



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:11 PM UTC

PDB ID : 4CQF / pdb_00004cqf
Title : Crystal structure of Schistosoma mansoni HDAC8 complexed with a mercaptoacetamide inhibitor
Authors : Marek, M.; Romier, C.
Deposited on : 2014-02-14
Resolution : 2.30 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

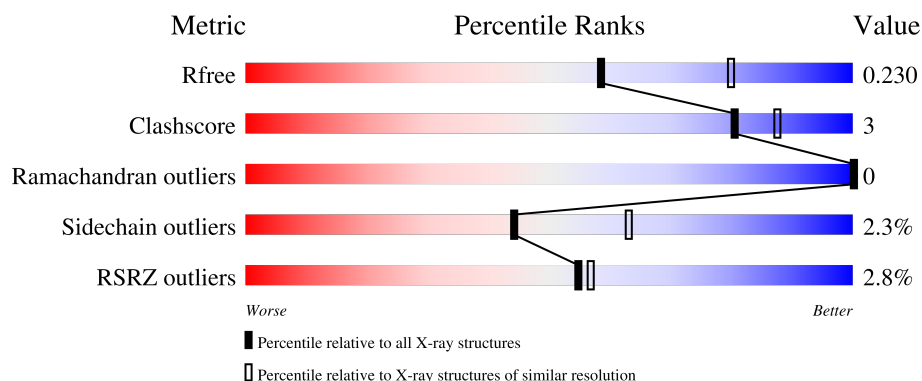
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	446	 3% 82% 7% 11%
1	B	446	 % 85% 7% 7%
1	C	446	 2% 85% 9% 7%
1	D	446	 3% 80% 10% 10%

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
6	GOL	C	902	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13648 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 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	0	0
			3187	2055	531	586	15			
1	B	413	Total	C	N	O	S	0	0	0
			3293	2120	552	605	16			
1	C	417	Total	C	N	O	S	0	1	0
			3331	2144	560	610	17			
1	D	400	Total	C	N	O	S	0	0	0
			3201	2063	534	590	14			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	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	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
D	441	GLY	-	expression tag	UNP A5H660
D	442	SER	-	expression tag	UNP A5H660
D	443	LEU	-	expression tag	UNP A5H660

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Chain	Residue	Modelled	Actual	Comment	Reference
D	444	VAL	-	expression tag	UNP A5H660
D	445	PRO	-	expression tag	UNP A5H660
D	446	ARG	-	expression tag	UNP A5H660

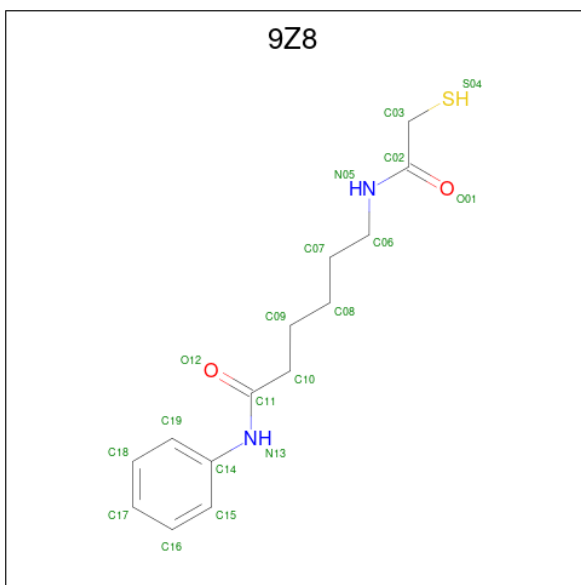
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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).

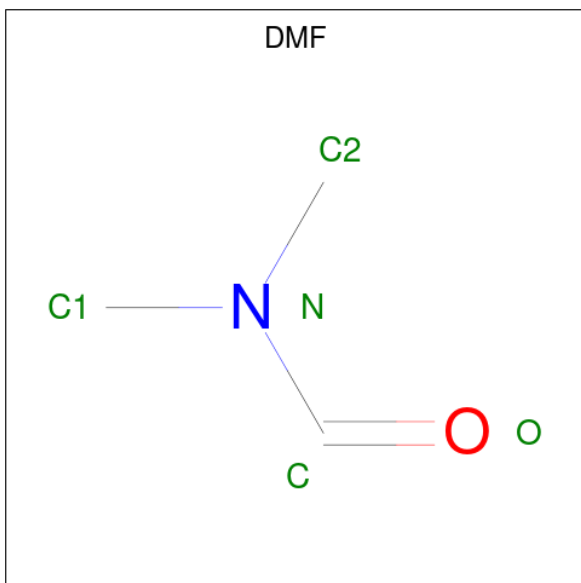
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total K 2 2	0	0
3	B	2	Total K 2 2	0	0
3	C	2	Total K 2 2	0	0
3	D	2	Total K 2 2	0	0

- Molecule 4 is 6-(2-Mercaptoacetyl-amino)-N-phenylhexanamide (CCD ID: 9Z8) (formula: C₁₄H₂₀N₂O₂S).



