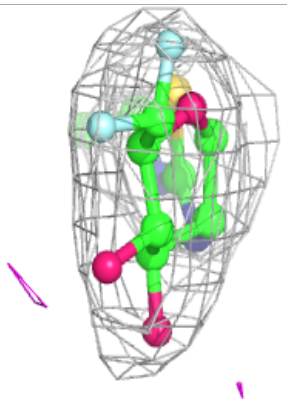


Electron density around OQ1 D 501:

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

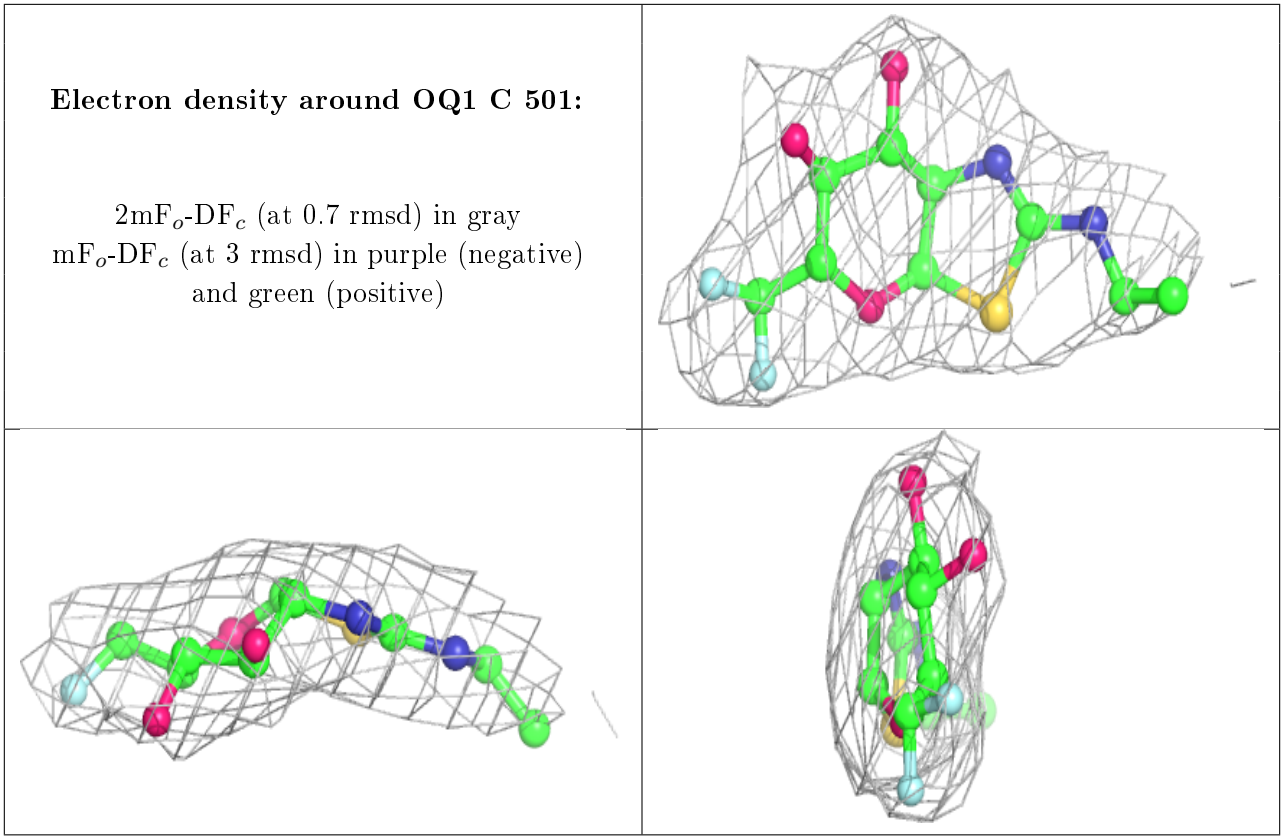






Electron density around OQ1 C 501:

$2mF_o$-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.