



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2021 – 04:24 PM BST

PDB ID : 7P3S
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 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 : 2.23.1
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) : 2.23.1

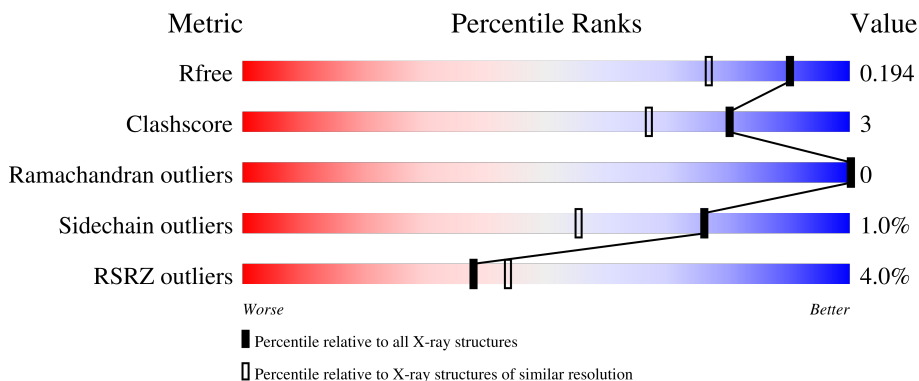
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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}	130704	2556 (1.56-1.52)
Clashscore	141614	2634 (1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)
RSRZ outliers	127900	2524 (1.56-1.52)

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	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 5px;">5% 85% • 11%</p>
1	B	447	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 5px;">2% 86% 5% 9%</p>
1	C	447	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 5px;">3% 86% 6% 8%</p>
1	D	447	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 83%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 5px;">4% 83% 7% 11%</p>

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 i

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

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 (three-letter code: 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 (three-letter code: K) (formula: K).

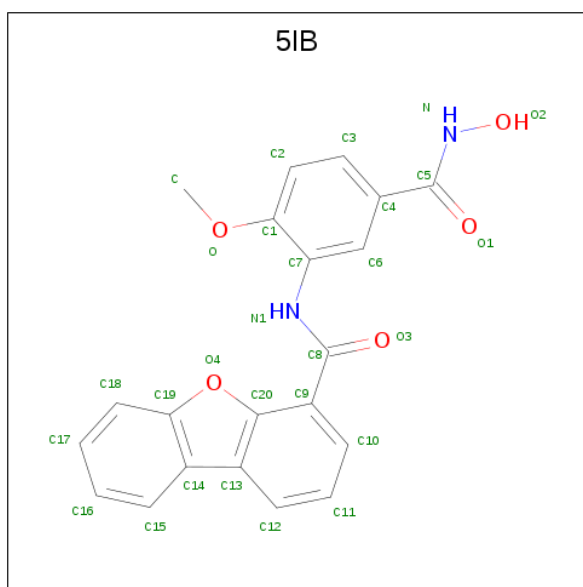
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total K 2 2	0	0
3	B	2	Total K 2 2	0	0
3	C	2	Total K 2 2	0	0
3	D	2	Total K 2 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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



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

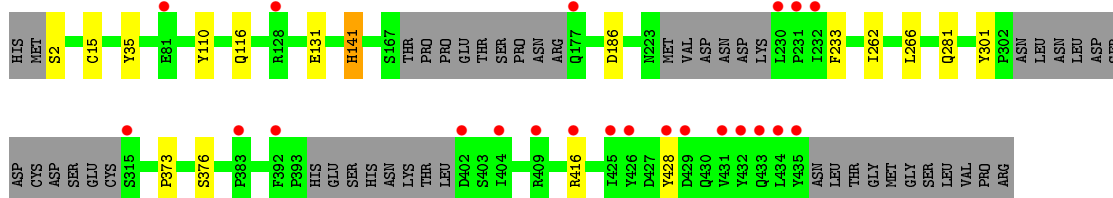
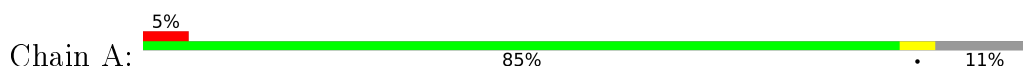
- Molecule 6 is water.

