



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:24 PM UTC

PDB ID : 6HSH / pdb_00006hsh
Title : Crystal structure of Schistosoma mansoni HDAC8 complexed with Quisinostat
Authors : Shaik, T.B.; Marek, M.; Romier, C.
Deposited on : 2018-10-01
Resolution : 1.54 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

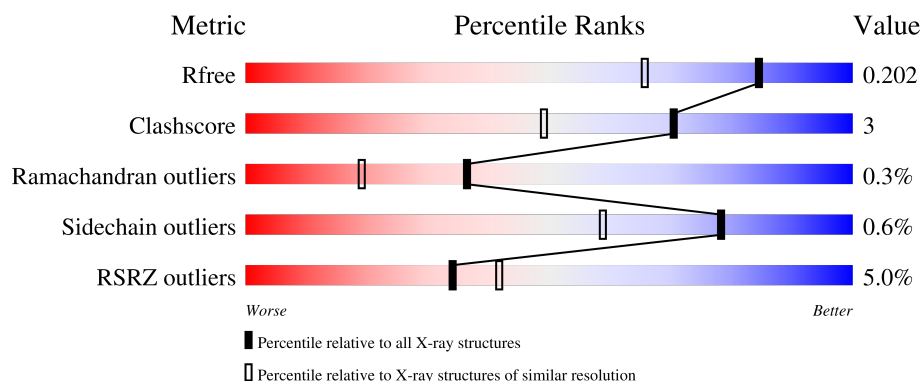
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

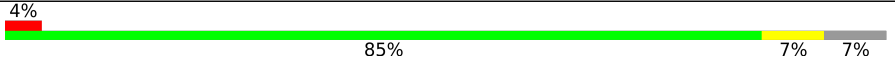
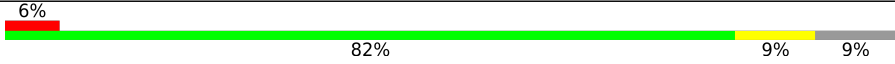
The reported resolution of this entry is 1.54 Å.

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	
1	B	447	
1	C	447	
1	D	447	

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
5	DMF	A	510	-	-	X	-
5	DMF	C	507	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14595 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	404	Total	C	N	O	S	0	4	0
			3247	2089	542	599	17			
1	B	410	Total	C	N	O	S	0	6	0
			3300	2128	550	605	17			
1	C	415	Total	C	N	O	S	0	3	0
			3319	2139	553	610	17			
1	D	405	Total	C	N	O	S	0	5	0
			3258	2104	540	596	18			

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).

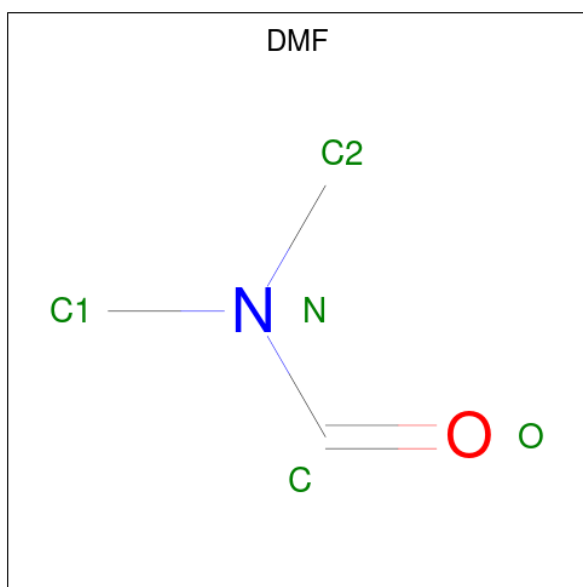
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- 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 2-[4-[[[(1-methylindol-3-yl)methylamino]methyl]piperidin-1-yl]- {N}-oxidanyl-pyrimidine-5-carboxamide (CCD ID: GOK) (formula: C₂₁H₂₆N₆O₂).





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	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	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	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		

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

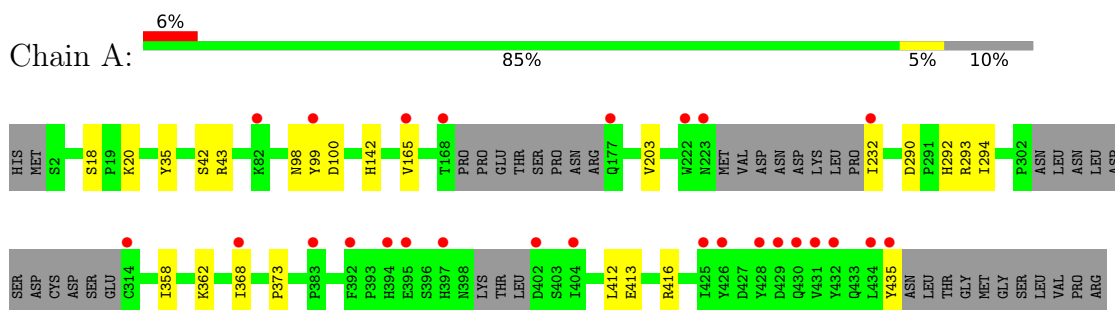
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	272	Total	O	0	0
			272	272		
7	B	304	Total	O	0	0
			304	304		
7	C	291	Total	O	0	0
			291	291		
7	D	235	Total	O	0	0
			235	235		

