Full wwPDB X-ray Structure Validation Report (i)

Jan 13, 2024 – 11:28 pm GMT

PDB ID	:	6HSH
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 (i) symbol.

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

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

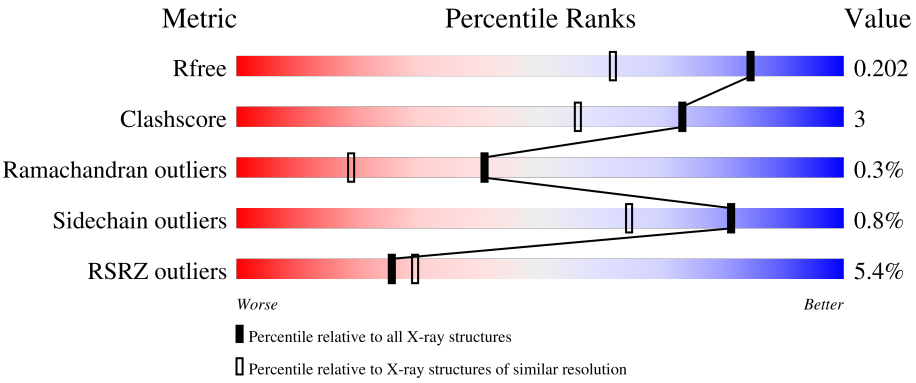
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.54 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}	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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	447	6% 85% 5% 10%
1	B	447	3% 87% . 8%
1	C	447	4% 85% 7% 7%
1	D	447	7% 82% 9% 9%

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 (i)

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

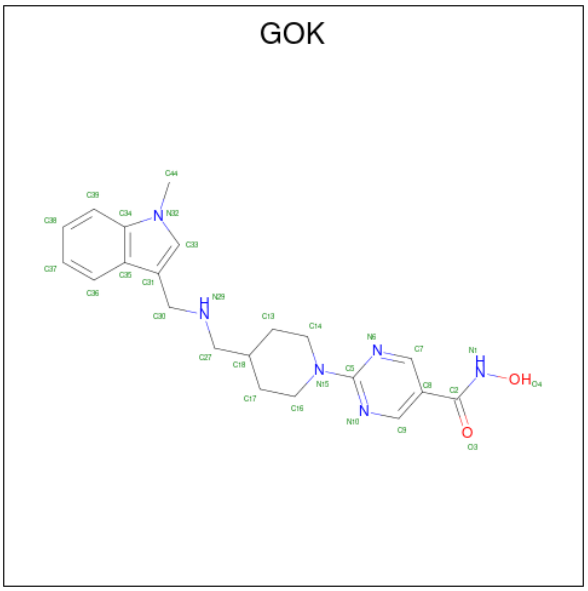
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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).

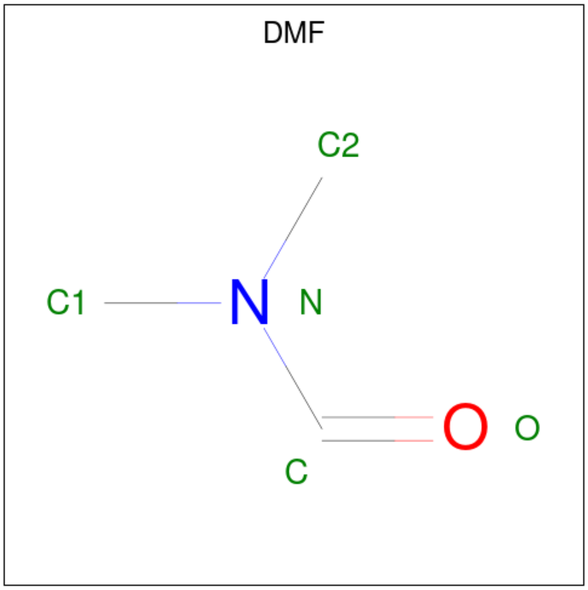
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total K 2 2	0	0
3	B	2	Total K 2 2	0	0
3	C	2	Total K 2 2	0	0
3	D	2	Total K 2 2	0	0

- Molecule 4 is 2-[4-[[(1-methylindol-3-yl)methylamino]methyl]piperidin-1-yl]- {N}-oxidanyl-pyrimidine-5-carboxamide (three-letter code: GOK) (formula: $C_{21}H_{26}N_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			29	21	6	2		
4	B	1	Total	C	N	O	0	0
			29	21	6	2		
4	B	1	Total	C	N	O	0	0
			29	21	6	2		
4	C	1	Total	C	N	O	0	0
			29	21	6	2		
4	C	1	Total	C	N	O	0	0
			29	21	6	2		
4	D	1	Total	C	N	O	0	0
			29	21	6	2		

- Molecule 5 is DIMETHYLFORMAMIDE (three-letter code: DMF) (formula: C_3H_7NO).



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

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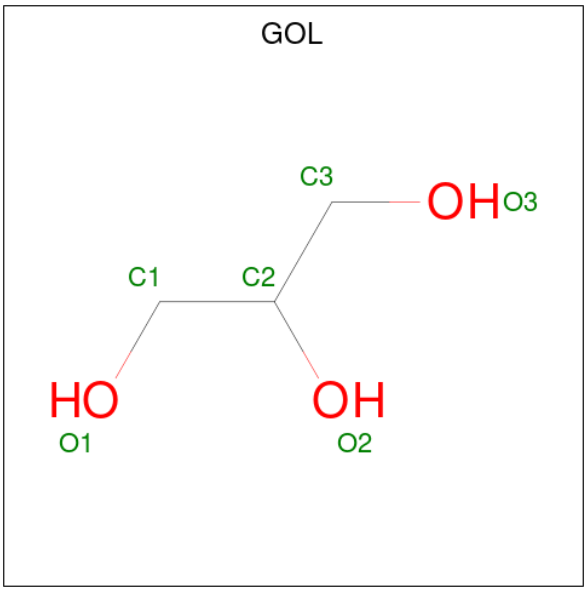
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C N O 5 3 1 1	0	0
5	C	1	Total C N O 5 3 1 1	0	0
5	C	1	Total C N O 5 3 1 1	0	0
5	C	1	Total C N O 5 3 1 1	0	0
5	C	1	Total C N O 5 3 1 1	0	0
5	C	1	Total C N O 5 3 1 1	0	0
5	C	1	Total C N O 5 3 1 1	0	0
5	D	1	Total C N O 5 3 1 1	0	0
5	D	1	Total C N O 5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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is water.

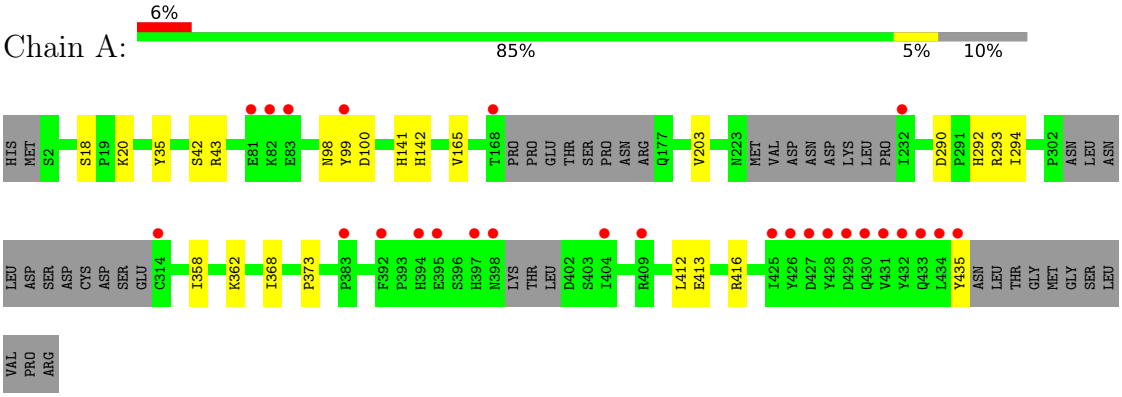
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	272	Total O 272 272	0	0
7	B	304	Total O 304 304	0	0
7	C	291	Total O 291 291	0	0
7	D	235	Total O 235 235	0	0

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.

