



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:01 PM UTC

PDB ID : 7P3S / pdb_00007p3s
Title : Crystal structure of Schistosoma mansoni HDAC8 complexed with a benzohydroxamate inhibitor 12
Authors : Shaik, T.B.; Romier, C.
Deposited on : 2021-07-08
Resolution : 1.55 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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

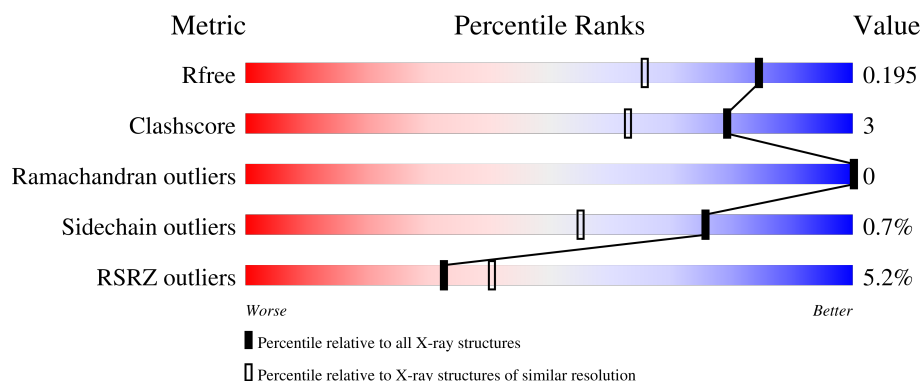
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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}	180053	1003 (1.54-1.54)
Clashscore	190562	1025 (1.54-1.54)
Ramachandran outliers	187476	1007 (1.54-1.54)
Sidechain outliers	187428	1007 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)

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	447	6% 86% 11%
1	B	447	3% 86% 6% 9%
1	C	447	3% 85% 7% 8%
1	D	447	7% 83% 6% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	C	505	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14397 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 Histone deacetylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	13	0
			3248	2105	533	595	15			
1	B	409	Total	C	N	O	S	0	9	0
			3295	2129	546	603	17			
1	C	412	Total	C	N	O	S	0	10	0
			3327	2147	553	610	17			
1	D	400	Total	C	N	O	S	0	7	0
			3231	2089	533	593	16			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP A5H660
A	441	GLY	-	expression tag	UNP A5H660
A	442	SER	-	expression tag	UNP A5H660
A	443	LEU	-	expression tag	UNP A5H660
A	444	VAL	-	expression tag	UNP A5H660
A	445	PRO	-	expression tag	UNP A5H660
A	446	ARG	-	expression tag	UNP A5H660
B	0	HIS	-	expression tag	UNP A5H660
B	441	GLY	-	expression tag	UNP A5H660
B	442	SER	-	expression tag	UNP A5H660
B	443	LEU	-	expression tag	UNP A5H660
B	444	VAL	-	expression tag	UNP A5H660
B	445	PRO	-	expression tag	UNP A5H660
B	446	ARG	-	expression tag	UNP A5H660
C	0	HIS	-	expression tag	UNP A5H660
C	441	GLY	-	expression tag	UNP A5H660
C	442	SER	-	expression tag	UNP A5H660
C	443	LEU	-	expression tag	UNP A5H660
C	444	VAL	-	expression tag	UNP A5H660
C	445	PRO	-	expression tag	UNP A5H660
C	446	ARG	-	expression tag	UNP A5H660

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	expression tag	UNP A5H660
D	441	GLY	-	expression tag	UNP A5H660
D	442	SER	-	expression tag	UNP A5H660
D	443	LEU	-	expression tag	UNP A5H660
D	444	VAL	-	expression tag	UNP A5H660
D	445	PRO	-	expression tag	UNP A5H660
D	446	ARG	-	expression tag	UNP A5H660

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

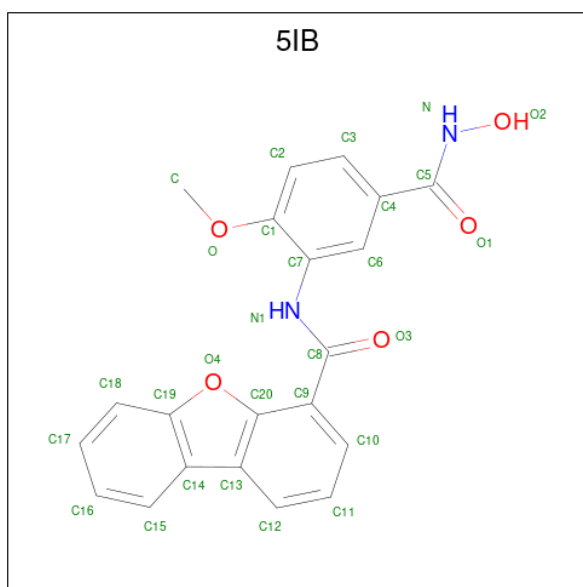
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total K 2 2	0	0
3	B	2	Total K 2 2	0	0
3	C	2	Total K 2 2	0	0
3	D	2	Total K 2 2	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is {N}-[2-methoxy-5-(oxidanylcabamoyl)phenyl]dibenzofuran-4-carboxamide (CCD ID: 5IB) (formula: C₂₁H₁₆N₂O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			28	21	2	5		
5	B	1	Total	C	N	O	0	0
			28	21	2	5		
5	C	1	Total	C	N	O	0	0
			28	21	2	5		
5	D	1	Total	C	N	O	0	0
			28	21	2	5		

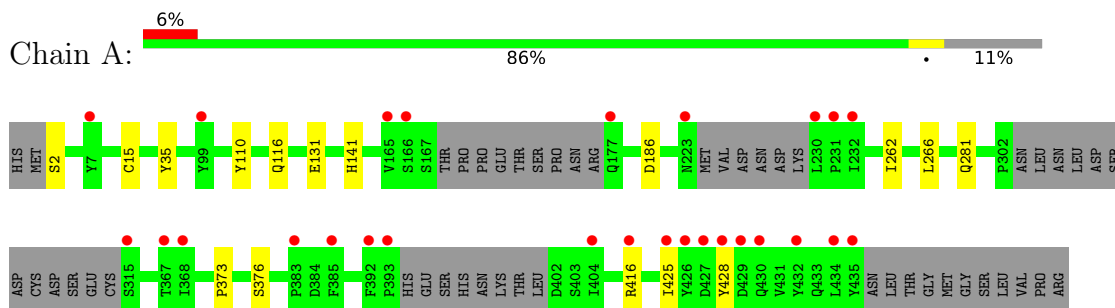
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	247	Total	O	0	0
			247	247		
6	B	302	Total	O	0	0
			302	302		
6	C	309	Total	O	0	0
			309	309		
6	D	266	Total	O	0	0
			266	266		

