Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 11:10 PM EDT

PDB ID	:	6S4Q
Title	:	scdSav(SASK) - Engineering Single-Chain Dimeric Streptavidin as Host for Artificial Metalloenzymes
Authors	:	Rebelein, J.G.
Deposited on	:	2019-06-28
Resolution	:	1.85 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

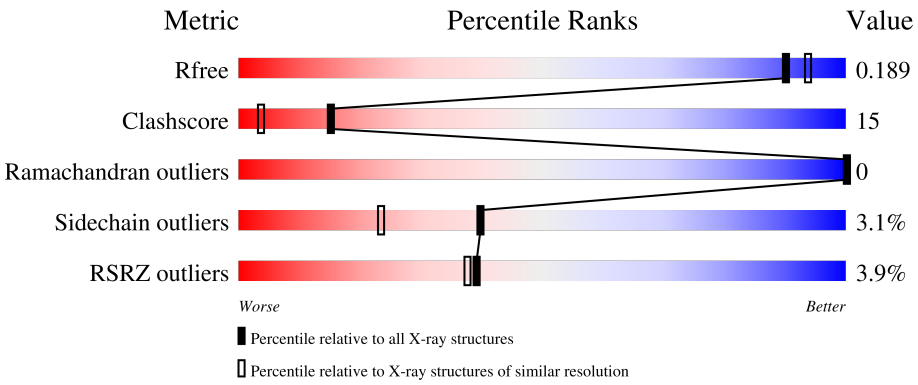
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	343	2% 57% 13% 29%
1	B	343	3% 60% 11% 29%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4171 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 Streptavidin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	243	1832	1140	318	373	1	0	5	0
1	B	244	1855	1153	323	378	1	0	6	0

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P22629
A	2	ALA	-	expression tag	UNP P22629
A	3	SER	-	expression tag	UNP P22629
A	4	MET	-	expression tag	UNP P22629
A	5	THR	-	expression tag	UNP P22629
A	6	GLY	-	expression tag	UNP P22629
A	7	GLY	-	expression tag	UNP P22629
A	8	GLN	-	expression tag	UNP P22629
A	9	GLN	-	expression tag	UNP P22629
A	10	MET	-	expression tag	UNP P22629
A	11	GLY	-	expression tag	UNP P22629
A	12	ARG	-	expression tag	UNP P22629
A	13	ASP	-	expression tag	UNP P22629
A	14	GLN	-	expression tag	UNP P22629
A	121	ALA	LYS	conflict	UNP P22629
A	160	GLY	-	linker	UNP P22629
A	161	SER	-	linker	UNP P22629
A	162	GLY	-	linker	UNP P22629
A	163	GLY	-	linker	UNP P22629
A	164	GLY	-	linker	UNP P22629
A	165	ASN	-	linker	UNP P22629
A	166	GLY	-	linker	UNP P22629
A	167	GLY	-	linker	UNP P22629
A	168	GLY	-	linker	UNP P22629
A	169	ASN	-	linker	UNP P22629

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Chain	Residue	Modelled	Actual	Comment	Reference
A	170	GLY	-	linker	UNP P22629
A	171	GLY	-	linker	UNP P22629
A	172	GLY	-	linker	UNP P22629
A	173	ASN	-	linker	UNP P22629
A	174	GLY	-	linker	UNP P22629
A	175	GLY	-	linker	UNP P22629
A	176	GLY	-	linker	UNP P22629
A	177	ASN	-	linker	UNP P22629
A	178	ILE	-	linker	UNP P22629
A	179	ASP	-	linker	UNP P22629
A	180	GLY	-	linker	UNP P22629
A	181	ARG	-	linker	UNP P22629
A	182	GLY	-	linker	UNP P22629
A	183	GLY	-	linker	UNP P22629
A	184	GLY	-	linker	UNP P22629
A	185	ASN	-	linker	UNP P22629
A	186	ALA	-	linker	UNP P22629
A	187	SER	-	linker	UNP P22629
A	188	MET	-	linker	UNP P22629
A	189	THR	-	linker	UNP P22629
A	190	GLY	-	linker	UNP P22629
A	191	GLY	-	linker	UNP P22629
A	192	GLN	-	linker	UNP P22629
A	193	GLN	-	linker	UNP P22629
A	194	MET	-	linker	UNP P22629
A	195	GLY	-	linker	UNP P22629
A	196	ARG	-	linker	UNP P22629
A	197	ASP	-	linker	UNP P22629
A	198	GLN	-	linker	UNP P22629
A	228	VAL	GLU	conflict	UNP P22629
A	229	THR	SER	conflict	UNP P22629
A	231	ARG	VAL	conflict	UNP P22629
A	311	CYS	HIS	conflict	UNP P22629
B	1	MET	-	initiating methionine	UNP P22629
B	2	ALA	-	expression tag	UNP P22629
B	3	SER	-	expression tag	UNP P22629
B	4	MET	-	expression tag	UNP P22629
B	5	THR	-	expression tag	UNP P22629
B	6	GLY	-	expression tag	UNP P22629
B	7	GLY	-	expression tag	UNP P22629
B	8	GLN	-	expression tag	UNP P22629
B	9	GLN	-	expression tag	UNP P22629

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Chain	Residue	Modelled	Actual	Comment	Reference
B	10	MET	-	expression tag	UNP P22629
B	11	GLY	-	expression tag	UNP P22629
B	12	ARG	-	expression tag	UNP P22629
B	13	ASP	-	expression tag	UNP P22629
B	14	GLN	-	expression tag	UNP P22629
B	121	ALA	LYS	conflict	UNP P22629
B	160	GLY	-	linker	UNP P22629
B	161	SER	-	linker	UNP P22629
B	162	GLY	-	linker	UNP P22629
B	163	GLY	-	linker	UNP P22629
B	164	GLY	-	linker	UNP P22629
B	165	ASN	-	linker	UNP P22629
B	166	GLY	-	linker	UNP P22629
B	167	GLY	-	linker	UNP P22629
B	168	GLY	-	linker	UNP P22629
B	169	ASN	-	linker	UNP P22629
B	170	GLY	-	linker	UNP P22629
B	171	GLY	-	linker	UNP P22629
B	172	GLY	-	linker	UNP P22629
B	173	ASN	-	linker	UNP P22629
B	174	GLY	-	linker	UNP P22629
B	175	GLY	-	linker	UNP P22629
B	176	GLY	-	linker	UNP P22629
B	177	ASN	-	linker	UNP P22629
B	178	ILE	-	linker	UNP P22629
B	179	ASP	-	linker	UNP P22629
B	180	GLY	-	linker	UNP P22629
B	181	ARG	-	linker	UNP P22629
B	182	GLY	-	linker	UNP P22629
B	183	GLY	-	linker	UNP P22629
B	184	GLY	-	linker	UNP P22629
B	185	ASN	-	linker	UNP P22629
B	186	ALA	-	linker	UNP P22629
B	187	SER	-	linker	UNP P22629
B	188	MET	-	linker	UNP P22629
B	189	THR	-	linker	UNP P22629
B	190	GLY	-	linker	UNP P22629
B	191	GLY	-	linker	UNP P22629
B	192	GLN	-	linker	UNP P22629
B	193	GLN	-	linker	UNP P22629
B	194	MET	-	linker	UNP P22629
B	195	GLY	-	linker	UNP P22629

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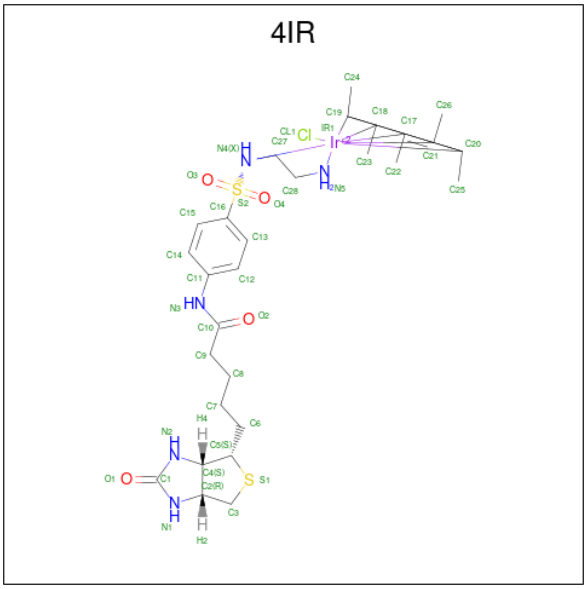
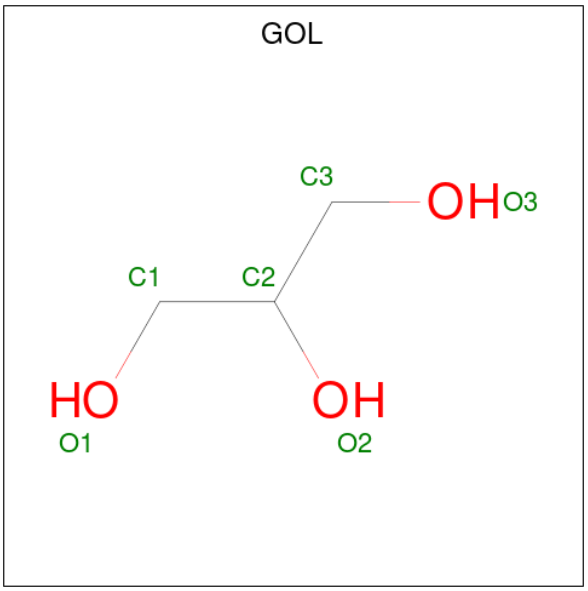
Chain	Residue	Modelled	Actual	Comment	Reference
B	196	ARG	-	linker	UNP P22629
B	197	ASP	-	linker	UNP P22629
B	198	GLN	-	linker	UNP P22629
B	228	VAL	GLU	conflict	UNP P22629
B	229	THR	SER	conflict	UNP P22629
B	231	ARG	VAL	conflict	UNP P22629
B	311	CYS	HIS	conflict	UNP P22629

- Molecule 2 is {N-(4-{[2-(amino-kappaN)ethyl]sulfamoyl-kappaN}phenyl)-5-[(3aS,4S,6aR)-2-oxohexahydro-1H-thieno[3,4-d]imidazol-4-yl]pentanamide}(chloro)[(1,2,3,4,5-eta)-1,2,3,4,5-pentamethylcyclopentadienyl]iridium(III) (three-letter code: 4IR) (formula: $C_{28}H_{45}ClIrN_5O_4S_2$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	Cl	Ir	N	O	S		
2	A	1	82	56	2	2	10	8	4	0	1
			Total	C	Cl	Ir	N	O	S		
2	A	1	82	56	2	2	10	8	4	0	1
			Total	C	Cl	Ir	N	O	S		
2	B	1	82	56	2	2	10	8	4	0	1
			Total	C	Cl	Ir	N	O	S		
2	B	1	82	56	2	2	10	8	4	0	1

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	B	1	6	3	3	0	0
			Total	C	O		
3	B	1	6	3	3	0	0

- Molecule 4 is water.

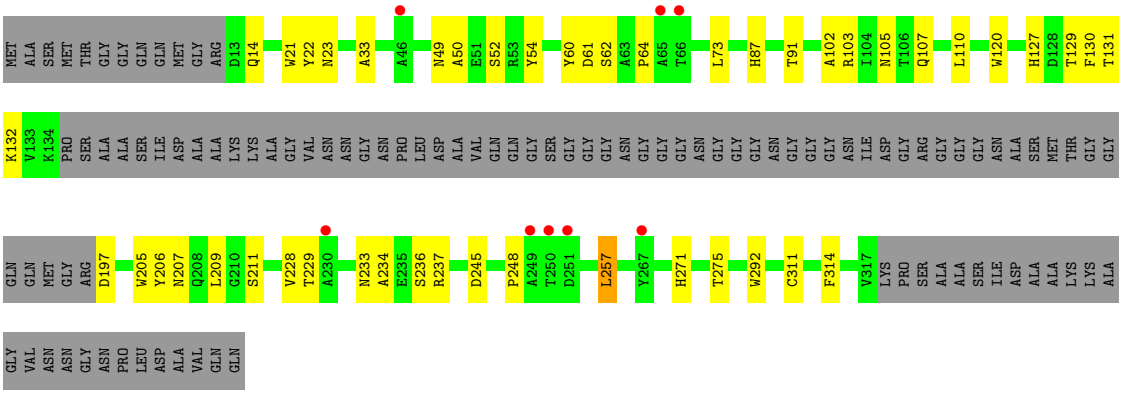
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	62	62	62	0	0
			Total	O		
4	B	64	64	64	0	0

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.