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

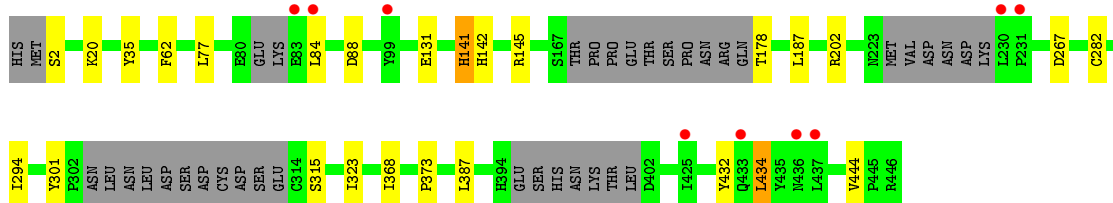
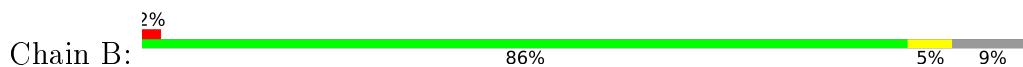
3 Residue-property plots [i](#)

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.

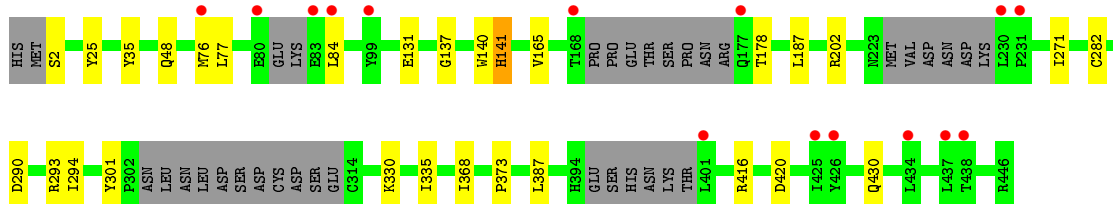
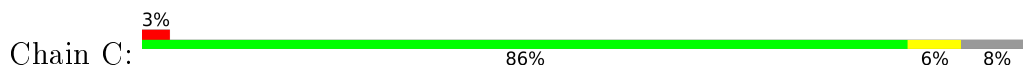
- Molecule 1: Histone deacetylase



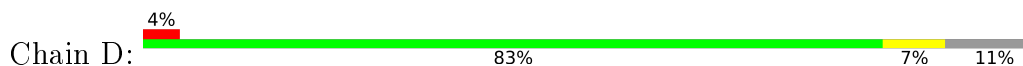
- Molecule 1: Histone deacetylase

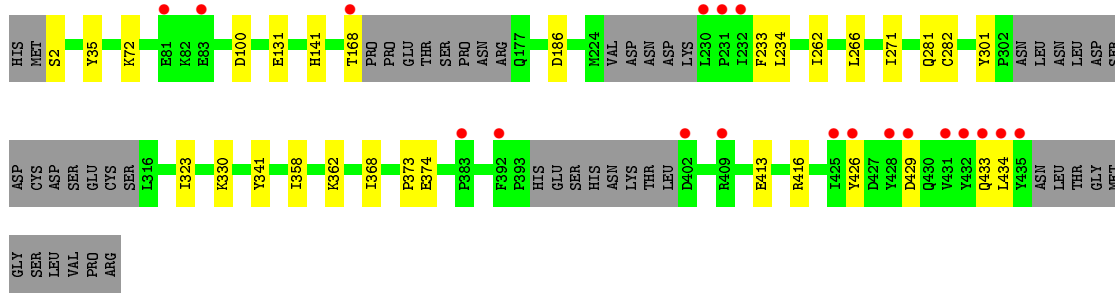


- Molecule 1: Histone deacetylase



- 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 46.51 – 1.55	Depositor EDS
% Data completeness (in resolution range)	90.2 (46.52-1.55) 90.2 (46.51-1.55)	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 0.169 , 0.194	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 , 50.8	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: ZN, 5IB, K, GOL