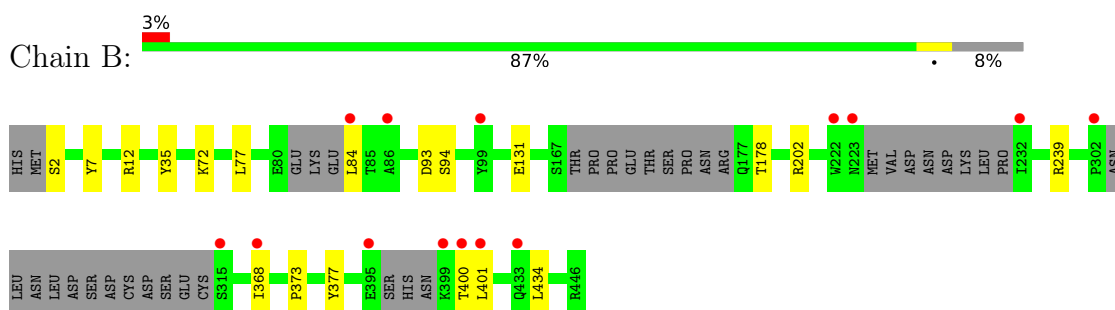
3 Residue-property plots [i](#)

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.

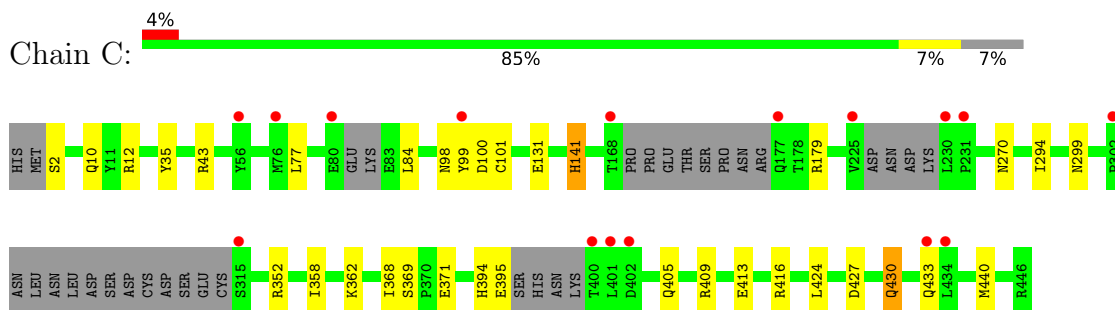
• Molecule 1: Histone deacetylase



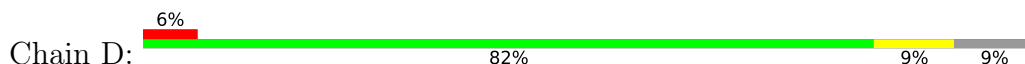
• Molecule 1: Histone deacetylase

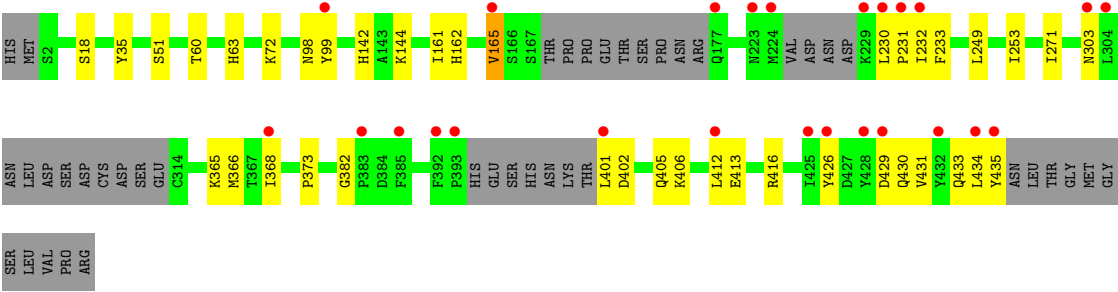


• Molecule 1: Histone deacetylase



• 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	70.75Å 70.80Å 97.82Å 78.03° 75.67° 85.74°	Depositor
Resolution (Å)	46.47 – 1.54 46.47 – 1.54	Depositor EDS
% Data completeness (in resolution range)	82.8 (46.47-1.54) 82.8 (46.47-1.54)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 1.55Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.168 , 0.202 0.169 , 0.202	Depositor DCC
R_{free} test set	10917 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.095 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14595	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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: K, ZN, GOK, GOL, DMF

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	0.32	0/3350	0.51	0/4556
1	B	0.36	0/3406	0.54	0/4631
1	C	0.34	0/3419	0.52	0/4651
1	D	0.32	0/3363	0.50	0/4573
All	All	0.34	0/13538	0.52	0/18411

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	3247	0	3131	16	0
1	B	3300	0	3203	18	0
1	C	3319	0	3221	30	0
1	D	3258	0	3172	27	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	29	0	0	2	0
4	B	58	0	0	1	0
4	C	58	0	0	1	0
4	D	29	0	0	1	0
5	A	30	0	42	5	0
5	B	30	0	40	2	0
5	C	45	0	63	8	0
5	D	30	0	42	2	0
6	A	6	0	8	0	0
6	B	12	0	15	3	0
6	C	18	0	24	3	0
6	D	12	0	16	0	0
7	A	272	0	0	1	0
7	B	304	0	0	1	0
7	C	291	0	0	2	1
7	D	235	0	0	4	1
All	All	14595	0	12977	90	1