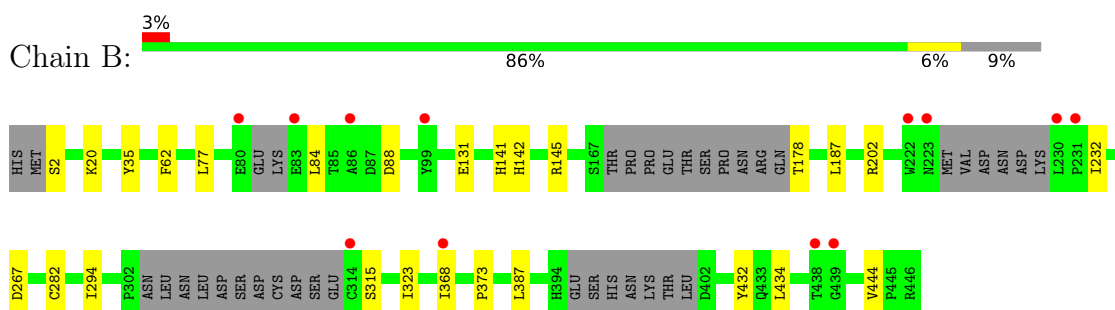
3 Residue-property plots [i](#)

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.

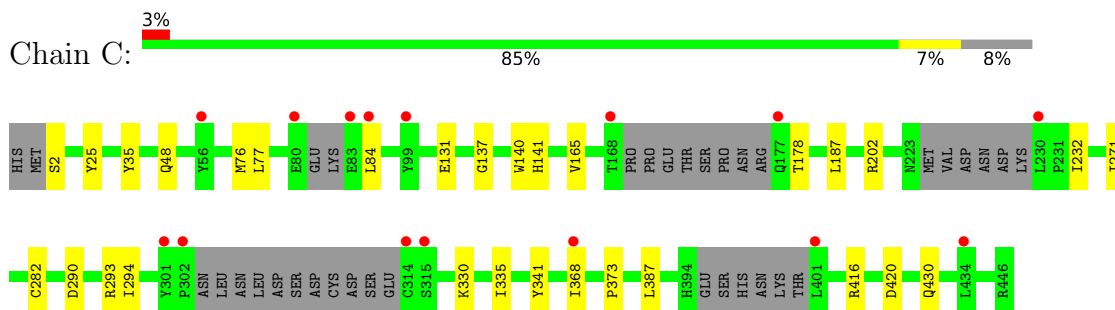
• Molecule 1: Histone deacetylase



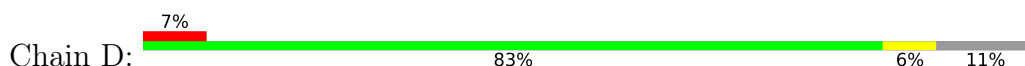
• Molecule 1: Histone deacetylase

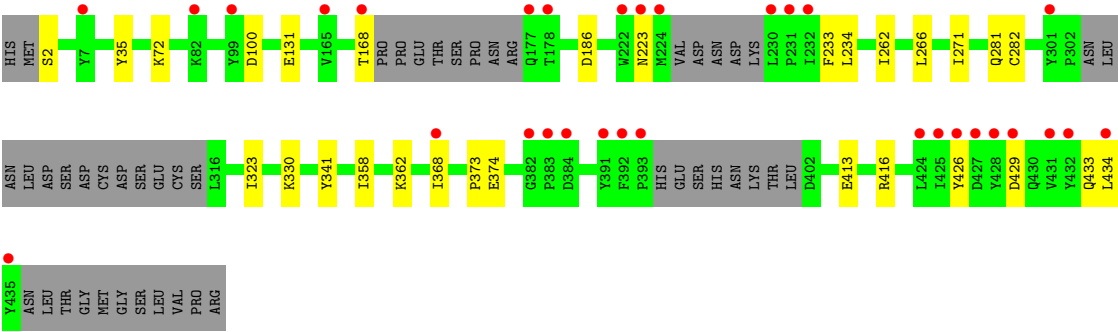


• Molecule 1: Histone deacetylase



• Molecule 1: Histone deacetylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	70.39Å 70.39Å 97.94Å 78.05° 75.57° 85.69°	Depositor
Resolution (Å)	46.52 – 1.55 46.52 – 1.55	Depositor EDS
% Data completeness (in resolution range)	90.2 (46.52-1.55) 90.2 (46.52-1.55)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 1.55Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.169 , 0.193 0.170 , 0.195	Depositor DCC
R_{free} test set	11752 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.097 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14397	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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: GOL, ZN, K, 5IB

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	0.25	0/3377	0.47	0/4593
1	B	0.29	0/3413	0.50	0/4641
1	C	0.28	0/3448	0.50	0/4688
1	D	0.26	0/3342	0.47	0/4546
All	All	0.27	0/13580	0.49	0/18468

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	3248	0	3186	11	0
1	B	3295	0	3217	18	0
1	C	3327	0	3249	23	0
1	D	3231	0	3145	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	18	0	24	6	0
4	B	6	0	8	0	0
4	C	12	0	16	4	0
4	D	12	0	16	1	0
5	A	28	0	0	0	0
5	B	28	0	0	3	0
5	C	28	0	0	1	0
5	D	28	0	0	1	0
6	A	247	0	0	1	0
6	B	302	0	0	1	0
6	C	309	0	0	2	0
6	D	266	0	0	4	0
All	All	14397	0	12861	70	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 3.