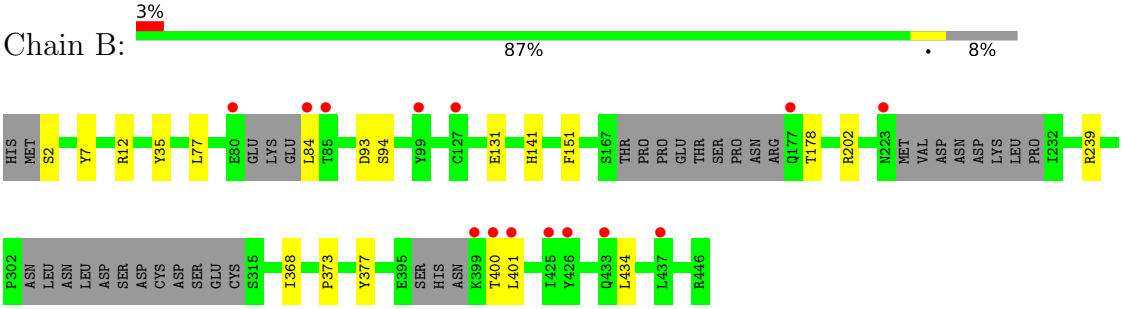
• Molecule 1: Histone deacetylase

Chain A:



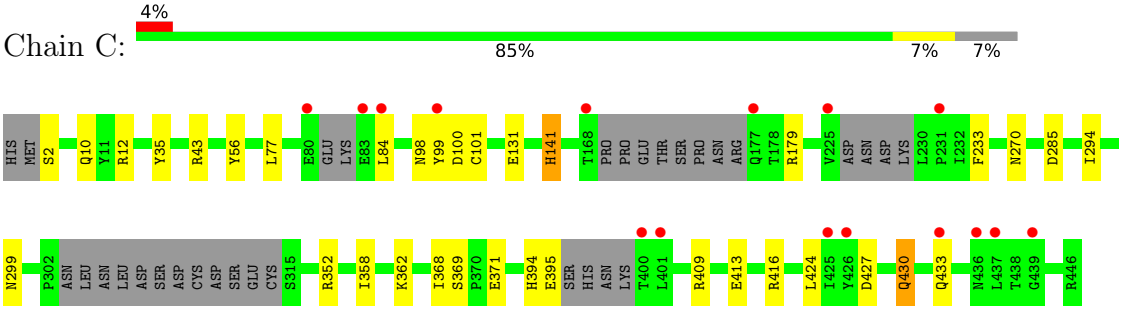
• Molecule 1: Histone deacetylase

Chain B:



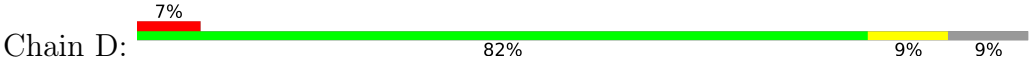
• Molecule 1: Histone deacetylase

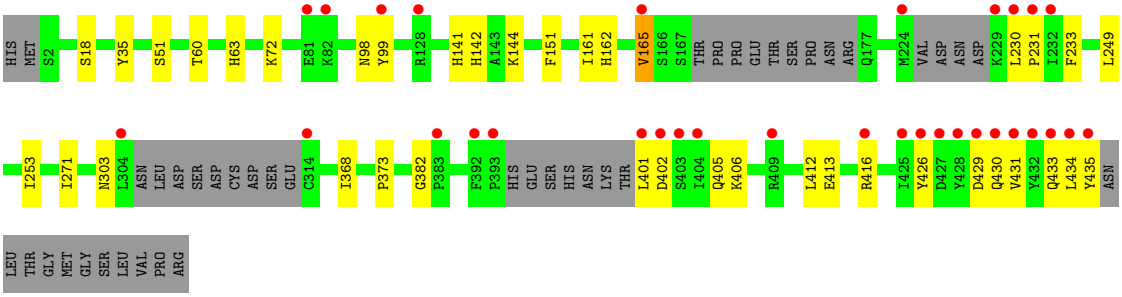
Chain C:



• Molecule 1: Histone deacetylase

Chain D:




HIS MET S2 S18 Y35 S51 T60 H63 K72 E81 K82 N98 Y99 R128 H141 H142 A143 K144 F151 I161 H162 V165 S166 S167 THR PRO PRO GLU THR SER PRO ASN ARG Q177 M224 VAL ASP ASN ASP K229 L230 P231 I232 F233 L249
I253 I271 N303 L304 ASN LEU ASP SER ASP CYS ASP SER GLU C314 I368 P373 G382 P383 F392 P393 HIS GLU SER HIS ASN LYS THR L401 D402 S403 I404 Q405 K406 R409 L412 E413 R416 I425 Y426 D427 Y428 D429 Q430 V431 Y432 Q433 L434 Y435 ASN
LEU THR GLY MET GLY SER LEU VAL PRO ARG

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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)	0.38 , 52.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.38	0/3350	0.54	0/4556
1	B	0.41	0/3406	0.58	1/4631 (0.0%)
1	C	0.40	0/3419	0.56	1/4651 (0.0%)
1	D	0.38	0/3363	0.54	0/4573
All	All	0.40	0/13538	0.55	2/18411 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	434	LEU	CA-CB-CG	6.43	130.09	115.30
1	C	285	ASP	CB-CG-OD1	5.12	122.91	118.30

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	3247	0	3131	16	0
1	B	3300	0	3203	18	0
1	C	3319	0	3221	29	0
1	D	3258	0	3172	25	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	87	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 (87) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:7[B]:TYR:OH	1:B:12:ARG:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:C:427:ASP:CG	1:C:430:GLN:HB2	2.41	0.41
1:C:77:LEU:HD13	1:C:84:LEU:HG	2.03	0.41
1:C:413:GLU:CD	1:C:416:ARG:HH21	2.23	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 (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	398/447 (89%)	392 (98%)	5 (1%)	1 (0%)	41 19
1	B	404/447 (90%)	398 (98%)	6 (2%)	0	100 100
1	C	406/447 (91%)	402 (99%)	3 (1%)	1 (0%)	47 24
1	D	400/447 (90%)	395 (99%)	3 (1%)	2 (0%)	29 9
All	All	1608/1788 (90%)	1587 (99%)	17 (1%)	4 (0%)	41 24

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 (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	355/392 (91%)	353 (99%)	2 (1%)	86 72
1	B	361/392 (92%)	359 (99%)	2 (1%)	86 72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	363/392 (93%)	359 (99%)	4 (1%)	73 51
1	D	357/392 (91%)	353 (99%)	4 (1%)	73 51
All	All	1436/1568 (92%)	1424 (99%)	12 (1%)	81 64

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

Mol	Chain	Res	Type
1	A	20	LYS
1	A	141	HIS
1	B	141	HIS
1	B	151	PHE
1	C	56	TYR
1	C	141	HIS
1	C	233	PHE
1	C	430	GLN
1	D	141	HIS
1	D	151	PHE
1	D	165	VAL
1	D	233	PHE

