Full wwPDB X-ray Structure Validation Report ⓘ

Jan 13, 2024 – 05:15 pm GMT

PDB ID	:	6HT8
Title	:	Crystal structure of Schistosoma mansoni HDAC8 complexed with a benzohydroxamate inhibitor 3
Authors	:	Marek, M.; Shaik, T.B.; Romier, C.
Deposited on	:	2018-10-03
Resolution	:	2.50 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:

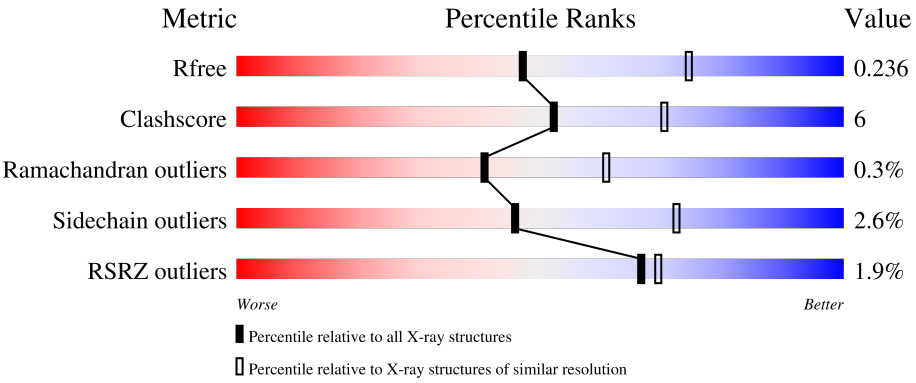
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	3% 77% 11% • 11%
1	B	447	% 80% 11% • 7%
1	C	447	81% 10% • 8%
1	D	447	2% 75% 13% • 11%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	A	505	-	-	X	-
5	GOL	A	506	-	-	X	-
5	GOL	B	506	-	-	X	-
5	GOL	B	508	-	-	X	-
5	GOL	C	505	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 13631 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	398	Total	C	N	O	S	0	0	0
			3188	2058	531	585	14			
1	B	414	Total	C	N	O	S	0	0	0
			3305	2128	553	609	15			
1	C	411	Total	C	N	O	S	0	1	0
			3289	2124	550	600	15			
1	D	398	Total	C	N	O	S	0	1	0
			3191	2060	531	585	15			

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

Continued on next page...

Continued from previous page...

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

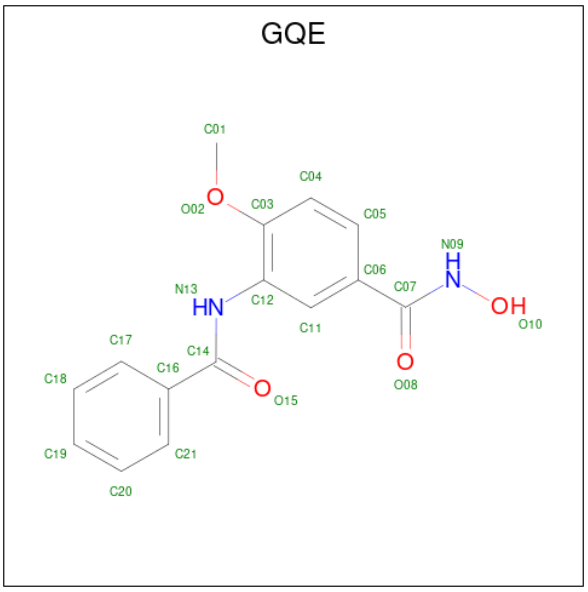
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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).

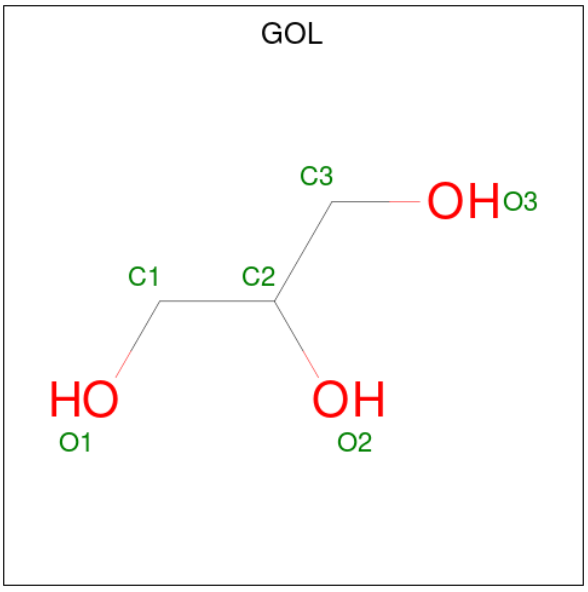
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total K 2 2	0	0
3	B	2	Total K 2 2	0	0
3	C	2	Total K 2 2	0	0
3	D	2	Total K 2 2	0	0

- Molecule 4 is 3-benzamido-4-methoxy- {N}-oxidanyl-benzamide (three-letter code: GQE) (formula: $C_{15}H_{14}N_2O_4$).