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	0.33	0/3377	0.52	0/4593
1	B	0.37	0/3413	0.55	1/4641 (0.0%)
1	C	0.36	0/3448	0.54	0/4688
1	D	0.34	0/3342	0.51	0/4546
All	All	0.35	0/13580	0.53	1/18468 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	434	LEU	CA-CB-CG	5.40	127.71	115.30

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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	0	0
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	0	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:D:330:LYS:NZ	6:D:608:HOH:O	2.36	0.57
1:B:187:LEU:HD21	1:B:294:ILE:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:330:LYS:NZ	6:C:609:HOH:O	2.41	0.53
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
4:A:505:GOL:O3	6:A:601:HOH:O	2.00	0.49
1:A:186:ASP:HB2	1:A:281:GLN:OE1	2.12	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:C:76:MET:HE2	1:C:77:LEU:HD23	1.97	0.46
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:413:GLU:HG3	1:D:416:ARG:NH2	2.35	0.42
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%)	355 (99%)	4 (1%)	73	51
1	B	363/392 (93%)	360 (99%)	3 (1%)	81	64
1	C	367/392 (94%)	364 (99%)	3 (1%)	81	64
1	D	354/392 (90%)	350 (99%)	4 (1%)	73	51
All	All	1443/1568 (92%)	1429 (99%)	14 (1%)	76	55

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	HIS
1	A	233	PHE
1	A	301	TYR
1	A	376	SER
1	B	141	HIS
1	B	301	TYR
1	B	315	SER
1	C	141	HIS
1	C	165	VAL
1	C	301	TYR
1	D	141	HIS
1	D	168	THR
1	D	233	PHE
1	D	301	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

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	27,31,31	0.70	0	34,44,44	0.95	2 (5%)
4	GOL	A	504	-	5,5,5	0.34	0	5,5,5	0.98	0
4	GOL	C	506	-	5,5,5	0.34	0	5,5,5	0.44	0
5	5IB	B	501	2	27,31,31	0.74	0	34,44,44	1.30	3 (8%)
4	GOL	A	505	-	5,5,5	0.46	0	5,5,5	0.78	0
4	GOL	A	506	-	5,5,5	0.39	0	5,5,5	0.48	0
5	5IB	C	501	2	27,31,31	0.73	0	34,44,44	1.28	3 (8%)
4	GOL	D	505	-	5,5,5	0.42	0	5,5,5	1.66	2 (40%)
5	5IB	A	507	2	27,31,31	0.71	1 (3%)	34,44,44	0.88	2 (5%)
4	GOL	C	505	-	5,5,5	0.62	0	5,5,5	0.93	0
4	GOL	B	505	-	5,5,5	0.32	0	5,5,5	0.59	0
4	GOL	D	506	-	5,5,5	0.34	0	5,5,5	0.41	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	-	3/16/16/16	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	504	-	-	2/4/4/4	-
4	GOL	C	506	-	-	1/4/4/4	-
5	5IB	B	501	2	-	2/16/16/16	0/4/4/4
4	GOL	A	505	-	-	2/4/4/4	-
4	GOL	A	506	-	-	3/4/4/4	-
5	5IB	C	501	2	-	2/16/16/16	0/4/4/4
4	GOL	D	505	-	-	3/4/4/4	-
5	5IB	A	507	2	-	0/16/16/16	0/4/4/4
4	GOL	C	505	-	-	4/4/4/4	-
4	GOL	B	505	-	-	2/4/4/4	-
4	GOL	D	506	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	507	5IB	C14-C19	-2.02	1.39	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	B	501	5IB	C7-N1-C8	4.47	139.19	126.93
5	C	501	5IB	C7-N1-C8	4.36	138.90	126.93
5	C	501	5IB	C1-C7-N1	3.75	123.39	116.66
5	B	501	5IB	C1-C7-N1	3.74	123.36	116.66
5	B	501	5IB	C15-C14-C19	-3.58	118.12	120.38
5	D	501	5IB	C15-C14-C19	-3.53	118.15	120.38
5	A	507	5IB	C15-C14-C19	-3.29	118.30	120.38
5	C	501	5IB	C15-C14-C19	-3.21	118.35	120.38
4	D	505	GOL	O2-C2-C3	2.75	121.23	109.12
5	D	501	5IB	C9-C8-N1	2.50	118.52	114.79
5	A	507	5IB	C9-C8-N1	2.29	118.22	114.79
4	D	505	GOL	O1-C1-C2	-2.28	99.29	110.20