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 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	C	511	-	4,4,4	0.37	0	4,4,4	0.49	0
5	DMF	C	510	-	4,4,4	0.26	0	4,4,4	0.49	0
5	DMF	A	506	-	4,4,4	0.33	0	4,4,4	0.44	0
4	GOK	C	505	2	28,32,32	0.48	0	37,44,44	0.67	1 (2%)
5	DMF	D	506	-	4,4,4	0.34	0	4,4,4	0.42	0
5	DMF	C	513	-	4,4,4	0.27	0	4,4,4	0.38	0
5	DMF	D	509	-	4,4,4	0.33	0	4,4,4	0.43	0
5	DMF	D	507	-	4,4,4	0.32	0	4,4,4	0.42	0
6	GOL	D	512	-	5,5,5	0.31	0	5,5,5	0.50	0
5	DMF	B	506	-	4,4,4	0.33	0	4,4,4	0.41	0
5	DMF	B	507	-	4,4,4	0.32	0	4,4,4	0.46	0
5	DMF	C	509	-	4,4,4	0.36	0	4,4,4	0.37	0
6	GOL	B	513	5	5,5,5	0.41	0	5,5,5	1.27	0
4	GOK	C	506	-	28,32,32	0.47	0	37,44,44	0.60	1 (2%)
5	DMF	C	501	-	4,4,4	0.31	0	4,4,4	0.34	0
5	DMF	C	507	-	4,4,4	0.36	0	4,4,4	0.36	0
5	DMF	B	509	-	4,4,4	0.37	0	4,4,4	0.44	0
5	DMF	A	507	-	4,4,4	0.37	0	4,4,4	0.51	0
6	GOL	C	516	-	5,5,5	0.34	0	5,5,5	0.37	0
5	DMF	A	510	-	4,4,4	0.29	0	4,4,4	0.29	0
6	GOL	C	515	-	5,5,5	0.28	0	5,5,5	0.50	0
4	GOK	B	505	-	28,32,32	0.47	0	37,44,44	0.59	1 (2%)
4	GOK	B	504	2	28,32,32	0.47	0	37,44,44	0.67	1 (2%)
5	DMF	A	508	-	4,4,4	0.35	0	4,4,4	0.40	0
6	GOL	D	511	-	5,5,5	0.37	0	5,5,5	0.31	0
5	DMF	D	505	-	4,4,4	0.30	0	4,4,4	0.47	0
5	DMF	B	510	-	4,4,4	0.37	0	4,4,4	0.23	0
5	DMF	C	508	-	4,4,4	0.32	0	4,4,4	0.56	0
5	DMF	A	505	-	4,4,4	0.30	0	4,4,4	0.28	0
4	GOK	A	504	2	28,32,32	0.46	0	37,44,44	0.63	1 (2%)
5	DMF	C	514	-	4,4,4	0.43	0	4,4,4	0.22	0
5	DMF	B	511	6	4,4,4	0.45	0	4,4,4	0.44	0
5	DMF	C	512	-	4,4,4	0.31	0	4,4,4	0.37	0
5	DMF	D	510	-	4,4,4	0.29	0	4,4,4	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	GOL	A	509	-	5,5,5	0.31	0	5,5,5	0.27	0
6	GOL	B	512	-	5,5,5	0.29	0	5,5,5	0.36	0
6	GOL	C	517	-	5,5,5	0.39	0	5,5,5	0.24	0
5	DMF	A	511	-	4,4,4	0.30	0	4,4,4	0.31	0
4	GOK	D	504	2	28,32,32	0.47	0	37,44,44	0.67	1 (2%)
5	DMF	D	508	-	4,4,4	0.35	0	4,4,4	0.40	0
5	DMF	B	508	-	4,4,4	0.34	0	4,4,4	0.35	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	C	511	-	-	2/2/2/2	-
5	DMF	C	510	-	-	0/2/2/2	-
5	DMF	A	506	-	-	0/2/2/2	-
4	GOK	C	505	2	-	0/14/38/38	0/4/4/4
5	DMF	D	506	-	-	2/2/2/2	-
5	DMF	C	513	-	-	0/2/2/2	-
5	DMF	D	509	-	-	2/2/2/2	-
5	DMF	D	507	-	-	2/2/2/2	-
6	GOL	D	512	-	-	2/4/4/4	-
5	DMF	B	506	-	-	0/2/2/2	-
5	DMF	B	507	-	-	0/2/2/2	-
5	DMF	C	509	-	-	2/2/2/2	-
6	GOL	B	513	5	-	1/4/4/4	-
4	GOK	C	506	-	-	3/14/38/38	0/4/4/4
5	DMF	C	501	-	-	0/2/2/2	-
5	DMF	C	507	-	-	2/2/2/2	-
5	DMF	B	509	-	-	2/2/2/2	-
5	DMF	A	507	-	-	2/2/2/2	-
6	GOL	C	516	-	-	4/4/4/4	-
5	DMF	A	510	-	-	0/2/2/2	-
6	GOL	C	515	-	-	3/4/4/4	-
4	GOK	B	505	-	-	2/14/38/38	0/4/4/4
4	GOK	B	504	2	-	0/14/38/38	0/4/4/4
5	DMF	A	508	-	-	0/2/2/2	-
6	GOL	D	511	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMF	D	505	-	-	0/2/2/2	-
5	DMF	B	510	-	-	2/2/2/2	-
5	DMF	C	508	-	-	2/2/2/2	-
5	DMF	A	505	-	-	0/2/2/2	-
4	GOK	A	504	2	-	0/14/38/38	0/4/4/4
5	DMF	C	514	-	-	0/2/2/2	-
5	DMF	B	511	6	-	0/2/2/2	-
5	DMF	C	512	-	-	0/2/2/2	-
5	DMF	D	510	-	-	2/2/2/2	-
6	GOL	A	509	-	-	0/4/4/4	-
6	GOL	B	512	-	-	0/4/4/4	-
6	GOL	C	517	-	-	0/4/4/4	-
5	DMF	A	511	-	-	2/2/2/2	-
4	GOK	D	504	2	-	0/14/38/38	0/4/4/4
5	DMF	D	508	-	-	0/2/2/2	-
5	DMF	B	508	-	-	0/2/2/2	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	504	GOK	C39-C34-N32	-2.22	130.23	132.14
4	D	504	GOK	C39-C34-N32	-2.13	130.31	132.14
4	B	505	GOK	C39-C34-N32	-2.13	130.31	132.14
4	C	505	GOK	C39-C34-N32	-2.09	130.35	132.14
4	A	504	GOK	C39-C34-N32	-2.07	130.37	132.14
4	C	506	GOK	C39-C34-N32	-2.04	130.39	132.14

There are no chirality outliers.

All (39) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
5	A	511	DMF	O-C-N-C1
5	A	511	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
4	B	505	GOK	C31-C30-N29-C27
5	D	509	DMF	O-C-N-C1
5	C	509	DMF	O-C-N-C1
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	B	510	DMF	O-C-N-C2
6	D	512	GOL	O1-C1-C2-O2
5	A	507	DMF	O-C-N-C1
5	C	508	DMF	O-C-N-C2
5	C	509	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
5	C	507	DMF	O-C-N-C2
4	C	506	GOK	C13-C18-C27-N29
6	C	516	GOL	O1-C1-C2-O2
4	C	506	GOK	C18-C27-N29-C30
6	B	513	GOL	O2-C2-C3-O3
6	C	515	GOL	O1-C1-C2-C3
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	C	511	DMF	1	0
5	A	506	DMF	1	0
4	C	505	GOK	1	0
5	B	507	DMF	2	0
6	B	513	GOL	3	0
5	C	507	DMF	4	0