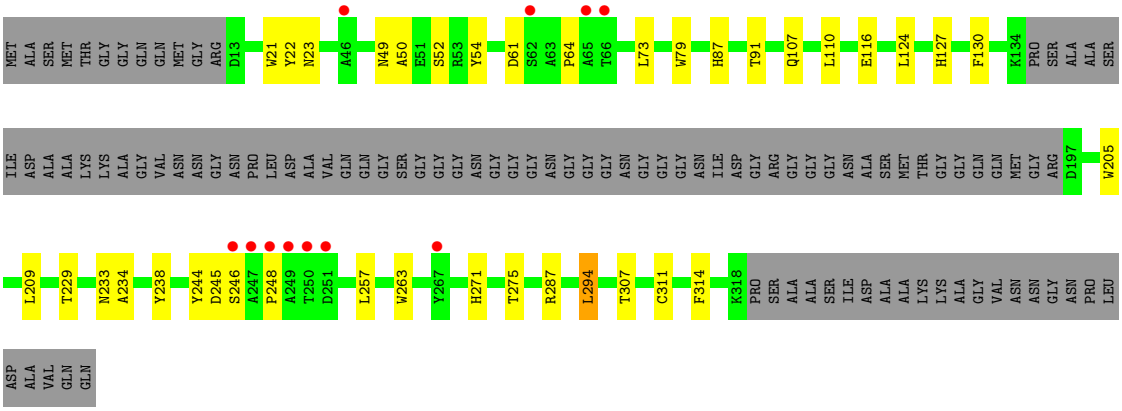
• Molecule 1: Streptavidin

Chain A:



• Molecule 1: Streptavidin

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	184.22Å 57.20Å 57.20Å 90.00° 108.09° 90.00°	Depositor
Resolution (Å)	43.82 – 1.85 43.78 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.82-1.85) 99.7 (43.78-1.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.195 , 0.231 0.204 , 0.189	Depositor DCC
R_{free} test set	2887 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	21.8	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 30.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.480 for -h-k-l,l,k 0.487 for -h+k-l,-l,-k 0.479 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4171	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 4IR

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	0.72	0/1891	0.93	0/2590
1	B	0.70	0/1910	0.92	0/2614
All	All	0.71	0/3801	0.93	0/5204

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	1832	0	1713	45	0
1	B	1855	0	1733	39	0
2	A	164	0	96	29	0
2	B	164	0	96	32	0
3	A	18	0	24	3	0
3	B	12	0	16	3	0
4	A	62	0	0	1	0
4	B	64	0	0	1	0
All	All	4171	0	3678	115	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 15.

All (115) 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:87:HIS:HB2	2:A:401[B]:4IR:H28A	1.24	1.14
1:B:87:HIS:HB2	2:B:401[B]:4IR:H28A	1.18	1.11
1:A:271:HIS:HB2	2:A:402[B]:4IR:H28A	1.34	1.07
1:B:271:HIS:HB2	2:B:402[B]:4IR:H28A	1.32	1.06
2:B:401[B]:4IR:H15	2:B:401[B]:4IR:H27A	1.39	1.03
2:A:402[B]:4IR:O3	2:A:402[B]:4IR:C24	2.08	1.01
1:A:107[A]:GLN:HE22	1:B:107[A]:GLN:HE22	1.11	0.99
1:B:233:ASN:HB3	2:B:402[B]:4IR:H14	1.46	0.97
1:A:49:ASN:HB3	2:A:401[B]:4IR:H14	1.49	0.95
1:A:107[A]:GLN:HE22	1:B:107[A]:GLN:NE2	1.64	0.95
2:B:402[A]:4IR:C25	2:B:402[A]:4IR:O3	2.15	0.94
2:A:401[A]:4IR:C25	2:B:402[A]:4IR:C26	2.47	0.92
2:B:402[B]:4IR:H27	2:B:402[B]:4IR:C13	2.02	0.89
2:A:401[A]:4IR:C25	2:B:402[A]:4IR:CL1	2.57	0.89
2:B:401[B]:4IR:C27	2:B:401[B]:4IR:C15	2.55	0.85
1:A:311:CYS:HG	1:B:311:CYS:HG	1.21	0.85
2:B:401[B]:4IR:H15	2:B:401[B]:4IR:C27	2.05	0.85
2:A:402[B]:4IR:O3	2:A:402[B]:4IR:C25	2.28	0.81
1:A:233:ASN:HB3	2:A:402[B]:4IR:H12	1.65	0.78
2:B:402[B]:4IR:C27	2:B:402[B]:4IR:H13	2.13	0.78
2:B:401[B]:4IR:H27A	2:B:401[B]:4IR:C15	2.17	0.74
2:B:402[B]:4IR:C13	2:B:402[B]:4IR:C27	2.64	0.74
2:A:402[A]:4IR:C26	2:A:402[A]:4IR:CL1	2.72	0.74
2:A:402[A]:4IR:CL1	2:A:402[A]:4IR:O4	2.43	0.73
2:B:401[B]:4IR:C26	2:B:401[B]:4IR:CL1	2.75	0.72
2:B:401[A]:4IR:C25	2:B:401[A]:4IR:O4	2.36	0.72
2:A:402[B]:4IR:C26	2:A:402[B]:4IR:CL1	2.75	0.71
1:A:197:ASP:OD2	1:A:248:PRO:HG3	1.91	0.70
2:A:402[A]:4IR:H28	1:B:124:LEU:HD21	1.74	0.70
2:B:401[A]:4IR:C26	2:B:401[A]:4IR:CL1	2.76	0.70
1:A:245:ASP:O	1:A:248:PRO:HD3	1.93	0.69
2:A:401[B]:4IR:C13	2:A:401[B]:4IR:C27	2.71	0.68
2:B:402[B]:4IR:C26	2:B:402[B]:4IR:CL1	2.78	0.68
1:B:233:ASN:CB	2:B:402[B]:4IR:H14	2.24	0.67
2:B:401[B]:4IR:C25	2:B:401[B]:4IR:O4	2.42	0.67
1:A:107[A]:GLN:NE2	1:B:107[A]:GLN:HE22	1.90	0.67
2:A:401[B]:4IR:H27A	2:A:401[B]:4IR:H13	1.77	0.67
2:A:401[A]:4IR:H28	2:A:401[A]:4IR:CL1	2.33	0.65
2:A:401[B]:4IR:C13	2:A:401[B]:4IR:H27	2.26	0.64
2:B:402[A]:4IR:C26	2:B:402[A]:4IR:CL1	2.83	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:401[A]:4IR:CL1	2:A:401[A]:4IR:C26	2.84	0.63
2:B:402[B]:4IR:H13	2:B:402[B]:4IR:H27A	1.79	0.63
1:B:229:THR:HG23	1:B:234:ALA:HB3	1.79	0.63
2:B:401[B]:4IR:C15	2:B:401[B]:4IR:H27	2.27	0.62
1:B:87:HIS:CB	2:B:401[B]:4IR:H28A	2.12	0.62
2:A:401[B]:4IR:C27	2:A:401[B]:4IR:H13	2.31	0.61
1:A:61:ASP:O	1:A:64:PRO:HD3	2.01	0.60
1:B:87:HIS:HB2	2:B:401[B]:4IR:C28	2.13	0.60
1:B:229:THR:CG2	1:B:234:ALA:CB	2.79	0.60
1:A:229:THR:HG23	1:A:234:ALA:HB3	1.84	0.59
1:A:102:ALA:HB3	1:A:132:LYS:HE2	1.84	0.59
2:A:401[B]:4IR:C26	2:A:401[B]:4IR:CL1	2.88	0.59
1:B:116:GLU:HA	1:B:116:GLU:OE1	2.02	0.59
1:A:229:THR:CG2	1:A:234:ALA:CB	2.82	0.58
1:B:233:ASN:HB3	2:B:402[B]:4IR:C14	2.30	0.57
1:A:87:HIS:HB2	2:A:401[B]:4IR:C28	2.16	0.56
1:A:271:HIS:HB2	2:A:402[B]:4IR:C28	2.22	0.55
1:A:120:TRP:CZ3	2:B:402[B]:4IR:H5	2.42	0.55
1:B:271:HIS:HB2	2:B:402[B]:4IR:C28	2.22	0.55
1:A:49:ASN:CB	2:A:401[B]:4IR:H14	2.32	0.54
1:B:79:TRP:CD2	2:B:401[A]:4IR:H8A	2.45	0.52
1:B:229:THR:HG23	1:B:234:ALA:CB	2.38	0.52
2:A:402[B]:4IR:O3	2:A:402[B]:4IR:C19	2.57	0.51
1:A:22:TYR:O	1:A:130:PHE:HA	2.10	0.51
1:B:49:ASN:HB3	2:B:401[B]:4IR:H12	1.92	0.50
1:B:205:TRP:HB3	1:B:314:PHE:HB3	1.94	0.50
1:A:228:VAL:CG2	1:A:237:ARG:HG2	2.42	0.49
1:A:233:ASN:H	2:A:402[B]:4IR:H9A	1.77	0.49
1:A:311:CYS:O	3:A:403:GOL:C1	2.61	0.49
1:A:49:ASN:HB3	2:A:401[B]:4IR:C14	2.32	0.49
1:A:205:TRP:HB3	1:A:314:PHE:HB3	1.95	0.49
1:B:127:HIS:CE1	3:B:403:GOL:H32	2.49	0.48
1:B:257:LEU:C	1:B:257:LEU:HD12	2.34	0.48
1:A:197:ASP:OD2	1:A:248:PRO:CG	2.60	0.48
1:A:229:THR:HG23	1:A:234:ALA:CB	2.43	0.48
2:A:401[B]:4IR:O4	2:A:401[B]:4IR:C25	2.59	0.48
1:A:257:LEU:C	1:A:257:LEU:HD12	2.34	0.47
1:A:311:CYS:CB	1:B:311:CYS:HG	2.28	0.47
1:B:61:ASP:O	1:B:64:PRO:HD3	2.14	0.47
1:A:91:THR:HB	1:A:275:THR:HB	1.97	0.47
1:A:311:CYS:O	3:A:403:GOL:H12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:402[B]:4IR:O3	2:A:402[B]:4IR:C20	2.62	0.47
1:B:244:TYR:CE2	1:B:246:SER:HA	2.49	0.46
1:A:103:ARG:HD3	1:A:131:THR:HG22	1.97	0.46
2:A:401[A]:4IR:CL1	2:B:402[A]:4IR:O4	2.71	0.46
2:A:402[A]:4IR:CL1	2:B:401[A]:4IR:C26	3.02	0.45
1:A:257:LEU:HD12	1:A:257:LEU:O	2.16	0.45
1:A:211:SER:OG	1:A:229:THR:HA	2.17	0.45
1:A:105:ASN:ND2	1:A:129[A]:THR:HG23	2.31	0.44
1:A:105:ASN:ND2	1:A:129[B]:THR:HG23	2.31	0.44
1:B:50:ALA:HA	1:B:54:TYR:OH	2.17	0.44
1:B:229:THR:CG2	1:B:234:ALA:HB3	2.44	0.44
1:A:21:TRP:HB3	1:A:130:PHE:HB3	1.99	0.44
1:B:21:TRP:HB3	1:B:130:PHE:HB3	1.98	0.44
1:B:91:THR:HB	1:B:275:THR:HB	1.99	0.44
1:A:60:TYR:CE2	1:A:62:SER:HA	2.53	0.43
1:B:127:HIS:CE1	3:B:403:GOL:C3	3.01	0.43
3:B:403:GOL:H31	4:B:556:HOH:O	2.18	0.43
1:B:23:ASN:HB3	1:B:130:PHE:CE1	2.54	0.43
1:A:311:CYS:O	3:A:403:GOL:H2	2.19	0.42
1:A:50:ALA:HA	1:A:54:TYR:OH	2.19	0.42
1:A:127:HIS:HE1	4:A:558:HOH:O	2.02	0.42
1:B:234:ALA:HA	1:B:238:TYR:OH	2.19	0.42
1:A:14:GLN:HG3	1:A:33:ALA:O	2.20	0.42
1:A:207:ASN:HB3	1:A:314:PHE:CE1	2.55	0.41
1:A:23:ASN:HB3	1:A:130:PHE:CE2	2.55	0.41
1:A:206:TYR:O	1:A:314:PHE:HA	2.19	0.41
1:B:245[A]:ASP:O	1:B:248:PRO:HD3	2.20	0.41
1:A:275:THR:O	1:A:292:TRP:HA	2.19	0.41
1:B:257:LEU:HD12	1:B:257:LEU:O	2.20	0.41
1:B:22:TYR:O	1:B:130:PHE:HA	2.21	0.41
1:B:110:LEU:C	1:B:110:LEU:HD23	2.41	0.41
1:B:294:LEU:O	1:B:307:THR:HA	2.21	0.41
1:B:263:TRP:CD2	2:B:402[A]:4IR:H8A	2.56	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	244/343 (71%)	231 (95%)	13 (5%)	0	100	100
1	B	246/343 (72%)	235 (96%)	11 (4%)	0	100	100
All	All	490/686 (71%)	466 (95%)	24 (5%)	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	183/237 (77%)	176 (96%)	7 (4%)	33	16
1	B	185/237 (78%)	180 (97%)	5 (3%)	44	29
All	All	368/474 (78%)	356 (97%)	12 (3%)	40	21