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 (90) 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:12:ARG:HH21	6:B:513:GOL:H31	1.42	0.84
1:A:42:SER:HA	5:A:510:DMF:H13	1.61	0.82
1:C:43:ARG:HE	5:C:508:DMF:H12	1.49	0.77
1:D:429:ASP:OD1	1:D:430:GLN:N	2.21	0.74
1:A:98:ASN:OD1	7:A:601:HOH:O	2.10	0.69
1:D:144:LYS:NZ	7:D:601:HOH:O	2.10	0.69
1:C:43:ARG:HE	5:C:508:DMF:C1	2.07	0.68
1:B:2:SER:N	1:B:131:GLU:OE2	2.29	0.66
1:C:12:ARG:HH21	5:C:507:DMF:H23	1.60	0.66
1:C:369:SER:OG	1:C:371:GLU:OE1	2.15	0.65
5:A:510:DMF:H12	1:B:93:ASP:HB2	1.79	0.64
1:B:178:THR:HB	1:B:202:ARG:HH21	1.63	0.62
1:A:290:ASP:O	1:A:293:ARG:HG2	2.00	0.62
1:C:2:SER:N	1:C:131:GLU:OE2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:ARG:HH21	6:B:513:GOL:C3	2.14	0.61
1:C:294:ILE:HD11	1:D:51:SER:HB2	1.83	0.60
1:C:12:ARG:HE	5:C:507:DMF:H12	1.65	0.60
1:D:429:ASP:O	1:D:433:GLN:HG2	2.01	0.60
1:D:98:ASN:OD1	7:D:602:HOH:O	2.17	0.59
1:A:413:GLU:HG3	1:A:416:ARG:HH21	1.67	0.58
1:C:35:TYR:CE1	1:C:368:ILE:HG23	2.39	0.57
1:D:413:GLU:HG3	1:D:416:ARG:HH21	1.71	0.56
1:C:413:GLU:OE1	1:C:416:ARG:NH2	2.39	0.55
1:D:18:SER:HB2	5:D:505:DMF:H11	1.87	0.55
1:C:35:TYR:CD1	1:C:368:ILE:HG23	2.44	0.52
6:C:515:GOL:O3	7:C:601:HOH:O	2.19	0.52
1:D:35:TYR:CD1	1:D:368:ILE:HG23	2.45	0.51
1:B:35:TYR:CD1	1:B:368:ILE:HG23	2.45	0.51
1:C:294:ILE:HD11	1:D:51:SER:CB	2.40	0.51
1:A:43:ARG:H	5:A:510:DMF:H22	1.76	0.50
1:B:77:LEU:HD13	1:B:84:LEU:HG	1.93	0.50
1:D:72:LYS:NZ	7:D:607:HOH:O	2.39	0.50
1:C:98:ASN:O	1:C:100:ASP:N	2.44	0.50
1:B:131:GLU:OE1	4:B:505:GOK:N29	2.44	0.50
1:A:35:TYR:CE1	1:A:368:ILE:HG23	2.47	0.50
1:B:7[B]:TYR:CD2	5:B:507:DMF:H13	2.47	0.50
1:B:377:TYR:OH	6:B:513:GOL:H32	2.11	0.50
1:B:7[A]:TYR:CD1	5:B:507:DMF:H13	2.47	0.49
5:A:510:DMF:H23	1:B:94:SER:HA	1.94	0.49
1:B:35:TYR:CE1	1:B:368:ILE:HG23	2.48	0.48
1:C:433:GLN:OE1	7:C:602:HOH:O	2.19	0.48
1:C:43:ARG:NE	5:C:508:DMF:H12	2.25	0.48
1:B:239:ARG:NH1	7:B:602:HOH:O	2.23	0.47
1:C:179:ARG:NH2	1:C:424:LEU:HD21	2.29	0.47
1:D:35:TYR:CZ	1:D:373:PRO:HD3	2.50	0.47
1:D:162:HIS:CD2	5:D:510:DMF:H23	2.50	0.47
1:D:412:LEU:HD11	1:D:431:VAL:HG12	1.98	0.46
1:C:409:ARG:HH21	5:C:511:DMF:H12	1.80	0.46
1:D:401:LEU:HD12	1:D:405:GLN:HG3	1.97	0.46
1:D:412:LEU:HD13	1:D:435:TYR:CE1	2.51	0.46
1:C:405:GLN:HG2	1:C:440:MET:HE3	1.98	0.46
1:B:7[B]:TYR:OH	1:B:12:ARG:HD2	2.16	0.46
1:C:270:ASN:OD1	6:C:516:GOL:H31	2.15	0.46
1:D:271:ILE:HD12	1:D:434:LEU:HD11	1.98	0.46
1:C:427:ASP:CG	1:C:430:GLN:HB2	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:GLU:CD	1:C:416:ARG:HH21	2.23	0.45
1:C:141:HIS:CD2	1:C:141:HIS:H	2.34	0.45
1:A:18:SER:HB2	5:A:506:DMF:H11	1.99	0.45
1:B:35:TYR:CZ	1:B:373:PRO:HD3	2.52	0.44
1:C:12:ARG:NE	5:C:507:DMF:H12	2.32	0.44
1:C:299:ASN:O	1:C:352:ARG:HD2	2.18	0.44
1:D:161:ILE:O	1:D:165:VAL:HG22	2.17	0.44
1:C:10:GLN:HB3	6:C:515:GOL:H12	1.99	0.44
1:D:230:LEU:HG	1:D:231:PRO:HD2	2.00	0.44
1:C:12:ARG:NH2	5:C:507:DMF:H23	2.32	0.43
1:C:100:ASP:OD1	4:C:505:GOK:N29	2.52	0.43
1:D:249:LEU:HD13	1:D:253:ILE:HD13	2.00	0.43
1:D:402:ASP:O	1:D:406:LYS:HG3	2.19	0.43
1:A:142:HIS:NE2	4:A:504:GOK:N1	2.68	0.42
1:C:98:ASN:O	1:C:101:CYS:N	2.46	0.42
1:A:165:VAL:HG11	1:A:203:VAL:CG2	2.49	0.42
1:D:429:ASP:CG	1:D:430:GLN:N	2.76	0.42
1:A:35:TYR:CD1	1:A:368:ILE:HG23	2.54	0.42
1:D:142:HIS:NE2	4:D:504:GOK:N1	2.67	0.42
1:A:35:TYR:CZ	1:A:373:PRO:HD3	2.55	0.42
1:A:412:LEU:HD21	1:A:435:TYR:CE1	2.55	0.42
1:C:394:HIS:O	1:C:395:GLU:HG2	2.19	0.41
1:B:178:THR:HB	1:B:202:ARG:NH2	2.34	0.41
1:D:35:TYR:CE1	1:D:368:ILE:HG23	2.55	0.41
1:A:292:HIS:HB3	1:A:294:ILE:HG12	2.02	0.41
1:A:100:ASP:OD1	4:A:504:GOK:N29	2.54	0.41
1:B:400:THR:HG23	1:B:401:LEU:HG	2.03	0.41
1:D:365:LYS:O	1:D:366:MET:HE2	2.21	0.41
1:C:77:LEU:HD13	1:C:84:LEU:HG	2.03	0.41
1:A:358:ILE:HG23	1:A:362:LYS:HE2	2.02	0.40
1:D:416:ARG:HG3	1:D:426:TYR:OH	2.21	0.40
1:C:358:ILE:HG23	1:C:362:LYS:HD3	2.03	0.40
1:D:382:GLY:O	7:D:603:HOH:O	2.22	0.40
1:A:98:ASN:O	1:A:100:ASP:N	2.55	0.40
1:D:60:THR:HA	1:D:63:HIS:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:861:HOH:O	7:D:681:HOH:O[1_545]	2.18	0.02