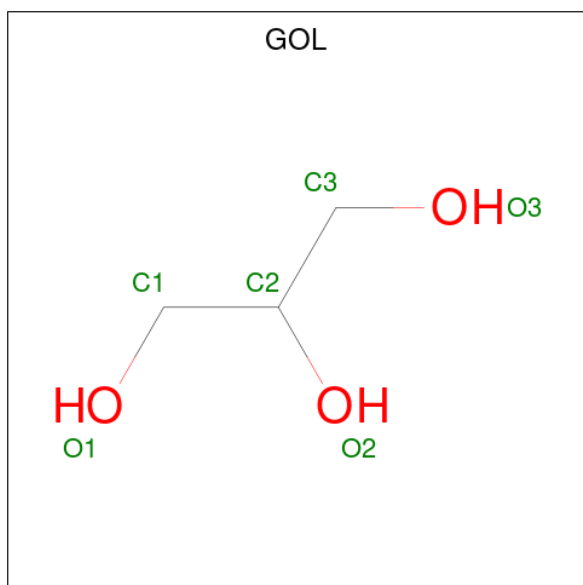
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			19	14	2	2	1		
4	B	1	Total	C	N	O	S	0	0
			19	14	2	2	1		
4	C	1	Total	C	N	O	S	0	0
			19	14	2	2	1		
4	D	1	Total	C	N	O	S	0	0
			19	14	2	2	1		

- Molecule 5 is DIMETHYLFORMAMIDE (CCD ID: DMF) (formula: C_3H_7NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			5	3	1	1		
5	A	1	Total	C	N	O	0	0
			5	3	1	1		
5	B	1	Total	C	N	O	0	0
			5	3	1	1		
5	B	1	Total	C	N	O	0	0
			5	3	1	1		
5	B	1	Total	C	N	O	0	0
			5	3	1	1		
5	C	1	Total	C	N	O	0	0
			5	3	1	1		
5	C	1	Total	C	N	O	0	0
			5	3	1	1		
5	C	1	Total	C	N	O	0	0
			5	3	1	1		
5	C	1	Total	C	N	O	0	0
			5	3	1	1		
5	D	1	Total	C	N	O	0	0
			5	3	1	1		
5	D	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

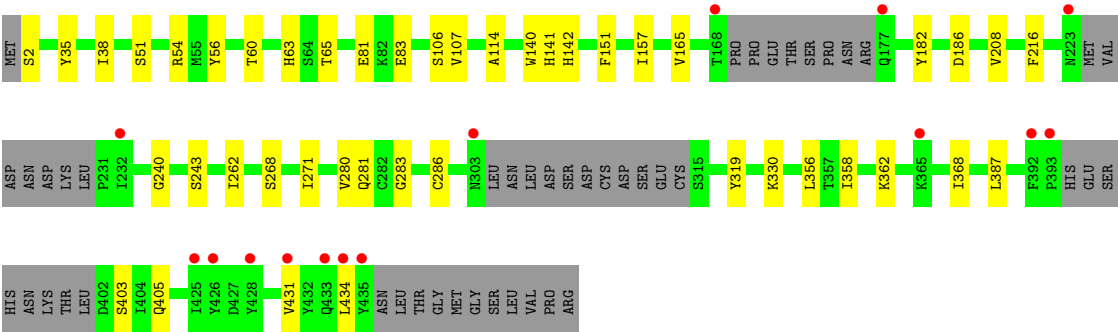
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	109	Total	O	0	0
			109	109		
7	B	116	Total	O	0	0
			116	116		
7	C	143	Total	O	0	0
			143	143		
7	D	83	Total	O	0	0
			83	83		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	70.78Å 70.81Å 98.02Å 77.79° 75.45° 85.40°	Depositor
Resolution (Å)	32.89 – 2.30 32.89 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (32.89-2.30) 99.7 (32.89-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.06 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.190 , 0.232 0.187 , 0.230	Depositor DCC
R_{free} test set	4059 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.149 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13648	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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, K, ZN, DMF, 9Z8

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	0.86	1/3276 (0.0%)	1.30	10/4454 (0.2%)
1	B	0.86	0/3384	1.30	9/4601 (0.2%)
1	C	0.87	1/3425 (0.0%)	1.28	8/4656 (0.2%)
1	D	0.86	1/3291 (0.0%)	1.32	7/4476 (0.2%)
All	All	0.86	3/13376 (0.0%)	1.30	34/18187 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	ILE	CA-CB	7.17	1.57	1.54
1	D	38	ILE	CA-CB	6.92	1.57	1.54
1	C	38	ILE	CA-CB	6.12	1.57	1.54

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	37	LEU	CA-C-N	6.34	126.52	120.43
1	C	37	LEU	C-N-CA	6.34	126.52	120.43
1	D	141	HIS	N-CA-C	6.30	120.06	112.38
1	A	141	HIS	N-CA-C	5.91	119.59	112.38
1	D	403	SER	N-CA-C	-5.79	104.56	111.69
1	C	141	HIS	N-CA-C	5.76	119.41	112.38
1	B	410	ARG	CA-C-N	5.64	127.78	120.56
1	B	410	ARG	C-N-CA	5.64	127.78	120.56
1	A	300	PHE	CA-CB-CG	5.64	119.44	113.80
1	D	107	VAL	N-CA-C	5.56	116.20	110.36
1	C	140	TRP	CA-C-N	5.55	129.48	120.60
1	C	140	TRP	C-N-CA	5.55	129.48	120.60
1	D	140	TRP	CA-C-N	5.47	129.35	120.60
1	D	140	TRP	C-N-CA	5.47	129.35	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	ILE	N-CA-C	5.43	116.92	111.00
1	D	114	ALA	CA-C-N	5.42	127.39	120.56
1	D	114	ALA	C-N-CA	5.42	127.39	120.56
1	A	140	TRP	CA-C-N	5.40	129.24	120.60
1	A	140	TRP	C-N-CA	5.40	129.24	120.60
1	B	197	PHE	CA-C-N	5.32	127.67	120.38
1	B	197	PHE	C-N-CA	5.32	127.67	120.38
1	A	114	ALA	CA-C-N	5.24	127.16	120.56
1	A	114	ALA	C-N-CA	5.24	127.16	120.56
1	B	272	VAL	N-CA-C	5.17	115.39	110.53
1	B	140	TRP	CA-C-N	5.17	129.35	120.72
1	B	140	TRP	C-N-CA	5.17	129.35	120.72
1	A	420	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	418	TYR	CA-C-N	5.14	127.12	120.44
1	A	418	TYR	C-N-CA	5.14	127.12	120.44
1	C	107	VAL	N-CA-C	5.14	115.76	110.36
1	B	61	ALA	N-CA-C	-5.06	106.36	112.54
1	B	141	HIS	N-CA-C	5.03	118.68	112.54
1	C	194	GLU	CA-C-N	5.02	126.96	120.44
1	C	194	GLU	C-N-CA	5.02	126.96	120.44