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	SER
1	A	73	LEU
1	A	110	LEU
1	A	209	LEU
1	A	236[A]	SER
1	A	236[B]	SER
1	A	257	LEU
1	B	52	SER

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Mol	Chain	Res	Type
1	B	73	LEU
1	B	209	LEU
1	B	287	ARG
1	B	294	LEU

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

Mol	Chain	Res	Type
1	A	82	ASN
1	A	105	ASN
1	A	266	ASN
1	B	82	ASN
1	B	127	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)

13 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	$\#\|Z\| > 2$
2	4IR	B	401[A]	-	31,49,49	1.98	3 (9%)	43,104,104	2.42	17 (39%)
3	GOL	A	403	-	5,5,5	0.13	0	5,5,5	0.43	0
3	GOL	A	405	-	5,5,5	0.16	0	5,5,5	0.40	0
2	4IR	A	401[B]	-	31,49,49	1.94	4 (12%)	43,104,104	2.58	18 (41%)
3	GOL	B	404	-	5,5,5	0.08	0	5,5,5	0.25	0
2	4IR	B	401[B]	-	31,49,49	2.10	3 (9%)	43,104,104	2.79	17 (39%)
2	4IR	A	402[A]	-	31,49,49	1.94	5 (16%)	43,104,104	2.52	17 (39%)
2	4IR	B	402[A]	-	31,49,49	1.91	3 (9%)	43,104,104	2.52	19 (44%)
3	GOL	A	404	-	5,5,5	1.09	1 (20%)	5,5,5	0.64	0
3	GOL	B	403	-	5,5,5	0.16	0	5,5,5	0.51	0
2	4IR	A	402[B]	-	31,49,49	2.13	3 (9%)	43,104,104	2.50	12 (27%)
2	4IR	A	401[A]	-	31,49,49	1.78	4 (12%)	43,104,104	3.69	22 (51%)
2	4IR	B	402[B]	-	31,49,49	2.04	2 (6%)	43,104,104	2.73	19 (44%)

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	4IR	B	401[A]	-	-	5/20/204/204	0/10/9/9
3	GOL	A	403	-	-	2/4/4/4	-
3	GOL	A	405	-	-	2/4/4/4	-
2	4IR	A	401[B]	-	-	8/20/204/204	0/10/9/9
3	GOL	B	404	-	-	4/4/4/4	-
2	4IR	B	401[B]	-	-	8/20/204/204	0/10/9/9
2	4IR	A	402[A]	-	-	3/20/204/204	0/10/9/9
2	4IR	B	402[A]	-	-	6/20/204/204	0/10/9/9
3	GOL	A	404	-	-	4/4/4/4	-
3	GOL	B	403	-	-	4/4/4/4	-
2	4IR	A	402[B]	-	-	4/20/204/204	0/10/9/9
2	4IR	A	401[A]	-	-	6/20/204/204	0/10/9/9
2	4IR	B	402[B]	-	-	8/20/204/204	0/10/9/9

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	402[B]	4IR	C16-S2	-10.36	1.62	1.76
2	B	401[B]	4IR	C16-S2	-10.33	1.62	1.76
2	B	402[B]	4IR	C16-S2	-10.06	1.62	1.76
2	A	401[B]	4IR	C16-S2	-8.81	1.64	1.76
2	B	401[A]	4IR	C16-S2	-8.63	1.64	1.76
2	B	402[A]	4IR	C16-S2	-8.50	1.64	1.76
2	A	402[A]	4IR	C16-S2	-7.87	1.65	1.76
2	A	401[A]	4IR	C16-S2	-7.83	1.65	1.76
2	A	401[B]	4IR	C5-S1	-3.58	1.76	1.82
2	B	402[B]	4IR	C5-S1	-3.42	1.77	1.82
2	B	401[A]	4IR	C5-S1	-3.39	1.77	1.82
2	A	402[B]	4IR	C5-S1	-3.31	1.77	1.82
2	B	401[B]	4IR	C5-S1	-3.30	1.77	1.82
2	A	401[A]	4IR	C5-S1	-3.25	1.77	1.82
2	A	402[A]	4IR	C27-N4	-3.16	1.45	1.48
2	B	402[A]	4IR	C5-S1	-2.94	1.77	1.82
2	B	401[A]	4IR	C27-N4	-2.91	1.45	1.48
2	B	402[A]	4IR	C27-N4	-2.86	1.45	1.48
2	A	402[A]	4IR	C5-S1	-2.83	1.78	1.82
2	A	402[B]	4IR	C27-N4	-2.59	1.45	1.48
2	A	402[A]	4IR	C13-C12	2.48	1.43	1.38
2	A	401[B]	4IR	C13-C16	2.28	1.42	1.38
3	A	404	GOL	O2-C2	2.27	1.50	1.43
2	A	402[A]	4IR	C1-N1	-2.22	1.31	1.35
2	A	401[A]	4IR	C15-C14	2.18	1.42	1.38
2	B	401[B]	4IR	C27-N4	-2.12	1.46	1.48
2	A	401[A]	4IR	C27-N4	-2.05	1.46	1.48
2	A	401[B]	4IR	C13-C12	2.02	1.42	1.38