There are no chirality outliers.

All (24) 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

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

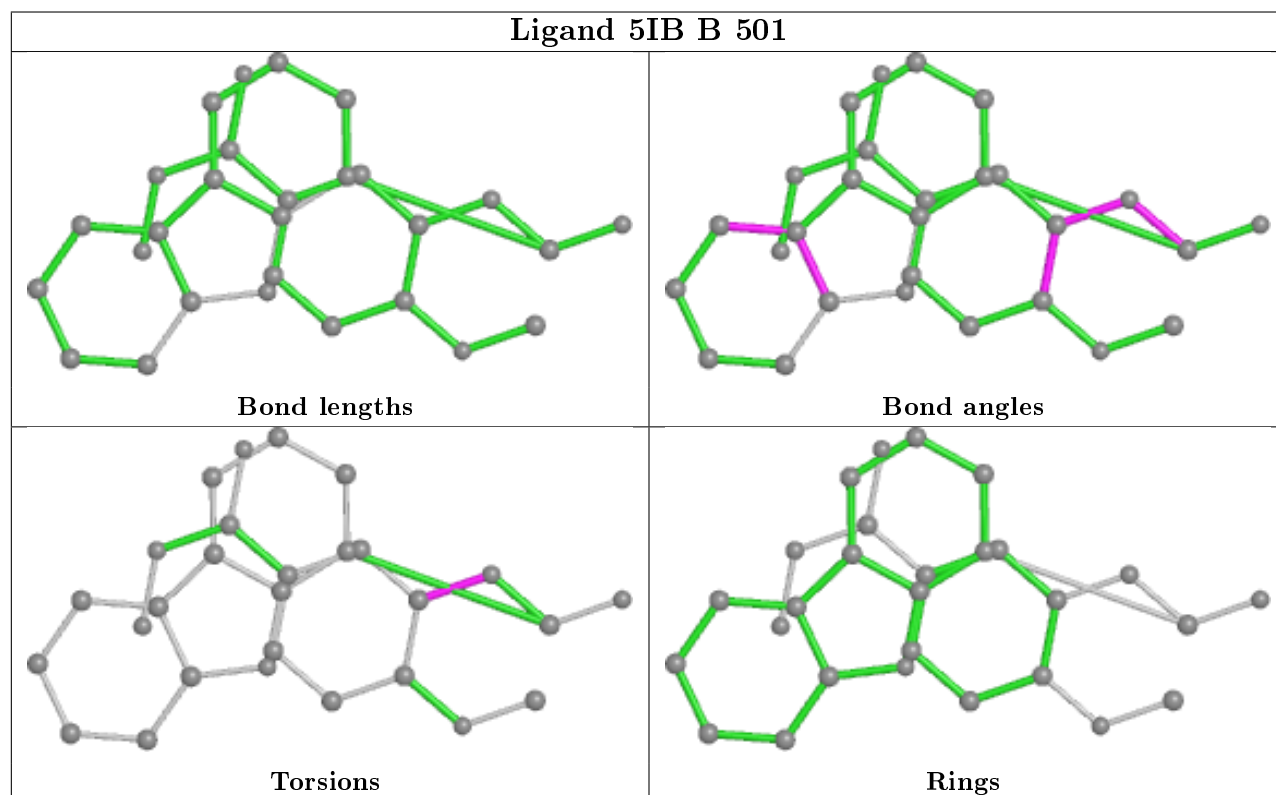
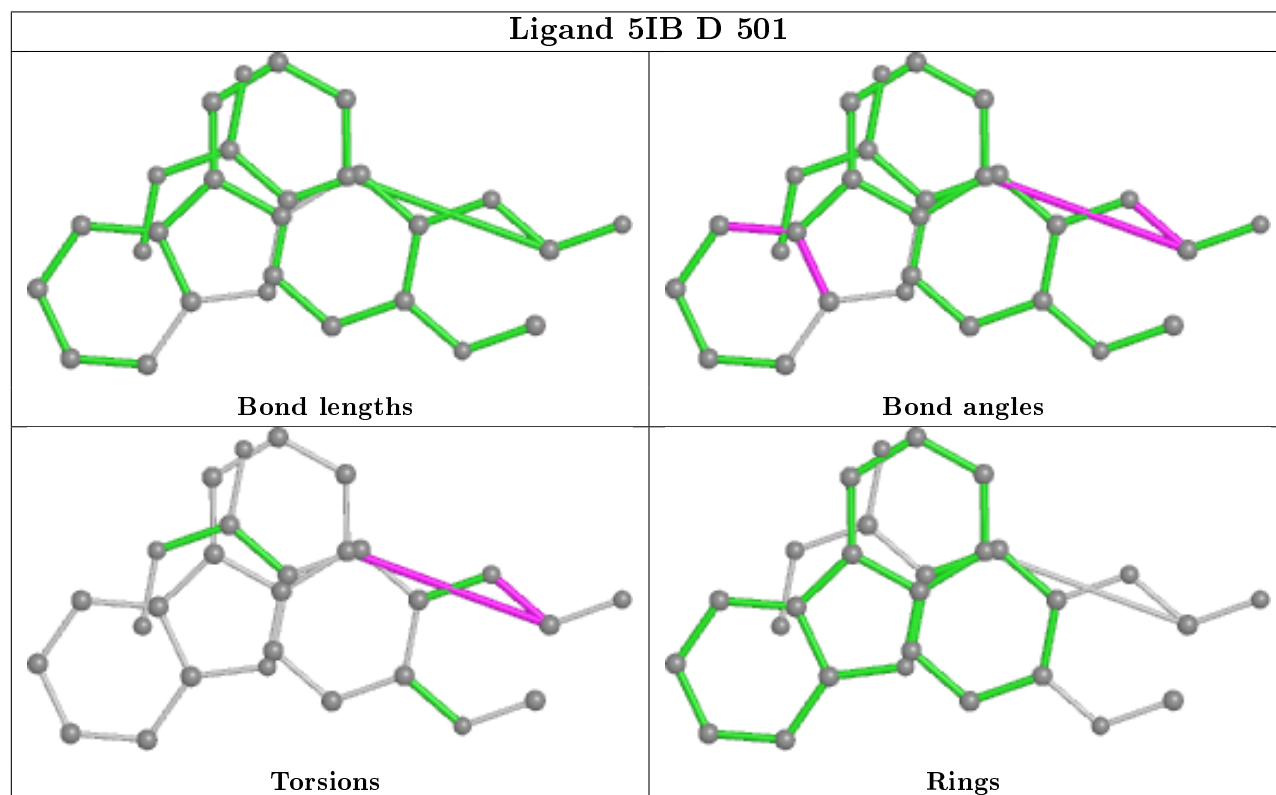
There are no ring outliers.