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3187	0	3077	11	0
1	B	3293	0	3185	13	0
1	C	3331	0	3233	22	0
1	D	3201	0	3090	24	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	19	0	19	1	0
4	B	19	0	19	1	0
4	C	19	0	19	2	0
4	D	19	0	19	3	0
5	A	10	0	14	1	0
5	B	15	0	21	1	0
5	C	20	0	28	0	0
5	D	10	0	14	1	0
6	B	12	0	16	0	0
6	C	18	0	24	5	0
6	D	12	0	16	1	0
7	A	109	0	0	0	0
7	B	116	0	0	0	0
7	C	143	0	0	0	0
7	D	83	0	0	0	0
All	All	13648	0	12794	68	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 (68) 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:B:368:ILE:HG21	1:B:387:LEU:CD2	1.99	0.92
1:C:21:PHE:HB3	6:C:900:GOL:H32	1.52	0.90
1:C:368:ILE:HG21	1:C:387:LEU:CD2	2.04	0.87
1:C:24:ARG:HB3	6:C:900:GOL:H31	1.59	0.83
1:B:368:ILE:HG21	1:B:387:LEU:HD22	1.66	0.78
1:D:54:ARG:HE	6:D:901:GOL:H31	1.50	0.76
1:C:368:ILE:HG21	1:C:387:LEU:HD22	1.72	0.69
1:C:368:ILE:CG2	1:C:387:LEU:HD22	2.22	0.69
1:B:368:ILE:CG2	1:B:387:LEU:HD22	2.22	0.69
1:D:368:ILE:HG21	1:D:387:LEU:CD2	2.23	0.69
1:C:368:ILE:CG2	1:C:387:LEU:CD2	2.72	0.67
1:B:368:ILE:CG2	1:B:387:LEU:CD2	2.73	0.66
1:C:224:MET:HG3	1:D:106:SER:HB3	1.78	0.64
1:D:56:TYR:HE2	1:D:65:THR:HG23	1.61	0.64
1:C:358:ILE:HG23	1:C:362:LYS:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:TYR:CE1	1:B:368:ILE:HG23	2.36	0.61
1:D:330:LYS:HD3	5:D:801:DMF:H13	1.82	0.59
1:D:56:TYR:CE2	1:D:65:THR:HG23	2.37	0.59
1:C:301:TYR:CD2	6:C:902:GOL:H2	2.39	0.58
1:D:186:ASP:HB2	1:D:281:GLN:OE1	2.03	0.57
1:D:368:ILE:CG2	1:D:387:LEU:HD22	2.36	0.55
1:A:186:ASP:HB2	1:A:281:GLN:OE1	2.07	0.55
1:C:186:ASP:HB2	1:C:281:GLN:OE1	2.08	0.54
1:C:50:ASP:HB2	1:C:54:ARG:HD3	1.90	0.53
1:B:186:ASP:HB2	1:B:281:GLN:OE1	2.09	0.52
1:B:151:PHE:HB3	5:B:800:DMF:H22	1.92	0.52
1:C:35:TYR:CE1	1:C:368:ILE:HG23	2.44	0.52
1:B:358:ILE:HG23	1:B:362:LYS:HD3	1.91	0.51
1:B:299:ASN:O	1:B:352:ARG:HD2	2.12	0.49
1:B:68:VAL:HG12	1:B:72:LYS:HE3	1.95	0.49
1:C:24:ARG:HD2	1:C:346:THR:HG21	1.95	0.49
1:A:142:HIS:CD2	4:A:700:9Z8:H032	2.48	0.48
1:D:60:THR:HA	1:D:63:HIS:O	2.13	0.48
1:B:142:HIS:CD2	4:B:700:9Z8:H032	2.49	0.48
1:C:368:ILE:HG21	1:C:387:LEU:HD21	1.91	0.48
1:D:368:ILE:HG21	1:D:387:LEU:HD22	1.91	0.48
1:B:267:ASP:HB3	1:B:434:LEU:HD11	1.96	0.47
1:D:358:ILE:HG23	1:D:362:LYS:HD3	1.97	0.47
1:A:151:PHE:HB3	5:A:800:DMF:H22	1.96	0.47
1:A:60:THR:HA	1:A:63:HIS:O	2.15	0.47
1:A:286:CYS:HB2	1:A:319:TYR:OH	2.15	0.46
1:A:292:HIS:HB3	1:A:294:ILE:HD12	1.98	0.46
1:C:294:ILE:HD11	1:D:51:SER:HA	1.97	0.46
1:D:208:VAL:HG11	1:D:262:ILE:HD12	1.97	0.46
1:A:157:ILE:HG21	1:A:182:TYR:CE1	2.51	0.46
1:D:368:ILE:CG2	1:D:387:LEU:CD2	2.91	0.46
1:A:334:LEU:HD22	1:A:336:LEU:HD21	1.99	0.45
1:A:249:LEU:HD13	1:A:253:ILE:HD13	1.97	0.45
1:C:216:PHE:CD1	4:C:700:9Z8:H071	2.52	0.44
1:D:268:SER:HB2	1:D:431:VAL:HG13	2.00	0.44
1:D:271:ILE:HD12	1:D:434:LEU:HD11	2.00	0.44
1:D:286:CYS:HB2	1:D:319:TYR:OH	2.19	0.43
1:D:35:TYR:CE1	1:D:368:ILE:HG23	2.53	0.43
1:D:157:ILE:HG21	1:D:182:TYR:CE1	2.54	0.43
1:C:24:ARG:HH21	6:C:900:GOL:H11	1.84	0.43
1:D:240:GLY:O	1:D:243:SER:OG	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:VAL:HG22	1:C:347:ALA:HA	2.01	0.42
1:D:216:PHE:CD1	4:D:700:9Z8:H062	2.54	0.42
1:D:151:PHE:CE2	4:D:700:9Z8:H071	2.55	0.42
1:A:204:VAL:HG21	1:A:273:ILE:HG12	2.01	0.42
1:C:253:ILE:HG22	1:C:295:PHE:CD1	2.55	0.42
1:A:35:TYR:CZ	1:A:373:PRO:HD3	2.56	0.41
1:D:142:HIS:CD2	4:D:700:9Z8:H032	2.55	0.41
1:D:186:ASP:OD2	1:D:283:GLY:HA3	2.20	0.41
1:C:178:THR:HB	1:C:202:ARG:HH21	1.85	0.41
1:B:178:THR:HB	1:B:202:ARG:HH21	1.86	0.40
1:C:142:HIS:CD2	4:C:700:9Z8:H032	2.56	0.40
1:C:366:MET:O	6:C:902:GOL:H31	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	388/446 (87%)	383 (99%)	5 (1%)	0	100	100
1	B	401/446 (90%)	391 (98%)	10 (2%)	0	100	100
1	C	406/446 (91%)	399 (98%)	7 (2%)	0	100	100
1	D	390/446 (87%)	382 (98%)	8 (2%)	0	100	100
All	All	1585/1784 (89%)	1555 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/391 (88%)	340 (99%)	5 (1%)	59	76
1	B	358/391 (92%)	348 (97%)	10 (3%)	38	56
1	C	363/391 (93%)	353 (97%)	10 (3%)	38	56
1	D	347/391 (89%)	340 (98%)	7 (2%)	48	67
All	All	1413/1564 (90%)	1381 (98%)	32 (2%)	44	63

