



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 2, 2022 – 10:26 AM JST

PDB ID : 7WNA
Title : Crystal Structure of the second bromodomain of human BRD2 in complex with the inhibitor Y13120
Authors : Li, J.; Zhang, C.; Xu, H.; Zhuang, X.; Wu, X.; Zhang, Y.; Xu, Y.
Deposited on : 2022-01-17
Resolution : 2.60 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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

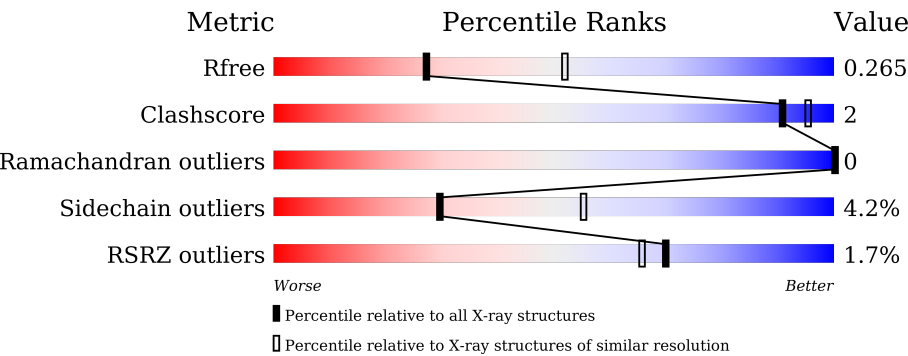
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	136	<div><div></div><div>77%</div><div>•</div><div>20%</div></div>
1	B	136	<div>4%</div> <div><div></div><div>72%</div><div>6%</div><div>•</div><div>21%</div></div>
1	C	136	<div><div></div><div>74%</div><div>6%</div><div></div><div>20%</div></div>
1	D	136	<div><div></div><div>75%</div><div>•</div><div>•</div><div>20%</div></div>
1	E	136	<div>%</div> <div><div></div><div>71%</div><div>8%</div><div></div><div>21%</div></div>
1	F	136	<div>3%</div> <div><div></div><div>65%</div><div>12%</div><div></div><div>22%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5727 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 Isoform 4 of Bromodomain-containing protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	109	Total	C	N	O	S	0	1	0
			908	582	159	160	7			
1	B	107	Total	C	N	O	S	0	0	0
			888	569	156	156	7			
1	C	109	Total	C	N	O	S	0	0	0
			902	578	158	159	7			
1	D	109	Total	C	N	O	S	0	0	0
			902	578	158	159	7			
1	E	108	Total	C	N	O	S	0	0	0
			896	573	157	159	7			
1	F	106	Total	C	N	O	S	0	0	0
			879	564	155	153	7			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	320	GLU	-	expression tag	UNP P25440
A	321	GLY	-	expression tag	UNP P25440
A	322	ASP	-	expression tag	UNP P25440
A	323	ILE	-	expression tag	UNP P25440
A	324	HIS	-	expression tag	UNP P25440
A	325	MET	-	expression tag	UNP P25440
A	326	LYS	-	expression tag	UNP P25440
A	327	LYS	-	expression tag	UNP P25440
A	328	GLY	-	expression tag	UNP P25440
A	329	HIS	-	expression tag	UNP P25440
A	330	HIS	-	expression tag	UNP P25440
A	331	HIS	-	expression tag	UNP P25440
A	332	HIS	-	expression tag	UNP P25440
A	333	HIS	-	expression tag	UNP P25440
A	334	HIS	-	expression tag	UNP P25440
A	335	GLU	-	expression tag	UNP P25440
A	336	ASN	-	expression tag	UNP P25440

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Chain	Residue	Modelled	Actual	Comment	Reference
A	337	LEU	-	expression tag	UNP P25440
A	338	TYR	-	expression tag	UNP P25440
A	339	PHE	-	expression tag	UNP P25440
A	340	GLN	-	expression tag	UNP P25440
A	341	GLY	-	expression tag	UNP P25440
A	342	GLY	-	expression tag	UNP P25440
A	343	SER	-	expression tag	UNP P25440
B	320	GLU	-	expression tag	UNP P25440
B	321	GLY	-	expression tag	UNP P25440
B	322	ASP	-	expression tag	UNP P25440
B	323	ILE	-	expression tag	UNP P25440
B	324	HIS	-	expression tag	UNP P25440
B	325	MET	-	expression tag	UNP P25440
B	326	LYS	-	expression tag	UNP P25440
B	327	LYS	-	expression tag	UNP P25440
B	328	GLY	-	expression tag	UNP P25440
B	329	HIS	-	expression tag	UNP P25440
B	330	HIS	-	expression tag	UNP P25440
B	331	HIS	-	expression tag	UNP P25440
B	332	HIS	-	expression tag	UNP P25440
B	333	HIS	-	expression tag	UNP P25440
B	334	HIS	-	expression tag	UNP P25440
B	335	GLU	-	expression tag	UNP P25440
B	336	ASN	-	expression tag	UNP P25440
B	337	LEU	-	expression tag	UNP P25440
B	338	TYR	-	expression tag	UNP P25440
B	339	PHE	-	expression tag	UNP P25440
B	340	GLN	-	expression tag	UNP P25440
B	341	GLY	-	expression tag	UNP P25440
B	342	GLY	-	expression tag	UNP P25440
B	343	SER	-	expression tag	UNP P25440
C	320	GLU	-	expression tag	UNP P25440
C	321	GLY	-	expression tag	UNP P25440
C	322	ASP	-	expression tag	UNP P25440
C	323	ILE	-	expression tag	UNP P25440
C	324	HIS	-	expression tag	UNP P25440
C	325	MET	-	expression tag	UNP P25440
C	326	LYS	-	expression tag	UNP P25440
C	327	LYS	-	expression tag	UNP P25440
C	328	GLY	-	expression tag	UNP P25440
C	329	HIS	-	expression tag	UNP P25440
C	330	HIS	-	expression tag	UNP P25440

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Chain	Residue	Modelled	Actual	Comment	Reference
C	331	HIS	-	expression tag	UNP P25440
C	332	HIS	-	expression tag	UNP P25440
C	333	HIS	-	expression tag	UNP P25440
C	334	HIS	-	expression tag	UNP P25440
C	335	GLU	-	expression tag	UNP P25440
C	336	ASN	-	expression tag	UNP P25440
C	337	LEU	-	expression tag	UNP P25440
C	338	TYR	-	expression tag	UNP P25440
C	339	PHE	-	expression tag	UNP P25440
C	340	GLN	-	expression tag	UNP P25440
C	341	GLY	-	expression tag	UNP P25440
C	342	GLY	-	expression tag	UNP P25440
C	343	SER	-	expression tag	UNP P25440
D	320	GLU	-	expression tag	UNP P25440
D	321	GLY	-	expression tag	UNP P25440
D	322	ASP	-	expression tag	UNP P25440
D	323	ILE	-	expression tag	UNP P25440
D	324	HIS	-	expression tag	UNP P25440
D	325	MET	-	expression tag	UNP P25440
D	326	LYS	-	expression tag	UNP P25440
D	327	LYS	-	expression tag	UNP P25440
D	328	GLY	-	expression tag	UNP P25440
D	329	HIS	-	expression tag	UNP P25440
D	330	HIS	-	expression tag	UNP P25440
D	331	HIS	-	expression tag	UNP P25440
D	332	HIS	-	expression tag	UNP P25440
D	333	HIS	-	expression tag	UNP P25440
D	334	HIS	-	expression tag	UNP P25440
D	335	GLU	-	expression tag	UNP P25440
D	336	ASN	-	expression tag	UNP P25440
D	337	LEU	-	expression tag	UNP P25440
D	338	TYR	-	expression tag	UNP P25440
D	339	PHE	-	expression tag	UNP P25440
D	340	GLN	-	expression tag	UNP P25440
D	341	GLY	-	expression tag	UNP P25440
D	342	GLY	-	expression tag	UNP P25440
D	343	SER	-	expression tag	UNP P25440
E	320	GLU	-	expression tag	UNP P25440
E	321	GLY	-	expression tag	UNP P25440
E	322	ASP	-	expression tag	UNP P25440
E	323	ILE	-	expression tag	UNP P25440
E	324	HIS	-	expression tag	UNP P25440