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	398/447 (89%)	392 (98%)	5 (1%)	1 (0%)	36	19
1	B	404/447 (90%)	398 (98%)	6 (2%)	0	100	100
1	C	406/447 (91%)	402 (99%)	3 (1%)	1 (0%)	43	25
1	D	400/447 (90%)	395 (99%)	3 (1%)	2 (0%)	24	8
All	All	1608/1788 (90%)	1587 (99%)	17 (1%)	4 (0%)	36	25

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	99	TYR
1	A	99	TYR
1	D	99	TYR
1	D	303	ASN

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	355/392 (91%)	353 (99%)	2 (1%)	78	59
1	B	361/392 (92%)	359 (99%)	2 (1%)	78	59
1	C	363/392 (93%)	361 (99%)	2 (1%)	78	59
1	D	357/392 (91%)	354 (99%)	3 (1%)	73	51
All	All	1436/1568 (92%)	1427 (99%)	9 (1%)	78	59

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	232	ILE
1	B	72	LYS
1	B	434	LEU
1	C	141	HIS
1	C	430	GLN
1	D	165	VAL
1	D	232	ILE
1	D	233	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	394	HIS
1	B	177	GLN
1	B	430	GLN
1	C	129	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 53 ligands modelled in this entry, 12 are monoatomic - leaving 41 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	A	510	-	4,4,4	0.30	0	4,4,4	0.31	0
5	DMF	D	510	-	4,4,4	0.30	0	4,4,4	0.44	0
5	DMF	A	511	-	4,4,4	0.31	0	4,4,4	0.33	0
4	GOK	C	505	2	32,32,32	0.24	0	42,44,44	0.51	0
6	GOL	D	511	-	5,5,5	0.38	0	5,5,5	0.34	0
6	GOL	A	509	-	5,5,5	0.32	0	5,5,5	0.31	0
5	DMF	C	511	-	4,4,4	0.38	0	4,4,4	0.52	0
6	GOL	D	512	-	5,5,5	0.31	0	5,5,5	0.54	0
4	GOK	D	504	2	32,32,32	0.23	0	42,44,44	0.49	0
5	DMF	B	506	-	4,4,4	0.34	0	4,4,4	0.43	0
5	DMF	B	509	-	4,4,4	0.38	0	4,4,4	0.46	0
5	DMF	A	506	-	4,4,4	0.34	0	4,4,4	0.46	0
5	DMF	C	509	-	4,4,4	0.37	0	4,4,4	0.39	0
5	DMF	C	508	-	4,4,4	0.33	0	4,4,4	0.60	0
6	GOL	C	517	-	5,5,5	0.40	0	5,5,5	0.27	0
5	DMF	B	508	-	4,4,4	0.35	0	4,4,4	0.37	0
6	GOL	C	516	-	5,5,5	0.35	0	5,5,5	0.39	0
4	GOK	A	504	2	32,32,32	0.23	0	42,44,44	0.47	0
5	DMF	B	510	-	4,4,4	0.39	0	4,4,4	0.24	0
4	GOK	B	504	2	32,32,32	0.24	0	42,44,44	0.49	0
5	DMF	B	511	6	4,4,4	0.47	0	4,4,4	0.47	0
5	DMF	A	505	-	4,4,4	0.31	0	4,4,4	0.30	0
5	DMF	C	513	-	4,4,4	0.28	0	4,4,4	0.40	0
5	DMF	D	505	-	4,4,4	0.32	0	4,4,4	0.49	0
5	DMF	C	510	-	4,4,4	0.27	0	4,4,4	0.51	0
5	DMF	B	507	-	4,4,4	0.33	0	4,4,4	0.48	0
5	DMF	C	501	-	4,4,4	0.32	0	4,4,4	0.36	0
5	DMF	C	512	-	4,4,4	0.32	0	4,4,4	0.39	0
5	DMF	D	509	-	4,4,4	0.34	0	4,4,4	0.45	0
6	GOL	B	512	-	5,5,5	0.29	0	5,5,5	0.40	0
5	DMF	C	507	-	4,4,4	0.37	0	4,4,4	0.38	0
5	DMF	D	506	-	4,4,4	0.35	0	4,4,4	0.44	0
6	GOL	B	513	5	5,5,5	0.43	0	5,5,5	1.33	0
4	GOK	C	506	-	32,32,32	0.25	0	42,44,44	0.42	0
5	DMF	D	508	-	4,4,4	0.36	0	4,4,4	0.42	0
5	DMF	C	514	-	4,4,4	0.45	0	4,4,4	0.23	0