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	233	PHE
1	A	262	ILE
1	A	334	LEU
1	A	433	GLN
1	B	13	GLN
1	B	72	LYS
1	B	84	LEU
1	B	165	VAL
1	B	200	SER
1	B	233	PHE
1	B	369	SER
1	B	371	GLU
1	B	404	ILE
1	B	430	GLN
1	C	20	LYS
1	C	84	LEU
1	C	165	VAL
1	C	177	GLN
1	C	224	MET
1	C	233	PHE
1	C	314	CYS
1	C	371	GLU
1	C	434	LEU
1	C	438	THR
1	D	2	SER
1	D	81	GLU
1	D	83	GLU

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Mol	Chain	Res	Type
1	D	165	VAL
1	D	280	VAL
1	D	356	LEU
1	D	405	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	292	HIS
1	B	10	GLN
1	B	33	ASN
1	B	155	ASN
1	B	270	ASN
1	C	33	ASN
1	D	33	ASN
1	D	155	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 12 are monoatomic - leaving 22 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	DMF	B	802	-	4,4,4	0.69	0	4,4,4	0.45	0
4	9Z8	D	700	2	19,19,19	1.72	3 (15%)	20,22,22	1.27	3 (15%)
5	DMF	A	801	-	4,4,4	0.73	0	4,4,4	0.41	0
5	DMF	C	801	-	4,4,4	0.73	0	4,4,4	0.28	0
5	DMF	C	803	-	4,4,4	0.70	0	4,4,4	0.27	0
6	GOL	C	902	-	5,5,5	0.54	0	5,5,5	2.20	3 (60%)
4	9Z8	A	700	2	19,19,19	1.79	3 (15%)	20,22,22	1.34	4 (20%)
6	GOL	D	901	-	5,5,5	0.90	0	5,5,5	1.62	1 (20%)
4	9Z8	B	700	2	19,19,19	1.71	3 (15%)	20,22,22	0.96	1 (5%)
6	GOL	B	901	-	5,5,5	0.77	0	5,5,5	1.60	1 (20%)
6	GOL	C	900	-	5,5,5	0.66	0	5,5,5	1.67	1 (20%)
5	DMF	D	801	-	4,4,4	0.71	0	4,4,4	0.34	0
5	DMF	A	800	-	4,4,4	0.75	0	4,4,4	0.55	0
5	DMF	C	802	-	4,4,4	0.74	0	4,4,4	0.43	0
5	DMF	B	800	-	4,4,4	0.73	0	4,4,4	0.72	0
6	GOL	B	902	-	5,5,5	0.79	0	5,5,5	1.61	1 (20%)
4	9Z8	C	700	2	19,19,19	1.76	3 (15%)	20,22,22	0.87	0
5	DMF	B	801	-	4,4,4	0.68	0	4,4,4	0.43	0
6	GOL	C	901	-	5,5,5	0.74	0	5,5,5	1.06	0
5	DMF	D	800	-	4,4,4	0.76	0	4,4,4	0.54	0
6	GOL	D	900	-	5,5,5	0.85	0	5,5,5	0.98	0
5	DMF	C	800	-	4,4,4	0.71	0	4,4,4	0.64	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	DMF	B	802	-	-	0/2/2/2	-
4	9Z8	D	700	2	-	7/13/15/15	0/1/1/1
5	DMF	A	801	-	-	0/2/2/2	-
5	DMF	C	801	-	-	0/2/2/2	-
5	DMF	C	803	-	-	0/2/2/2	-
6	GOL	C	902	-	-	4/4/4/4	-
4	9Z8	A	700	2	-	8/13/15/15	0/1/1/1
6	GOL	D	901	-	-	1/4/4/4	-
4	9Z8	B	700	2	-	0/13/15/15	0/1/1/1
6	GOL	B	901	-	-	1/4/4/4	-
6	GOL	C	900	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMF	D	801	-	-	0/2/2/2	-
5	DMF	A	800	-	-	0/2/2/2	-
5	DMF	C	802	-	-	0/2/2/2	-
5	DMF	B	800	-	-	0/2/2/2	-
6	GOL	B	902	-	-	4/4/4/4	-
4	9Z8	C	700	2	-	3/13/15/15	0/1/1/1
5	DMF	B	801	-	-	0/2/2/2	-
6	GOL	C	901	-	-	0/4/4/4	-
5	DMF	D	800	-	-	0/2/2/2	-
6	GOL	D	900	-	-	0/4/4/4	-
5	DMF	C	800	-	-	0/2/2/2	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	700	9Z8	C02-N05	4.51	1.44	1.33
4	D	700	9Z8	C02-N05	4.38	1.43	1.33
4	A	700	9Z8	C11-N13	4.34	1.44	1.35
4	D	700	9Z8	C11-N13	4.25	1.44	1.35
4	C	700	9Z8	C11-N13	4.13	1.44	1.35
4	C	700	9Z8	C02-N05	3.99	1.42	1.33
4	B	700	9Z8	C02-N05	3.97	1.42	1.33
4	B	700	9Z8	C11-N13	3.87	1.43	1.35
4	B	700	9Z8	C03-S04	-3.54	1.76	1.82
4	C	700	9Z8	C03-S04	-3.49	1.76	1.82
4	A	700	9Z8	C03-S04	-3.11	1.76	1.82
4	D	700	9Z8	C03-S04	-2.70	1.77	1.82

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	700	9Z8	C10-C11-N13	3.07	119.93	114.59
4	D	700	9Z8	C10-C11-N13	2.94	119.70	114.59
6	C	900	GOL	O3-C3-C2	2.76	122.82	110.38
6	C	902	GOL	O3-C3-C2	2.64	122.25	110.38
6	B	902	GOL	O2-C2-C1	2.47	119.39	109.18
6	C	902	GOL	O1-C1-C2	2.43	121.34	110.38
4	A	700	9Z8	C08-C07-C06	2.39	124.58	113.56
4	D	700	9Z8	O12-C11-C10	-2.37	117.73	122.02
4	D	700	9Z8	C09-C10-C11	2.29	119.55	113.19
4	A	700	9Z8	O12-C11-C10	-2.28	117.88	122.02
4	A	700	9Z8	C09-C10-C11	2.27	119.50	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	901	GOL	O1-C1-C2	2.24	120.47	110.38
6	C	902	GOL	O2-C2-C3	2.15	118.08	109.18
4	B	700	9Z8	C10-C11-N13	2.15	118.33	114.59
6	D	901	GOL	O3-C3-C2	2.07	119.70	110.38

There are no chirality outliers.

All (32) torsion outliers are listed below:

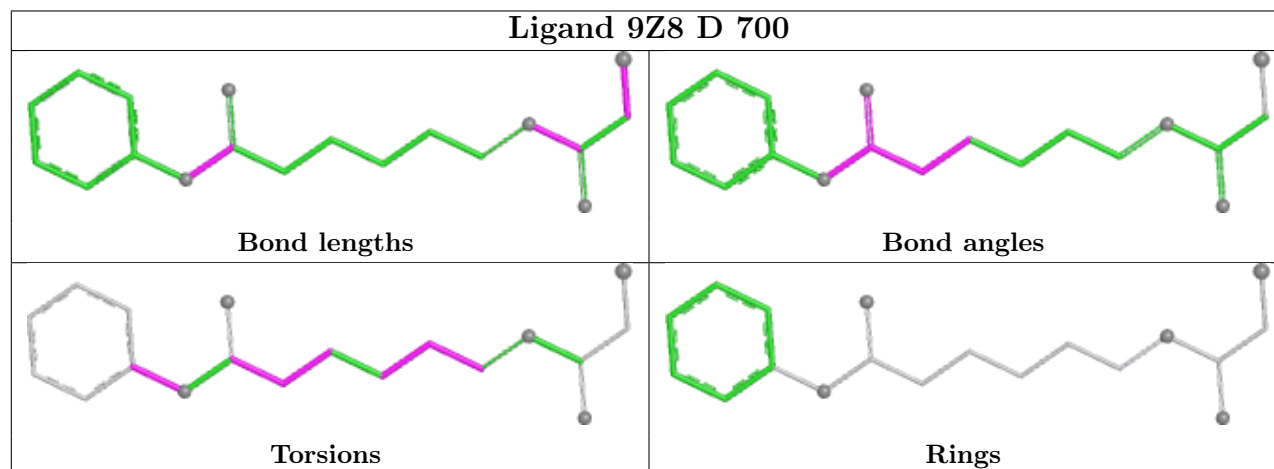
Mol	Chain	Res	Type	Atoms
6	B	902	GOL	O1-C1-C2-C3
6	B	902	GOL	O2-C2-C3-O3
6	C	900	GOL	C1-C2-C3-O3
6	C	902	GOL	C1-C2-C3-O3
4	C	700	9Z8	C08-C09-C10-C11
4	D	700	9Z8	C08-C09-C10-C11
4	C	700	9Z8	N05-C06-C07-C08
6	C	900	GOL	O2-C2-C3-O3
6	C	902	GOL	O2-C2-C3-O3
4	D	700	9Z8	N05-C06-C07-C08
4	A	700	9Z8	N05-C06-C07-C08
6	B	902	GOL	C1-C2-C3-O3
6	C	900	GOL	O1-C1-C2-C3
6	B	901	GOL	O2-C2-C3-O3
6	B	902	GOL	O1-C1-C2-O2
6	C	900	GOL	O1-C1-C2-O2
6	C	902	GOL	O1-C1-C2-O2