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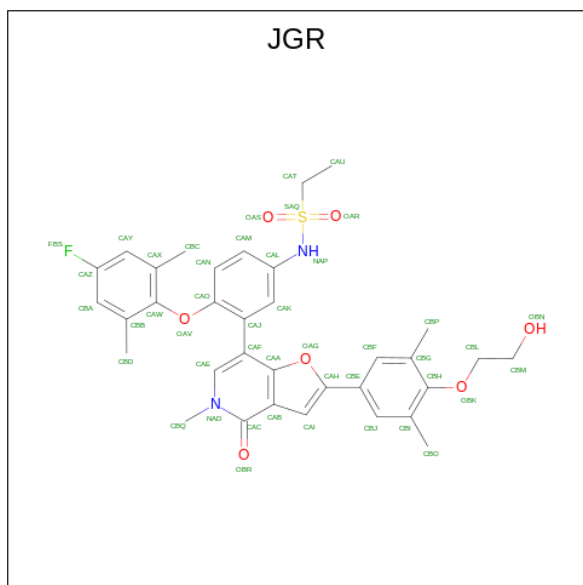
Chain	Residue	Modelled	Actual	Comment	Reference
E	325	MET	-	expression tag	UNP P25440
E	326	LYS	-	expression tag	UNP P25440
E	327	LYS	-	expression tag	UNP P25440
E	328	GLY	-	expression tag	UNP P25440
E	329	HIS	-	expression tag	UNP P25440
E	330	HIS	-	expression tag	UNP P25440
E	331	HIS	-	expression tag	UNP P25440
E	332	HIS	-	expression tag	UNP P25440
E	333	HIS	-	expression tag	UNP P25440
E	334	HIS	-	expression tag	UNP P25440
E	335	GLU	-	expression tag	UNP P25440
E	336	ASN	-	expression tag	UNP P25440
E	337	LEU	-	expression tag	UNP P25440
E	338	TYR	-	expression tag	UNP P25440
E	339	PHE	-	expression tag	UNP P25440
E	340	GLN	-	expression tag	UNP P25440
E	341	GLY	-	expression tag	UNP P25440
E	342	GLY	-	expression tag	UNP P25440
E	343	SER	-	expression tag	UNP P25440
F	320	GLU	-	expression tag	UNP P25440
F	321	GLY	-	expression tag	UNP P25440
F	322	ASP	-	expression tag	UNP P25440
F	323	ILE	-	expression tag	UNP P25440
F	324	HIS	-	expression tag	UNP P25440
F	325	MET	-	expression tag	UNP P25440
F	326	LYS	-	expression tag	UNP P25440
F	327	LYS	-	expression tag	UNP P25440
F	328	GLY	-	expression tag	UNP P25440
F	329	HIS	-	expression tag	UNP P25440
F	330	HIS	-	expression tag	UNP P25440
F	331	HIS	-	expression tag	UNP P25440
F	332	HIS	-	expression tag	UNP P25440
F	333	HIS	-	expression tag	UNP P25440
F	334	HIS	-	expression tag	UNP P25440
F	335	GLU	-	expression tag	UNP P25440
F	336	ASN	-	expression tag	UNP P25440
F	337	LEU	-	expression tag	UNP P25440
F	338	TYR	-	expression tag	UNP P25440
F	339	PHE	-	expression tag	UNP P25440
F	340	GLN	-	expression tag	UNP P25440
F	341	GLY	-	expression tag	UNP P25440
F	342	GLY	-	expression tag	UNP P25440

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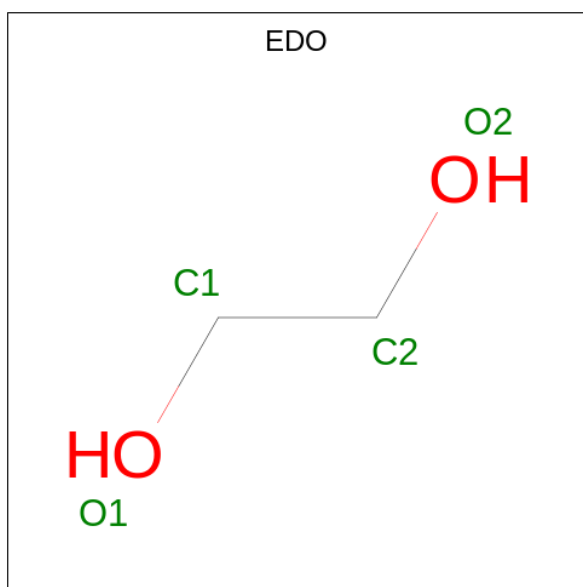
Chain	Residue	Modelled	Actual	Comment	Reference
F	343	SER	-	expression tag	UNP P25440

- Molecule 2 is {N}-[4-(4-fluoranyl-2,6-dimethyl-phenoxy)-3-[2-[4-(2-hydroxyethoxy)-3,5-dimethyl-phenyl]-5-methyl-4-oxidanylidene-furo[3,2-c]pyridin-7-yl]phenyl]ethanesulfonamide (three-letter code: JGR) (formula: C₃₄H₃₅FN₂O₇S) (labeled as "Ligand of Interest" by depositor).



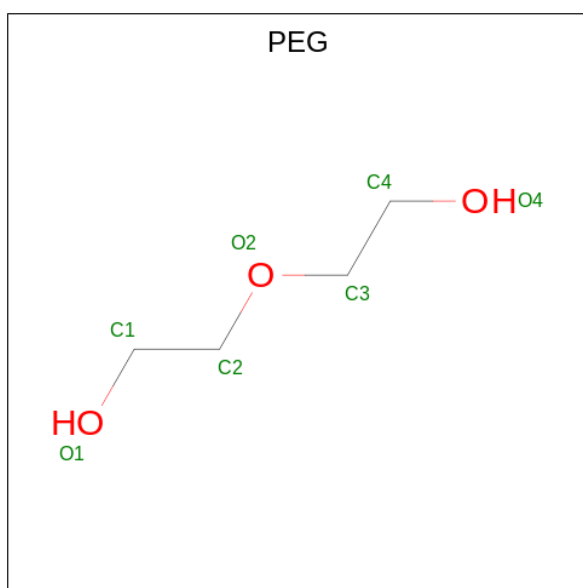
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			45	34	1	2	7	1		
2	B	1	Total	C	F	N	O	S	0	0
			45	34	1	2	7	1		
2	C	1	Total	C	F	N	O	S	0	0
			45	34	1	2	7	1		
2	D	1	Total	C	F	N	O	S	0	0
			45	34	1	2	7	1		
2	E	1	Total	C	F	N	O	S	0	0
			45	34	1	2	7	1		
2	F	1	Total	C	F	N	O	S	0	0
			45	34	1	2	7	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		


- Molecule 5 is water.

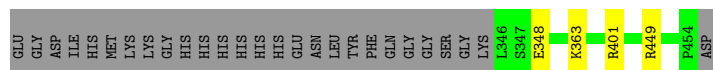
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	19	Total 19	O 19	0	0
5	B	6	Total 6	O 6	0	0
5	C	8	Total 8	O 8	0	0
5	D	15	Total 15	O 15	0	0
5	E	8	Total 8	O 8	0	0
5	F	4	Total 4	O 4	0	0

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

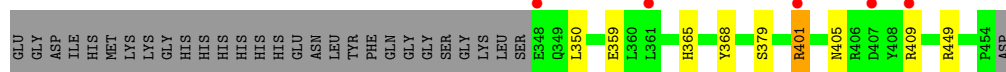
- Molecule 1: Isoform 4 of Bromodomain-containing protein 2

Chain A:  77% 20%



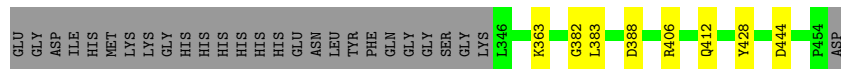
- Molecule 1: Isoform 4 of Bromodomain-containing protein 2

Chain B:  4% 72% 6% 21%




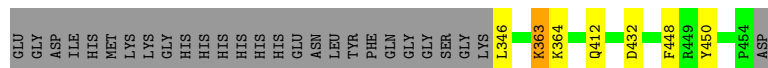
- Molecule 1: Isoform 4 of Bromodomain-containing protein 2

Chain C:  74% 6% 20%



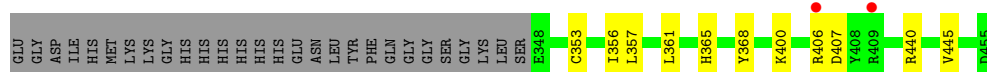
- Molecule 1: Isoform 4 of Bromodomain-containing protein 2