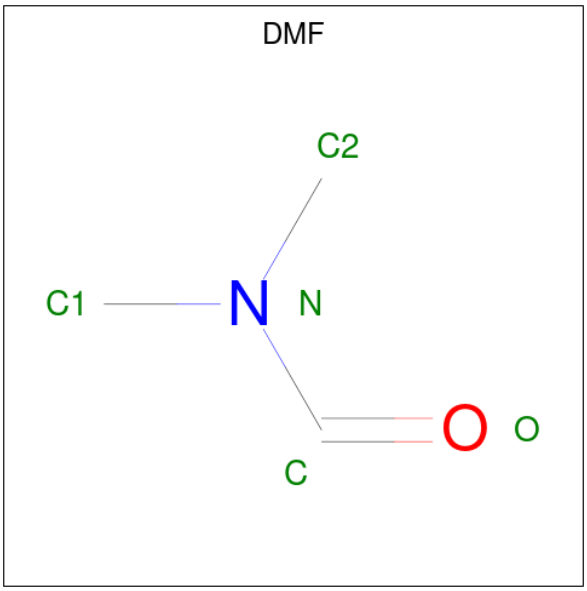
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			21	15	2	4		
4	B	1	Total	C	N	O	0	0
			21	15	2	4		
4	C	1	Total	C	N	O	0	0
			21	15	2	4		
4	D	1	Total	C	N	O	0	0
			21	15	2	4		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is DIMETHYLFORMAMIDE (three-letter code: DMF) (formula: C_3H_7NO).



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

Continued on next page...

Continued from previous page...

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

- Molecule 7 is water.

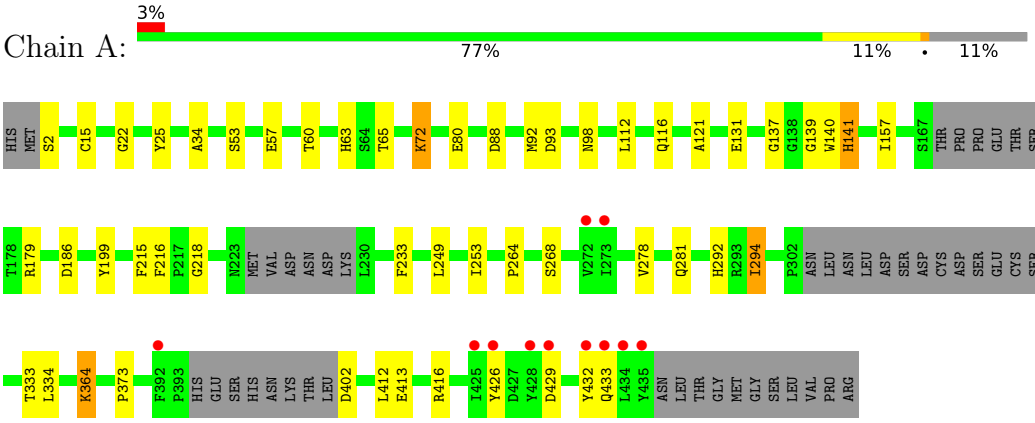
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	98	Total	O	0	0
			98	98		
7	B	133	Total	O	0	0
			133	133		
7	C	139	Total	O	0	0
			139	139		
7	D	104	Total	O	0	0
			104	104		

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.