4	A	700	9Z8	C07-C08-C09-C10
4	A	700	9Z8	C09-C10-C11-O12
4	D	700	9Z8	C09-C10-C11-N13
4	D	700	9Z8	C09-C10-C11-O12
4	A	700	9Z8	C09-C10-C11-N13
4	D	700	9Z8	C06-C07-C08-C09
4	A	700	9Z8	C08-C09-C10-C11
4	A	700	9Z8	C06-C07-C08-C09
4	D	700	9Z8	C19-C14-N13-C11
4	D	700	9Z8	C15-C14-N13-C11
6	D	901	GOL	O2-C2-C3-O3
4	A	700	9Z8	C15-C14-N13-C11
4	A	700	9Z8	C19-C14-N13-C11
4	C	700	9Z8	C15-C14-N13-C11
6	C	902	GOL	O1-C1-C2-C3

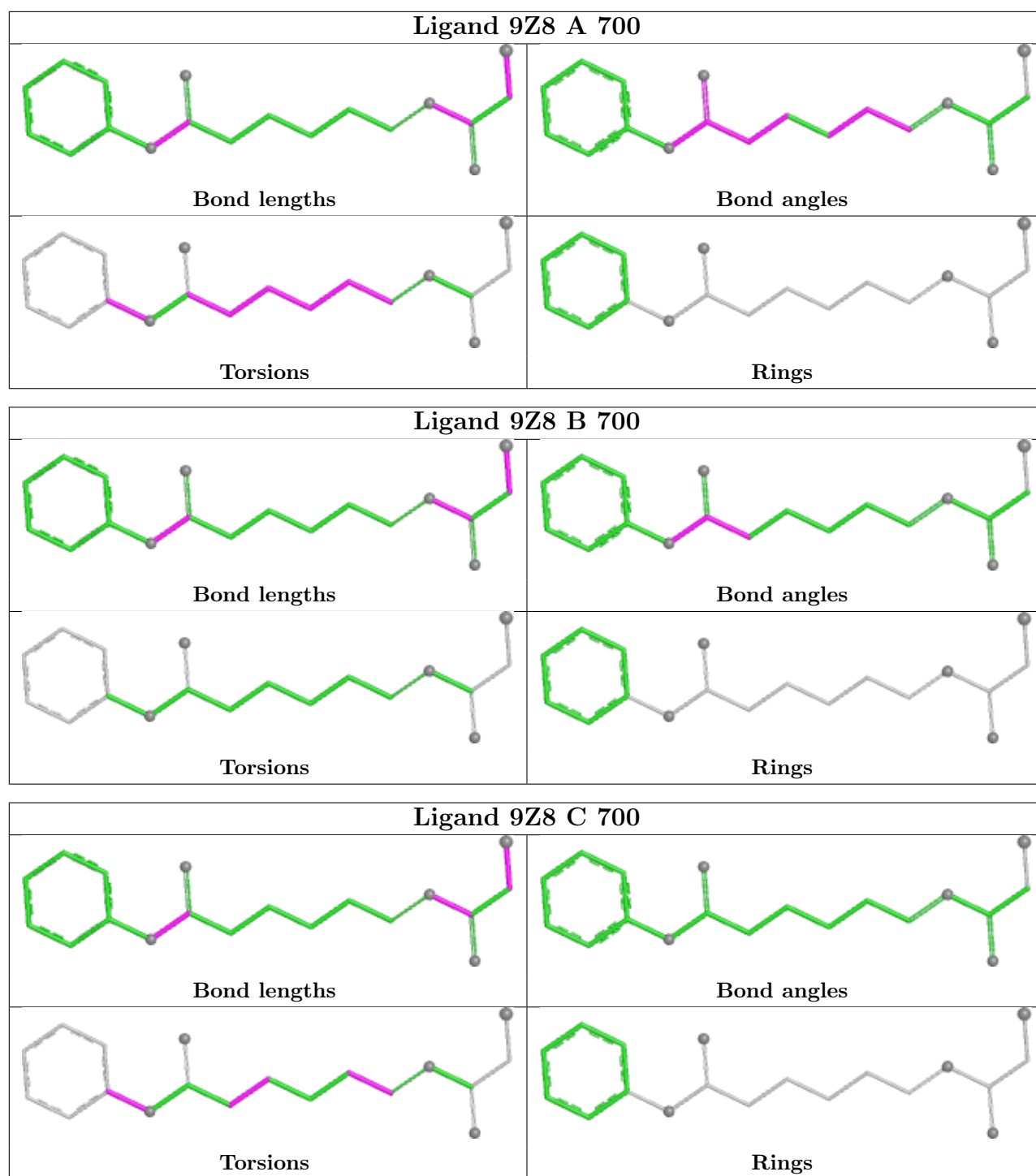
There are no ring outliers.