All (70) 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:C:25:TYR:HB2	4:C:505:GOL:H31	1.53	0.88
1:C:140:TRP:HZ2	4:C:505:GOL:H12	1.53	0.71
1:D:234:LEU:HB2	4:D:505:GOL:H32	1.73	0.71
1:D:374:GLU:OE2	6:D:601:HOH:O	2.09	0.69
1:B:88:ASP:OD2	6:B:601:HOH:O	2.14	0.66
1:D:2:SER:N	1:D:131:GLU:OE1	2.30	0.65
1:C:35:TYR:CE1	1:C:368[A]:ILE:HG23	2.32	0.64
1:B:35:TYR:CE1	1:B:368[A]:ILE:HG23	2.34	0.63
1:C:137:GLY:HA2	4:C:505:GOL:H11	1.82	0.62
1:A:116:GLN:HE22	4:A:506:GOL:H31	1.67	0.59
1:C:48:GLN:NE2	6:C:605:HOH:O	2.35	0.59
1:C:416:ARG:NH1	1:C:420[B]:ASP:OD1	2.35	0.59
1:B:20:LYS:NZ	5:B:501:5IB:O4	2.35	0.58
1:B:187:LEU:HD21	1:B:294:ILE:HD12	1.86	0.56
1:C:140:TRP:CZ2	4:C:505:GOL:H12	2.38	0.56
1:C:368[A]:ILE:HG21	1:C:387:LEU:HD22	1.89	0.55
1:C:2:SER:N	1:C:131:GLU:OE1	2.39	0.55
1:A:116:GLN:NE2	4:A:506:GOL:H31	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:LEU:HD13	1:C:84:LEU:HG	1.90	0.52
1:B:2:SER:N	1:B:131:GLU:OE2	2.42	0.52
1:D:358:ILE:HG23	1:D:362:LYS:HD3	1.91	0.51
1:D:341:TYR:OH	5:D:501:5IB:O1	2.18	0.50
1:D:35:TYR:CD1	1:D:368:ILE:HG23	2.48	0.49
1:B:77:LEU:HD13	1:B:84:LEU:HG	1.95	0.49
1:C:178:THR:HB	1:C:202:ARG:HH21	1.78	0.49
1:A:186:ASP:HB2	1:A:281:GLN:OE1	2.12	0.48
4:A:505:GOL:O3	6:A:601:HOH:O	2.00	0.48
1:D:72:LYS:NZ	6:D:614:HOH:O	2.44	0.48
1:D:429:ASP:O	1:D:433:GLN:HG2	2.12	0.48
1:A:15:CYS:SG	4:A:505:GOL:O1	2.71	0.48
1:D:262[B]:ILE:HG12	1:D:266:LEU:HG	1.95	0.48
1:B:35:TYR:CD1	1:B:368[B]:ILE:HG23	2.49	0.47
1:A:2:SER:N	1:A:131:GLU:OE2	2.46	0.47
1:C:187:LEU:HD21	1:C:294:ILE:HD12	1.95	0.47
1:B:368[A]:ILE:HG21	1:B:387:LEU:HD22	1.97	0.47
1:C:35:TYR:CD1	1:C:368[B]:ILE:HG23	2.50	0.47
1:C:290:ASP:O	1:C:293:ARG:HD3	2.15	0.47
1:A:116:GLN:HE22	4:A:506:GOL:C3	2.28	0.46
1:B:142:HIS:NE2	5:B:501:5IB:N	2.63	0.46
1:C:271:ILE:HD13	1:C:430:GLN:HG2	1.98	0.45
1:D:186:ASP:HB2	1:D:281:GLN:OE1	2.16	0.45
1:D:282[B]:CYS:SG	1:D:323:ILE:HD11	2.56	0.45
1:A:35:TYR:CZ	1:A:373:PRO:HD3	2.52	0.45
1:D:35:TYR:CZ	1:D:373:PRO:HD3	2.52	0.45
1:B:35:TYR:CZ	1:B:373:PRO:HD3	2.52	0.45
1:D:416:ARG:HG3	1:D:426:TYR:OH	2.17	0.44
1:B:368[A]:ILE:HG21	1:B:387:LEU:CD2	2.48	0.44
1:C:341:TYR:OH	5:C:501:5IB:O1	2.34	0.44
1:D:100:ASP:HB2	6:D:813:HOH:O	2.18	0.44
1:C:35:TYR:CE1	1:C:368[B]:ILE:HG23	2.53	0.44
1:A:141:HIS:H	1:A:141:HIS:CD2	2.35	0.44
1:D:271:ILE:HD12	1:D:434:LEU:HD11	2.00	0.44
1:C:35:TYR:CZ	1:C:373:PRO:HD3	2.53	0.43
1:A:416:ARG:HD2	1:A:428:TYR:CE1	2.53	0.43
1:B:178:THR:HB	1:B:202:ARG:HH21	1.84	0.43
1:B:432:TYR:HA	1:B:444:VAL:HG21	2.01	0.43
1:A:262[B]:ILE:HG12	1:A:266:LEU:HG	2.02	0.42
1:B:35:TYR:CD1	1:B:368[A]:ILE:HG23	2.55	0.42
1:C:330:LYS:NZ	6:C:609:HOH:O	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:413:GLU:HG3	1:D:416:ARG:NH2	2.35	0.42
1:D:330:LYS:NZ	6:D:608:HOH:O	2.36	0.41
1:B:282[B]:CYS:SG	1:B:323:ILE:HD11	2.60	0.41
1:B:62:PHE:O	1:B:145:ARG:HG3	2.21	0.41
1:C:368[A]:ILE:HG21	1:C:387:LEU:CD2	2.49	0.41
1:B:267:ASP:HB3	1:B:434:LEU:HD11	2.03	0.41
1:B:141:HIS:NE2	5:B:501:5IB:O2	2.35	0.40
1:C:282[B]:CYS:SG	1:C:335:ILE:HG23	2.61	0.40
1:A:110:TYR:CE1	4:A:505:GOL:H12	2.56	0.40
1:C:141:HIS:H	1:C:141:HIS:CD2	2.39	0.40
1:C:368[A]:ILE:CG2	1:C:387:LEU:HD22	2.50	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	402/447 (90%)	396 (98%)	6 (2%)	0	100	100
1	B	406/447 (91%)	401 (99%)	5 (1%)	0	100	100
1	C	410/447 (92%)	404 (98%)	6 (2%)	0	100	100
1	D	397/447 (89%)	393 (99%)	4 (1%)	0	100	100
All	All	1615/1788 (90%)	1594 (99%)	21 (1%)	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	359/392 (92%)	357 (99%)	2 (1%)	78	59
1	B	363/392 (93%)	361 (99%)	2 (1%)	78	59
1	C	367/392 (94%)	364 (99%)	3 (1%)	73	51
1	D	354/392 (90%)	351 (99%)	3 (1%)	73	51
All	All	1443/1568 (92%)	1433 (99%)	10 (1%)	76	55

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	376	SER
1	A	425	ILE
1	B	232	ILE
1	B	315	SER
1	C	76	MET
1	C	165	VAL
1	C	232	ILE
1	D	168	THR
1	D	223	ASN
1	D	233	PHE

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

Mol	Chain	Res	Type
1	C	48	GLN
1	C	129	HIS
1	C	274	GLN
1	D	223	ASN
1	D	405	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 for Mogul analysis.