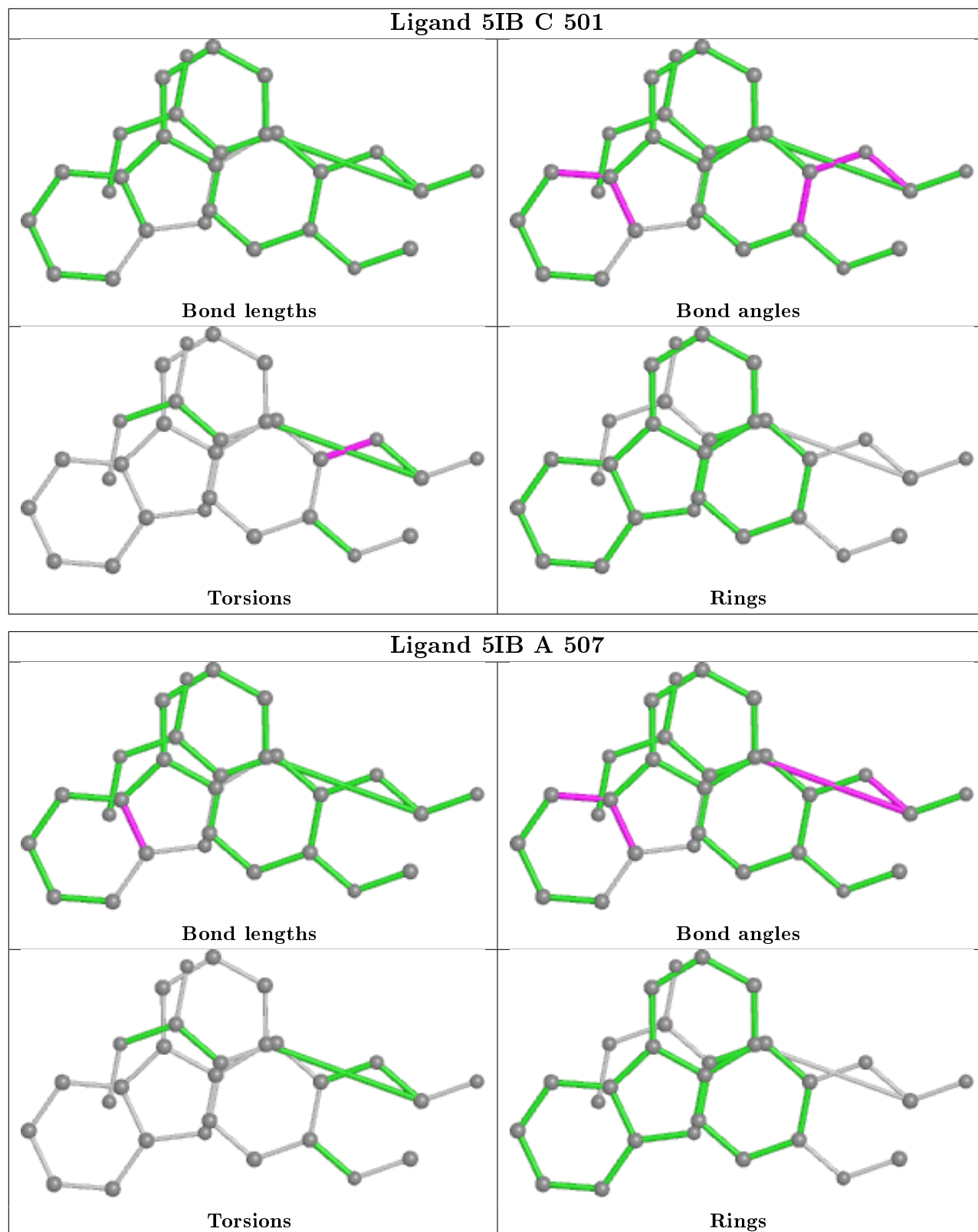
6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	501	5IB	1	0
5	B	501	5IB	3	0
4	A	505	GOL	3	0
4	A	506	GOL	3	0
4	D	505	GOL	1	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 [\(i\)](#)