10 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	700	9Z8	3	0
6	C	902	GOL	2	0
4	A	700	9Z8	1	0
6	D	901	GOL	1	0
4	B	700	9Z8	1	0
6	C	900	GOL	3	0
5	D	801	DMF	1	0
5	A	800	DMF	1	0
5	B	800	DMF	1	0
4	C	700	9Z8	2	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 [i](#)

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	398/446 (89%)	-0.01	15 (3%) 44 46	15, 24, 53, 77	0
1	B	413/446 (92%)	-0.26	6 (1%) 72 73	12, 21, 41, 80	0
1	C	417/446 (93%)	-0.21	9 (2%) 62 64	10, 21, 42, 85	1 (0%)
1	D	400/446 (89%)	-0.04	15 (3%) 44 46	15, 24, 53, 91	0
All	All	1628/1784 (91%)	-0.13	45 (2%) 55 57	10, 22, 49, 91	1 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	168	THR	6.1
1	D	168	THR	4.9
1	A	224	MET	4.7
1	A	435	TYR	4.5
1	D	393	PRO	4.4
1	D	428	TYR	4.4
1	A	425	ILE	4.3
1	A	426	TYR	4.2
1	D	303	ASN	4.0
1	A	315	SER	3.7
1	C	76	MET	3.5
1	D	435	TYR	3.5
1	D	425	ILE	3.4
1	D	392	PHE	3.4
1	A	428	TYR	3.4
1	D	426	TYR	3.4
1	C	224	MET	3.3
1	D	434	LEU	3.3
1	C	303	ASN	3.3
1	A	223	ASN	3.2
1	A	392	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	232	ILE	3.2
1	A	432	TYR	3.1
1	A	232	ILE	3.0
1	D	365	LYS	2.9
1	A	302	PRO	2.9
1	A	393	PRO	2.8
1	B	438	THR	2.7
1	C	401	LEU	2.7
1	B	230	LEU	2.6
1	D	431	VAL	2.6
1	A	434	LEU	2.5
1	B	229	LYS	2.5
1	C	230	LEU	2.5
1	C	312	SER	2.5
1	A	430	GLN	2.4
1	A	177	GLN	2.3
1	D	433	GLN	2.3
1	B	223	ASN	2.2
1	B	302	PRO	2.2
1	D	177	GLN	2.1
1	D	223	ASN	2.1
1	B	313	GLU	2.1
1	C	438	THR	2.0
1	C	80	GLU	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](#)