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401[A]	4IR	C16-S2-N4	14.34	128.91	107.54
2	A	401[B]	4IR	O4-S2-O3	-8.39	105.93	119.52
2	A	401[A]	4IR	C5-C4-N2	-8.07	105.90	113.13
2	A	401[A]	4IR	C3-C2-N1	-7.57	103.41	113.03
2	A	401[A]	4IR	O4-S2-O3	-7.11	108.00	119.52
2	B	401[B]	4IR	O4-S2-O3	-6.83	108.46	119.52
2	A	402[A]	4IR	O4-S2-O3	-6.76	108.57	119.52
2	B	402[B]	4IR	O4-S2-O3	-6.73	108.61	119.52
2	A	402[B]	4IR	O2-C10-N3	-6.40	111.96	123.63
2	B	401[B]	4IR	O2-C10-C9	-6.29	110.52	122.02
2	B	402[B]	4IR	O2-C10-N3	-6.29	112.16	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	402[B]	4IR	O2-C10-C9	-6.28	110.54	122.02
2	A	402[B]	4IR	O4-S2-O3	-6.14	109.57	119.52
2	B	401[A]	4IR	O2-C10-C9	-6.07	110.92	122.02
2	B	401[B]	4IR	O2-C10-N3	-6.00	112.69	123.63
2	A	402[B]	4IR	O2-C10-C9	-5.89	111.25	122.02
2	B	402[A]	4IR	O4-S2-O3	-5.83	110.08	119.52
2	B	401[B]	4IR	C5-C4-N2	-5.80	107.93	113.13
2	B	401[A]	4IR	O4-S2-O3	-5.51	110.60	119.52
2	A	401[A]	4IR	C3-C2-C4	-5.30	104.06	108.66
2	B	401[B]	4IR	C3-C2-C4	-5.29	104.06	108.66
2	B	401[A]	4IR	O2-C10-N3	-5.26	114.04	123.63
2	A	402[A]	4IR	C3-C2-N1	-5.14	106.50	113.03
2	A	402[B]	4IR	C3-C2-N1	-5.11	106.54	113.03
2	B	401[B]	4IR	C3-C2-N1	-5.03	106.63	113.03
2	A	402[A]	4IR	C12-C13-C16	4.90	124.52	119.45
2	A	401[B]	4IR	O2-C10-C9	-4.78	113.27	122.02
2	B	401[A]	4IR	C11-N3-C10	-4.74	119.20	127.50
2	B	402[A]	4IR	O2-C10-C9	-4.57	113.65	122.02
2	B	402[A]	4IR	C11-N3-C10	-4.52	119.59	127.50
2	B	402[B]	4IR	C5-C4-N2	-4.47	109.12	113.13
2	A	402[B]	4IR	C5-C4-N2	-4.46	109.13	113.13
2	B	402[B]	4IR	C11-N3-C10	-4.45	119.70	127.50
2	A	401[A]	4IR	C11-N3-C10	-4.39	119.81	127.50
2	B	402[A]	4IR	O2-C10-N3	-4.38	115.63	123.63
2	A	402[A]	4IR	C16-S2-N4	4.15	113.73	107.54
2	A	402[B]	4IR	C9-C10-N3	-4.15	107.29	114.59
2	B	402[A]	4IR	C3-C2-N1	-4.09	107.83	113.03
2	A	401[B]	4IR	O4-S2-C16	4.08	113.21	108.05
2	A	401[B]	4IR	C11-N3-C10	-4.03	120.44	127.50
2	B	402[A]	4IR	C5-C4-N2	-4.00	109.54	113.13
2	A	401[A]	4IR	C15-C16-C13	-3.99	114.87	120.44
2	A	402[A]	4IR	O2-C10-C9	-3.95	114.80	122.02
2	A	402[B]	4IR	C22-C17-C18	3.90	131.16	120.71
2	A	402[A]	4IR	C2-C3-S1	3.89	109.64	106.31
2	B	402[A]	4IR	C3-C2-C4	-3.85	105.32	108.66
2	B	401[B]	4IR	C11-N3-C10	-3.82	120.81	127.50
2	B	401[A]	4IR	C2-C3-S1	3.82	109.58	106.31
2	A	401[B]	4IR	C22-C17-C18	3.81	130.92	120.71
2	A	402[A]	4IR	C11-N3-C10	-3.80	120.86	127.50
2	B	402[A]	4IR	C14-C15-C16	3.74	123.32	119.45
2	B	401[B]	4IR	O4-S2-C16	3.72	112.76	108.05
2	B	401[B]	4IR	C22-C17-C18	3.72	130.68	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	402[B]	4IR	C2-C3-S1	3.70	109.48	106.31
2	A	401[B]	4IR	C13-C16-S2	3.70	123.65	119.76
2	B	402[B]	4IR	C22-C17-C18	3.68	130.57	120.71
2	B	402[B]	4IR	C13-C16-S2	3.68	123.63	119.76
2	B	402[B]	4IR	O3-S2-C16	3.64	112.65	108.05
2	B	402[B]	4IR	C2-C3-S1	3.62	109.41	106.31
2	B	402[B]	4IR	C16-S2-N4	3.60	112.91	107.54
2	A	401[A]	4IR	O2-C10-N3	-3.59	117.08	123.63
2	A	402[A]	4IR	C15-C16-C13	-3.55	115.49	120.44
2	A	401[B]	4IR	C2-C3-S1	3.51	109.31	106.31
2	A	401[B]	4IR	C3-C2-N1	-3.50	108.58	113.03
2	B	402[A]	4IR	C16-S2-N4	3.50	112.76	107.54
2	A	401[A]	4IR	C12-C13-C16	3.47	123.04	119.45
2	A	401[A]	4IR	O3-S2-C16	-3.43	103.70	108.05
2	B	401[A]	4IR	C15-C16-S2	3.42	123.36	119.76
2	B	402[A]	4IR	C15-C16-C13	-3.41	115.69	120.44
2	B	402[A]	4IR	C13-C16-S2	3.40	123.34	119.76
2	A	401[A]	4IR	N2-C1-N1	3.31	111.87	108.76
2	B	401[A]	4IR	C27-N4-S2	-3.26	111.76	118.89
2	A	401[A]	4IR	C13-C16-S2	3.25	123.18	119.76
2	A	402[A]	4IR	C13-C16-S2	3.23	123.16	119.76
2	B	402[B]	4IR	C3-C2-N1	-3.22	108.94	113.03
2	A	401[B]	4IR	C15-C14-C11	3.20	124.00	120.30
2	B	401[A]	4IR	C12-C13-C16	3.17	122.73	119.45
2	B	401[A]	4IR	C3-C2-C4	-3.16	105.92	108.66
2	B	402[B]	4IR	C28-C27-N4	3.16	113.03	107.27
2	A	402[A]	4IR	O2-C10-N3	-3.11	117.96	123.63
2	A	402[A]	4IR	C4-C2-N1	3.10	105.73	102.43
2	B	402[A]	4IR	O3-S2-C16	-3.09	104.14	108.05
2	B	401[A]	4IR	C15-C16-C13	-3.04	116.20	120.44
2	A	401[B]	4IR	C15-C16-C13	-3.03	116.21	120.44
2	A	402[B]	4IR	N2-C1-N1	3.02	111.60	108.76
2	B	402[A]	4IR	C2-C3-S1	2.99	108.87	106.31
2	B	401[B]	4IR	C2-C3-S1	2.99	108.86	106.31
2	A	401[B]	4IR	O2-C10-N3	-2.99	118.18	123.63
2	A	401[B]	4IR	C27-N4-S2	-2.98	112.36	118.89
2	A	401[B]	4IR	C12-C13-C16	2.98	122.53	119.45
2	B	401[A]	4IR	C3-C2-N1	-2.97	109.25	113.03
2	B	402[B]	4IR	C27-N4-S2	-2.95	112.43	118.89
2	A	401[A]	4IR	C14-C15-C16	2.95	122.50	119.45
2	A	401[A]	4IR	C27-N4-S2	-2.90	112.55	118.89
2	B	401[B]	4IR	C9-C10-N3	-2.86	109.55	114.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	402[A]	4IR	C5-C4-N2	-2.83	110.59	113.13
2	A	401[A]	4IR	O2-C10-C9	-2.82	116.87	122.02
2	B	402[A]	4IR	C27-N4-S2	-2.79	112.77	118.89
2	A	402[A]	4IR	O4-S2-C16	-2.73	104.59	108.05
2	B	401[A]	4IR	C4-C2-N1	2.71	105.31	102.43
2	A	401[A]	4IR	O4-S2-C16	-2.70	104.62	108.05
2	B	401[B]	4IR	N2-C1-N1	2.70	111.29	108.76
2	A	401[B]	4IR	C16-S2-N4	2.57	111.36	107.54
2	A	401[B]	4IR	C28-C27-N4	2.56	111.95	107.27
2	B	402[A]	4IR	O4-S2-C16	2.55	111.28	108.05
2	A	401[B]	4IR	C14-C11-C12	-2.54	115.55	119.03
2	B	401[B]	4IR	C27-N4-S2	-2.52	113.37	118.89
2	B	402[A]	4IR	C22-C17-C18	2.52	127.46	120.71
2	A	402[A]	4IR	O1-C1-N1	-2.50	122.35	125.94
2	A	402[A]	4IR	C2-C4-N2	-2.49	99.99	102.67
2	B	402[B]	4IR	C7-C6-C5	-2.41	108.98	113.86
2	A	401[A]	4IR	C4-N2-C1	-2.39	110.39	112.62
2	A	401[A]	4IR	C2-C3-S1	2.34	108.31	106.31
2	B	402[B]	4IR	C26-C21-C20	2.34	126.97	120.71
2	B	402[B]	4IR	C9-C10-N3	-2.30	110.54	114.59
2	A	401[A]	4IR	O1-C1-N1	-2.29	122.65	125.94
2	B	401[B]	4IR	C5-C4-C2	2.29	111.59	108.94
2	A	401[B]	4IR	N2-C1-N1	2.29	110.91	108.76
2	B	402[B]	4IR	C15-C14-C11	2.28	122.94	120.30
2	A	402[B]	4IR	C27-N4-S2	2.28	123.89	118.89
2	B	401[B]	4IR	C4-C5-S1	-2.28	103.03	105.20
2	B	402[B]	4IR	C3-C2-C4	-2.27	106.69	108.66
2	B	401[A]	4IR	C14-C11-C12	-2.26	115.94	119.03
2	B	402[B]	4IR	N2-C1-N1	2.26	110.88	108.76
2	B	402[A]	4IR	C14-C11-C12	-2.24	115.97	119.03
2	B	402[A]	4IR	C13-C12-C11	2.23	122.88	120.30
2	A	401[A]	4IR	C14-C11-C12	-2.23	115.98	119.03
2	B	401[A]	4IR	C16-S2-N4	2.23	110.86	107.54
2	A	402[A]	4IR	C4-C5-S1	2.23	107.33	105.20
2	B	401[A]	4IR	C15-C14-C11	2.22	122.86	120.30
2	A	402[B]	4IR	C13-C16-S2	2.20	122.08	119.76
2	B	401[B]	4IR	C14-C15-C16	2.20	121.73	119.45
2	A	401[A]	4IR	C4-C5-S1	-2.14	103.16	105.20
2	A	401[B]	4IR	C26-C21-C20	2.14	126.44	120.71
2	A	401[A]	4IR	C26-C21-C20	2.13	126.43	120.71
2	A	402[A]	4IR	C15-C14-C11	2.09	122.72	120.30
2	B	401[B]	4IR	C16-S2-N4	2.08	110.65	107.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401[A]	4IR	O1-C1-N1	-2.06	122.98	125.94
2	B	402[A]	4IR	N2-C1-N1	2.03	110.67	108.76
2	A	402[B]	4IR	C3-C2-C4	-2.02	106.91	108.66
2	B	401[A]	4IR	C22-C17-C18	2.01	126.08	120.71

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401[A]	4IR	C27-N4-S2-O3
2	A	401[A]	4IR	C27-N4-S2-C16
2	A	401[B]	4IR	C27-N4-S2-O3
2	A	401[B]	4IR	C27-N4-S2-O4
2	A	401[B]	4IR	C27-N4-S2-C16
2	A	402[B]	4IR	C9-C10-N3-C11
2	B	401[B]	4IR	C27-N4-S2-O3
2	B	401[B]	4IR	C27-N4-S2-O4
2	B	401[B]	4IR	C27-N4-S2-C16
2	B	401[B]	4IR	O2-C10-N3-C11
2	B	402[A]	4IR	S1-C5-C6-C7
2	B	402[A]	4IR	C4-C5-C6-C7
2	B	402[B]	4IR	C27-N4-S2-O3
2	B	402[B]	4IR	C27-N4-S2-O4
2	B	402[B]	4IR	C27-N4-S2-C16
2	B	402[B]	4IR	O2-C10-N3-C11
3	A	404	GOL	O1-C1-C2-C3
3	B	404	GOL	O1-C1-C2-C3
3	B	404	GOL	C1-C2-C3-O3
2	A	401[B]	4IR	O2-C10-N3-C11
2	B	401[B]	4IR	C7-C8-C9-C10
2	A	402[A]	4IR	O2-C10-N3-C11
2	B	401[A]	4IR	C7-C8-C9-C10
2	B	402[B]	4IR	C7-C8-C9-C10
2	B	402[A]	4IR	O2-C10-N3-C11
2	B	401[A]	4IR	O2-C10-N3-C11
3	A	404	GOL	O1-C1-C2-O2
3	B	404	GOL	O1-C1-C2-O2
2	A	401[B]	4IR	C7-C8-C9-C10
3	A	403	GOL	O1-C1-C2-C3
3	A	405	GOL	O1-C1-C2-C3
3	B	403	GOL	O1-C1-C2-C3
3	B	403	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	B	402[A]	4IR	C7-C8-C9-C10
2	A	402[B]	4IR	C6-C7-C8-C9
3	A	403	GOL	O1-C1-C2-O2
2	A	401[B]	4IR	C13-C16-S2-O3
2	B	401[B]	4IR	C15-C16-S2-O3
2	B	401[B]	4IR	C13-C16-S2-O3
2	A	401[B]	4IR	C15-C16-S2-O3
2	A	401[A]	4IR	O2-C10-N3-C11
2	B	402[B]	4IR	C15-C16-S2-O3
2	A	401[A]	4IR	C12-C11-N3-C10
2	B	402[B]	4IR	C13-C16-S2-O3
3	A	405	GOL	O1-C1-C2-O2
3	B	404	GOL	O2-C2-C3-O3
2	A	401[A]	4IR	C14-C11-N3-C10
2	B	402[B]	4IR	C9-C10-N3-C11
2	A	401[B]	4IR	C9-C10-N3-C11
3	A	404	GOL	C1-C2-C3-O3
2	A	401[A]	4IR	C27-N4-S2-O4
3	A	404	GOL	O2-C2-C3-O3
3	B	403	GOL	O1-C1-C2-O2
2	A	402[A]	4IR	C15-C16-S2-O4
2	B	402[A]	4IR	C13-C16-S2-O3
2	B	401[B]	4IR	C9-C10-N3-C11
2	B	401[A]	4IR	C6-C7-C8-C9
2	B	402[A]	4IR	C15-C16-S2-O3
2	A	402[A]	4IR	C13-C16-S2-O4
2	B	401[A]	4IR	C15-C16-S2-O4
2	B	401[A]	4IR	C13-C16-S2-O4
2	A	402[B]	4IR	C12-C11-N3-C10
2	A	402[B]	4IR	C14-C11-N3-C10
3	B	403	GOL	O2-C2-C3-O3

There are no ring outliers.

10 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401[A]	4IR	4	0
3	A	403	GOL	3	0
2	A	401[B]	4IR	11	0
2	B	401[B]	4IR	11	0
2	A	402[A]	4IR	4	0
2	B	402[A]	4IR	6	0