Chain D:  75% 20%

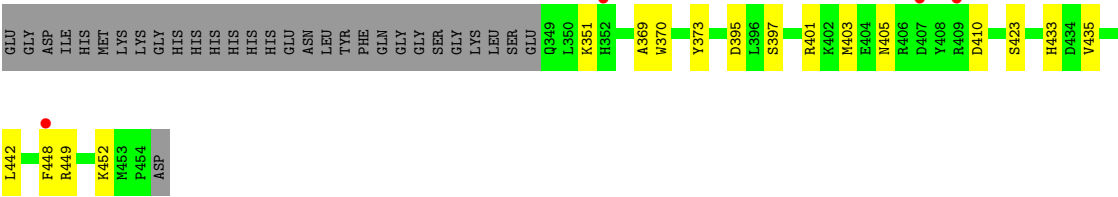


- Molecule 1: Isoform 4 of Bromodomain-containing protein 2

Chain E:  71% 8% 21%



- Molecule 1: Isoform 4 of Bromodomain-containing protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	106.63Å 106.63Å 87.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	106.63 – 2.60 29.57 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (106.63-2.60) 98.7 (29.57-2.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.208 , 0.268 0.215 , 0.265	Depositor DCC
R_{free} test set	1562 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 22.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.326 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5727	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: JGR, EDO, PEG

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	0.66	0/936	0.77	0/1261
1	B	0.64	0/913	0.81	1/1230 (0.1%)
1	C	0.64	0/927	0.78	1/1249 (0.1%)
1	D	0.67	0/927	0.77	0/1249
1	E	0.59	0/921	0.73	0/1241
1	F	0.61	0/904	0.74	0/1218
All	All	0.63	0/5528	0.76	2/7448 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	444	ASP	CB-CG-OD1	5.27	123.04	118.30
1	B	401	ARG	NE-CZ-NH1	5.14	122.87	120.30

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	908	0	893	1	0
1	B	888	0	869	3	0
1	C	902	0	885	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	902	0	885	2	0
1	E	896	0	873	5	0
1	F	879	0	863	7	0
2	A	45	0	0	0	0
2	B	45	0	0	0	0
2	C	45	0	0	0	0
2	D	45	0	0	0	0
2	E	45	0	0	0	0
2	F	45	0	0	0	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0
4	A	7	0	10	1	0
4	D	7	0	10	0	0
5	A	19	0	0	0	0
5	B	6	0	0	0	0
5	C	8	0	0	0	0
5	D	15	0	0	0	0
5	E	8	0	0	0	0
5	F	4	0	0	0	0
All	All	5727	0	5300	19	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 2.

All (19) 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:F:369:ALA:HB2	1:F:442:LEU:HD13	1.76	0.66
1:F:370:TRP:HA	1:F:373:TYR:CD2	2.37	0.60
1:F:370:TRP:HA	1:F:373:TYR:CE2	2.38	0.59
1:F:395:ASP:OD2	1:F:397:SER:OG	2.20	0.56
1:E:365:HIS:CD2	1:E:445:VAL:HG21	2.45	0.51
1:B:405:ASN:ND2	1:C:388:ASP:OD2	2.44	0.51
1:B:365:HIS:HB3	1:B:368:TYR:CE2	2.47	0.49
1:C:382:GLY:HA3	1:D:363:LYS:HG2	1.95	0.48
1:F:369:ALA:HB2	1:F:442:LEU:CD1	2.42	0.47
1:B:350:LEU:HD11	1:B:409:ARG:O	2.15	0.47
1:F:433:HIS:ND1	1:F:435:VAL:HG12	2.31	0.46
1:E:365:HIS:HD2	1:E:368:TYR:OH	1.99	0.45
1:C:406:ARG:NH1	1:E:361:LEU:O	2.50	0.45
1:E:353:CYS:HA	1:E:356:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:401:ARG:O	1:F:405:ASN:ND2	2.52	0.43
1:E:357:LEU:HD21	1:E:400:LYS:HA	2.00	0.43
1:D:412:GLN:NE2	1:D:450:TYR:OH	2.53	0.41
1:A:401:ARG:HE	4:A:503:PEG:H31	1.86	0.41
1:C:383:LEU:HD22	1:C:428:TYR:OH	2.20	0.41

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	108/136 (79%)	105 (97%)	3 (3%)	0	100	100
1	B	105/136 (77%)	101 (96%)	4 (4%)	0	100	100
1	C	107/136 (79%)	107 (100%)	0	0	100	100
1	D	107/136 (79%)	102 (95%)	5 (5%)	0	100	100
1	E	106/136 (78%)	101 (95%)	5 (5%)	0	100	100
1	F	104/136 (76%)	97 (93%)	7 (7%)	0	100	100
All	All	637/816 (78%)	613 (96%)	24 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	97/118 (82%)	94 (97%)	3 (3%)	40	66
1	B	94/118 (80%)	90 (96%)	4 (4%)	29	54
1	C	96/118 (81%)	94 (98%)	2 (2%)	53	77
1	D	96/118 (81%)	91 (95%)	5 (5%)	23	46
1	E	95/118 (80%)	92 (97%)	3 (3%)	39	65
1	F	93/118 (79%)	86 (92%)	7 (8%)	13	27
All	All	571/708 (81%)	547 (96%)	24 (4%)	30	55

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	348	GLU
1	A	363	LYS
1	A	449	ARG
1	B	359	GLU
1	B	379	SER
1	B	401	ARG
1	B	449	ARG
1	C	363	LYS
1	C	412	GLN
1	D	346	LEU
1	D	363	LYS
1	D	364	LYS
1	D	432	ASP
1	D	448	PHE
1	E	406	ARG
1	E	407	ASP
1	E	440	ARG
1	F	351	LYS
1	F	403	MET
1	F	410	ASP
1	F	423	SER
1	F	448	PHE
1	F	449	ARG
1	F	452	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	349	GLN

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Mol	Chain	Res	Type
1	C	412	GLN
1	D	412	GLN
1	E	365	HIS
1	F	354	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 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	EDO	A	502	-	3,3,3	0.49	0	2,2,2	0.36	0
2	JGR	F	501	-	43,49,49	3.05	14 (32%)	57,73,73	1.60	10 (17%)
3	EDO	B	502	-	3,3,3	0.46	0	2,2,2	0.48	0
2	JGR	E	501	-	43,49,49	3.24	16 (37%)	57,73,73	1.92	12 (21%)
4	PEG	A	503	-	6,6,6	0.95	0	5,5,5	0.96	0
2	JGR	D	501	-	43,49,49	3.05	15 (34%)	57,73,73	1.52	9 (15%)
2	JGR	B	501	-	43,49,49	2.87	12 (27%)	57,73,73	1.52	10 (17%)
2	JGR	A	501	-	43,49,49	3.25	16 (37%)	57,73,73	1.31	6 (10%)
4	PEG	D	502	-	6,6,6	0.56	0	5,5,5	1.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	JGR	C	501	-	43,49,49	2.98	14 (32%)	57,73,73	1.47	7 (12%)

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	EDO	A	502	-	-	0/1/1/1	-
2	JGR	F	501	-	-	3/22/24/24	0/5/5/5
3	EDO	B	502	-	-	0/1/1/1	-
2	JGR	E	501	-	-	1/22/24/24	0/5/5/5
4	PEG	A	503	-	-	3/4/4/4	-
2	JGR	D	501	-	-	3/22/24/24	0/5/5/5
2	JGR	B	501	-	-	3/22/24/24	0/5/5/5
2	JGR	A	501	-	-	2/22/24/24	0/5/5/5
4	PEG	D	502	-	-	2/4/4/4	-
2	JGR	C	501	-	-	3/22/24/24	0/5/5/5