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
5	5IB	D	501	2	31,31,31	0.26	0	44,44,44	0.64	0
5	5IB	A	507	2	31,31,31	0.26	0	44,44,44	0.61	0
4	GOL	A	504	-	5,5,5	0.34	0	5,5,5	1.04	1 (20%)
4	GOL	D	506	-	5,5,5	0.34	0	5,5,5	0.45	0
4	GOL	A	506	-	5,5,5	0.39	0	5,5,5	0.52	0
4	GOL	B	505	-	5,5,5	0.33	0	5,5,5	0.63	0
4	GOL	D	505	-	5,5,5	0.43	0	5,5,5	1.77	2 (40%)
5	5IB	C	501	2	31,31,31	0.31	0	44,44,44	1.08	3 (6%)
4	GOL	C	506	-	5,5,5	0.34	0	5,5,5	0.49	0
4	GOL	A	505	-	5,5,5	0.47	0	5,5,5	0.85	0
5	5IB	B	501	2	31,31,31	0.37	0	44,44,44	1.08	3 (6%)
4	GOL	C	505	-	5,5,5	0.64	0	5,5,5	1.00	0

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
5	5IB	D	501	2	-	4/16/16/16	0/4/4/4
5	5IB	A	507	2	-	2/16/16/16	0/4/4/4
4	GOL	A	504	-	-	2/4/4/4	-
4	GOL	D	506	-	-	0/4/4/4	-
4	GOL	A	506	-	-	3/4/4/4	-
4	GOL	B	505	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	505	-	-	3/4/4/4	-
5	5IB	C	501	2	-	6/16/16/16	0/4/4/4
4	GOL	C	506	-	-	1/4/4/4	-
4	GOL	A	505	-	-	2/4/4/4	-
5	5IB	B	501	2	-	6/16/16/16	0/4/4/4
4	GOL	C	505	-	-	4/4/4/4	-

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	5IB	C7-N1-C8	4.42	139.19	126.90
5	C	501	5IB	C7-N1-C8	4.31	138.90	126.90
5	C	501	5IB	C1-C7-N1	3.58	123.39	116.73
5	B	501	5IB	C1-C7-N1	3.56	123.36	116.73
4	D	505	GOL	O2-C2-C3	2.91	121.23	109.18
4	D	505	GOL	O1-C1-C2	-2.46	99.29	110.38
5	B	501	5IB	O4-C20-C9	2.14	127.60	124.55
4	A	504	GOL	C3-C2-C1	-2.09	104.12	111.80
5	C	501	5IB	O4-C20-C9	2.08	127.52	124.55

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	504	GOL	C1-C2-C3-O3
4	A	505	GOL	O1-C1-C2-C3
4	A	506	GOL	C1-C2-C3-O3
4	A	506	GOL	O2-C2-C3-O3
4	B	505	GOL	C1-C2-C3-O3
4	C	505	GOL	O1-C1-C2-C3
4	C	505	GOL	C1-C2-C3-O3
4	D	505	GOL	O1-C1-C2-C3
5	B	501	5IB	C1-C7-N1-C8
5	B	501	5IB	N1-C8-C9-C20
5	B	501	5IB	O3-C8-C9-C20
5	C	501	5IB	C1-C7-N1-C8
5	C	501	5IB	N1-C8-C9-C20
5	C	501	5IB	O3-C8-C9-C20
5	B	501	5IB	C6-C7-N1-C8

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Mol	Chain	Res	Type	Atoms
5	C	501	5IB	C6-C7-N1-C8
4	D	505	GOL	O1-C1-C2-O2
4	A	505	GOL	O1-C1-C2-O2
4	B	505	GOL	O2-C2-C3-O3
4	C	505	GOL	O1-C1-C2-O2
4	A	504	GOL	O2-C2-C3-O3
4	C	505	GOL	O2-C2-C3-O3
4	D	505	GOL	O2-C2-C3-O3
5	A	507	5IB	O3-C8-C9-C20
5	A	507	5IB	N1-C8-C9-C20
5	C	501	5IB	O3-C8-C9-C10
5	B	501	5IB	O3-C8-C9-C10
5	D	501	5IB	N1-C8-C9-C20
5	D	501	5IB	O3-C8-N1-C7
5	D	501	5IB	O3-C8-C9-C20
4	A	506	GOL	O1-C1-C2-O2
5	D	501	5IB	C9-C8-N1-C7
5	B	501	5IB	N1-C8-C9-C10
5	C	501	5IB	N1-C8-C9-C10
4	C	506	GOL	O1-C1-C2-O2