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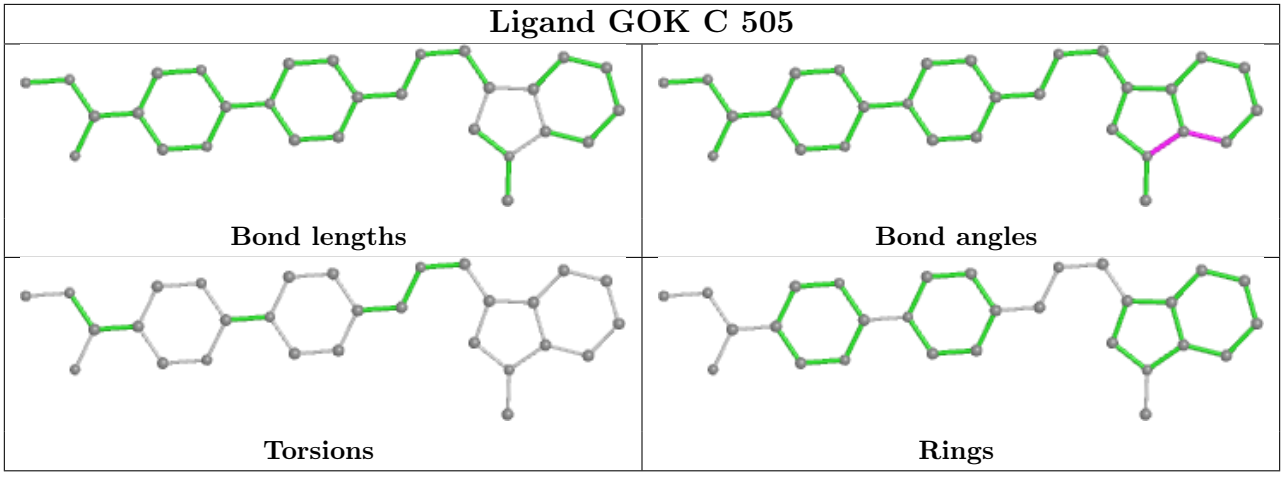
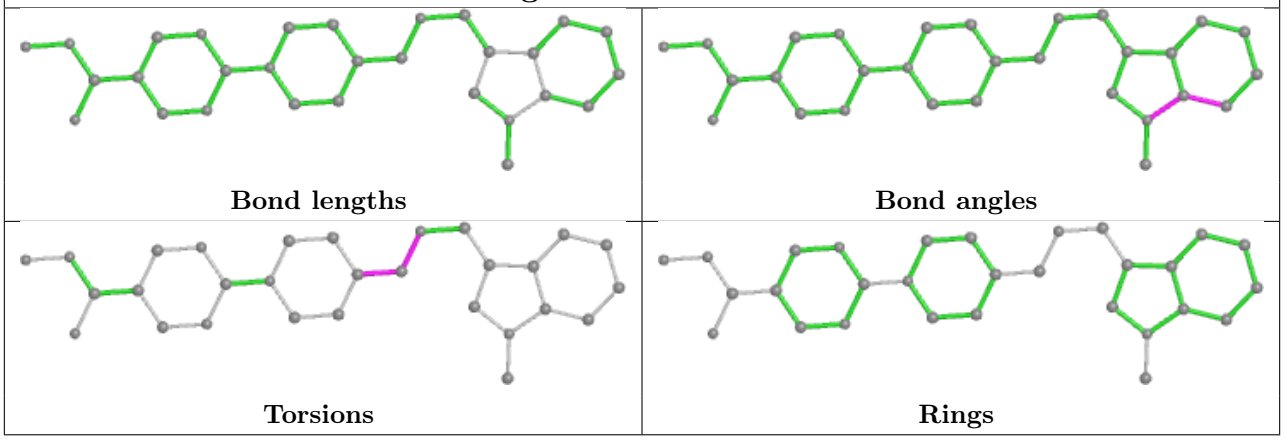
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	516	GOL	1	0
5	A	510	DMF	4	0
6	C	515	GOL	2	0
4	B	505	GOK	1	0
5	D	505	DMF	1	0
5	C	508	DMF	3	0
4	A	504	GOK	2	0
5	D	510	DMF	1	0
4	D	504	GOK	1	0

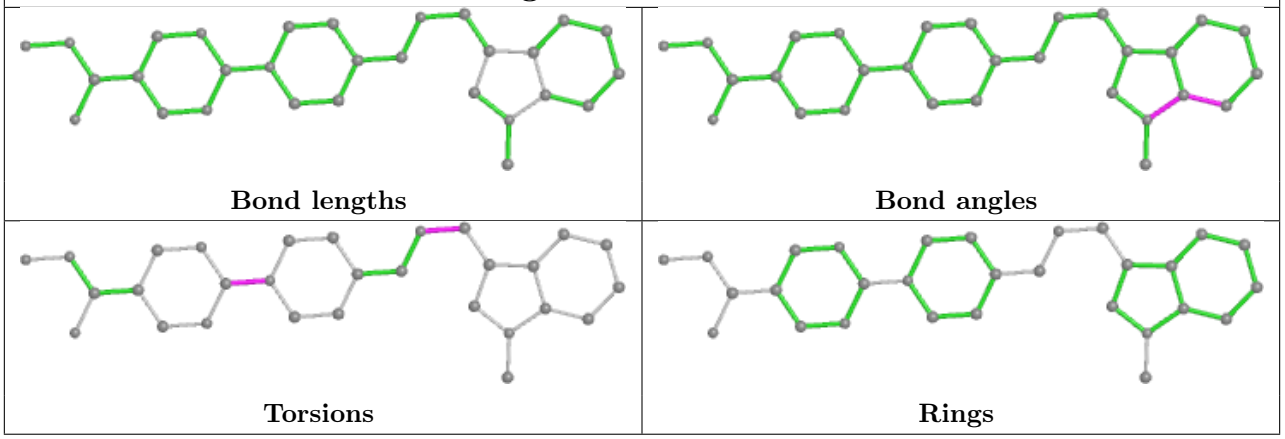
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