4	GOK	B	505	-	32,32,32	0.23	0	42,44,44	0.39	0
6	GOL	C	515	-	5,5,5	0.29	0	5,5,5	0.53	0
5	DMF	A	507	-	4,4,4	0.38	0	4,4,4	0.54	0
5	DMF	D	507	-	4,4,4	0.33	0	4,4,4	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMF	A	508	-	4,4,4	0.36	0	4,4,4	0.42	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	A	510	-	-	0/2/2/2	-
5	DMF	D	510	-	-	2/2/2/2	-
5	DMF	A	511	-	-	2/2/2/2	-
4	GOK	C	505	2	-	0/16/38/38	0/4/4/4
6	GOL	D	511	-	-	0/4/4/4	-
6	GOL	A	509	-	-	0/4/4/4	-
5	DMF	C	511	-	-	2/2/2/2	-
6	GOL	D	512	-	-	2/4/4/4	-
4	GOK	D	504	2	-	0/16/38/38	0/4/4/4
5	DMF	B	506	-	-	0/2/2/2	-
5	DMF	B	509	-	-	2/2/2/2	-
5	DMF	A	506	-	-	0/2/2/2	-
5	DMF	C	509	-	-	2/2/2/2	-
5	DMF	C	508	-	-	2/2/2/2	-
6	GOL	C	517	-	-	0/4/4/4	-
5	DMF	B	508	-	-	0/2/2/2	-
6	GOL	C	516	-	-	4/4/4/4	-
4	GOK	A	504	2	-	0/16/38/38	0/4/4/4
5	DMF	B	510	-	-	2/2/2/2	-
4	GOK	B	504	2	-	0/16/38/38	0/4/4/4
5	DMF	B	511	6	-	0/2/2/2	-
5	DMF	A	505	-	-	0/2/2/2	-
5	DMF	C	513	-	-	0/2/2/2	-
5	DMF	D	505	-	-	0/2/2/2	-
5	DMF	C	510	-	-	0/2/2/2	-
5	DMF	B	507	-	-	0/2/2/2	-
5	DMF	C	501	-	-	0/2/2/2	-
5	DMF	C	512	-	-	0/2/2/2	-
5	DMF	D	509	-	-	2/2/2/2	-
6	GOL	B	512	-	-	0/4/4/4	-
5	DMF	C	507	-	-	2/2/2/2	-
5	DMF	D	506	-	-	2/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	B	513	5	-	1/4/4/4	-
4	GOK	C	506	-	-	4/16/38/38	0/4/4/4
5	DMF	D	508	-	-	0/2/2/2	-
5	DMF	C	514	-	-	0/2/2/2	-
4	GOK	B	505	-	-	3/16/38/38	0/4/4/4
6	GOL	C	515	-	-	2/4/4/4	-
5	DMF	A	507	-	-	2/2/2/2	-
5	DMF	D	507	-	-	2/2/2/2	-
5	DMF	A	508	-	-	0/2/2/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	505	GOK	C31-C30-N29-C27
4	B	505	GOK	N29-C30-C31-C35
4	C	506	GOK	C17-C18-C27-N29
4	C	506	GOK	N29-C30-C31-C35
6	C	515	GOL	O2-C2-C3-O3
6	D	512	GOL	O1-C1-C2-C3
5	B	509	DMF	O-C-N-C2
5	B	509	DMF	O-C-N-C1
5	D	507	DMF	O-C-N-C2
5	D	507	DMF	O-C-N-C1
5	A	511	DMF	O-C-N-C1
5	A	511	DMF	O-C-N-C2
5	D	510	DMF	O-C-N-C2
5	C	511	DMF	O-C-N-C1
5	D	506	DMF	O-C-N-C1
5	D	510	DMF	O-C-N-C1
5	C	511	DMF	O-C-N-C2
5	D	506	DMF	O-C-N-C2
5	D	509	DMF	O-C-N-C2
6	C	515	GOL	C1-C2-C3-O3
6	C	516	GOL	O1-C1-C2-C3
6	C	516	GOL	C1-C2-C3-O3
5	D	509	DMF	O-C-N-C1
5	C	509	DMF	O-C-N-C1

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Mol	Chain	Res	Type	Atoms
6	D	512	GOL	O1-C1-C2-O2
5	B	510	DMF	O-C-N-C2
5	A	507	DMF	O-C-N-C1
5	C	509	DMF	O-C-N-C2
5	C	508	DMF	O-C-N-C2
5	B	510	DMF	O-C-N-C1
6	C	516	GOL	O2-C2-C3-O3
5	A	507	DMF	O-C-N-C2
5	C	508	DMF	O-C-N-C1
5	C	507	DMF	O-C-N-C1
4	C	506	GOK	C13-C18-C27-N29
5	C	507	DMF	O-C-N-C2
6	C	516	GOL	O1-C1-C2-O2
4	C	506	GOK	C18-C27-N29-C30
6	B	513	GOL	O2-C2-C3-O3
4	B	505	GOK	N10-C5-N15-C16