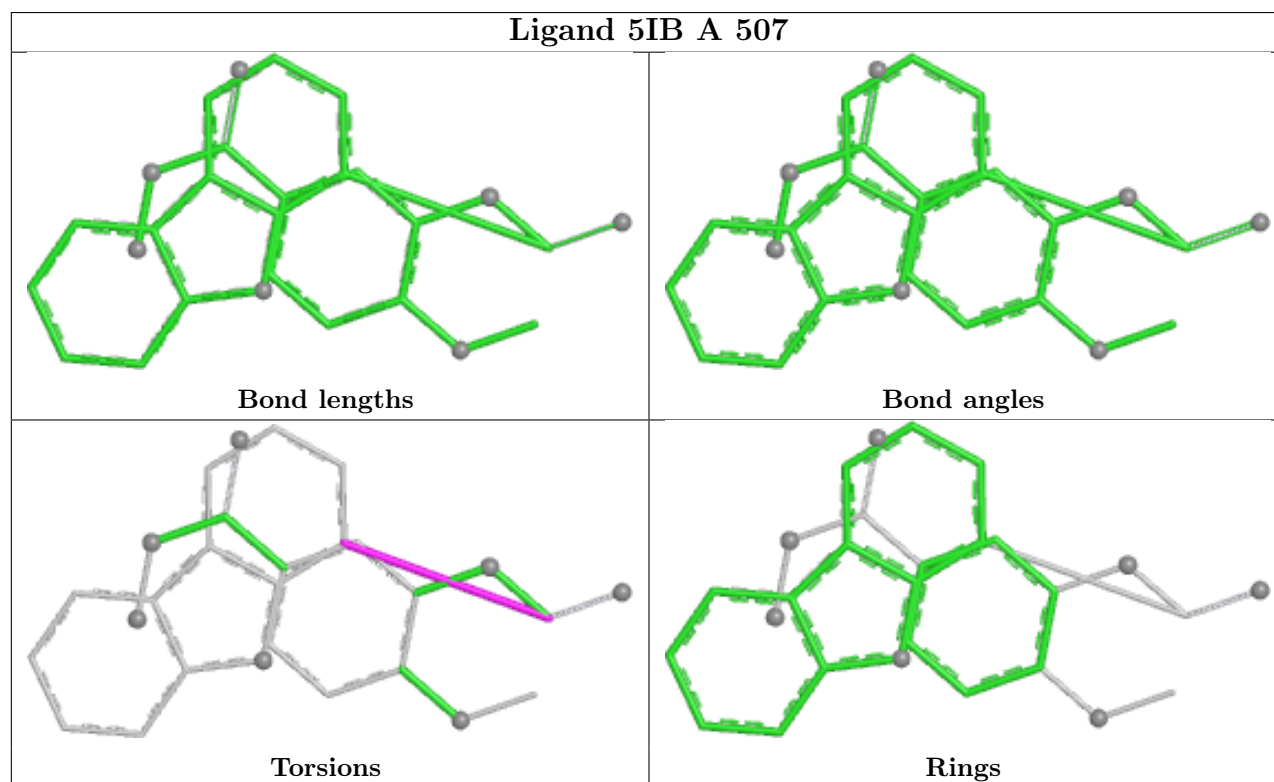
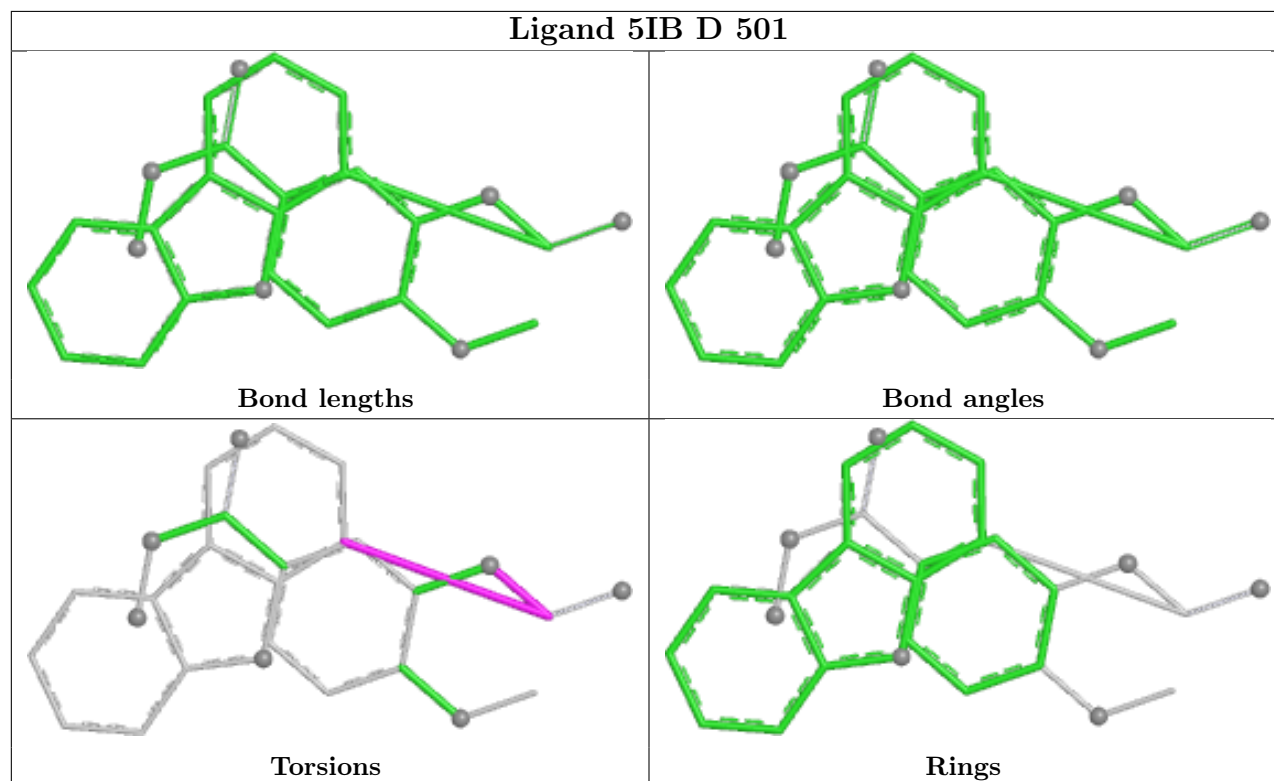
There are no ring outliers.