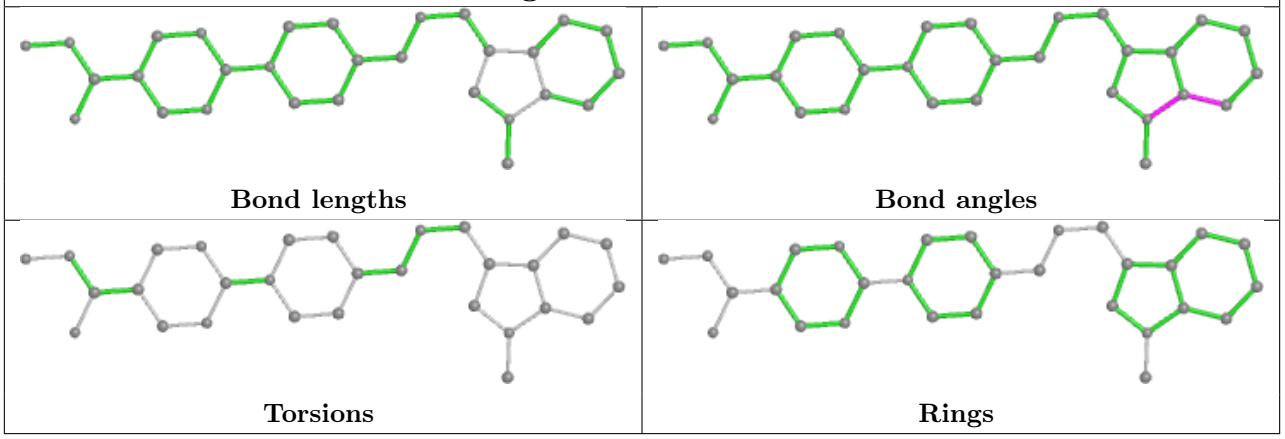
Ligand GOK C 506

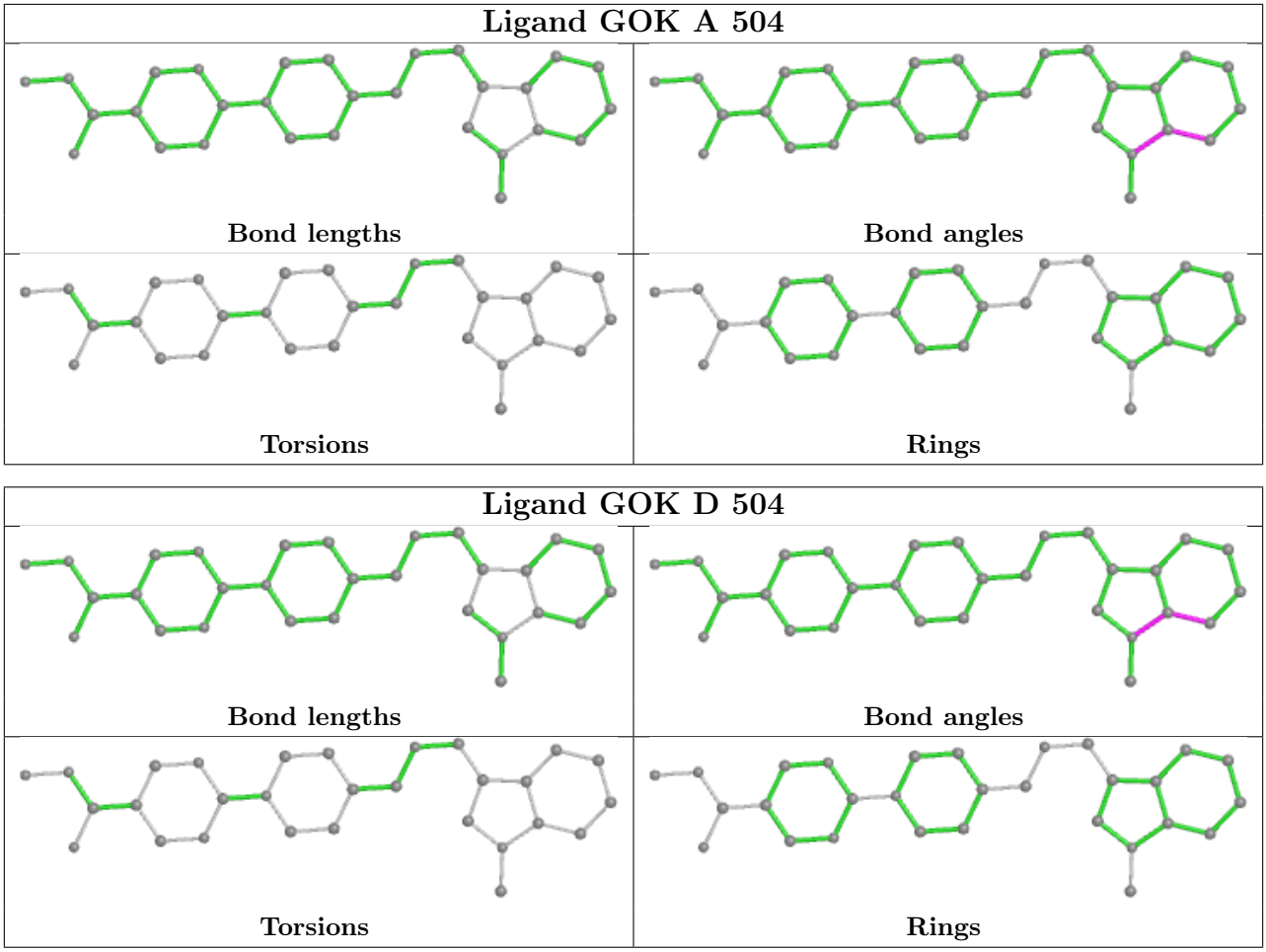


Ligand GOK B 505



Ligand GOK B 504





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, 95^{th} 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%)	0.07	26 (6%)	19	22	17, 25, 59, 95	0
1	B	410/447 (91%)	-0.05	14 (3%)	45	51	16, 22, 42, 83	0
1	C	415/447 (92%)	-0.01	16 (3%)	39	45	16, 23, 45, 90	0
1	D	405/447 (90%)	0.14	32 (7%)	12	14	18, 25, 60, 97	0
All	All	1634/1788 (91%)	0.04	88 (5%)	25	29	16, 24, 51, 97	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	432	TYR	11.7
1	D	401	LEU	11.3
1	A	432	TYR	11.1
1	D	426	TYR	8.5
1	D	425	ILE	8.1
1	A	428	TYR	7.9
1	D	435	TYR	7.9
1	D	434	LEU	7.2
1	A	434	LEU	6.7
1	A	426	TYR	6.5
1	B	99	TYR	6.4
1	D	428	TYR	6.1
1	A	425	ILE	5.9
1	C	83	GLU	5.7
1	A	433	GLN	5.7
1	D	230	LEU	5.5
1	A	435	TYR	5.4
1	D	429	ASP	5.2
1	A	81	GLU	5.2
1	C	168	THR	5.1
1	A	392	PHE	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	429	ASP	4.9
1	B	401	LEU	4.9
1	A	314	CYS	4.9
1	C	225	VAL	4.8
1	A	383	PRO	4.8
1	A	431	VAL	4.7
1	C	425	ILE	4.7
1	D	392	PHE	4.7
1	A	398	ASN	4.6
1	C	99	TYR	4.4
1	A	395	GLU	4.3
1	B	437	LEU	4.2
1	C	177	GLN	4.1
1	D	433	GLN	4.1
1	A	394	HIS	4.1
1	D	431	VAL	3.7
1	D	304	LEU	3.6
1	C	401	LEU	3.5
1	C	433	GLN	3.3
1	C	437	LEU	3.3
1	A	232	ILE	3.2
1	B	177	GLN	3.2
1	D	99	TYR	3.1
1	B	425	ILE	3.1
1	A	404	ILE	3.1
1	D	128	ARG	2.9
1	A	83	GLU	2.9
1	D	231	PRO	2.9
1	B	433	GLN	2.9
1	A	430	GLN	2.8
1	A	427	ASP	2.7
1	D	427	ASP	2.7
1	D	314	CYS	2.7
1	D	81	GLU	2.7
1	D	409	ARG	2.6
1	D	402	ASP	2.6
1	A	82	LYS	2.6
1	B	85	THR	2.6
1	C	439	GLY	2.5
1	A	409	ARG	2.5
1	B	223	ASN	2.5
1	D	383	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	416	ARG	2.5
1	C	80	GLU	2.5
1	C	426	TYR	2.5
1	D	229	LYS	2.5
1	C	84	LEU	2.5
1	A	397	HIS	2.5
1	D	82	LYS	2.5
1	A	99	TYR	2.4
1	B	399	LYS	2.4
1	C	231	PRO	2.4
1	B	84	LEU	2.4
1	D	404	ILE	2.4
1	B	426	TYR	2.4
1	D	165	VAL	2.3
1	D	224	MET	2.3
1	B	80	GLU	2.3
1	C	400	THR	2.3
1	C	436	ASN	2.3
1	A	168	THR	2.3
1	B	127[A]	CYS	2.1
1	D	393	PRO	2.0
1	D	430	GLN	2.0
1	D	232	ILE	2.0
1	B	400	THR	2.0
1	D	403	SER	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, 95^{th} 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
6	GOL	B	513	6/6	0.55	0.19	53,56,58,68	0
5	DMF	B	509	5/5	0.66	0.18	48,56,62,63	0
5	DMF	D	506	5/5	0.67	0.16	62,63,68,71	0
5	DMF	B	508	5/5	0.75	0.19	44,55,55,56	0
5	DMF	A	510	5/5	0.77	0.20	43,48,56,61	0
5	DMF	B	511	5/5	0.79	0.23	61,63,66,68	0
5	DMF	D	505	5/5	0.81	0.17	32,32,36,40	0
6	GOL	C	515	6/6	0.82	0.12	38,41,45,48	0
5	DMF	D	508	5/5	0.83	0.14	63,65,69,69	0
5	DMF	C	501	5/5	0.83	0.13	35,37,44,44	0
5	DMF	C	507	5/5	0.83	0.16	48,55,57,61	0
6	GOL	C	516	6/6	0.83	0.22	34,42,49,59	0
4	GOK	C	506	29/29	0.84	0.16	35,45,61,64	0
5	DMF	C	514	5/5	0.84	0.13	33,40,43,47	0
5	DMF	C	508	5/5	0.85	0.11	33,33,44,45	0
4	GOK	B	505	29/29	0.86	0.24	29,64,75,78	0
5	DMF	A	505	5/5	0.86	0.13	60,62,63,65	0
5	DMF	C	511	5/5	0.87	0.20	46,52,56,59	0
5	DMF	A	506	5/5	0.87	0.14	35,40,43,45	0
5	DMF	D	510	5/5	0.88	0.12	49,50,52,53	0
5	DMF	C	513	5/5	0.88	0.15	48,49,50,55	0
5	DMF	A	511	5/5	0.89	0.11	32,39,46,49	0
5	DMF	C	509	5/5	0.89	0.13	63,64,65,70	0
6	GOL	D	512	6/6	0.89	0.14	41,46,53,56	0
4	GOK	C	505	29/29	0.90	0.12	24,35,48,51	0
6	GOL	B	512	6/6	0.91	0.08	28,28,32,33	0
5	DMF	A	508	5/5	0.91	0.09	41,44,47,48	0
5	DMF	C	512	5/5	0.91	0.13	34,40,44,48	0
5	DMF	B	506	5/5	0.91	0.10	31,32,45,49	0
4	GOK	D	504	29/29	0.91	0.10	27,36,46,47	0
4	GOK	A	504	29/29	0.92	0.11	24,31,50,50	0
4	GOK	B	504	29/29	0.93	0.11	24,33,43,43	0
5	DMF	A	507	5/5	0.93	0.10	39,40,48,54	0
5	DMF	B	510	5/5	0.93	0.12	29,31,38,39	0
5	DMF	B	507	5/5	0.93	0.11	42,44,47,53	0
6	GOL	C	517	6/6	0.93	0.07	25,29,30,32	0
6	GOL	D	511	6/6	0.93	0.07	28,32,32,35	0
6	GOL	A	509	6/6	0.93	0.09	24,29,31,33	0
5	DMF	D	507	5/5	0.94	0.12	42,47,49,56	0
5	DMF	C	510	5/5	0.95	0.07	33,36,41,42	0
5	DMF	D	509	5/5	0.97	0.08	46,47,54,58	0
3	K	A	503	1/1	1.00	0.09	18,18,18,18	0
3	K	B	502	1/1	1.00	0.08	20,20,20,20	0