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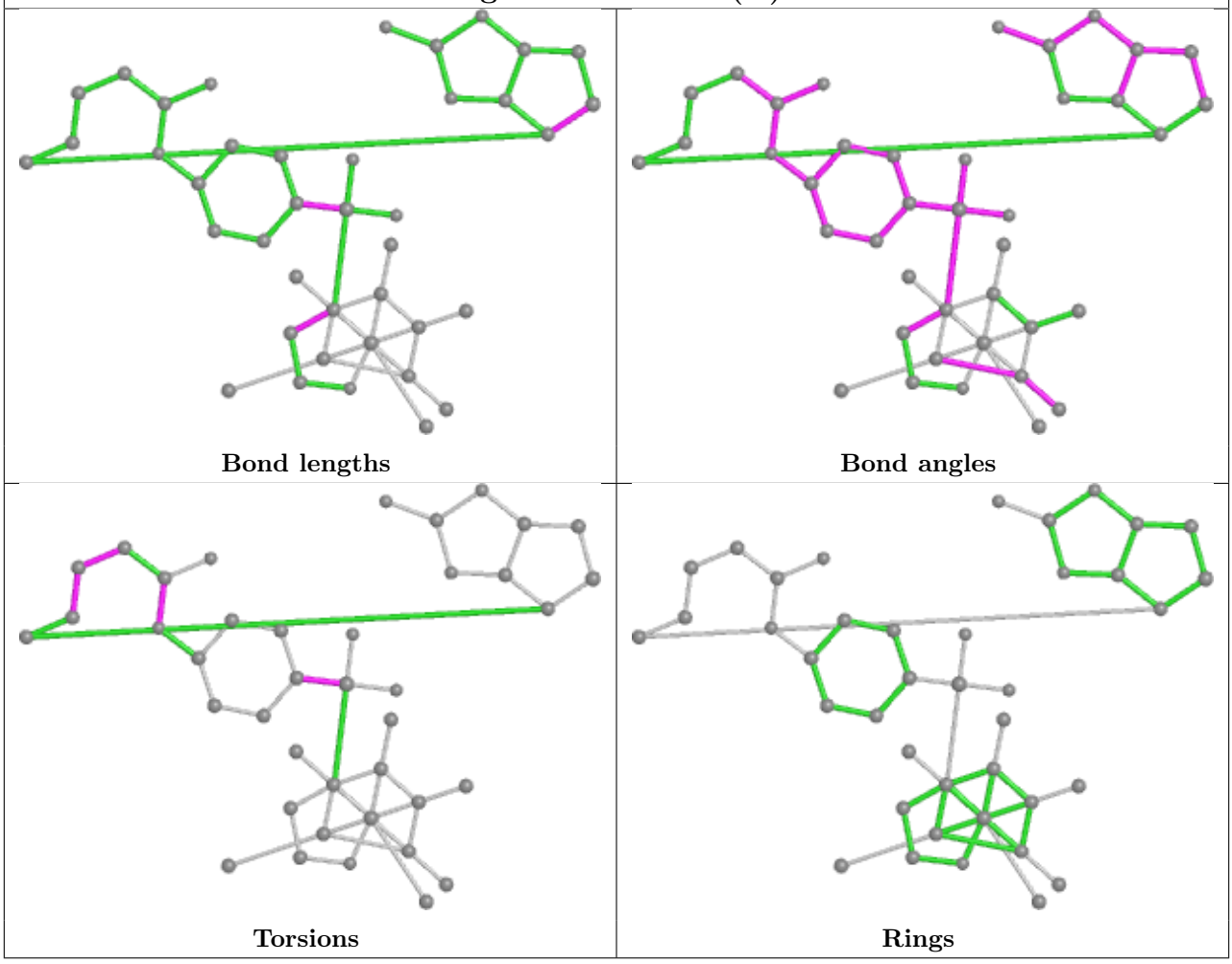
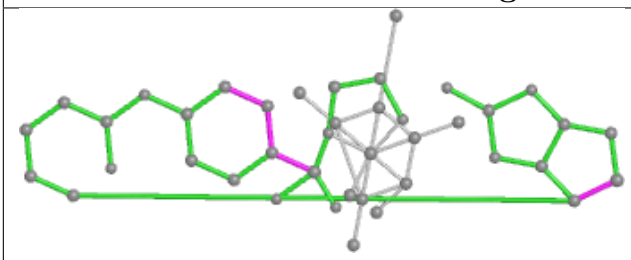
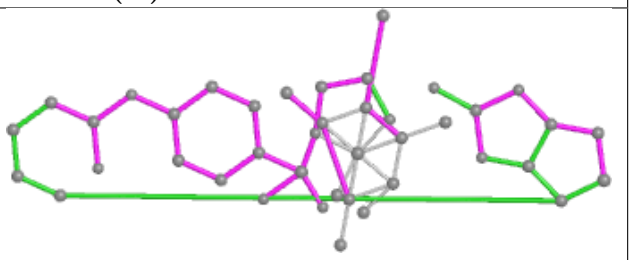
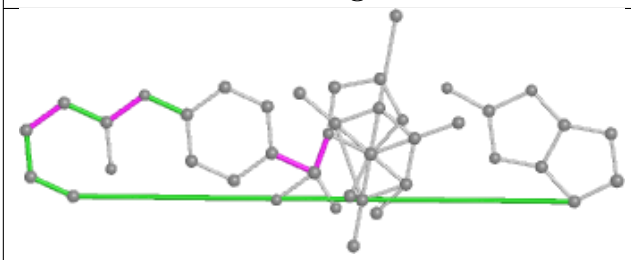
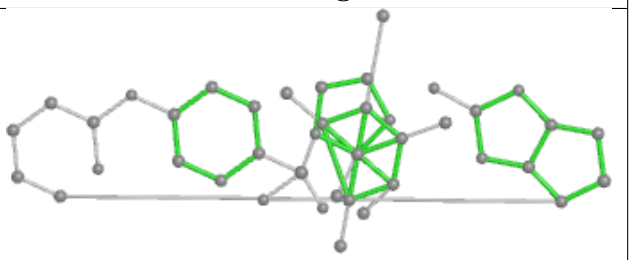
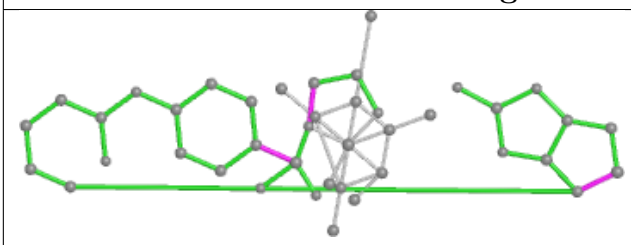
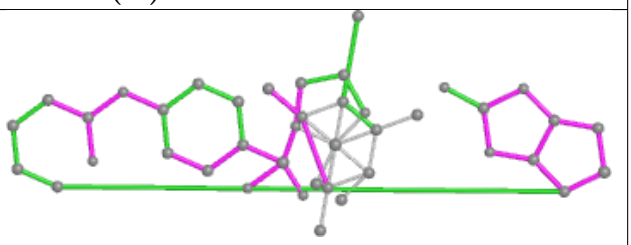
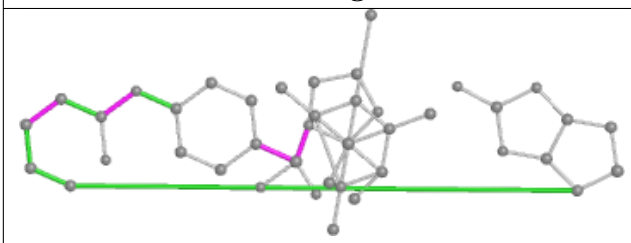
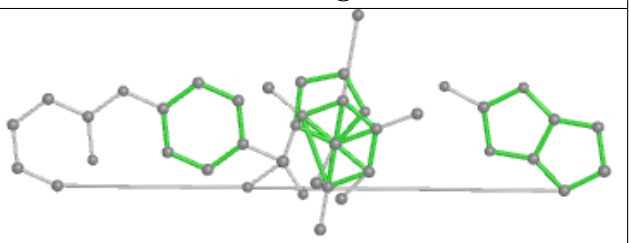
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	403	GOL	3	0
2	A	402[B]	4IR	9	0
2	A	401[A]	4IR	5	0
2	B	402[B]	4IR	11	0

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.

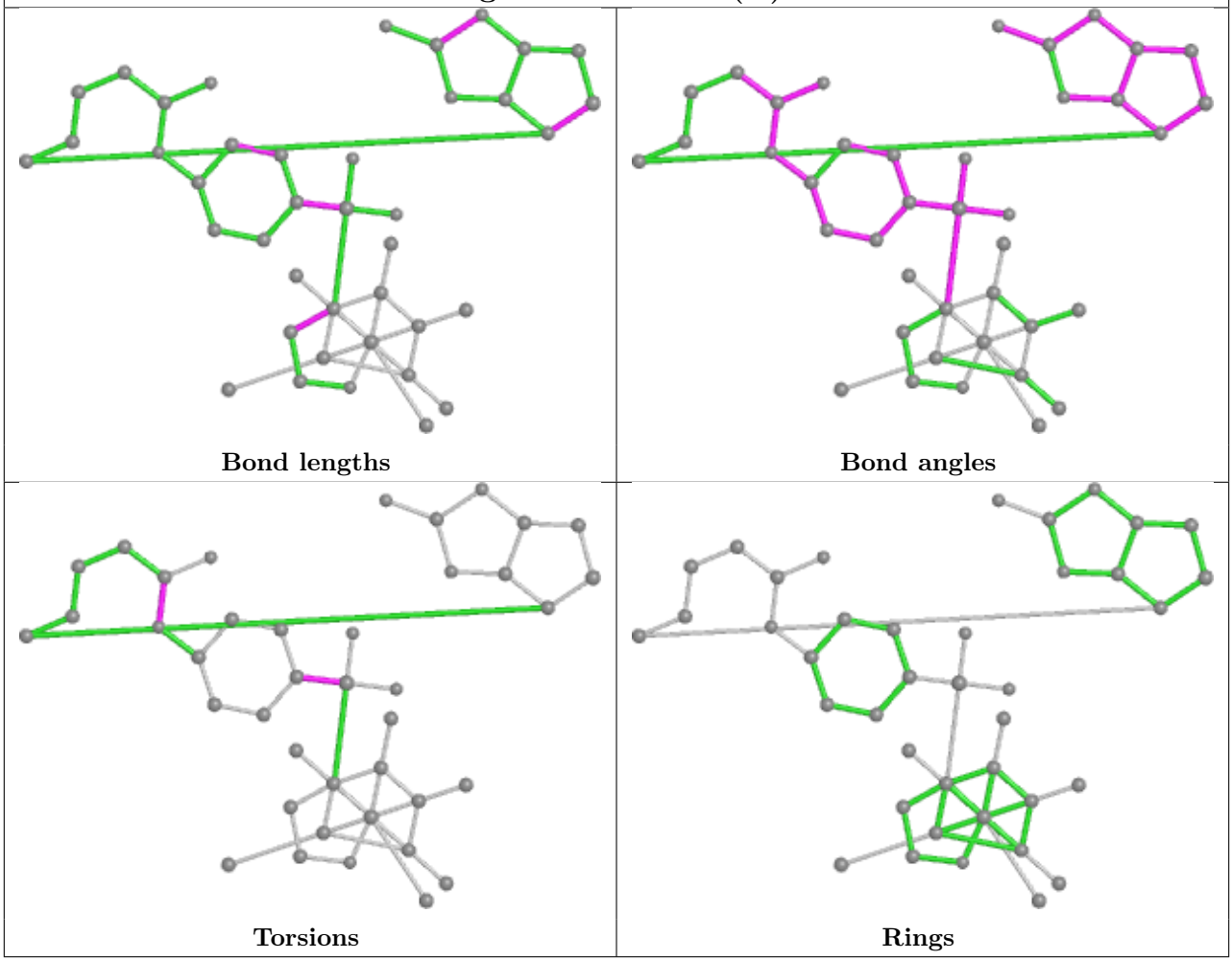
Ligand 4IR B 401 (A)



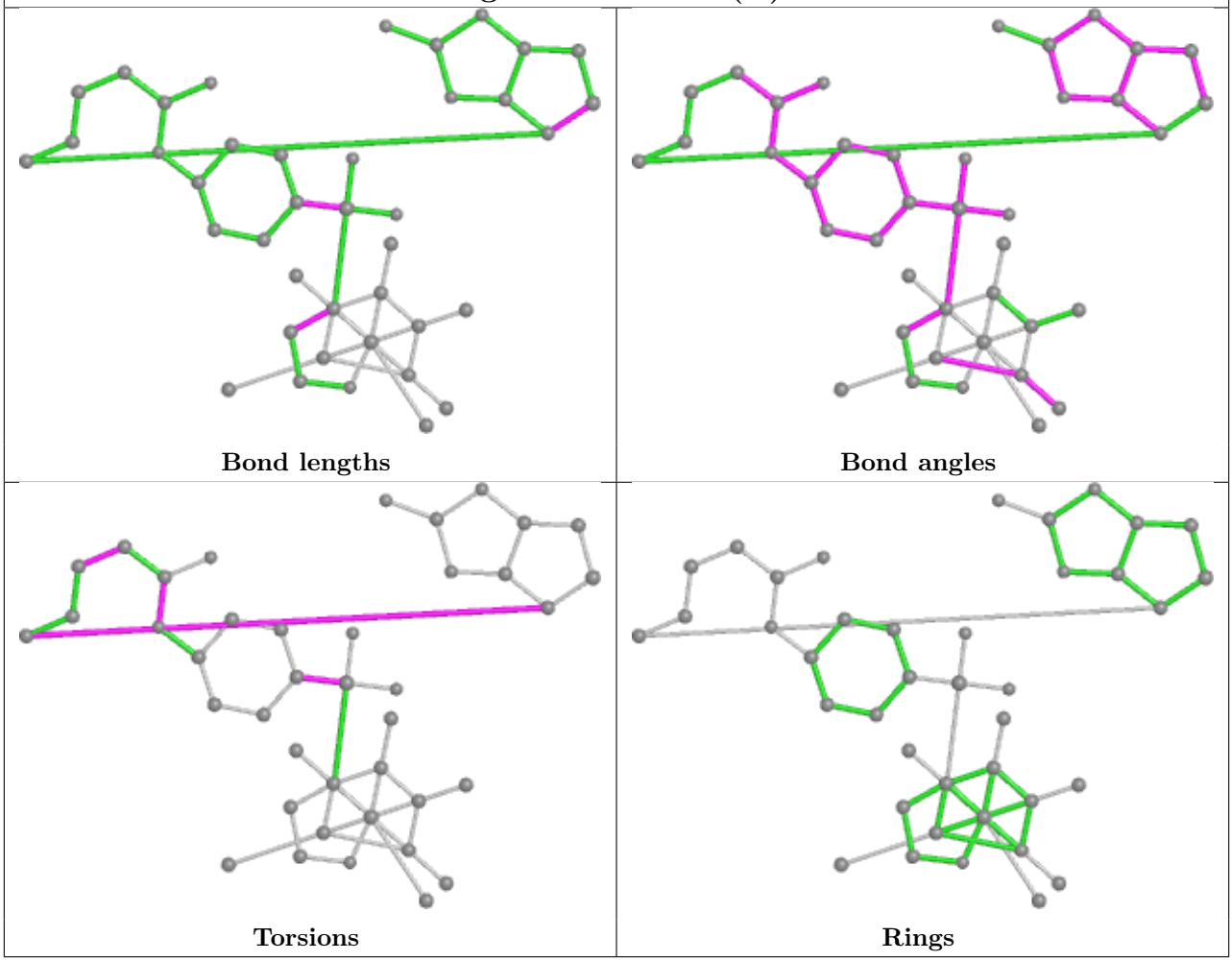
Ligand 4IR A 401 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 4IR B 401 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings