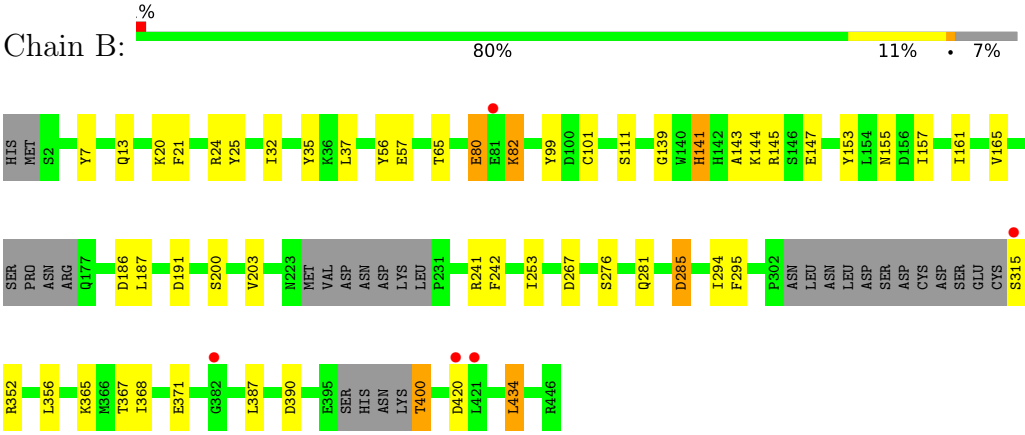
• Molecule 1: Histone deacetylase

Chain A:



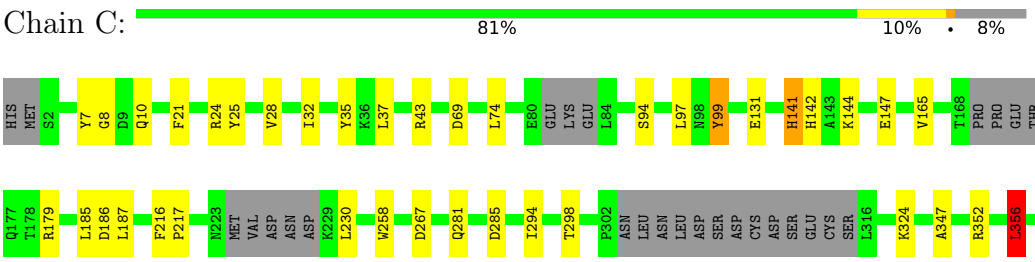
• Molecule 1: Histone deacetylase

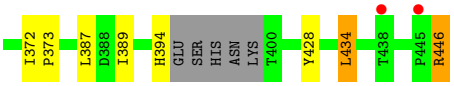
Chain B:



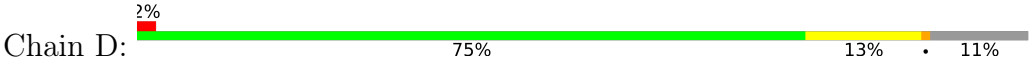
• Molecule 1: Histone deacetylase

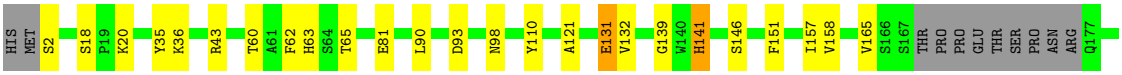
Chain C:

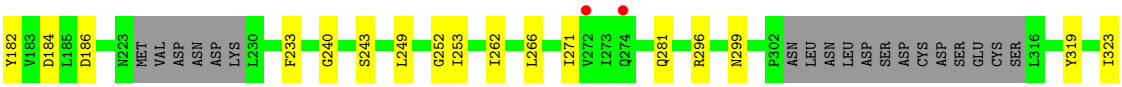


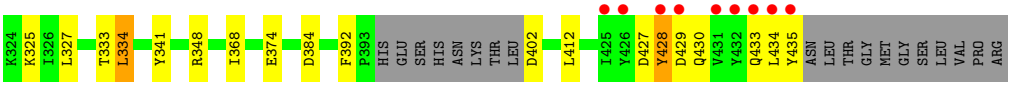


• Molecule 1: Histone deacetylase









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	70.79Å 70.92Å 98.34Å 77.90° 75.58° 85.33°	Depositor
Resolution (Å)	35.62 – 2.50 49.88 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.7 (35.62-2.50) 97.8 (49.88-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 2.48Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.158 , 0.235 0.158 , 0.236	Depositor DCC
R_{free} test set	3125 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	25.7	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 62.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.116 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13631	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 4.85% 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: GQE, DMF, ZN, K, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.53	0/3278	0.65	0/4459
1	B	0.58	0/3397	0.68	1/4620 (0.0%)
1	C	0.59	0/3384	0.68	2/4603 (0.0%)
1	D	0.53	0/3284	0.65	1/4467 (0.0%)
All	All	0.56	0/13343	0.66	4/18149 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	356	LEU	CA-CB-CG	6.28	129.73	115.30
1	C	434	LEU	CB-CG-CD1	-5.25	102.08	111.00
1	B	434	LEU	CB-CG-CD2	-5.16	102.23	111.00
1	D	334	LEU	CA-CB-CG	5.07	126.96	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	400	THR	Peptide