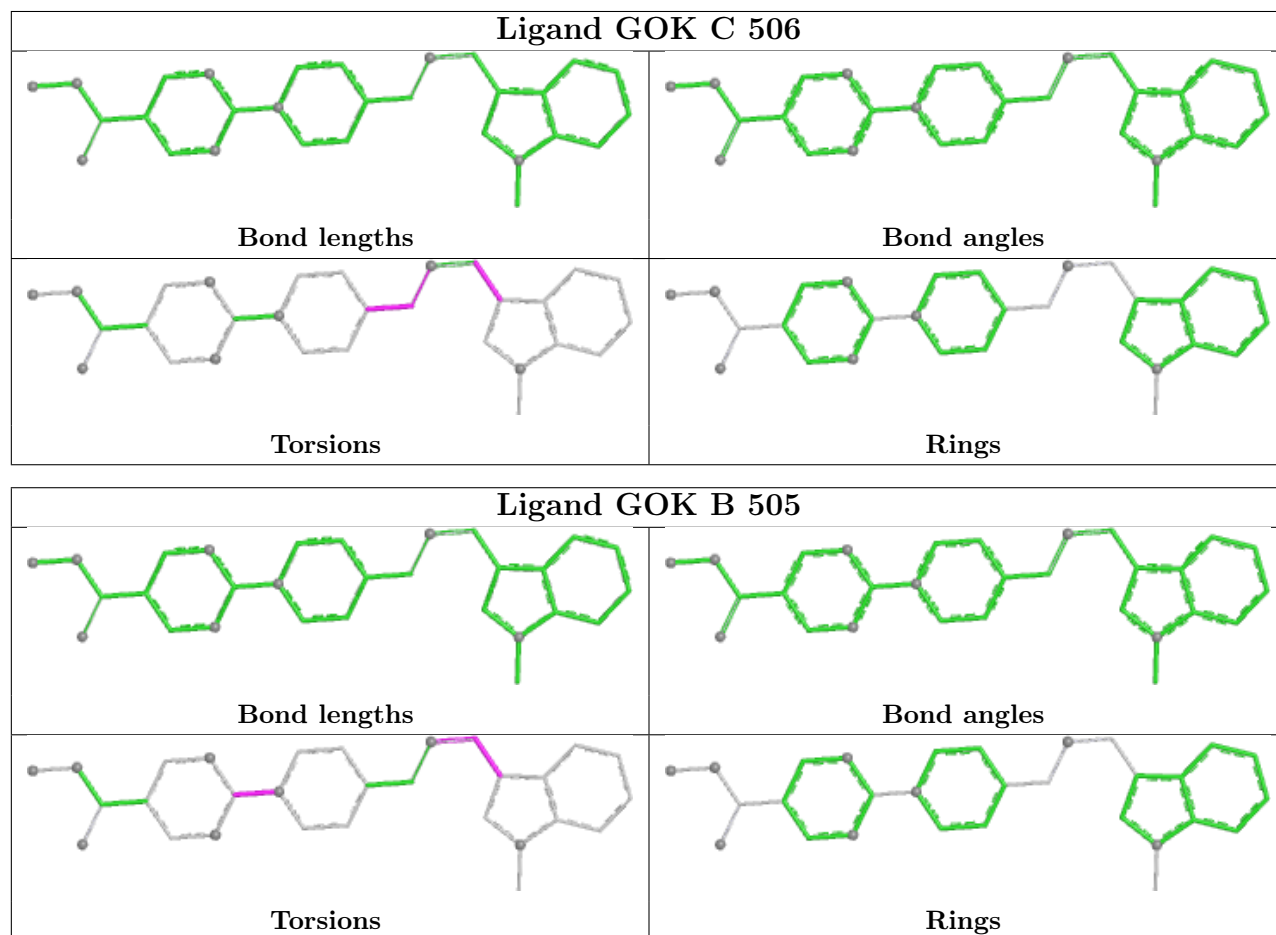
There are no ring outliers.

15 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	510	DMF	4	0
5	D	510	DMF	1	0
4	C	505	GOK	1	0
5	C	511	DMF	1	0
4	D	504	GOK	1	0
5	A	506	DMF	1	0
5	C	508	DMF	3	0
6	C	516	GOL	1	0
4	A	504	GOK	2	0
5	D	505	DMF	1	0
5	B	507	DMF	2	0
5	C	507	DMF	4	0
6	B	513	GOL	3	0
4	B	505	GOK	1	0
6	C	515	GOL	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 ⓘ