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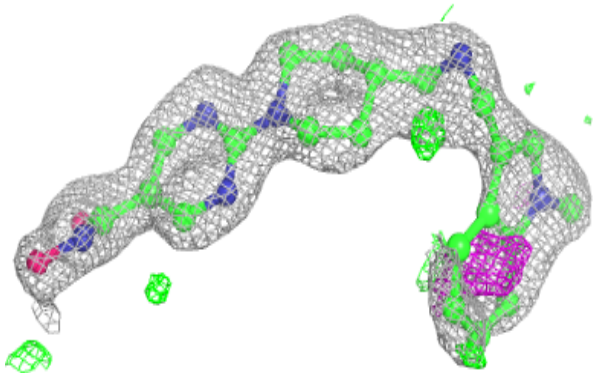
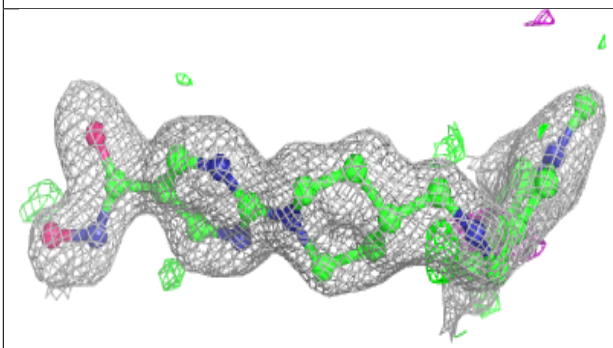
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	K	B	503	1/1	1.00	0.10	17,17,17,17	0
3	K	C	503	1/1	1.00	0.06	23,23,23,23	0
3	K	C	504	1/1	1.00	0.09	17,17,17,17	0
3	K	D	502	1/1	1.00	0.08	22,22,22,22	0
3	K	D	503	1/1	1.00	0.09	18,18,18,18	0
2	ZN	A	501	1/1	1.00	0.06	33,33,33,33	0
2	ZN	B	501	1/1	1.00	0.07	33,33,33,33	0
2	ZN	C	502	1/1	1.00	0.08	33,33,33,33	0
2	ZN	D	501	1/1	1.00	0.07	34,34,34,34	0
3	K	A	502	1/1	1.00	0.08	22,22,22,22	0

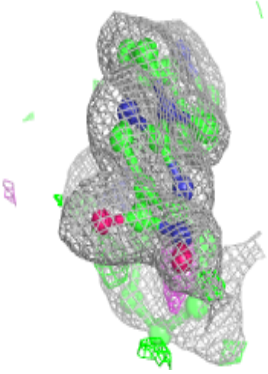
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