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	3188	0	3081	37	0
1	B	3305	0	3199	42	0
1	C	3289	0	3194	32	0
1	D	3191	0	3086	33	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
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	21	0	0	0	0
4	B	21	0	0	0	0
4	C	21	0	0	1	0
4	D	21	0	0	0	0
5	A	18	0	24	10	0
5	B	24	0	31	13	0
5	C	6	0	8	4	0
6	A	10	0	14	0	0
6	B	10	0	14	1	0
6	C	10	0	14	2	0
6	D	10	0	14	0	0
7	A	98	0	0	2	0
7	B	133	0	0	2	0
7	C	139	0	0	5	0
7	D	104	0	0	3	0
All	All	13631	0	12679	143	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 6.

All (143) 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:21:PHE:HB3	5:B:506:GOL:H11	1.48	0.94
1:C:24:ARG:HB3	5:C:505:GOL:H31	1.51	0.91
1:A:15:CYS:HB3	5:A:506:GOL:H32	1.65	0.79
1:B:24:ARG:HE	5:B:506:GOL:H32	1.45	0.79
1:B:24:ARG:HB3	5:B:506:GOL:H12	1.68	0.75
1:C:21:PHE:HB3	5:C:505:GOL:H32	1.68	0.75
1:A:249:LEU:HD13	1:A:253:ILE:HD13	1.68	0.74
1:A:216:PHE:O	5:A:505:GOL:H32	1.85	0.73
1:C:69:ASP:OD2	7:C:601:HOH:O	2.04	0.73
1:A:137:GLY:HA2	5:A:506:GOL:H31	1.73	0.71
1:C:230:LEU:HD21	1:D:81:GLU:HG3	1.72	0.71
1:D:374:GLU:OE2	7:D:601:HOH:O	2.12	0.67
1:B:20:LYS:HE2	1:B:341:TYR:HE2	1.59	0.67
1:A:25:TYR:HB2	5:A:506:GOL:H11	1.77	0.65
5:C:505:GOL:O1	7:C:602:HOH:O	2.12	0.64
1:D:412:LEU:HD21	1:D:428:TYR:HE1	1.63	0.64
1:C:131:GLU:HB3	6:C:506:DMF:H12	1.80	0.64
1:B:191:ASP:OD2	7:B:601:HOH:O	2.15	0.63
1:C:35:TYR:CE1	1:C:368:ILE:HG23	2.33	0.63
1:D:2:SER:N	1:D:131:GLU:OE2	2.32	0.62
1:B:35:TYR:CE1	1:B:368:ILE:HG23	2.34	0.62
1:B:267:ASP:HB3	1:B:434:LEU:HD21	1.82	0.61
1:C:186:ASP:HB2	1:C:281:GLN:OE1	2.02	0.60
1:B:24:ARG:HB3	5:B:506:GOL:C1	2.31	0.60
1:A:218:GLY:HA2	5:A:505:GOL:H12	1.85	0.59
1:A:264:PRO:O	1:A:268:SER:OG	2.21	0.58
1:D:252:GLY:O	1:D:296:ARG:HD2	2.02	0.58
1:C:187:LEU:HD21	1:C:294:ILE:HD12	1.86	0.57
1:A:139:GLY:HA2	1:A:157:ILE:HD11	1.86	0.57
1:A:317:SER:HB3	1:A:320:LEU:HG	1.86	0.57
1:A:177:GLN:HE21	1:A:179:ARG:HH11	1.51	0.57
1:D:249:LEU:HD13	1:D:253:ILE:HD13	1.87	0.56
1:C:144:LYS:HB2	1:C:147:GLU:HB3	1.88	0.56
1:B:24:ARG:NE	5:B:506:GOL:H32	2.20	0.56
1:B:143:ALA:HB3	1:B:155:ASN:HB2	1.88	0.56
1:A:429:ASP:O	1:A:433:GLN:HG2	2.06	0.56
1:B:20:LYS:HE2	1:B:341:TYR:CE2	2.41	0.56
1:A:218:GLY:CA	5:A:505:GOL:H12	2.36	0.55
1:D:412:LEU:HD12	1:D:435:TYR:CE1	2.41	0.55
1:C:25:TYR:HB2	5:C:505:GOL:H2	1.88	0.54
1:B:186:ASP:HB2	1:B:281:GLN:OE1	2.08	0.54