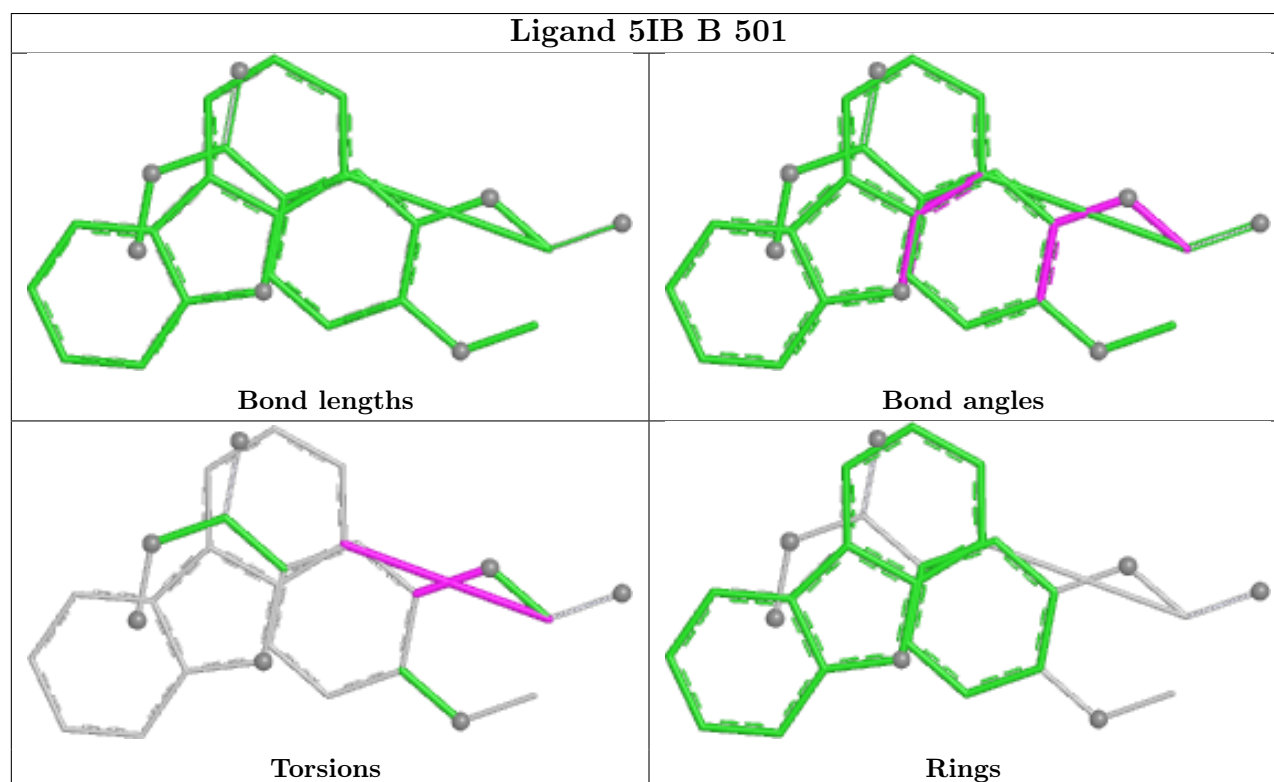
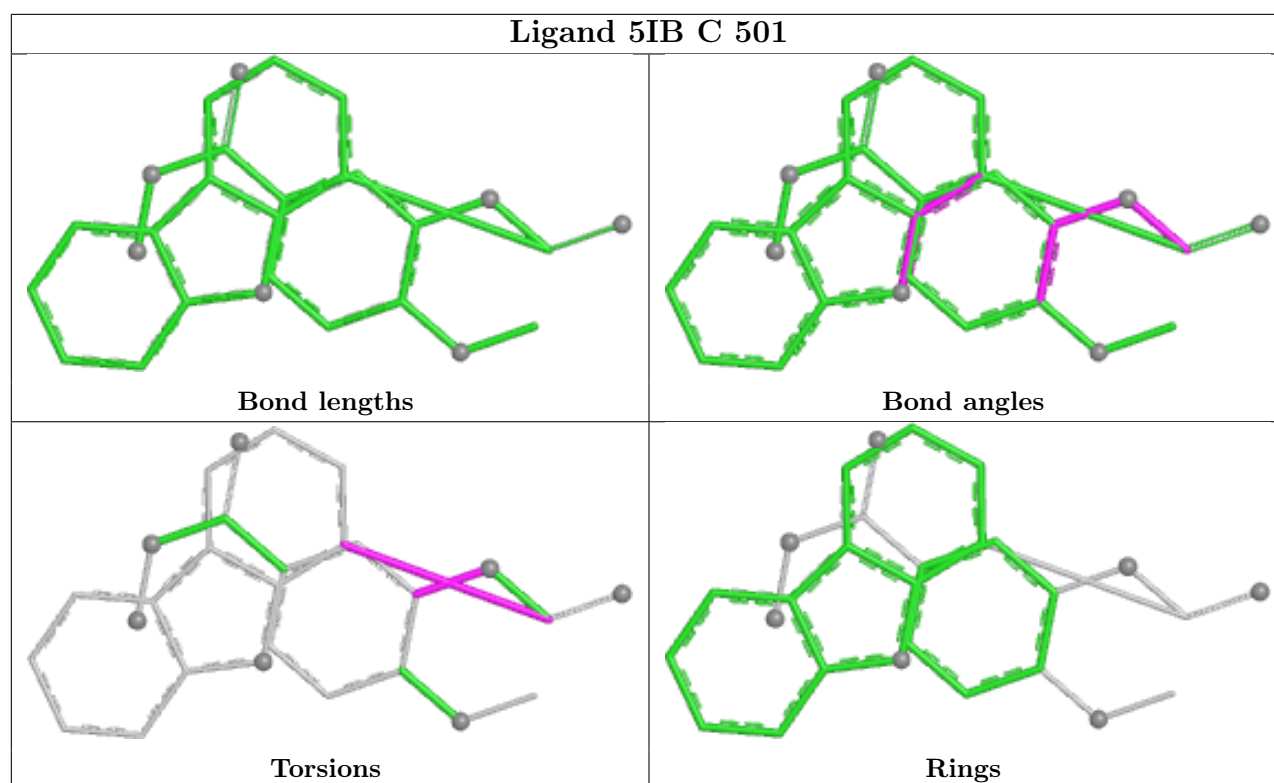
7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	501	5IB	1	0
4	A	506	GOL	3	0
4	D	505	GOL	1	0
5	C	501	5IB	1	0
4	A	505	GOL	3	0
5	B	501	5IB	3	0
4	C	505	GOL	4	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 ⓘ