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	404/447 (90%)	0.15	26 (6%)	25 32	14, 25, 59, 95	4 (0%)
1	B	410/447 (91%)	-0.03	14 (3%)	48 57	10, 22, 42, 83	6 (1%)
1	C	415/447 (92%)	0.05	16 (3%)	43 52	12, 23, 45, 90	3 (0%)
1	D	405/447 (90%)	0.23	25 (6%)	26 34	14, 25, 60, 97	5 (1%)
All	All	1634/1788 (91%)	0.10	81 (4%)	34 42	10, 24, 51, 97	18 (1%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	401	LEU	5.7
1	A	432	TYR	5.5
1	A	428	TYR	5.3
1	B	401	LEU	5.3
1	C	225	VAL	5.1
1	A	426	TYR	5.1
1	D	230	LEU	5.0
1	D	426	TYR	4.9
1	A	232	ILE	4.9
1	A	435	TYR	4.7
1	C	99	TYR	4.5
1	D	401	LEU	4.4
1	D	304	LEU	4.3
1	B	223	ASN	4.2
1	D	432	TYR	4.1
1	C	230	LEU	4.0
1	D	425	ILE	3.9
1	B	232	ILE	3.8
1	C	231	PRO	3.6
1	A	99	TYR	3.6
1	D	435	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	428	TYR	3.5
1	A	425	ILE	3.5
1	D	434	LEU	3.5
1	A	223	ASN	3.5
1	A	431	VAL	3.5
1	D	232	ILE	3.3
1	D	229	LYS	3.3
1	D	165	VAL	3.3
1	A	314	CYS	3.3
1	A	392	PHE	3.3
1	D	231	PRO	3.2
1	D	392	PHE	3.2
1	C	168	THR	3.2
1	B	315	SER	3.1
1	B	99	TYR	3.1
1	B	433	GLN	3.1
1	A	434	LEU	3.0
1	D	368	ILE	3.0
1	D	393	PRO	3.0
1	B	395	GLU	2.9
1	A	394	HIS	2.8
1	D	224	MET	2.8
1	B	399	LYS	2.8
1	A	395	GLU	2.7
1	D	99	TYR	2.6
1	C	400	THR	2.6
1	C	402	ASP	2.6
1	C	433	GLN	2.6
1	C	56	TYR	2.6
1	C	80	GLU	2.6
1	B	84	LEU	2.5
1	C	177	GLN	2.5
1	A	168	THR	2.5
1	A	404	ILE	2.4
1	A	177	GLN	2.4
1	C	302	PRO	2.4
1	B	400	THR	2.4
1	D	385	PHE	2.4
1	A	402	ASP	2.3
1	D	303	ASN	2.3
1	D	429	ASP	2.3
1	D	177	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	223	ASN	2.2
1	A	383	PRO	2.2
1	A	430	GLN	2.2
1	A	397	HIS	2.2
1	B	368	ILE	2.2
1	C	76	MET	2.2
1	D	383	PRO	2.1
1	C	434	LEU	2.1
1	A	368	ILE	2.1
1	A	222	TRP	2.1
1	A	82	LYS	2.0
1	A	165	VAL	2.0
1	B	86	ALA	2.0
1	D	412	LEU	2.0
1	C	315	SER	2.0
1	A	429	ASP	2.0
1	B	302	PRO	2.0
1	B	222	TRP	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	DMF	B	511	5/5	0.77	0.16	61,63,66,68	0
5	DMF	C	511	5/5	0.78	0.19	46,52,56,59	0
5	DMF	C	501	5/5	0.83	0.17	35,37,44,44	0
5	DMF	D	510	5/5	0.84	0.17	49,50,52,53	0
5	DMF	A	510	5/5	0.85	0.18	43,48,56,61	0