1:A:2:SER:N	1:A:131:GLU:OE1	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:SER:O	1:A:57:GLU:HG3	2.09	0.53
1:D:20:LYS:HE2	1:D:341:TYR:CE1	2.44	0.53
1:B:101:CYS:HB3	1:B:153:TYR:CE2	2.44	0.52
1:B:420:ASP:OD2	7:B:602:HOH:O	2.19	0.52
1:D:427:ASP:OD2	1:D:430:GLN:N	2.29	0.52
1:D:429:ASP:O	1:D:433:GLN:HG2	2.10	0.51
1:A:215:PHE:HD2	5:A:505:GOL:H31	1.76	0.51
1:D:43:ARG:O	7:D:602:HOH:O	2.18	0.51
1:B:267:ASP:CB	1:B:434:LEU:HD21	2.40	0.50
1:A:60:THR:HA	1:A:63:HIS:O	2.11	0.50
1:A:121:ALA:HB1	1:A:334:LEU:HD11	1.93	0.50
1:A:186:ASP:HB2	1:A:281:GLN:OE1	2.12	0.50
1:B:35:TYR:CD1	1:B:368:ILE:HG23	2.46	0.50
1:B:80:GLU:HB2	1:B:82:LYS:H	1.77	0.49
1:A:215:PHE:CD2	5:A:505:GOL:H31	2.47	0.49
1:C:74:LEU:HD22	1:C:97:LEU:HD13	1.95	0.49
1:A:292:HIS:HB3	1:A:294:ILE:HG13	1.94	0.49
1:D:186:ASP:HB2	1:D:281:GLN:OE1	2.12	0.49
1:D:299:ASN:ND2	1:D:348:ARG:HB3	2.28	0.49
1:A:413:GLU:HG3	1:A:416:ARG:HH21	1.78	0.49
1:A:93:ASP:HA	1:A:98:ASN:ND2	2.28	0.48
1:C:359:GLU:OE1	7:C:604:HOH:O	2.20	0.48
1:B:187:LEU:HD21	1:B:294:ILE:HD12	1.94	0.48
1:B:111:SER:OG	1:B:153:TYR:HB2	2.14	0.47
1:B:390:ASP:HB2	5:B:508:GOL:H32	1.96	0.47
1:B:80:GLU:HB2	1:B:82:LYS:HB2	1.97	0.47
1:C:141:HIS:CD2	1:C:141:HIS:H	2.32	0.47
1:D:141:HIS:H	1:D:141:HIS:CD2	2.33	0.47
1:A:72:LYS:O	1:A:72:LYS:HD3	2.13	0.47
1:C:356:LEU:HD22	1:C:360:GLU:HG2	1.96	0.47
1:B:25:TYR:HB2	5:B:506:GOL:H2	1.97	0.47
1:D:60:THR:HA	1:D:63:HIS:O	2.15	0.47
1:B:7:TYR:CD2	6:B:509:DMF:H13	2.50	0.47
1:B:141:HIS:HB3	1:B:157:ILE:HD12	1.98	0.46
1:B:352:ARG:NH2	5:B:507:GOL:O3	2.48	0.46
1:B:390:ASP:CB	5:B:508:GOL:H32	2.46	0.46
1:B:161:ILE:HG21	1:B:203:VAL:HG11	1.98	0.46
1:D:384:ASP:HB2	7:D:666:HOH:O	2.14	0.46
1:C:32:ILE:HG23	1:C:37:LEU:HB2	1.98	0.46
1:C:216:PHE:HA	1:C:217:PRO:HA	1.74	0.45
1:C:267:ASP:HB3	1:C:434:LEU:HD11	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ARG:HG3	1:A:426:TYR:OH	2.17	0.45
1:B:253:ILE:HG22	1:B:295:PHE:CD1	2.51	0.45
1:D:62:PHE:CD1	1:D:158:VAL:HG11	2.51	0.45
1:A:141:HIS:H	1:A:141:HIS:CD2	2.35	0.45
1:B:139:GLY:HA2	1:B:157:ILE:HD11	1.98	0.45
1:B:390:ASP:H	5:B:508:GOL:C3	2.29	0.45
1:C:428:TYR:CD1	1:C:446:ARG:HA	2.52	0.45
1:A:80:GLU:HB2	7:A:648:HOH:O	2.16	0.45
1:D:132:VAL:HA	1:D:333:THR:O	2.17	0.45
1:A:199:TYR:CG	1:C:394:HIS:HA	2.52	0.44
1:D:18:SER:HB3	1:D:110:TYR:CE1	2.51	0.44
1:D:139:GLY:HA2	1:D:157:ILE:HD11	1.99	0.44
1:A:60:THR:HG21	1:A:65:THR:HB	1.99	0.44
1:A:88:ASP:O	1:A:92:MET:HG2	2.17	0.44