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	JGR	OAR-SAQ	7.92	1.54	1.43
2	A	501	JGR	FBS-CAZ	7.24	1.53	1.36
2	C	501	JGR	OAR-SAQ	7.20	1.53	1.43
2	E	501	JGR	FBS-CAZ	6.89	1.53	1.36
2	D	501	JGR	OAR-SAQ	6.86	1.53	1.43
2	B	501	JGR	OAR-SAQ	6.82	1.53	1.43
2	F	501	JGR	OAS-SAQ	6.55	1.52	1.43
2	E	501	JGR	OAR-SAQ	6.48	1.52	1.43
2	A	501	JGR	CAA-CAF	-6.45	1.32	1.47
2	E	501	JGR	CAT-SAQ	6.44	1.84	1.76
2	D	501	JGR	CAT-SAQ	6.36	1.84	1.76
2	F	501	JGR	OAR-SAQ	6.35	1.52	1.43
2	E	501	JGR	CBE-CAH	-6.26	1.35	1.46
2	A	501	JGR	CBD-CBB	-6.03	1.39	1.51
2	C	501	JGR	CAA-CAF	-6.02	1.33	1.47
2	C	501	JGR	CBP-CBG	-5.98	1.39	1.51
2	D	501	JGR	CBD-CBB	-5.97	1.39	1.51
2	A	501	JGR	CBP-CBG	-5.96	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	JGR	CBD-CBB	-5.95	1.39	1.51
2	F	501	JGR	CBE-CAH	-5.87	1.36	1.46
2	B	501	JGR	CAA-CAF	-5.85	1.33	1.47
2	F	501	JGR	CAA-CAF	-5.83	1.33	1.47
2	A	501	JGR	CBE-CAH	-5.68	1.36	1.46
2	C	501	JGR	CAT-SAQ	5.65	1.83	1.76
2	E	501	JGR	CAL-NAP	-5.65	1.34	1.43
2	F	501	JGR	CBO-CBI	-5.58	1.39	1.51
2	D	501	JGR	CBE-CAH	-5.55	1.36	1.46
2	D	501	JGR	CBC-CAX	-5.54	1.39	1.51
2	E	501	JGR	CBD-CBB	-5.53	1.39	1.51
2	A	501	JGR	CBC-CAX	-5.50	1.40	1.51
2	E	501	JGR	CBC-CAX	-5.49	1.40	1.51
2	E	501	JGR	CAB-CAC	-5.49	1.36	1.47
2	E	501	JGR	CAA-CAF	-5.48	1.34	1.47
2	B	501	JGR	OAS-SAQ	5.47	1.51	1.43
2	C	501	JGR	CAB-CAC	-5.38	1.36	1.47
2	A	501	JGR	CAT-SAQ	5.37	1.83	1.76
2	D	501	JGR	OAS-SAQ	5.32	1.51	1.43
2	D	501	JGR	CBP-CBG	-5.27	1.40	1.51
2	C	501	JGR	CBO-CBI	-5.24	1.40	1.51
2	D	501	JGR	CAA-CAF	-5.24	1.35	1.47
2	C	501	JGR	CBE-CAH	-5.24	1.37	1.46
2	F	501	JGR	CAJ-CAF	-5.22	1.40	1.49
2	F	501	JGR	CAB-CAC	-5.19	1.37	1.47
2	B	501	JGR	CBC-CAX	-5.12	1.40	1.51
2	B	501	JGR	CBE-CAH	-5.10	1.37	1.46
2	F	501	JGR	CBP-CBG	-5.08	1.40	1.51
2	A	501	JGR	CBO-CBI	-5.08	1.40	1.51
2	B	501	JGR	CBD-CBB	-5.08	1.40	1.51
2	E	501	JGR	OAS-SAQ	5.03	1.50	1.43
2	C	501	JGR	CBD-CBB	-5.03	1.41	1.51
2	D	501	JGR	CAL-NAP	-5.01	1.35	1.43
2	E	501	JGR	CAJ-CAF	-5.00	1.40	1.49
2	B	501	JGR	CBP-CBG	-4.98	1.41	1.51
2	B	501	JGR	CAL-NAP	-4.84	1.35	1.43
2	B	501	JGR	CBO-CBI	-4.84	1.41	1.51
2	F	501	JGR	CBC-CAX	-4.82	1.41	1.51
2	E	501	JGR	CBO-CBI	-4.81	1.41	1.51
2	D	501	JGR	CBO-CBI	-4.79	1.41	1.51
2	F	501	JGR	CAT-SAQ	4.74	1.82	1.76
2	F	501	JGR	CAL-NAP	-4.71	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	JGR	CAB-CAC	-4.64	1.38	1.47
2	C	501	JGR	OAS-SAQ	4.62	1.50	1.43
2	B	501	JGR	CAT-SAQ	4.56	1.82	1.76
2	A	501	JGR	CAL-NAP	-4.49	1.35	1.43
2	A	501	JGR	CAB-CAC	-4.48	1.38	1.47
2	D	501	JGR	CAB-CAC	-4.45	1.38	1.47
2	C	501	JGR	CAL-NAP	-4.40	1.36	1.43
2	E	501	JGR	CBP-CBG	-4.39	1.42	1.51
2	D	501	JGR	CAJ-CAF	-4.36	1.41	1.49
2	C	501	JGR	CBC-CAX	-4.32	1.42	1.51
2	A	501	JGR	CAJ-CAF	-3.86	1.42	1.49
2	C	501	JGR	CAJ-CAF	-3.66	1.43	1.49
2	A	501	JGR	OAS-SAQ	3.49	1.48	1.43
2	B	501	JGR	CAJ-CAF	-3.34	1.43	1.49
2	D	501	JGR	FBS-CAZ	3.27	1.44	1.36
2	C	501	JGR	FBS-CAZ	-2.73	1.29	1.36
2	C	501	JGR	CAI-CAB	-2.39	1.35	1.40
2	E	501	JGR	SAQ-NAP	-2.38	1.58	1.62
2	F	501	JGR	FBS-CAZ	2.35	1.42	1.36
2	E	501	JGR	CAI-CAB	-2.34	1.35	1.40
2	F	501	JGR	SAQ-NAP	-2.32	1.58	1.62
2	D	501	JGR	CAK-CAL	2.27	1.43	1.39
2	D	501	JGR	CAY-CAZ	2.18	1.41	1.37
2	E	501	JGR	CAE-NAD	2.16	1.42	1.36
2	A	501	JGR	SAQ-NAP	2.04	1.66	1.62
2	A	501	JGR	CAI-CAB	-2.01	1.36	1.40
2	A	501	JGR	OAV-CAO	-2.00	1.35	1.39

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	JGR	OAS-SAQ-OAR	-8.31	107.31	119.35
2	C	501	JGR	OAS-SAQ-OAR	-6.23	110.32	119.35
2	F	501	JGR	OAS-SAQ-OAR	-6.01	110.64	119.35
2	E	501	JGR	CAT-SAQ-NAP	5.75	115.10	106.83
2	F	501	JGR	CAT-SAQ-NAP	5.62	114.91	106.83
2	D	501	JGR	OAS-SAQ-OAR	-5.35	111.60	119.35
2	B	501	JGR	OAS-SAQ-OAR	-4.96	112.17	119.35
2	A	501	JGR	OAS-SAQ-OAR	-3.64	114.07	119.35
2	D	501	JGR	CAX-CAY-CAZ	3.60	121.86	119.26
2	E	501	JGR	FBS-CAZ-CAY	3.56	123.34	118.25
2	B	501	JGR	CAT-SAQ-NAP	3.44	111.77	106.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	JGR	CAK-CAL-NAP	3.29	128.36	119.93
2	A	501	JGR	CBA-CAZ-CAY	-3.20	119.47	123.52
2	E	501	JGR	CAF-CAE-NAD	-3.13	118.96	122.96
2	F	501	JGR	CBA-CAZ-CAY	-3.12	119.58	123.52
2	A	501	JGR	CAM-CAL-NAP	-3.11	113.37	120.09
2	E	501	JGR	CBL-OBK-CBH	3.04	123.42	114.23
2	D	501	JGR	CAF-CAE-NAD	-3.02	119.10	122.96
2	D	501	JGR	CBQ-NAD-CAE	-2.97	114.67	120.61
2	B	501	JGR	CAK-CAL-NAP	2.95	127.50	119.93
2	E	501	JGR	CBA-CAZ-CAY	-2.94	119.80	123.52
2	C	501	JGR	CAK-CAL-NAP	2.89	127.35	119.93
2	C	501	JGR	CAT-SAQ-NAP	2.87	110.96	106.83
2	D	501	JGR	CAT-SAQ-NAP	2.85	110.92	106.83
2	B	501	JGR	CBA-CAZ-CAY	-2.83	119.94	123.52
2	B	501	JGR	OAR-SAQ-NAP	2.80	114.09	107.28
2	F	501	JGR	CBQ-NAD-CAE	-2.77	115.06	120.61
2	F	501	JGR	CAK-CAL-NAP	2.76	127.02	119.93
2	E	501	JGR	CAM-CAL-NAP	-2.73	114.19	120.09
2	A	501	JGR	CAX-CAY-CAZ	2.73	121.23	119.26
2	E	501	JGR	CAK-CAL-NAP	2.69	126.83	119.93
2	C	501	JGR	CAM-CAL-NAP	-2.66	114.34	120.09
2	E	501	JGR	CBB-CBA-CAZ	2.64	121.16	119.26
2	B	501	JGR	CAX-CAY-CAZ	2.63	121.16	119.26
2	E	501	JGR	CAO-OAV-CAW	2.62	123.61	117.79
2	C	501	JGR	CBA-CAZ-CAY	-2.58	120.26	123.52
2	D	501	JGR	CAM-CAL-NAP	-2.55	114.57	120.09
2	F	501	JGR	CAX-CAY-CAZ	2.54	121.10	119.26
2	D	501	JGR	CAK-CAL-NAP	2.53	126.41	119.93
2	F	501	JGR	CAM-CAL-NAP	-2.51	114.66	120.09
2	B	501	JGR	FBS-CAZ-CBA	2.50	121.82	118.25
2	B	501	JGR	CBC-CAX-CAW	2.41	124.71	120.82
2	F	501	JGR	CAF-CAE-NAD	-2.41	119.88	122.96
2	B	501	JGR	CAM-CAL-NAP	-2.41	114.88	120.09
2	D	501	JGR	CBC-CAX-CAW	2.40	124.69	120.82
2	F	501	JGR	FBS-CAZ-CAY	2.36	121.63	118.25
2	D	501	JGR	CBA-CAZ-CAY	-2.36	120.53	123.52
2	C	501	JGR	FBS-CAZ-CAY	2.30	121.54	118.25
2	E	501	JGR	CBJ-CBE-CAH	2.26	123.28	120.42
2	B	501	JGR	CAU-CAT-SAQ	-2.25	109.77	112.93
2	A	501	JGR	CAT-SAQ-NAP	2.23	110.04	106.83
2	C	501	JGR	CBB-CBA-CAZ	2.22	120.87	119.26
2	F	501	JGR	CBJ-CBE-CAH	2.07	123.04	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	JGR	OAR-SAQ-NAP	2.03	112.22	107.28