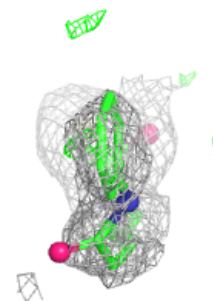
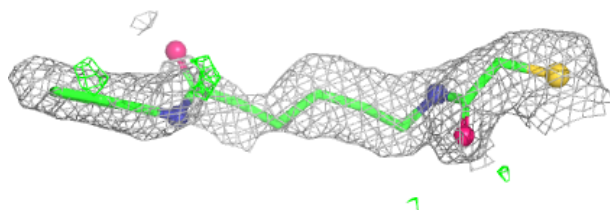
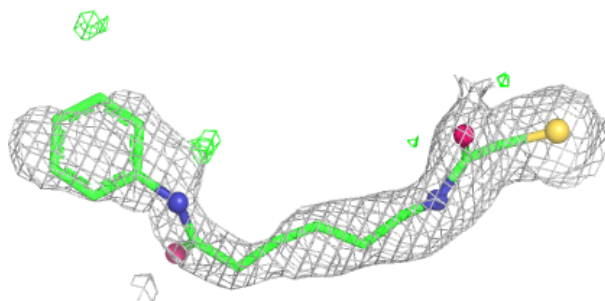
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GOL	C	902	6/6	0.74	0.20	32,36,38,39	0
5	DMF	D	801	5/5	0.78	0.16	38,38,40,42	0
6	GOL	B	901	6/6	0.79	0.21	39,48,48,51	0
5	DMF	C	800	5/5	0.79	0.17	31,36,38,42	0
6	GOL	D	901	6/6	0.79	0.18	48,52,54,56	0
5	DMF	B	801	5/5	0.85	0.14	29,29,33,37	0
5	DMF	C	803	5/5	0.85	0.13	35,36,39,42	0
5	DMF	A	801	5/5	0.86	0.12	36,39,43,44	0
5	DMF	D	800	5/5	0.86	0.15	32,36,39,43	0
5	DMF	B	800	5/5	0.86	0.14	31,35,37,38	0
5	DMF	C	801	5/5	0.89	0.13	37,41,42,44	0
5	DMF	C	802	5/5	0.89	0.16	31,34,38,40	0
6	GOL	C	900	6/6	0.90	0.16	22,34,36,38	0
5	DMF	A	800	5/5	0.90	0.13	37,40,41,42	0
6	GOL	B	902	6/6	0.90	0.11	25,31,33,34	0
5	DMF	B	802	5/5	0.91	0.13	28,32,34,34	0
4	9Z8	A	700	19/19	0.91	0.16	27,44,59,59	0
4	9Z8	D	700	19/19	0.92	0.16	26,53,66,66	0
6	GOL	C	901	6/6	0.92	0.09	17,28,30,31	0
4	9Z8	B	700	19/19	0.93	0.14	21,45,53,55	0
6	GOL	D	900	6/6	0.95	0.09	24,30,32,33	0
4	9Z8	C	700	19/19	0.95	0.12	20,43,55,56	0
3	K	C	601	1/1	0.98	0.05	24,24,24,24	0
3	K	D	600	1/1	0.99	0.02	27,27,27,27	0
3	K	D	601	1/1	0.99	0.02	16,16,16,16	0
2	ZN	C	500	1/1	0.99	0.02	24,24,24,24	0
3	K	A	600	1/1	0.99	0.02	23,23,23,23	0
3	K	A	601	1/1	0.99	0.02	18,18,18,18	0
3	K	B	600	1/1	0.99	0.03	23,23,23,23	0
3	K	B	601	1/1	0.99	0.03	16,16,16,16	0
2	ZN	B	500	1/1	0.99	0.01	24,24,24,24	0
2	ZN	D	500	1/1	1.00	0.02	25,25,25,25	0
3	K	C	600	1/1	1.00	0.02	13,13,13,13	0
2	ZN	A	500	1/1	1.00	0.01	28,28,28,28	0

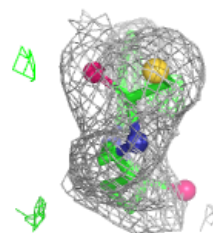
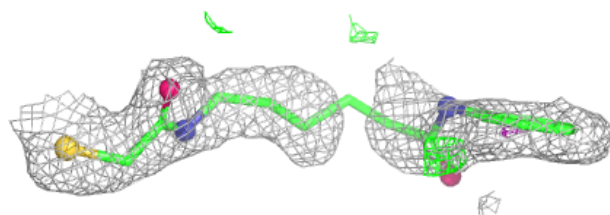
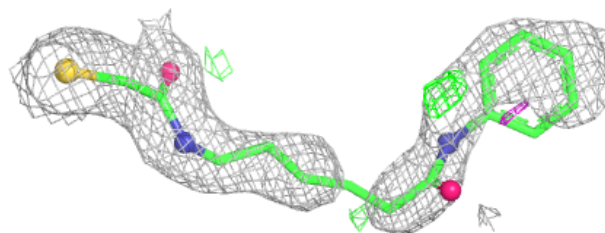
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 9Z8 A 700:

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

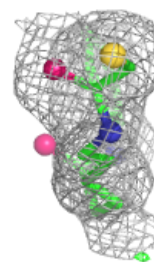
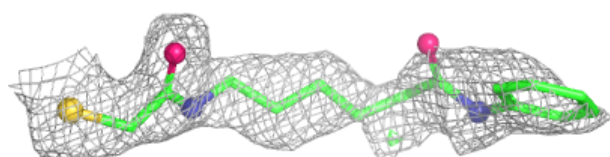
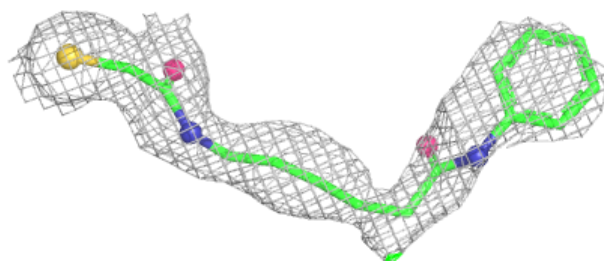
**Electron density around 9Z8 D 700:**

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

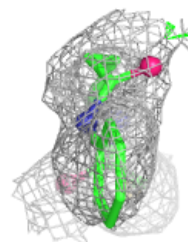
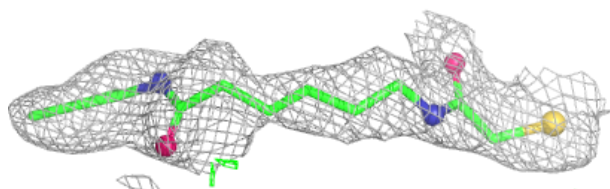
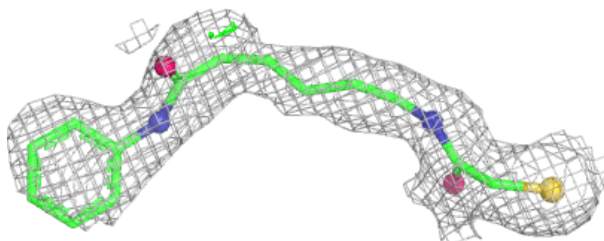


Electron density around 9Z8 B 700:

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

**Electron density around 9Z8 C 700:**

$2mF_o-DF_c$ (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.