1:C:267:ASP:CB	1:C:434:LEU:HD11	2.48	0.44
1:C:352:ARG:HD3	6:C:507:DMF:H11	1.99	0.44
1:B:365:LYS:HE3	1:B:367:THR:OG1	2.18	0.44
1:D:35:TYR:CE1	1:D:368:ILE:HG23	2.52	0.44
1:A:278:VAL:O	1:A:333:THR:HA	2.18	0.44
1:B:32:ILE:HG23	1:B:37:LEU:HB2	1.99	0.43
1:C:99:TYR:OH	7:C:603:HOH:O	2.15	0.43
1:D:319:TYR:O	1:D:323:ILE:HG12	2.19	0.43
1:B:241:ARG:HG2	1:B:242:PHE:CE2	2.53	0.43
1:D:62:PHE:CG	1:D:158:VAL:HG11	2.54	0.43
1:C:185:LEU:HD22	1:C:258:TRP:CH2	2.54	0.43
1:D:121:ALA:HB1	1:D:334:LEU:HD13	2.01	0.43
1:D:20:LYS:HD2	1:D:151:PHE:CG	2.54	0.42
1:A:215:PHE:O	5:A:505:GOL:H11	2.19	0.42
1:A:364:LYS:HA	7:A:656:HOH:O	2.18	0.42
1:D:93:ASP:HA	1:D:98:ASN:ND2	2.34	0.42
1:C:7[B]:TYR:CG	1:C:8:GLY:N	2.88	0.42
1:C:324:LYS:HB2	1:C:324:LYS:HE2	1.57	0.42
1:A:121:ALA:CB	1:A:334:LEU:HD11	2.50	0.42
1:D:240:GLY:O	1:D:243:SER:OG	2.37	0.42
1:B:24:ARG:HH21	5:B:506:GOL:H32	1.84	0.42
1:B:368:ILE:CG2	1:B:387:LEU:HD22	2.50	0.42
1:C:28:VAL:HG22	1:C:347:ALA:HA	2.01	0.42
1:C:142:HIS:NE2	4:C:504:GQE:N09	2.67	0.42
1:D:36:LYS:HA	1:D:36:LYS:HD3	1.88	0.41
1:B:390:ASP:H	5:B:508:GOL:H32	1.85	0.41
1:D:90:LEU:HD12	1:D:90:LEU:HA	1.78	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:TRP:HZ2	5:A:506:GOL:H2	1.85	0.41
1:B:144:LYS:HB2	1:B:147:GLU:HB3	2.03	0.41
1:C:298:THR:HA	1:C:389:ILE:HD11	2.02	0.41
1:C:372:ILE:HA	1:C:373:PRO:HD3	1.94	0.41
1:A:112:LEU:O	1:A:116:GLN:HG3	2.19	0.41
1:C:179:ARG:HD2	7:C:622:HOH:O	2.19	0.41
1:B:157:ILE:HG12	1:B:336:LEU:HD13	2.02	0.41
1:C:368:ILE:HG21	1:C:387:LEU:CD2	2.51	0.41
1:A:412:LEU:HD21	1:A:432:TYR:CD2	2.55	0.41
1:B:285:ASP:OD1	1:B:285:ASP:N	2.54	0.41
1:A:34:ALA:HB1	1:A:373:PRO:HG2	2.02	0.41
1:D:266:LEU:HD12	1:D:325:LYS:HD2	2.03	0.41
1:D:182:TYR:CE2	1:D:184:ASP:HB2	2.56	0.41
1:B:56:TYR:OH	1:B:65:THR:HB	2.21	0.40
1:D:327:LEU:HA	1:D:327:LEU:HD23	1.72	0.40
1:B:157:ILE:HG12	1:B:336:LEU:CD1	2.51	0.40
1:B:368:ILE:O	5:B:507:GOL:H11	2.21	0.40
1:D:271:ILE:HD12	1:D:434:LEU:HD11	2.02	0.40
1:C:7[A]:TYR:CE2	1:C:43:ARG:HD3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	388/447 (87%)	377 (97%)	10 (3%)	1 (0%)	41	61
1	B	404/447 (90%)	396 (98%)	6 (2%)	2 (0%)	29	48
1	C	400/447 (90%)	389 (97%)	10 (2%)	1 (0%)	41	61
1	D	389/447 (87%)	373 (96%)	16 (4%)	0	100	100
All	All	1581/1788 (88%)	1535 (97%)	42 (3%)	4 (0%)	41	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	99	TYR
1	B	82	LYS
1	C	99	TYR
1	A	22	GLY