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	501	JGR	CAU-CAT-SAQ-NAP
2	F	501	JGR	CAU-CAT-SAQ-OAR
4	A	503	PEG	O2-C3-C4-O4
2	C	501	JGR	OBK-CBL-CBM-OBN
2	D	501	JGR	OBK-CBL-CBM-OBN
4	D	502	PEG	O2-C3-C4-O4
4	A	503	PEG	O1-C1-C2-O2
2	B	501	JGR	CAA-CAF-CAJ-CAK
2	C	501	JGR	CAA-CAF-CAJ-CAK
2	B	501	JGR	OBK-CBL-CBM-OBN
2	E	501	JGR	OBK-CBL-CBM-OBN
4	A	503	PEG	C4-C3-O2-C2
4	D	502	PEG	O1-C1-C2-O2
2	B	501	JGR	CAA-CAF-CAJ-CAO
2	D	501	JGR	CAA-CAF-CAJ-CAK
2	F	501	JGR	CAA-CAF-CAJ-CAK
2	C	501	JGR	CAA-CAF-CAJ-CAO
2	D	501	JGR	CAA-CAF-CAJ-CAO
2	A	501	JGR	CAK-CAL-NAP-SAQ
2	A	501	JGR	CAA-CAF-CAJ-CAK

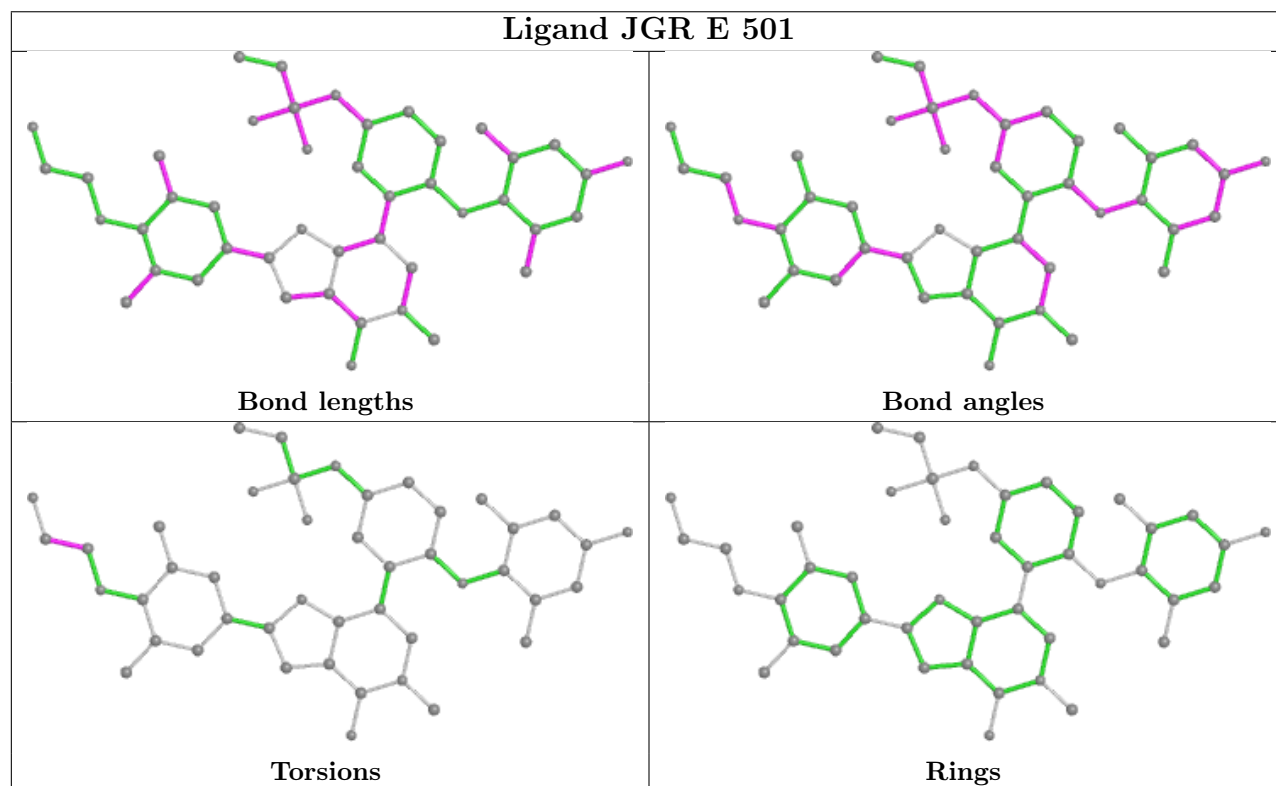
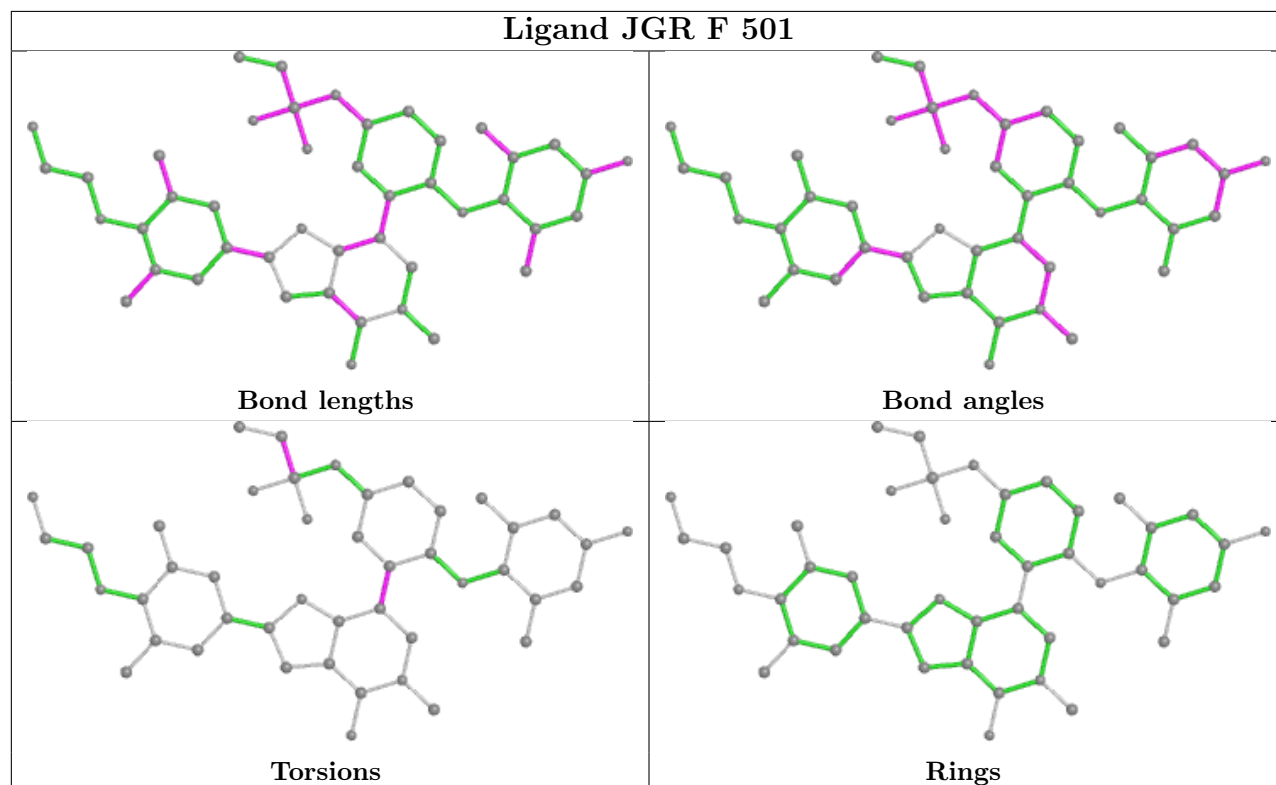
There are no ring outliers.