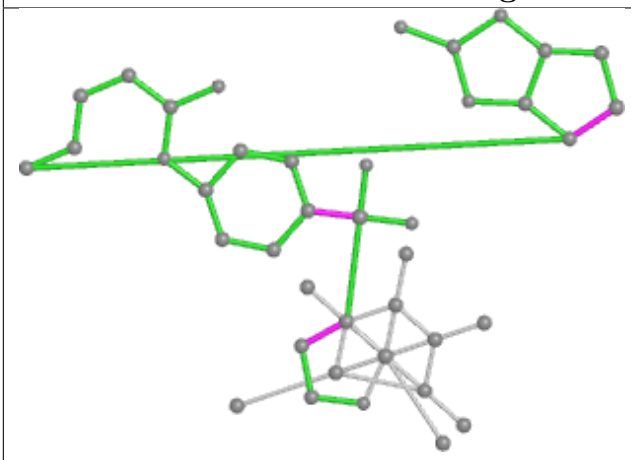
Ligand 4IR A 402 (A)



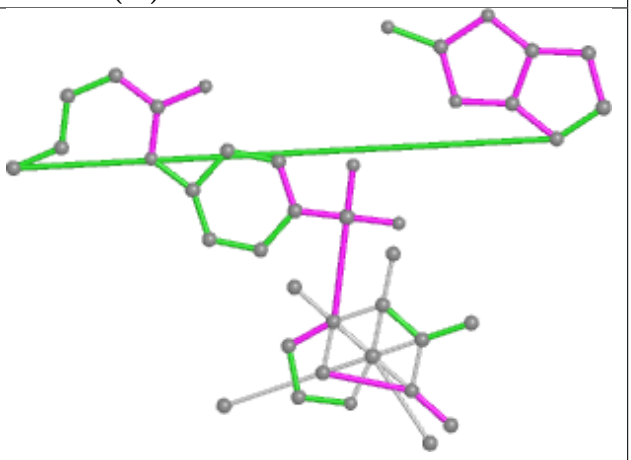
Ligand 4IR B 402 (A)



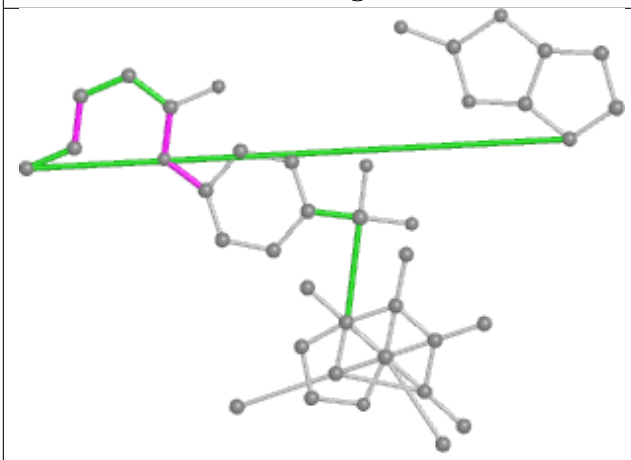
Ligand 4IR A 402 (B)



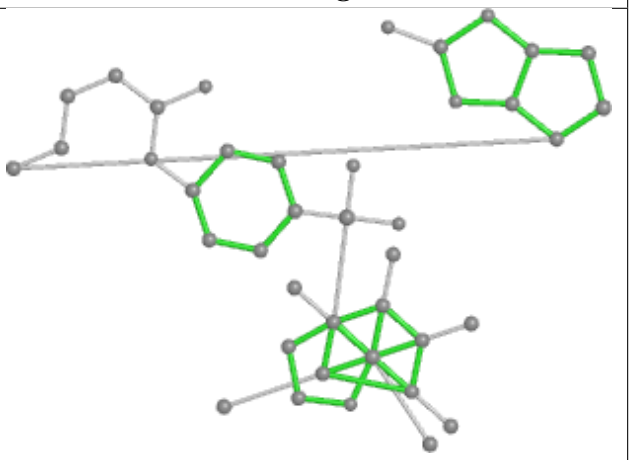
Bond lengths



Bond angles

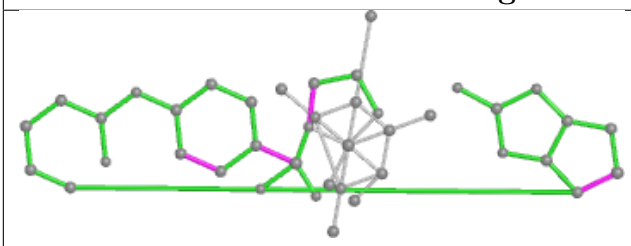


Torsions

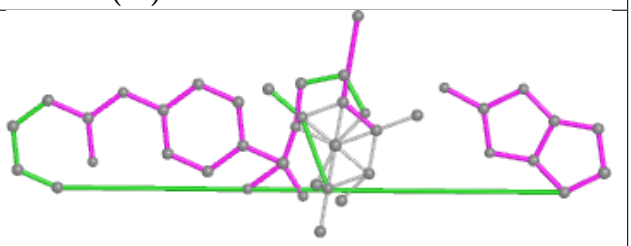


Rings

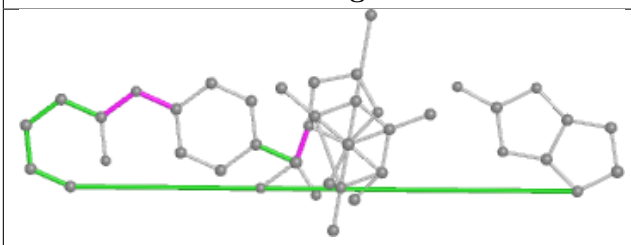
Ligand 4IR A 401 (A)



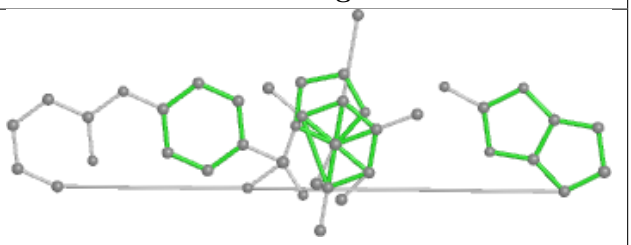
Bond lengths



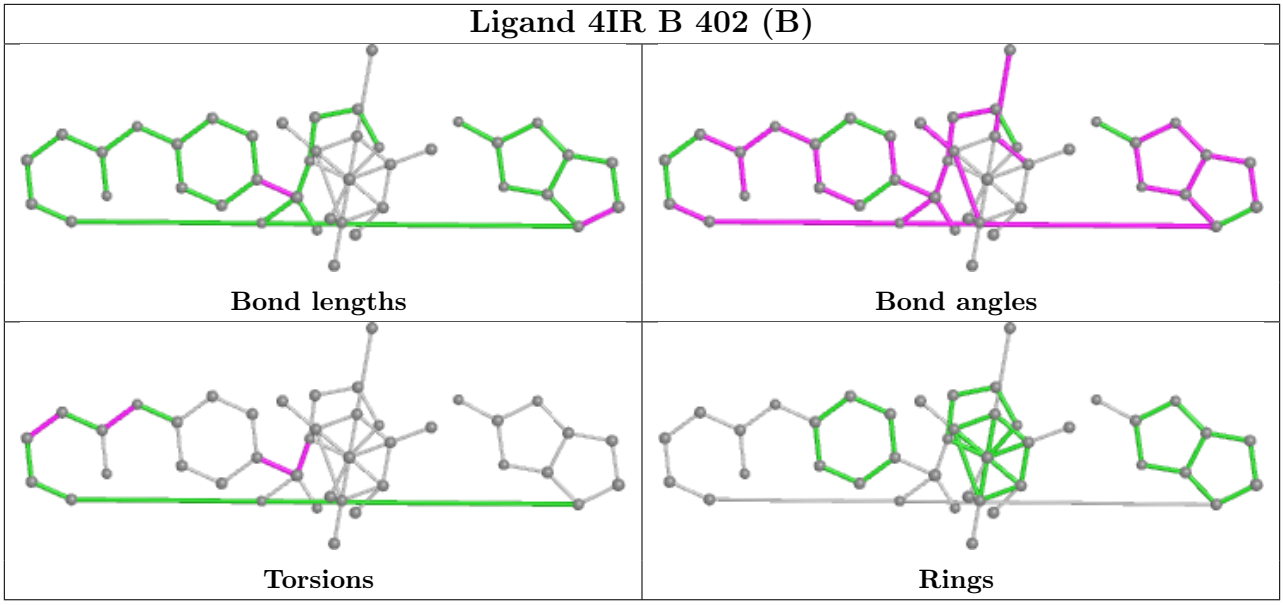
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	243/343 (70%)	-0.26	8 (3%)	46	44	17, 29, 56, 81	0
1	B	244/343 (71%)	-0.27	11 (4%)	33	32	18, 29, 59, 78	0
All	All	487/686 (70%)	-0.27	19 (3%)	39	38	17, 29, 57, 81	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	250	THR	6.0
1	A	66	THR	5.5
1	B	250	THR	5.0
1	B	249	ALA	5.0
1	B	65	ALA	4.0
1	A	46	ALA	3.5
1	B	46	ALA	3.5
1	B	248	PRO	3.2
1	B	66	THR	3.0
1	A	251	ASP	2.9
1	A	249	ALA	2.9
1	B	267	TYR	2.9
1	B	62	SER	2.8
1	A	65	ALA	2.7
1	B	247	ALA	2.6
1	A	267	TYR	2.4
1	A	230	ALA	2.3
1	B	251	ASP	2.2
1	B	246	SER	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)