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	345/392 (88%)	339 (98%)	6 (2%)	60	82
1	B	359/392 (92%)	346 (96%)	13 (4%)	35	61
1	C	357/392 (91%)	350 (98%)	7 (2%)	55	79
1	D	346/392 (88%)	336 (97%)	10 (3%)	42	69
All	All	1407/1568 (90%)	1371 (97%)	36 (3%)	46	72

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LYS
1	A	141	HIS
1	A	233	PHE
1	A	294	ILE
1	A	364	LYS
1	A	402	ASP
1	B	13	GLN
1	B	57	GLU
1	B	80	GLU
1	B	141	HIS
1	B	145	ARG
1	B	165	VAL
1	B	200	SER
1	B	276	SER
1	B	285	ASP
1	B	315	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	356	LEU
1	B	371	GLU
1	B	400	THR
1	C	10	GLN
1	C	94	SER
1	C	141	HIS
1	C	165	VAL
1	C	285	ASP
1	C	356	LEU
1	C	446	ARG
1	D	65	THR
1	D	131	GLU
1	D	141	HIS
1	D	146	SER
1	D	165	VAL
1	D	233	PHE
1	D	262	ILE
1	D	392	PHE
1	D	402	ASP
1	D	428	TYR

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 12 are monoatomic - leaving 20 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	$\#\|Z\| > 2$
4	GQE	A	504	2	22,22,22	2.17	3 (13%)	29,29,29	2.13	8 (27%)
5	GOL	A	506	-	5,5,5	0.45	0	5,5,5	0.78	0
6	DMF	A	508	-	4,4,4	0.33	0	4,4,4	0.26	0
6	DMF	B	510	-	4,4,4	0.35	0	4,4,4	0.19	0
4	GQE	B	504	2	22,22,22	2.30	4 (18%)	29,29,29	2.62	9 (31%)
6	DMF	D	505	-	4,4,4	0.37	0	4,4,4	0.41	0
5	GOL	A	505	-	5,5,5	0.58	0	5,5,5	1.47	1 (20%)
5	GOL	B	507	-	5,5,5	0.51	0	5,5,5	1.02	0
6	DMF	D	506	-	4,4,4	0.34	0	4,4,4	0.33	0
4	GQE	C	504	2	22,22,22	2.07	3 (13%)	29,29,29	2.42	6 (20%)
6	DMF	C	507	-	4,4,4	0.34	0	4,4,4	0.51	0
5	GOL	C	505	-	5,5,5	0.46	0	5,5,5	0.91	0
6	DMF	A	509	-	4,4,4	0.37	0	4,4,4	0.32	0
5	GOL	B	506	-	5,5,5	0.26	0	5,5,5	0.96	0
5	GOL	B	505	-	5,5,5	0.34	0	5,5,5	1.02	0
6	DMF	C	506	-	4,4,4	0.40	0	4,4,4	0.08	0
4	GQE	D	504	2	22,22,22	2.22	3 (13%)	29,29,29	1.82	5 (17%)
5	GOL	B	508	-	5,5,5	0.37	0	5,5,5	0.51	0
6	DMF	B	509	-	4,4,4	0.38	0	4,4,4	0.35	0
5	GOL	A	507	-	5,5,5	0.50	0	5,5,5	0.34	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
4	GQE	A	504	2	-	2/16/16/16	0/2/2/2
5	GOL	A	506	-	-	2/4/4/4	-
6	DMF	A	508	-	-	0/2/2/2	-
6	DMF	B	510	-	-	2/2/2/2	-
4	GQE	B	504	2	-	2/16/16/16	0/2/2/2
6	DMF	D	505	-	-	0/2/2/2	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	505	-	-	2/4/4/4	-
5	GOL	B	507	-	-	2/4/4/4	-
6	DMF	D	506	-	-	2/2/2/2	-
4	GQE	C	504	2	-	5/16/16/16	0/2/2/2
6	DMF	C	507	-	-	0/2/2/2	-
5	GOL	C	505	-	-	4/4/4/4	-
6	DMF	A	509	-	-	0/2/2/2	-
5	GOL	B	506	-	-	4/4/4/4	-
5	GOL	B	505	-	-	2/4/4/4	-
6	DMF	C	506	-	-	2/2/2/2	-
4	GQE	D	504	2	-	2/16/16/16	0/2/2/2
5	GOL	B	508	-	-	4/4/4/4	-
6	DMF	B	509	-	-	0/2/2/2	-
5	GOL	A	507	-	-	0/4/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	504	GQE	C07-N09	8.97	1.44	1.32
4	B	504	GQE	C07-N09	8.94	1.44	1.32
4	A	504	GQE	C07-N09	8.69	1.44	1.32
4	C	504	GQE	C07-N09	8.19	1.43	1.32
4	D	504	GQE	O10-N09	-3.66	1.30	1.40
4	B	504	GQE	O10-N09	-3.58	1.31	1.40
4	C	504	GQE	O10-N09	-3.52	1.31	1.40
4	B	504	GQE	C14-N13	3.49	1.45	1.35
4	A	504	GQE	O10-N09	-3.45	1.31	1.40
4	A	504	GQE	C14-N13	3.12	1.44	1.35
4	C	504	GQE	C14-N13	3.01	1.43	1.35
4	D	504	GQE	C14-N13	2.73	1.43	1.35
4	B	504	GQE	C12-N13	2.22	1.46	1.41