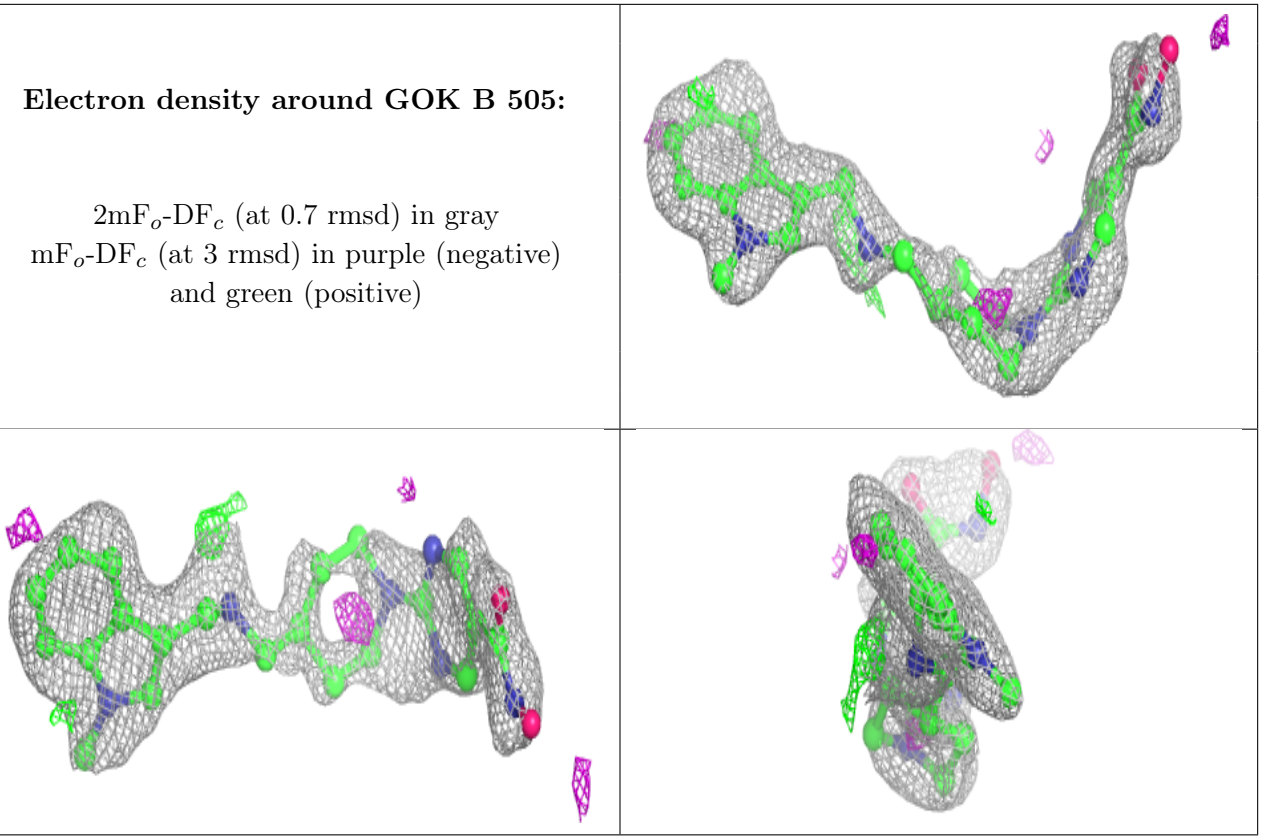






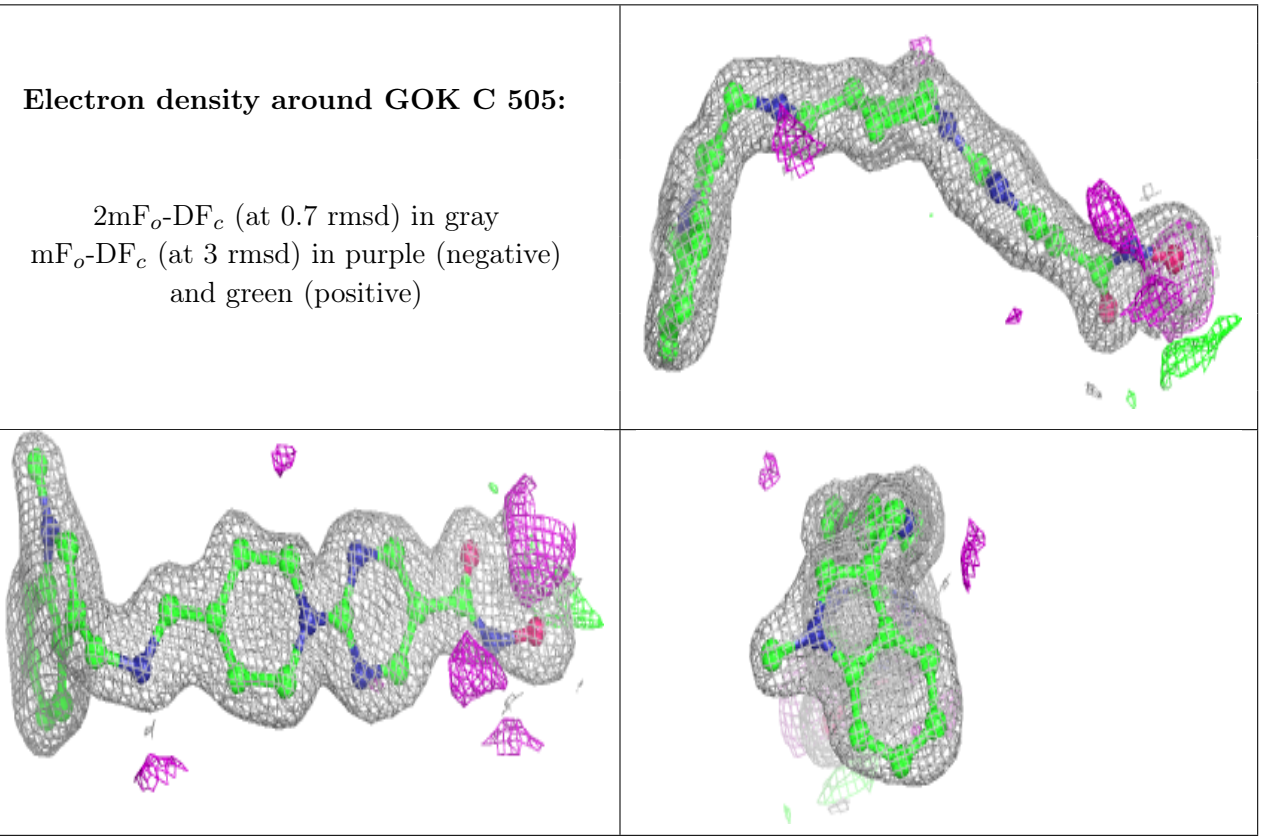
Electron density around GOK B 505:

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



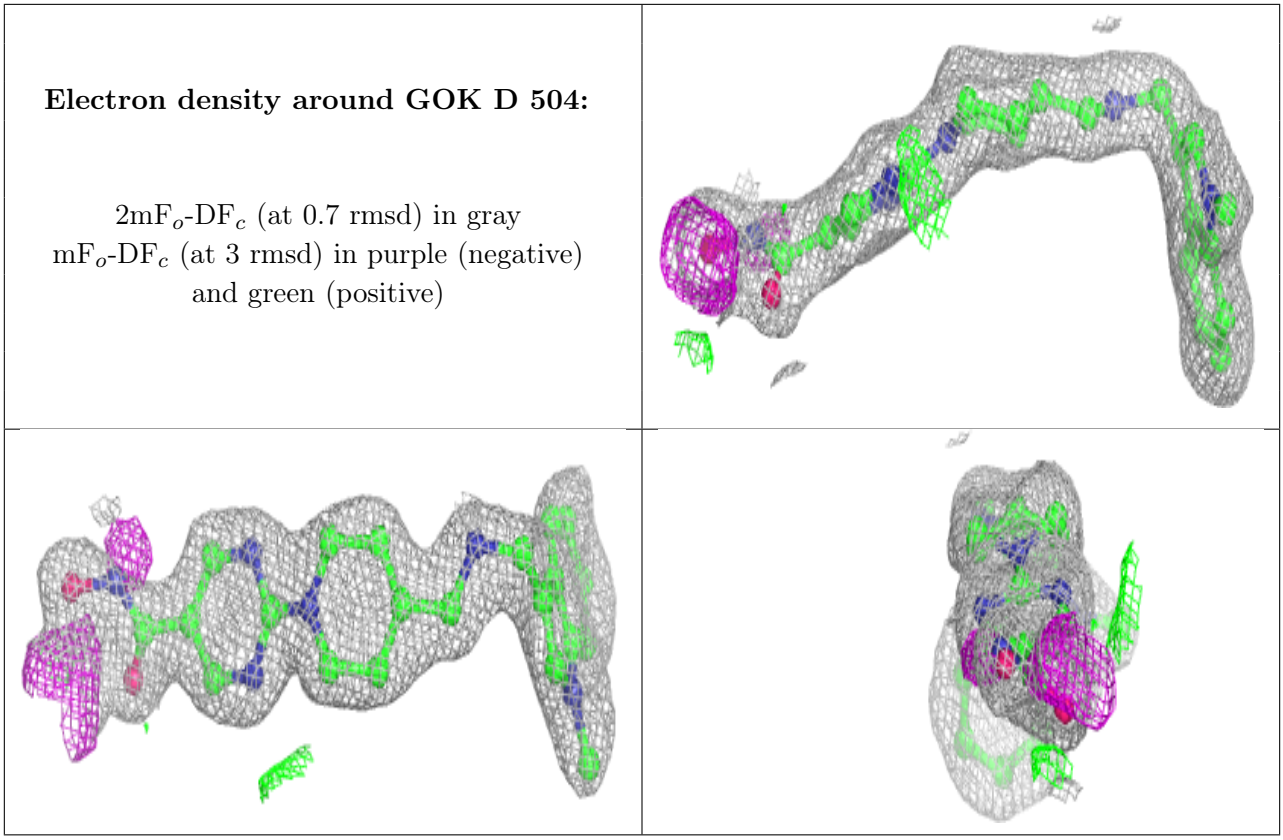
Electron density around GOK C 505:

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



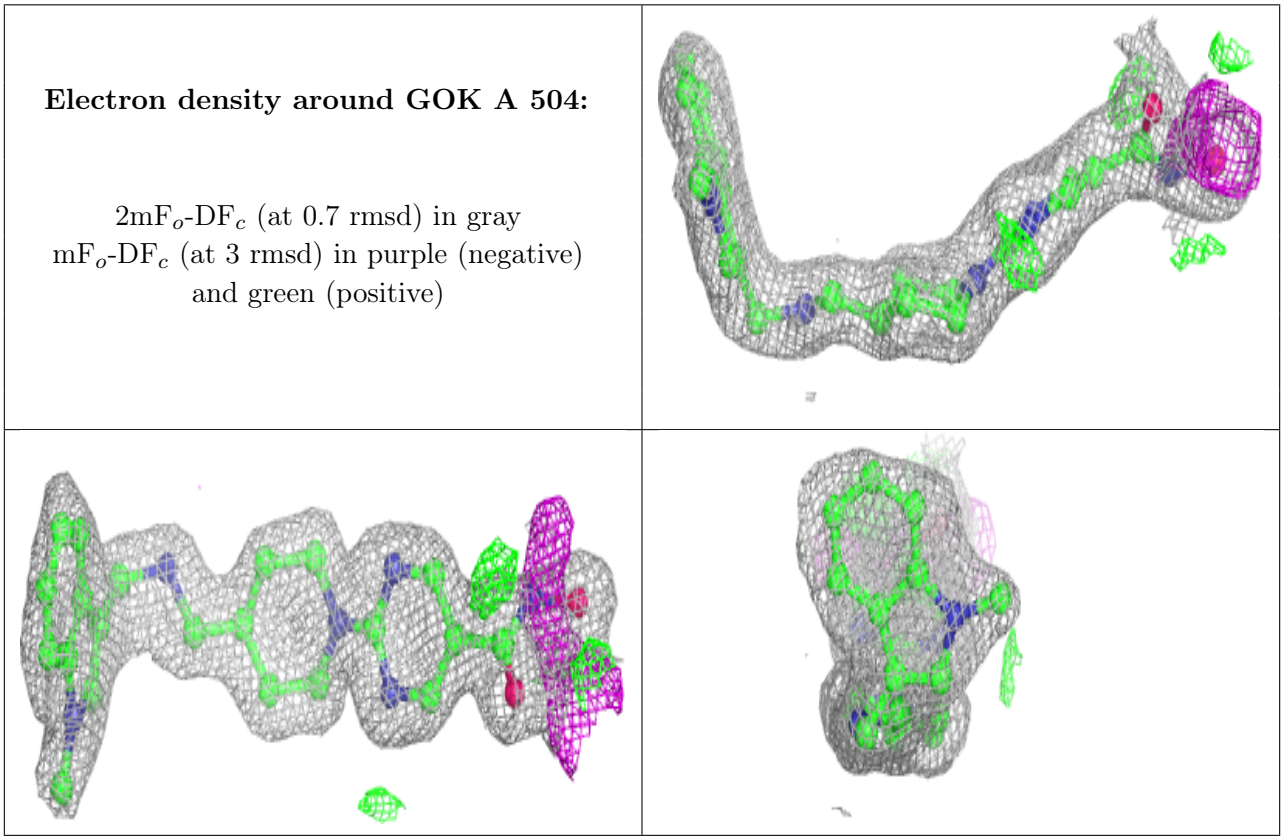
Electron density around GOK D 504:

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



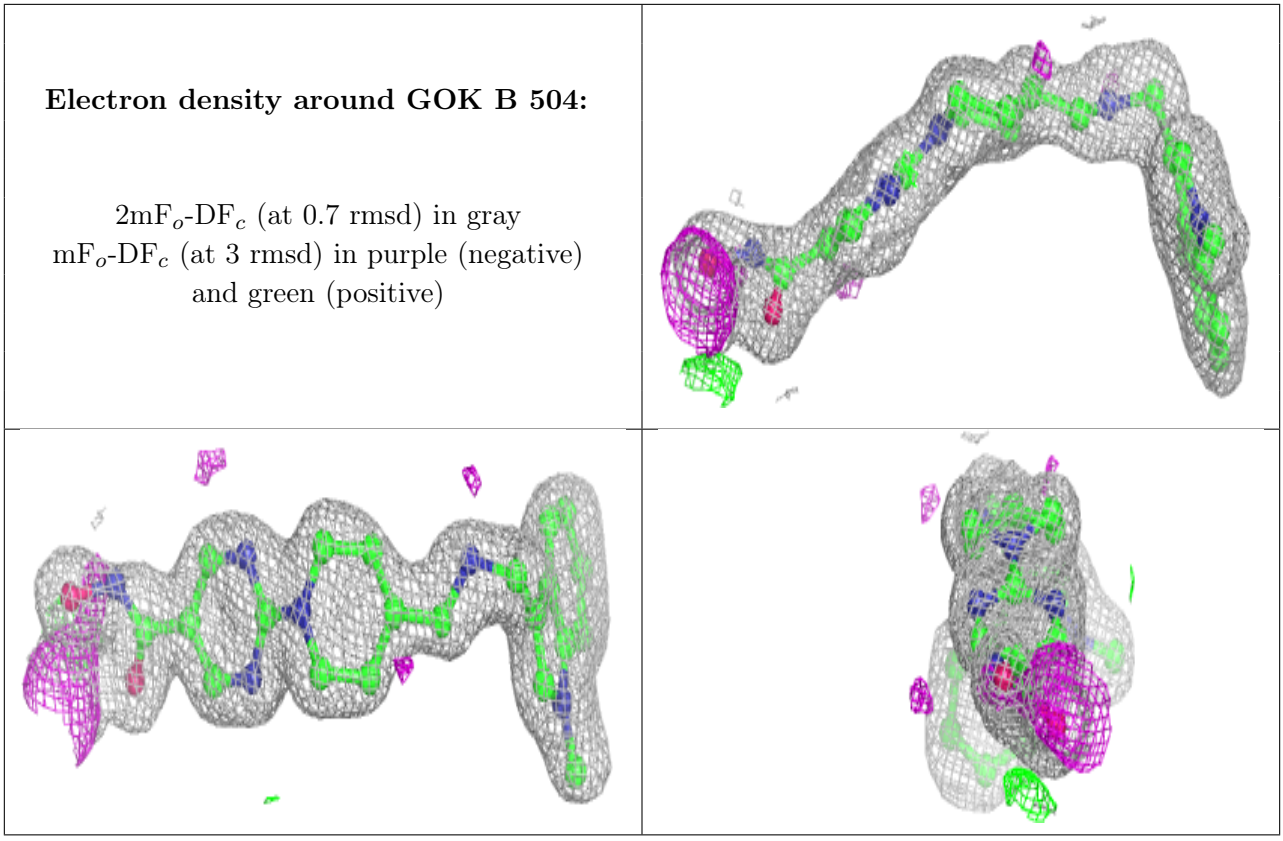
Electron density around GOK A 504:

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



Electron density around GOK B 504:

$2mF_o$-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.