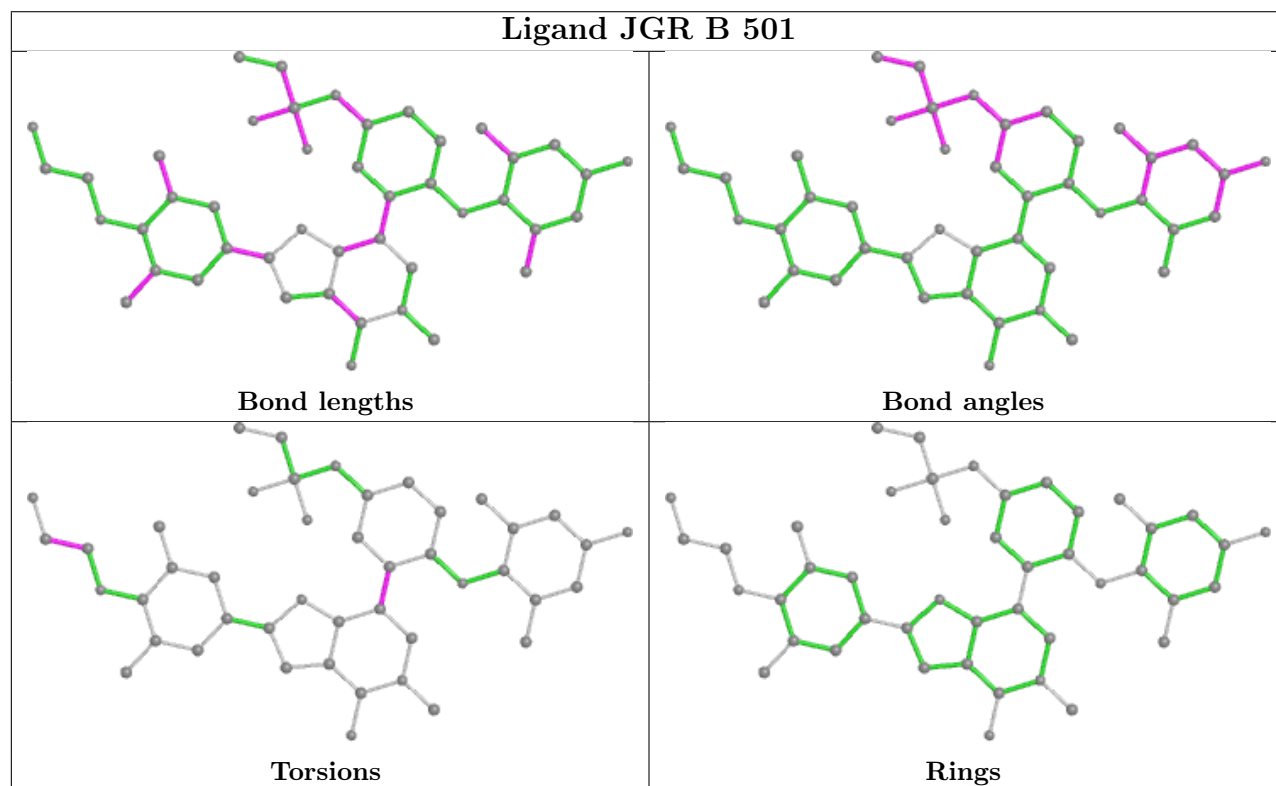
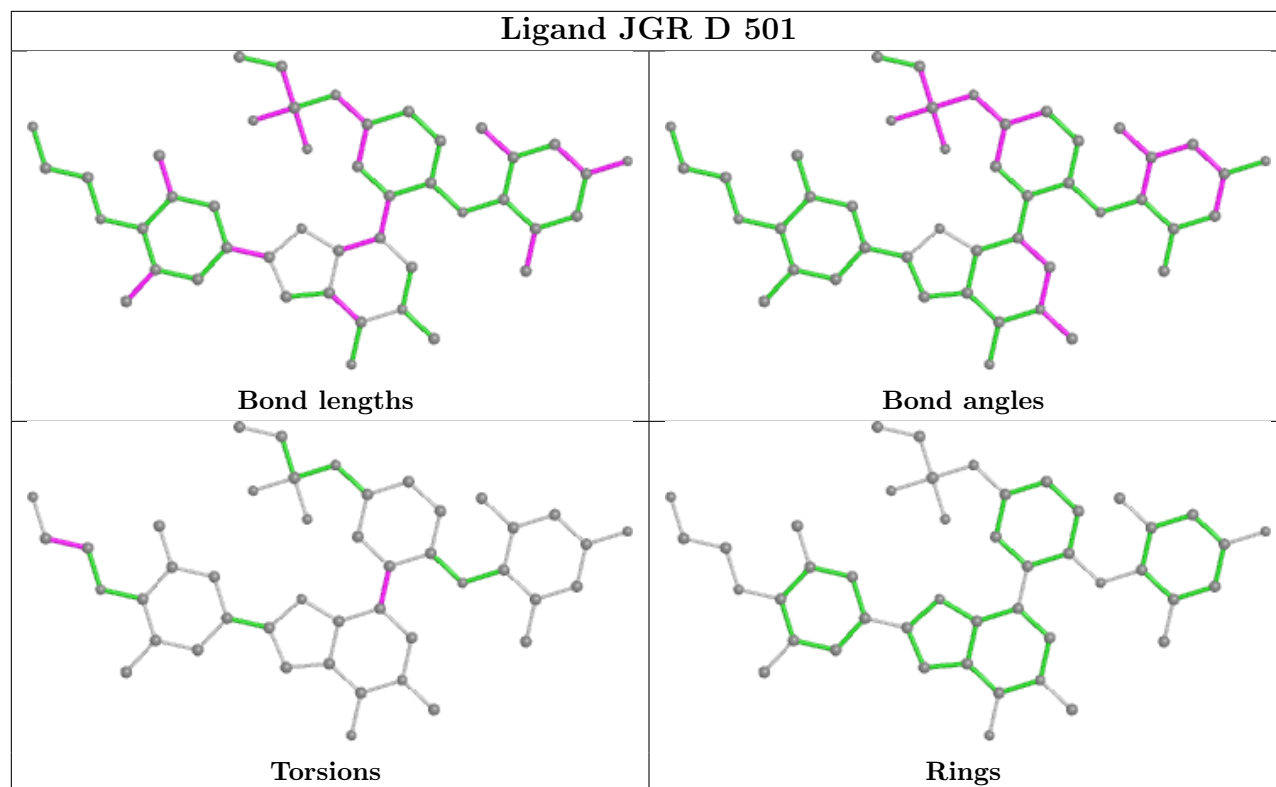
1 monomer is involved in 1 short contact:

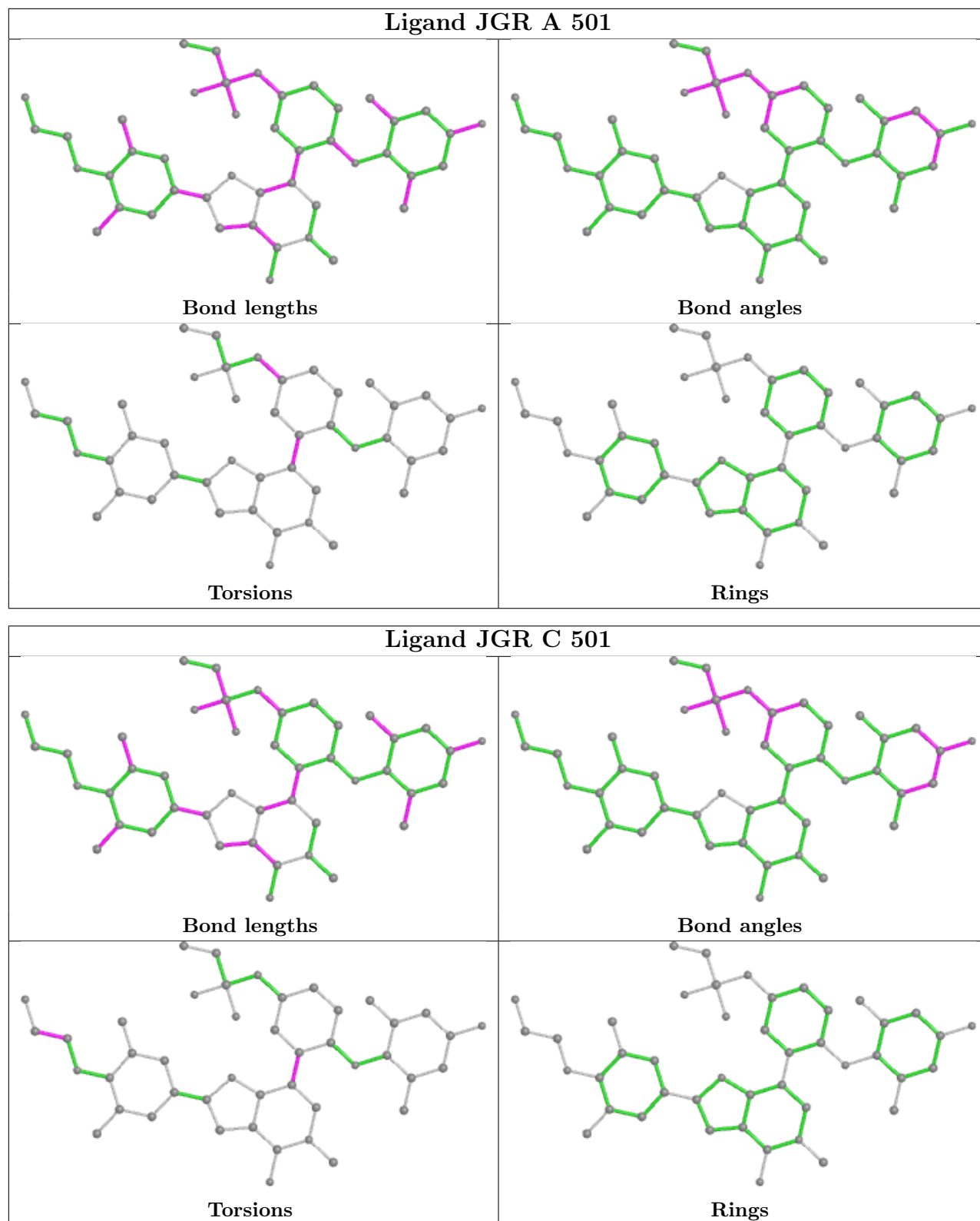
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	PEG	1	0