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

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%)	0.06	22 (5%) 25 28	13, 21, 53, 82	0
1	B	409/447 (91%)	-0.06	9 (2%) 62 67	12, 18, 36, 87	0
1	C	412/447 (92%)	-0.03	15 (3%) 42 49	12, 19, 38, 93	0
1	D	400/447 (89%)	0.05	19 (4%) 30 34	14, 21, 51, 85	0
All	All	1620/1788 (90%)	0.01	65 (4%) 38 44	12, 20, 45, 93	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	432	TYR	10.4
1	D	425	ILE	9.8
1	A	425	ILE	9.7
1	D	428	TYR	9.5
1	D	432	TYR	9.3
1	D	426	TYR	8.6
1	A	426	TYR	8.0
1	A	434	LEU	7.8
1	A	428	TYR	7.2
1	A	230	LEU	7.1
1	A	392	PHE	6.8
1	B	230	LEU	6.8
1	C	230	LEU	6.1
1	D	392	PHE	6.0
1	C	83	GLU	5.8
1	D	435	TYR	5.8
1	A	435	TYR	5.7
1	D	230	LEU	5.6
1	D	168	THR	5.6
1	D	429	ASP	5.2
1	B	83	GLU	5.1

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Mol	Chain	Res	Type	RSRZ
1	D	434	LEU	5.1
1	A	433	GLN	4.5
1	A	429	ASP	4.5
1	C	425	ILE	4.4
1	A	231	PRO	3.9
1	C	168	THR	3.8
1	B	425	ILE	3.8
1	D	433	GLN	3.7
1	D	232	ILE	3.7
1	A	128	ARG	3.5
1	B	99	TYR	3.5
1	C	437	LEU	3.3
1	A	409	ARG	3.3
1	C	99	TYR	3.3
1	D	402	ASP	3.3
1	D	81	GLU	3.2
1	C	84	LEU	3.0
1	A	232	ILE	2.9
1	B	84	LEU	2.9
1	A	383	PRO	2.8
1	C	231	PRO	2.8
1	A	177	GLN	2.7
1	B	437	LEU	2.7
1	B	231	PRO	2.6
1	C	401	LEU	2.6
1	C	426	TYR	2.5
1	C	438	THR	2.5
1	C	177	GLN	2.5
1	D	409	ARG	2.5
1	A	404	ILE	2.4
1	C	80	GLU	2.4
1	D	431	VAL	2.3
1	A	81	GLU	2.3
1	A	402	ASP	2.3
1	A	416	ARG	2.3
1	B	436	ASN	2.2
1	D	83	GLU	2.2
1	A	315	SER	2.1
1	C	434	LEU	2.1
1	B	433	GLN	2.0
1	C	76	MET	2.0
1	D	383	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	431	VAL	2.0
1	D	231	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 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
5	5IB	C	501	28/28	0.68	0.26	34,69,77,78	0
5	5IB	D	501	28/28	0.69	0.27	36,74,80,89	0
5	5IB	A	507	28/28	0.73	0.33	36,101,127,128	0
5	5IB	B	501	28/28	0.76	0.26	23,55,63,70	0
4	GOL	A	506	6/6	0.87	0.16	31,38,43,47	0
4	GOL	A	504	6/6	0.89	0.12	23,27,33,38	0
4	GOL	C	506	6/6	0.89	0.10	23,28,29,30	0
4	GOL	A	505	6/6	0.90	0.24	23,31,40,50	0
4	GOL	D	505	6/6	0.90	0.11	19,29,30,31	0
4	GOL	D	506	6/6	0.91	0.12	36,37,40,47	0
4	GOL	C	505	6/6	0.92	0.17	22,25,36,36	0
4	GOL	B	505	6/6	0.92	0.10	19,27,33,36	0
2	ZN	A	501	1/1	1.00	0.05	17,17,17,17	0
2	ZN	B	502	1/1	1.00	0.05	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	0.05	17,17,17,17	0
3	K	A	502	1/1	1.00	0.06	16,16,16,16	0
3	K	A	503	1/1	1.00	0.08	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	0.09	17,17,17,17	0
3	K	C	503	1/1	1.00	0.07	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	K	C	504	1/1	1.00	0.09	18,18,18,18	0
3	K	D	503	1/1	1.00	0.07	16,16,16,16	0
3	K	D	504	1/1	1.00	0.09	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.