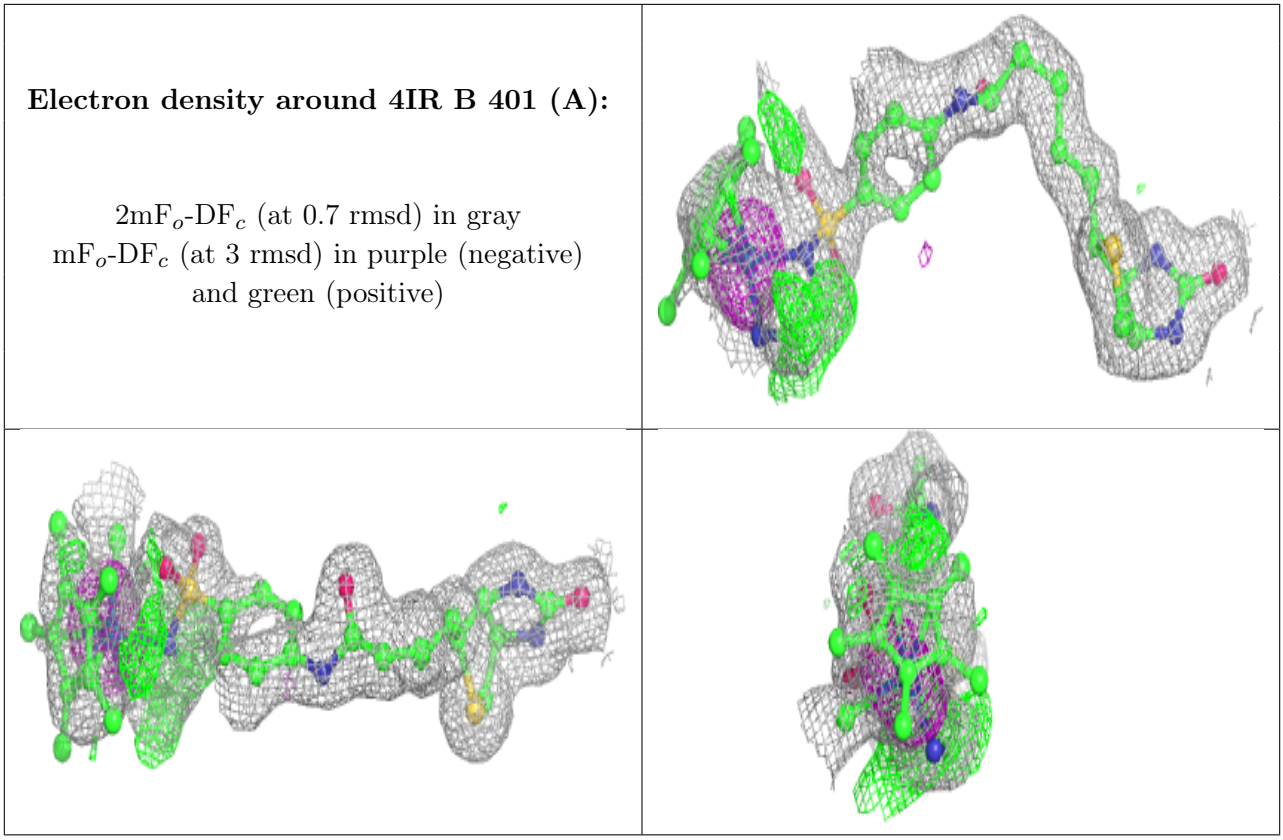
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	B	403	6/6	0.73	0.11	63,73,74,76	0
3	GOL	A	403	6/6	0.91	0.14	43,56,58,60	0
3	GOL	A	404	6/6	0.92	0.13	38,41,43,44	6
3	GOL	A	405	6/6	0.93	0.12	63,66,66,70	0
2	4IR	B	401[A]	41/41	0.96	0.14	19,30,48,54	41
2	4IR	B	401[B]	41/41	0.96	0.14	20,41,50,54	41
2	4IR	B	402[A]	41/41	0.96	0.14	15,30,47,51	41
2	4IR	B	402[B]	41/41	0.96	0.14	24,39,47,50	41
2	4IR	A	401[A]	41/41	0.96	0.13	17,33,49,57	41
2	4IR	A	401[B]	41/41	0.96	0.13	22,37,48,52	41
2	4IR	A	402[A]	41/41	0.96	0.14	14,30,46,56	41
2	4IR	A	402[B]	41/41	0.96	0.14	25,46,57,60	41
3	GOL	B	404	6/6	0.97	0.13	46,46,47,48	6

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.

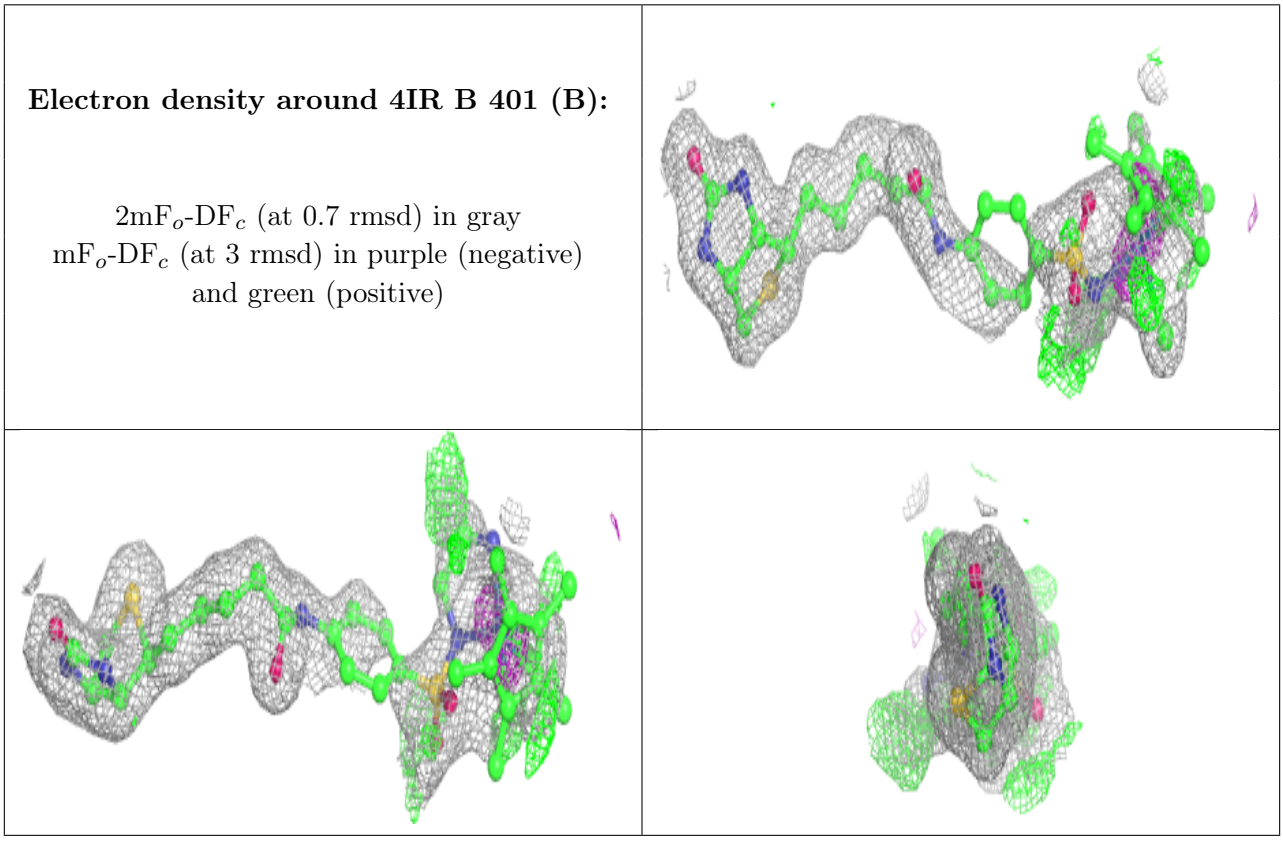
Electron density around 4IR B 401 (A):

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



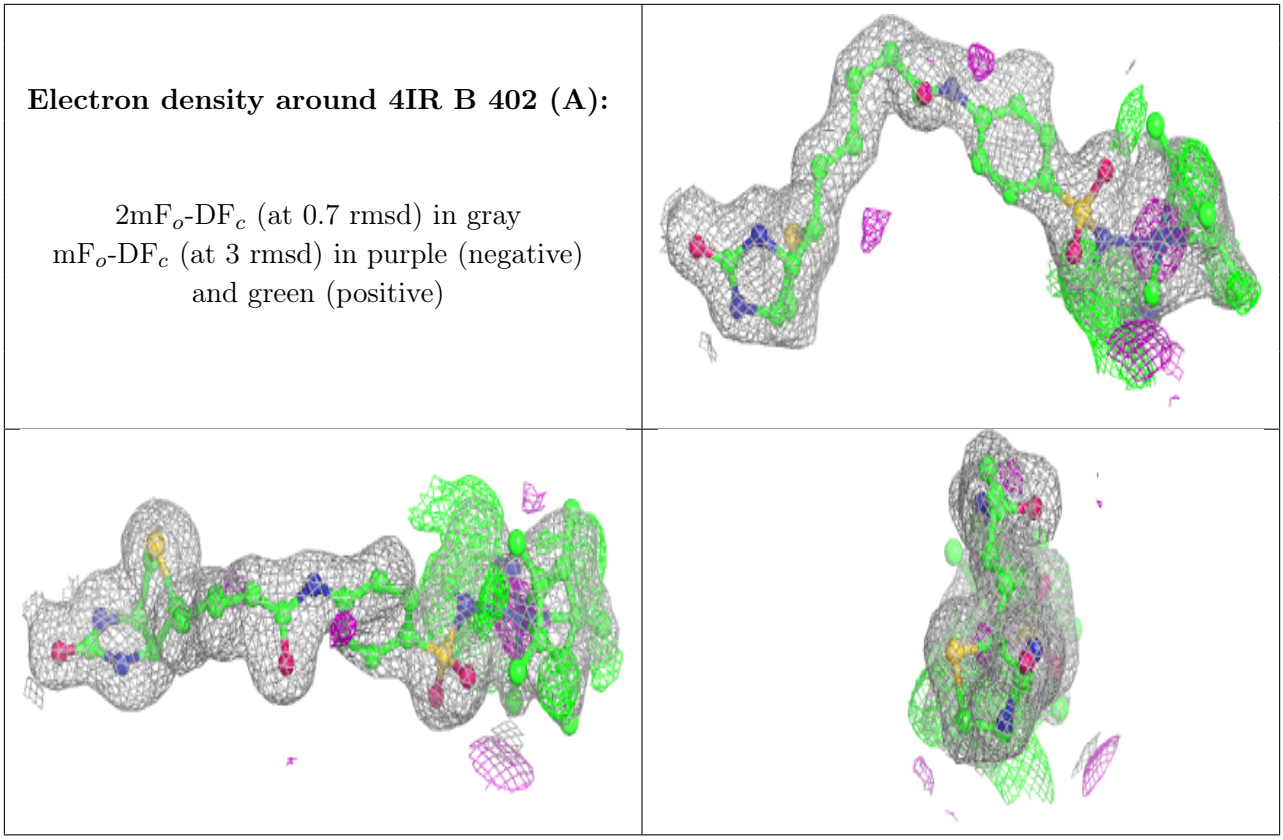
Electron density around 4IR B 401 (B):

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



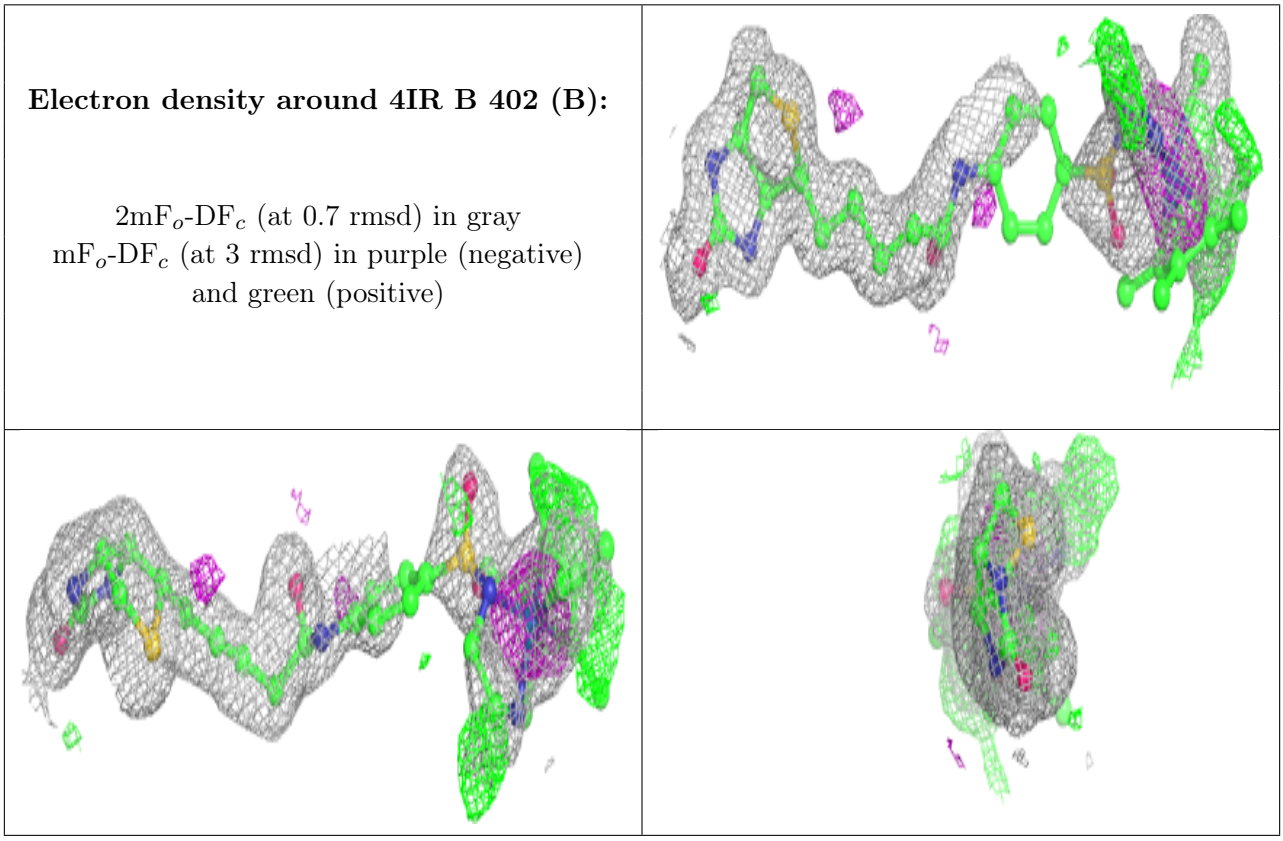
Electron density around 4IR B 402 (A):