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 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 ⓘ

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, 95th 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	109/136 (80%)	-0.20	0 100 100	24, 41, 69, 92	0
1	B	107/136 (78%)	0.19	5 (4%) 31 25	35, 58, 92, 105	0
1	C	109/136 (80%)	-0.11	0 100 100	34, 52, 75, 89	0
1	D	109/136 (80%)	-0.23	0 100 100	26, 39, 63, 78	0
1	E	108/136 (79%)	0.20	2 (1%) 66 62	44, 65, 94, 106	0
1	F	106/136 (77%)	0.43	4 (3%) 40 33	49, 72, 106, 140	0
All	All	648/816 (79%)	0.05	11 (1%) 70 66	24, 55, 93, 140	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	407	ASP	4.5
1	F	409	ARG	4.0
1	B	361	LEU	3.4
1	B	348	GLU	3.2
1	B	409	ARG	3.1
1	F	448	PHE	3.1
1	F	352	HIS	2.8
1	B	407	ASP	2.7
1	E	406	ARG	2.4
1	B	401	ARG	2.2
1	E	409	ARG	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 monosaccharides in this entry.

6.4 Ligands [i](#)

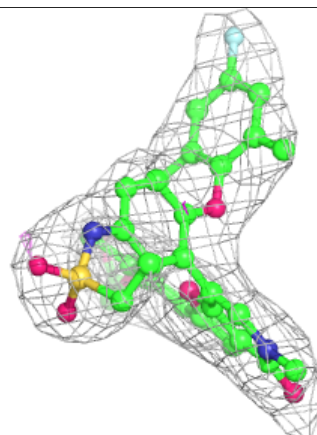
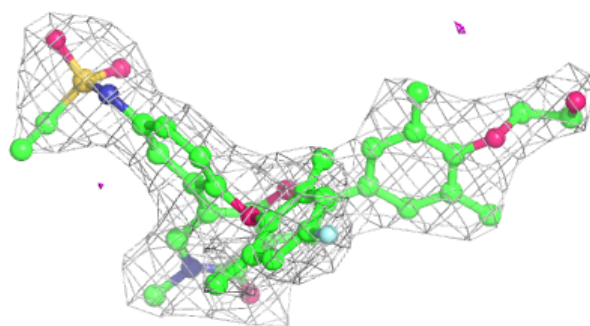
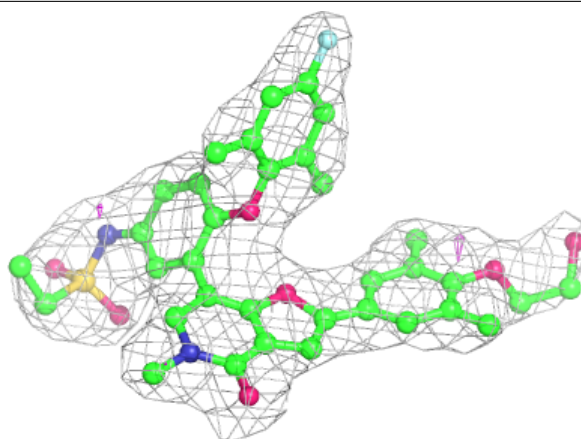
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	B	502	4/4	0.79	0.27	59,60,62,63	0
4	PEG	A	503	7/7	0.86	0.24	29,41,52,57	0
4	PEG	D	502	7/7	0.93	0.22	33,39,58,63	0
3	EDO	A	502	4/4	0.94	0.20	50,55,57,59	0
2	JGR	F	501	45/45	0.97	0.20	44,56,62,65	0
2	JGR	B	501	45/45	0.97	0.15	41,46,53,60	0
2	JGR	C	501	45/45	0.97	0.16	32,41,48,54	0
2	JGR	D	501	45/45	0.97	0.17	31,40,49,62	0
2	JGR	E	501	45/45	0.97	0.18	52,57,63,66	0
2	JGR	A	501	45/45	0.98	0.17	29,41,55,63	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.

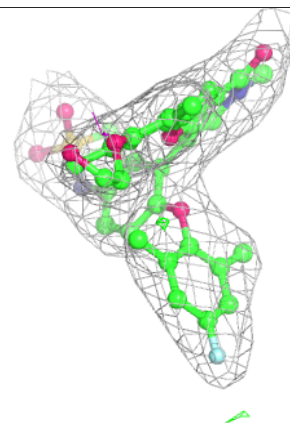
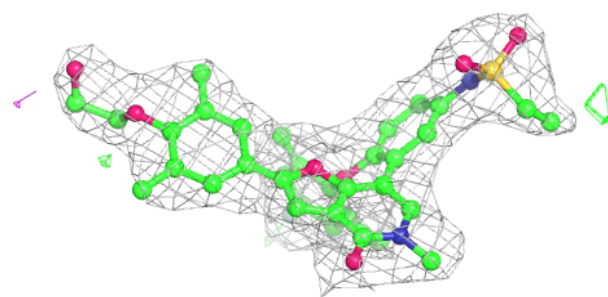
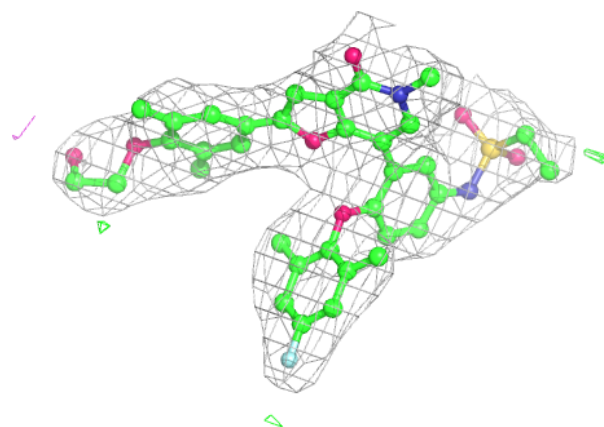
Electron density around JGR F 501:

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

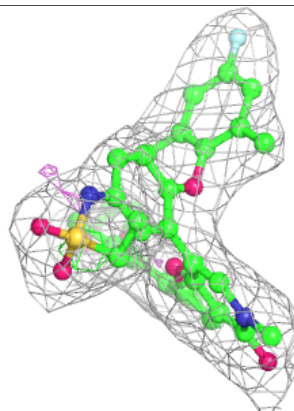
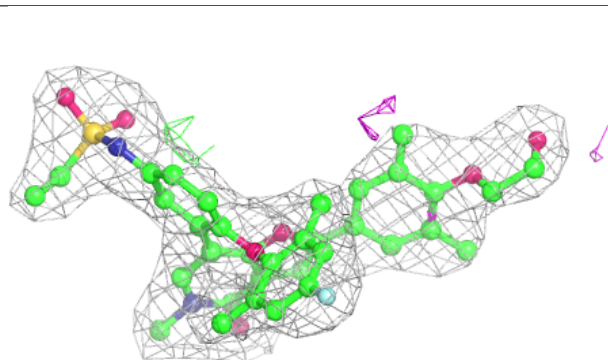
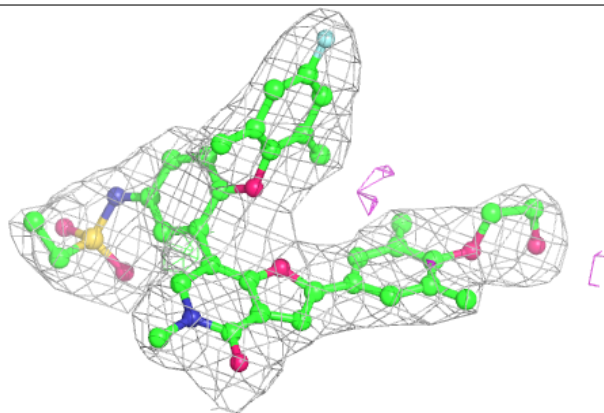