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, 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	399/447 (89%)	0.28	27 (6%)	23 29	10, 21, 53, 82	13 (3%)
1	B	409/447 (91%)	0.01	12 (2%)	53 62	8, 18, 36, 87	9 (2%)
1	C	412/447 (92%)	0.04	15 (3%)	46 54	8, 19, 38, 93	10 (2%)
1	D	400/447 (89%)	0.31	31 (7%)	19 23	10, 21, 51, 85	7 (1%)
All	All	1620/1788 (90%)	0.16	85 (5%)	33 40	8, 20, 45, 93	39 (2%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	425	ILE	6.8
1	D	230	LEU	5.9
1	A	230	LEU	5.9
1	D	392	PHE	5.8
1	D	426	TYR	5.8
1	D	428	TYR	5.7
1	A	392	PHE	5.4
1	A	425	ILE	5.3
1	A	432	TYR	5.1
1	A	426	TYR	5.0
1	C	168	THR	5.0
1	C	401	LEU	4.9
1	D	435	TYR	4.5
1	D	232	ILE	4.4
1	A	435	TYR	4.3
1	A	428	TYR	4.2
1	D	432	TYR	4.2
1	B	230	LEU	4.0
1	D	168	THR	4.0
1	A	223	ASN	3.9
1	D	393	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	232	ILE	3.8
1	A	177	GLN	3.7
1	A	434	LEU	3.7
1	C	315	SER	3.7
1	A	99	TYR	3.5
1	A	368	ILE	3.4
1	C	230	LEU	3.4
1	A	165	VAL	3.4
1	D	177	GLN	3.3
1	D	165	VAL	3.3
1	A	315	SER	3.2
1	A	429	ASP	3.2
1	A	367	THR	3.2
1	B	223	ASN	3.1
1	D	223	ASN	3.1
1	B	99	TYR	3.0
1	A	393	PRO	2.9
1	A	231	PRO	2.9
1	B	314	CYS	2.9
1	C	56	TYR	2.8
1	D	224	MET	2.8
1	B	80	GLU	2.7
1	C	368[A]	ILE	2.7
1	D	434	LEU	2.7
1	D	383	PRO	2.7
1	D	427	ASP	2.6
1	D	429	ASP	2.6
1	D	368	ILE	2.6
1	B	83	GLU	2.6
1	D	231	PRO	2.6
1	D	99	TYR	2.5
1	C	177	GLN	2.5
1	C	314	CYS	2.5
1	D	424	LEU	2.5
1	C	84	LEU	2.4
1	C	99	TYR	2.4
1	D	222	TRP	2.3
1	B	438	THR	2.3
1	D	178	THR	2.3
1	A	383	PRO	2.3
1	C	434	LEU	2.3
1	A	385	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	430	GLN	2.3
1	D	382	GLY	2.3
1	A	404	ILE	2.3
1	D	7	TYR	2.3
1	B	231	PRO	2.2
1	A	416	ARG	2.2
1	B	368[A]	ILE	2.2
1	B	222	TRP	2.2
1	C	301	TYR	2.2
1	A	166	SER	2.2
1	C	80	GLU	2.2
1	B	86	ALA	2.1
1	D	391	TYR	2.1
1	A	427	ASP	2.1
1	C	83	GLU	2.1
1	D	301	TYR	2.1
1	D	384	ASP	2.1
1	D	82	LYS	2.1
1	D	431	VAL	2.1
1	A	7	TYR	2.1
1	B	439	GLY	2.0
1	C	302	PRO	2.0

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 oligosaccharides 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
5	5IB	D	501	28/28	0.73	0.25	36,74,80,89	0

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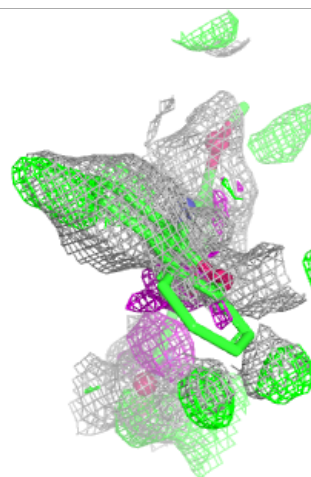
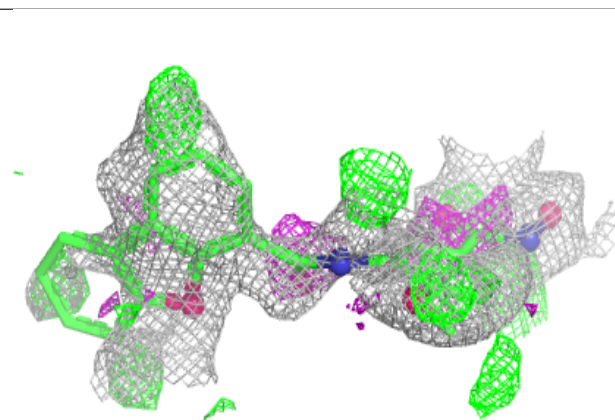
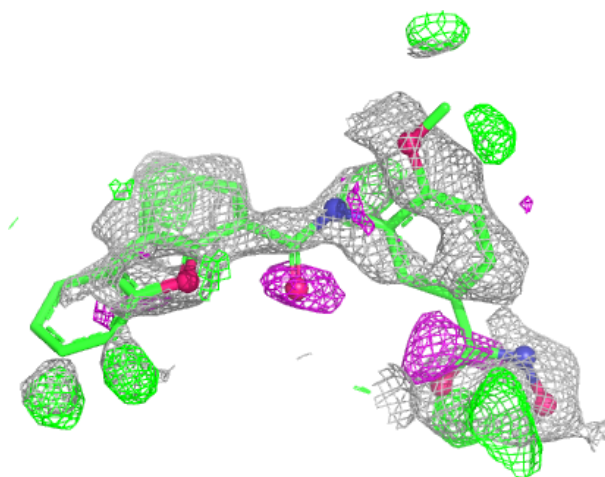
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	5IB	A	507	28/28	0.75	0.27	36,101,127,128	0
5	5IB	C	501	28/28	0.79	0.23	34,69,77,78	0
5	5IB	B	501	28/28	0.80	0.19	23,55,63,70	0
4	GOL	A	505	6/6	0.86	0.13	23,31,40,50	0
4	GOL	A	506	6/6	0.87	0.16	31,38,43,47	0
4	GOL	D	505	6/6	0.90	0.12	19,29,30,31	0
4	GOL	D	506	6/6	0.90	0.12	36,37,40,47	0
4	GOL	A	504	6/6	0.91	0.13	23,27,33,38	0
4	GOL	C	505	6/6	0.92	0.12	22,25,36,36	0
4	GOL	C	506	6/6	0.92	0.11	23,28,29,30	0
4	GOL	B	505	6/6	0.93	0.11	19,27,33,36	0
2	ZN	A	501	1/1	1.00	0.01	17,17,17,17	0
2	ZN	B	502	1/1	1.00	0.03	15,15,15,15	0
2	ZN	C	502	1/1	1.00	0.04	15,15,15,15	0
2	ZN	D	502	1/1	1.00	0.02	17,17,17,17	0
3	K	A	502	1/1	1.00	0.05	16,16,16,16	0
3	K	A	503	1/1	1.00	0.02	17,17,17,17	0
3	K	B	503	1/1	1.00	0.06	15,15,15,15	0
3	K	B	504	1/1	1.00	0.01	17,17,17,17	0
3	K	C	503	1/1	1.00	0.05	15,15,15,15	0
3	K	C	504	1/1	1.00	0.01	18,18,18,18	0
3	K	D	503	1/1	1.00	0.03	16,16,16,16	0
3	K	D	504	1/1	1.00	0.02	18,18,18,18	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.