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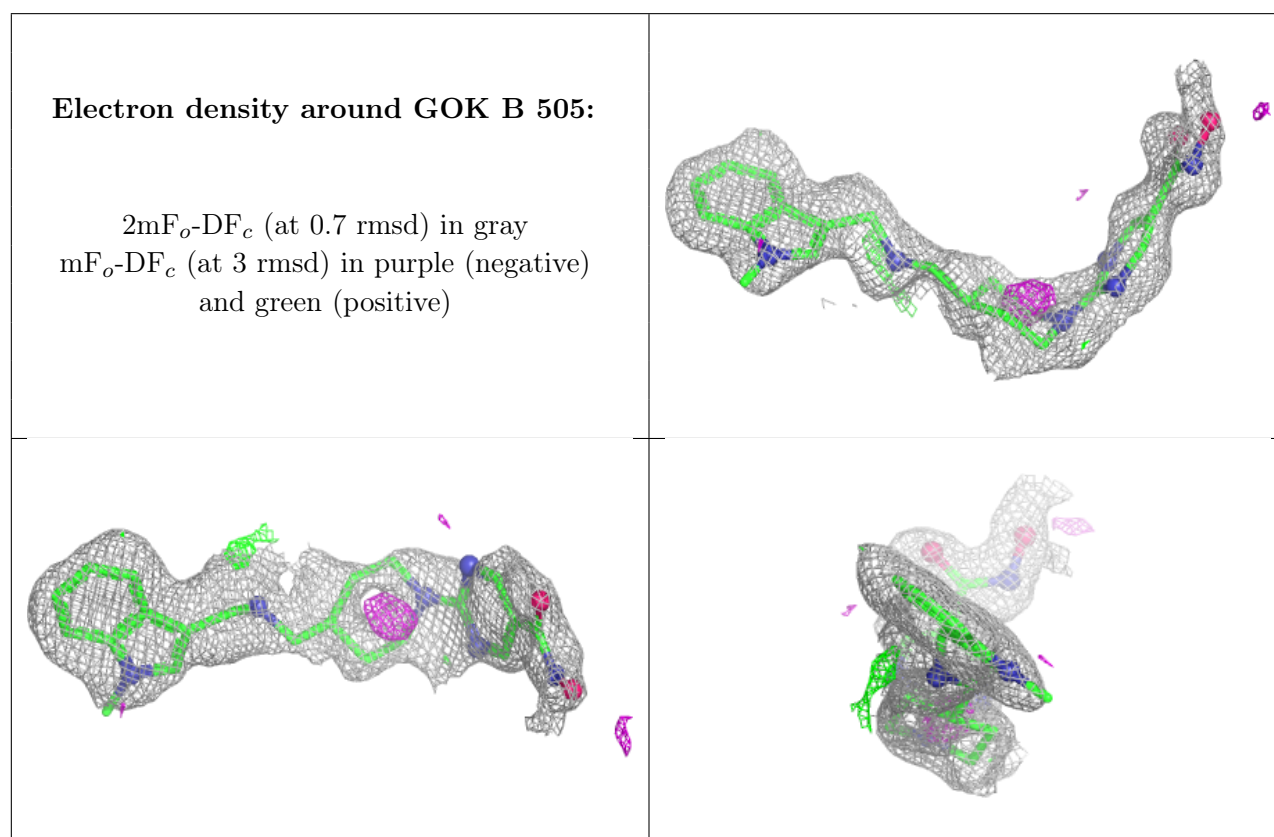
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMF	C	507	5/5	0.85	0.17	48,55,57,61	0
5	DMF	B	509	5/5	0.85	0.17	48,56,62,63	0
5	DMF	D	505	5/5	0.85	0.14	32,32,36,40	0
4	GOK	B	505	29/29	0.85	0.14	29,64,75,78	0
6	GOL	B	513	6/6	0.85	0.18	53,56,58,68	0
6	GOL	C	516	6/6	0.85	0.12	34,42,49,59	0
5	DMF	C	514	5/5	0.86	0.16	33,40,43,47	0
5	DMF	B	508	5/5	0.86	0.16	44,55,55,56	0
5	DMF	D	506	5/5	0.86	0.17	62,63,68,71	0
5	DMF	C	508	5/5	0.86	0.14	33,33,44,45	0
5	DMF	A	505	5/5	0.86	0.17	60,62,63,65	0
5	DMF	C	513	5/5	0.86	0.19	48,49,50,55	0
5	DMF	D	508	5/5	0.87	0.18	63,65,69,69	0
5	DMF	C	509	5/5	0.87	0.14	63,64,65,70	0
5	DMF	A	506	5/5	0.87	0.14	35,40,43,45	0
4	GOK	C	506	29/29	0.87	0.13	35,45,61,64	0
5	DMF	B	507	5/5	0.88	0.16	42,44,47,53	0
5	DMF	D	507	5/5	0.88	0.15	42,47,49,56	0
5	DMF	A	508	5/5	0.88	0.12	41,44,47,48	0
5	DMF	C	512	5/5	0.89	0.16	34,40,44,48	0
6	GOL	C	515	6/6	0.89	0.12	38,41,45,48	0
5	DMF	A	511	5/5	0.89	0.13	32,39,46,49	0
5	DMF	B	506	5/5	0.91	0.12	31,32,45,49	0
5	DMF	A	507	5/5	0.91	0.12	39,40,48,54	0
4	GOK	D	504	29/29	0.91	0.11	27,36,46,47	0
5	DMF	C	510	5/5	0.91	0.11	33,36,41,42	0
5	DMF	B	510	5/5	0.92	0.10	29,31,38,39	0
5	DMF	D	509	5/5	0.93	0.12	46,47,54,58	0
4	GOK	A	504	29/29	0.93	0.10	24,31,50,50	0
6	GOL	B	512	6/6	0.93	0.09	28,28,32,33	0
6	GOL	D	512	6/6	0.93	0.12	41,46,53,56	0
6	GOL	A	509	6/6	0.94	0.09	24,29,31,33	0
4	GOK	C	505	29/29	0.94	0.09	24,35,48,51	0
4	GOK	B	504	29/29	0.94	0.09	24,33,43,43	0
6	GOL	D	511	6/6	0.95	0.09	28,32,32,35	0
6	GOL	C	517	6/6	0.96	0.07	25,29,30,32	0
2	ZN	B	501	1/1	0.99	0.16	33,33,33,33	0
2	ZN	C	502	1/1	0.99	0.16	33,33,33,33	0
2	ZN	D	501	1/1	0.99	0.16	34,34,34,34	0
2	ZN	A	501	1/1	0.99	0.13	33,33,33,33	0
3	K	A	503	1/1	1.00	0.01	18,18,18,18	0
3	K	B	502	1/1	1.00	0.03	20,20,20,20	0

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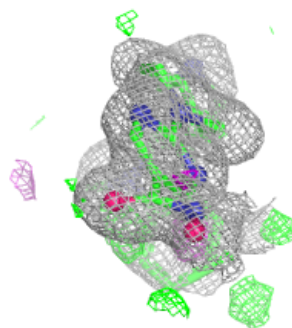
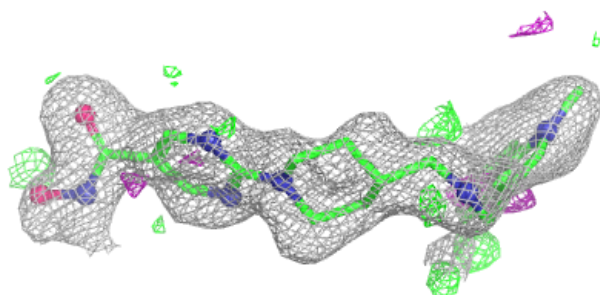
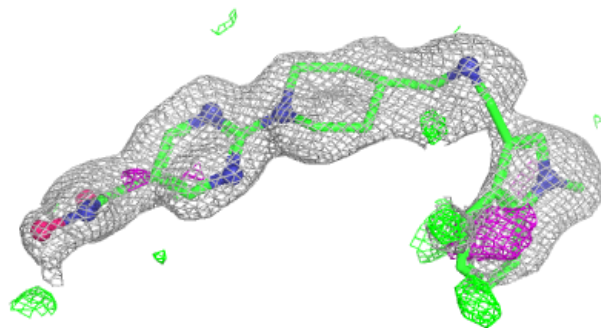
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	K	B	503	1/1	1.00	0.02	17,17,17,17	0
3	K	C	503	1/1	1.00	0.04	23,23,23,23	0
3	K	C	504	1/1	1.00	0.04	17,17,17,17	0
3	K	D	502	1/1	1.00	0.02	22,22,22,22	0
3	K	D	503	1/1	1.00	0.01	18,18,18,18	0
3	K	A	502	1/1	1.00	0.02	22,22,22,22	0

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 GOK C 506:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.