Electron density around JGR B 501:

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

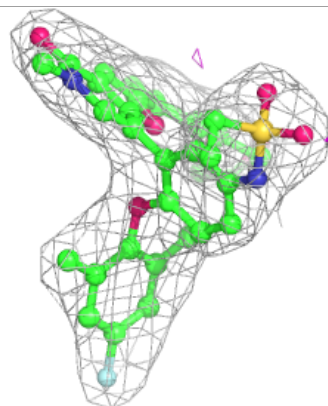
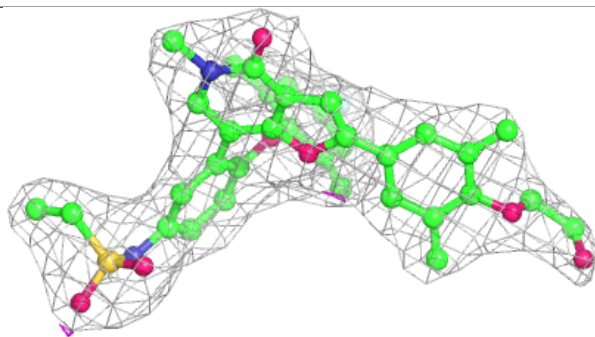
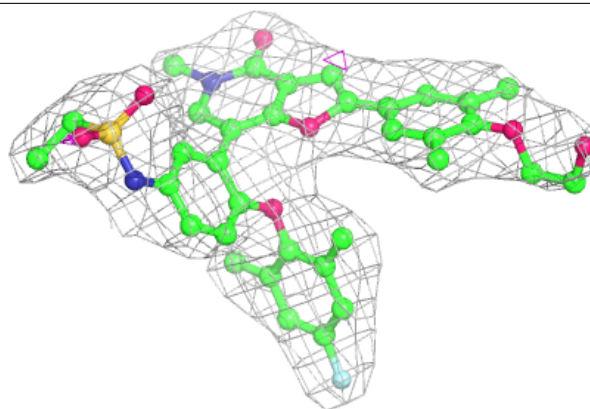
**Electron density around JGR C 501:**

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

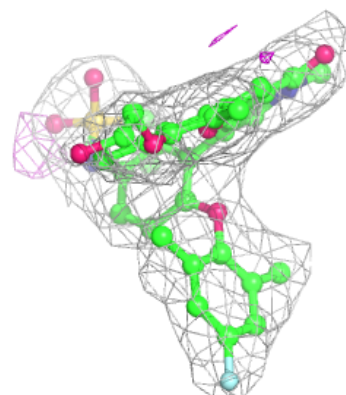
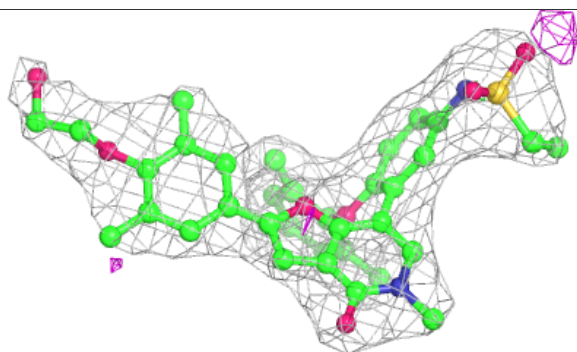
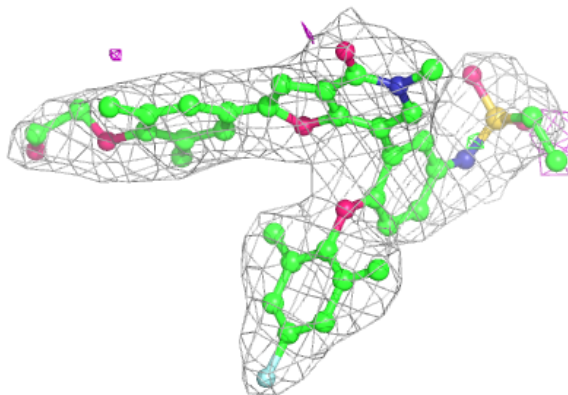


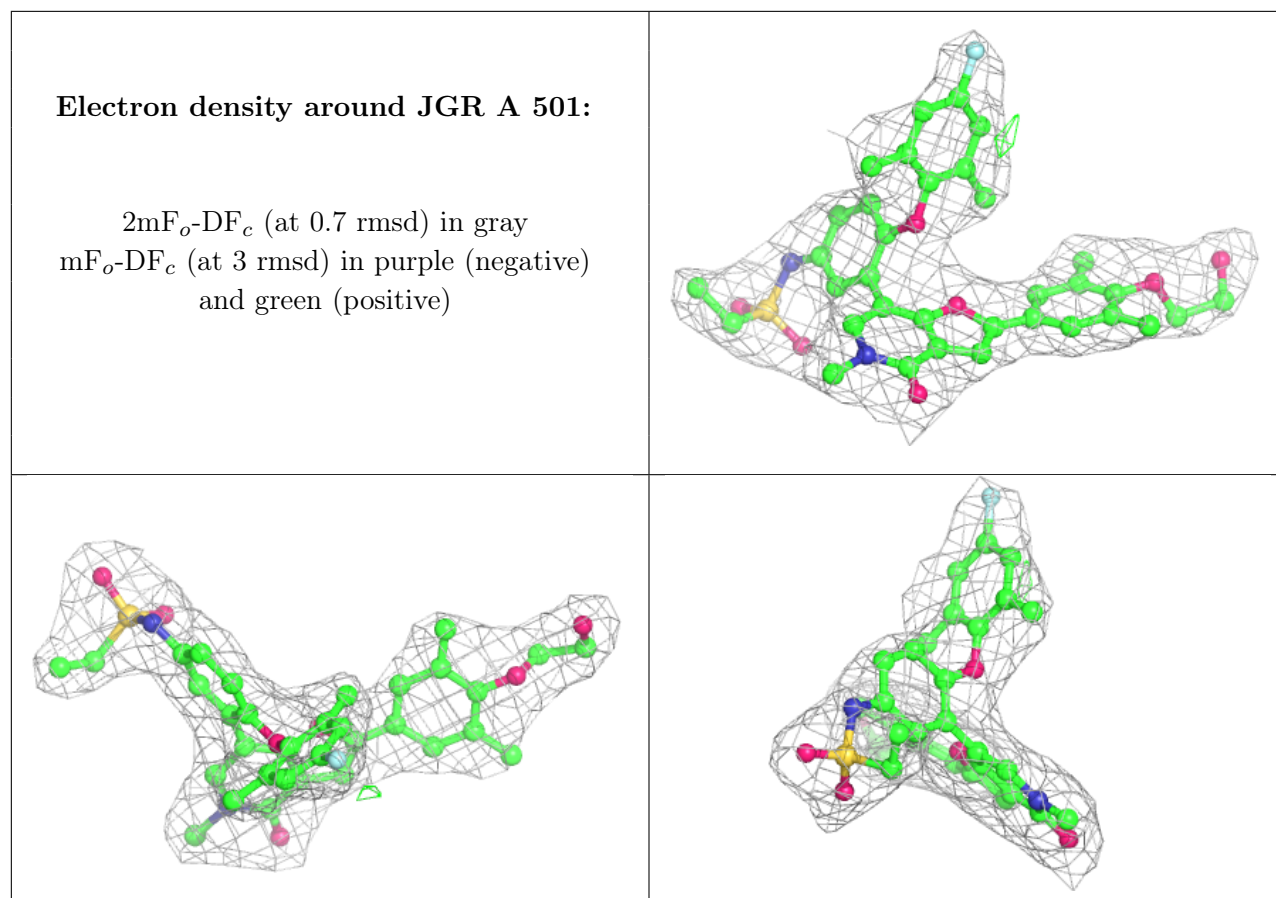
Electron density around JGR D 501:

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

**Electron density around JGR E 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 [i](#)

There are no such residues in this entry.