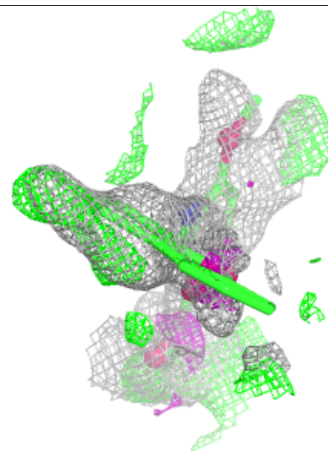
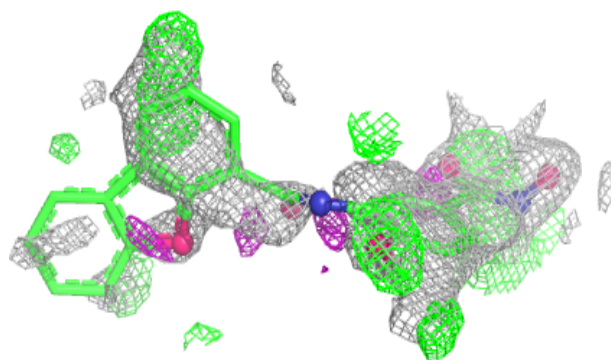
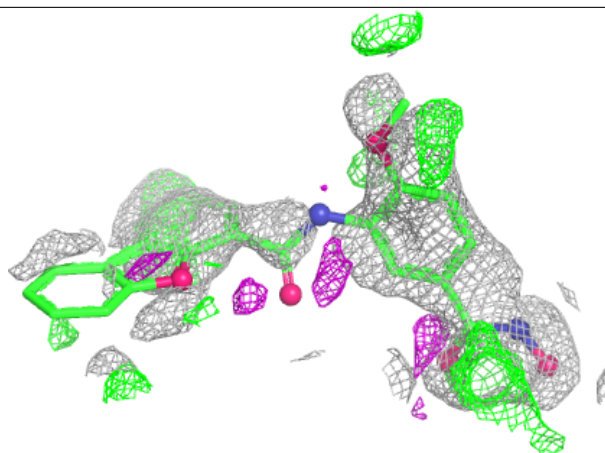
Electron density around 5IB D 501:

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



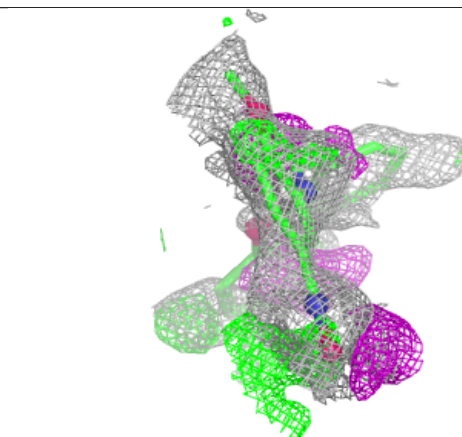
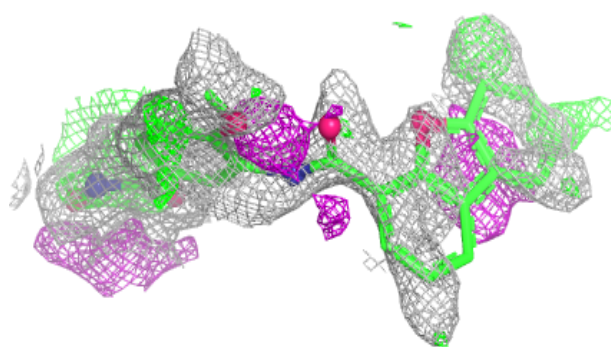
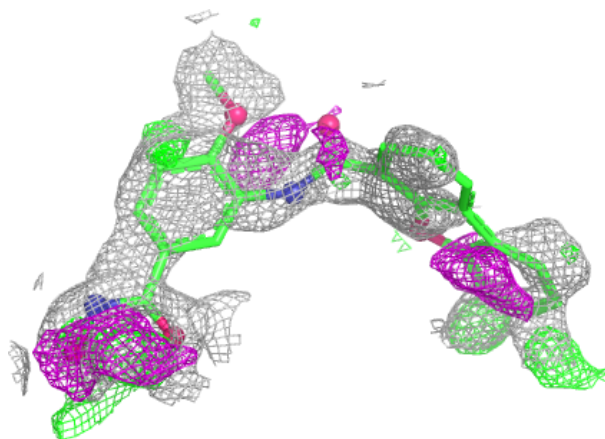
Electron density around 5IB A 507:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

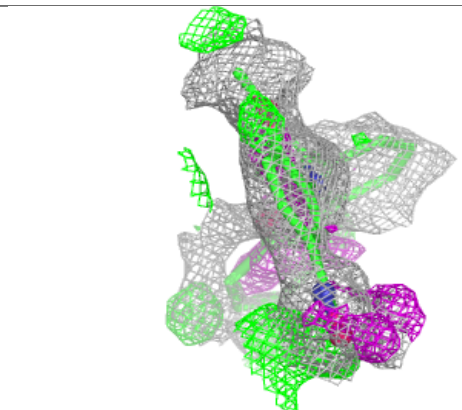
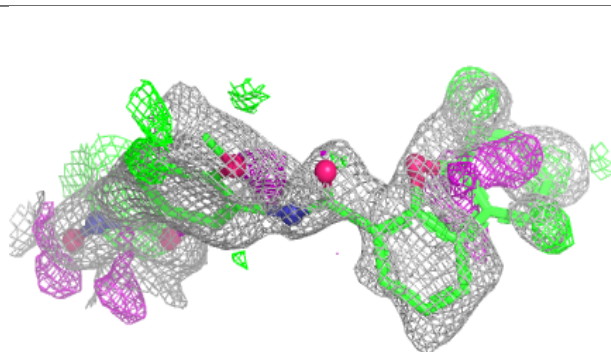
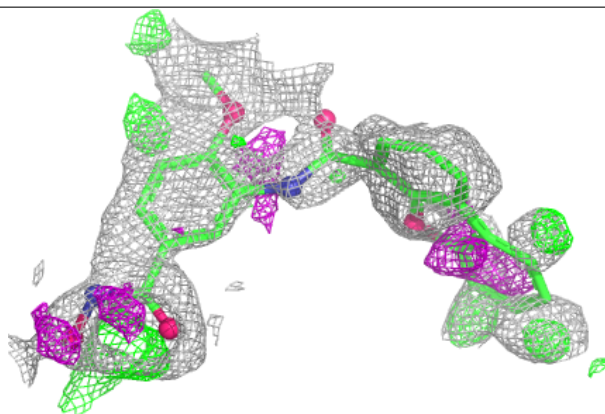


Electron density around 5IB C 501:

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

**Electron density around 5IB 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.