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



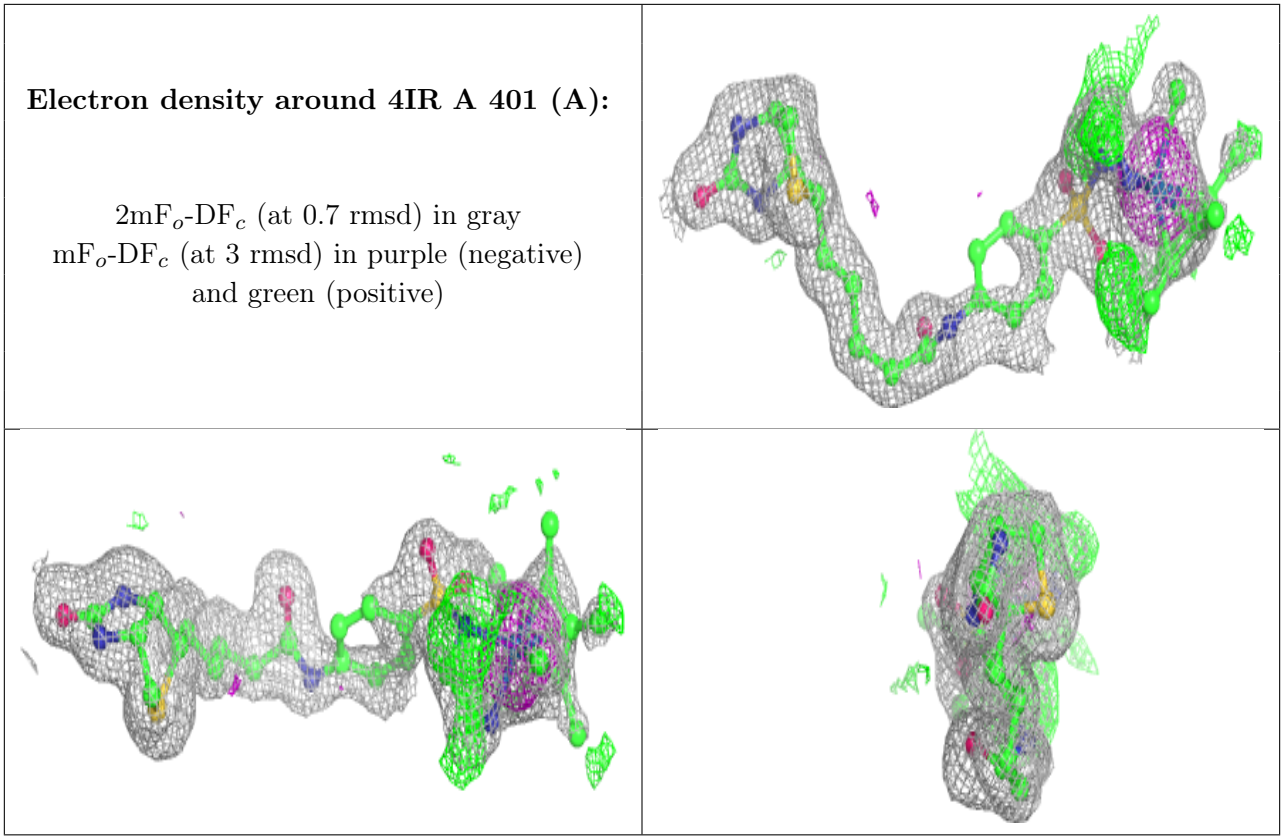
Electron density around 4IR B 402 (B):

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



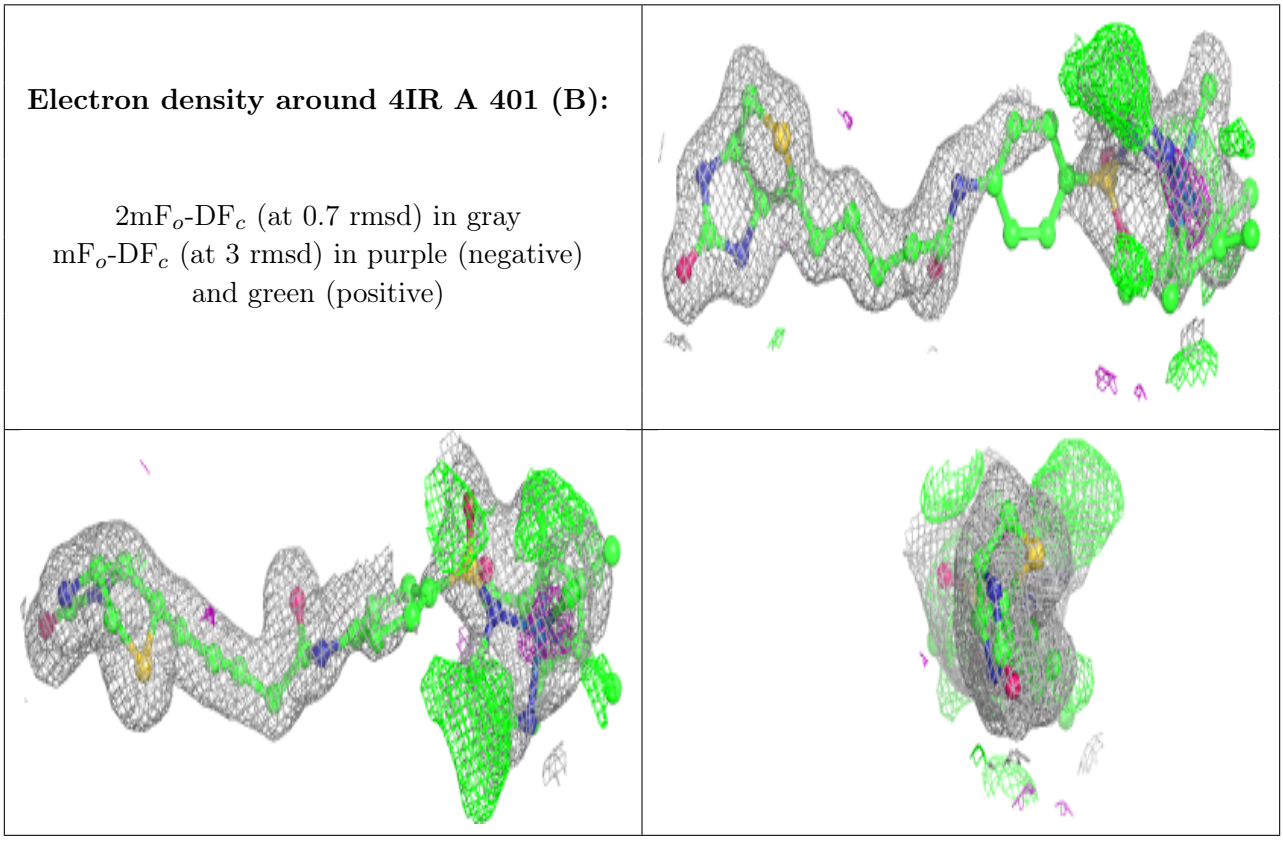
Electron density around 4IR A 401 (A):

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



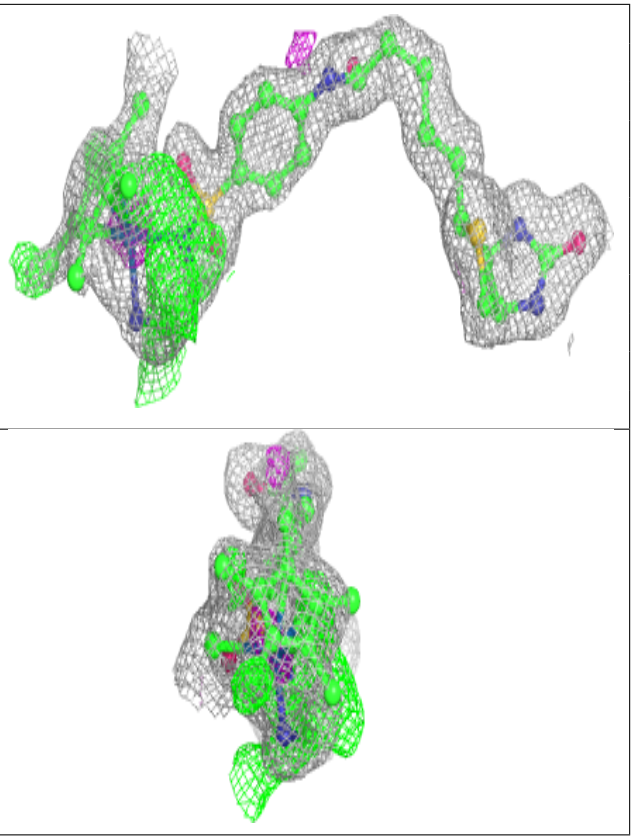
Electron density around 4IR A 401 (B):

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



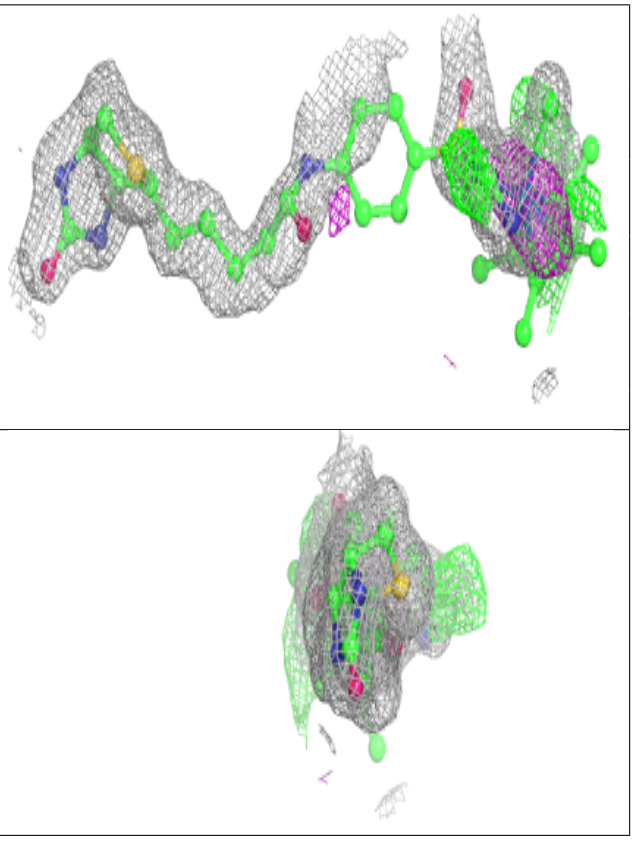
Electron density around 4IR A 402 (A):

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



Electron density around 4IR A 402 (B):

$2mF_o$-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.