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	504	GQE	O02-C03-C12	7.15	123.58	114.80
4	C	504	GQE	O02-C03-C12	7.12	123.54	114.80
4	B	504	GQE	C03-C12-N13	7.05	129.31	116.66
4	C	504	GQE	C03-C12-N13	6.80	128.85	116.66
4	A	504	GQE	C03-C12-N13	5.78	127.03	116.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	504	GQE	O02-C03-C12	5.45	121.49	114.80
4	D	504	GQE	C03-C12-N13	5.31	126.18	116.66
4	B	504	GQE	C06-C07-N09	4.89	124.00	116.16
4	D	504	GQE	O02-C03-C12	4.49	120.31	114.80
4	C	504	GQE	O02-C03-C04	-4.27	117.04	124.37
4	B	504	GQE	O02-C03-C04	-4.24	117.10	124.37
4	B	504	GQE	O08-C07-N09	-4.00	115.47	122.94
4	A	504	GQE	C06-C07-N09	3.87	122.36	116.16
4	B	504	GQE	C11-C12-N13	-3.53	112.56	121.90
4	C	504	GQE	C11-C12-N13	-3.48	112.70	121.90
4	A	504	GQE	O08-C07-N09	-3.23	116.92	122.94
4	D	504	GQE	C11-C12-N13	-3.21	113.42	121.90
4	A	504	GQE	C11-C12-N13	-3.19	113.48	121.90
4	C	504	GQE	C06-C07-N09	3.06	121.07	116.16
4	C	504	GQE	O08-C07-N09	-2.95	117.44	122.94
4	D	504	GQE	O08-C07-N09	-2.82	117.68	122.94
4	B	504	GQE	O15-C14-C16	-2.69	116.14	120.94
4	A	504	GQE	O02-C03-C04	-2.68	119.78	124.37
4	B	504	GQE	C16-C14-N13	2.68	121.81	115.92
4	D	504	GQE	C06-C07-N09	2.61	120.35	116.16
5	A	505	GOL	O3-C3-C2	2.59	122.61	110.20
4	A	504	GQE	C12-N13-C14	-2.57	119.89	126.93
4	B	504	GQE	C06-C11-C12	2.24	123.80	119.70
4	A	504	GQE	C16-C14-N13	2.21	120.79	115.92

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	505	GOL	O1-C1-C2-C3
5	B	505	GOL	O1-C1-C2-C3
5	B	506	GOL	O1-C1-C2-C3
5	B	508	GOL	O1-C1-C2-C3
5	B	508	GOL	C1-C2-C3-O3
5	C	505	GOL	O1-C1-C2-C3
5	C	505	GOL	C1-C2-C3-O3
5	C	505	GOL	O2-C2-C3-O3
6	B	510	DMF	O-C-N-C1
5	B	506	GOL	O1-C1-C2-O2
5	B	508	GOL	O2-C2-C3-O3
6	B	510	DMF	O-C-N-C2
6	C	506	DMF	O-C-N-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	506	GOL	O1-C1-C2-C3
5	B	506	GOL	C1-C2-C3-O3
5	B	507	GOL	O1-C1-C2-C3
6	C	506	DMF	O-C-N-C2
5	A	505	GOL	O1-C1-C2-O2
5	B	506	GOL	O2-C2-C3-O3
5	B	508	GOL	O1-C1-C2-O2
5	C	505	GOL	O1-C1-C2-O2
4	A	504	GQE	C03-C12-N13-C14
4	C	504	GQE	C03-C12-N13-C14
4	B	504	GQE	C03-C12-N13-C14
5	A	506	GOL	O1-C1-C2-O2
5	B	505	GOL	O1-C1-C2-O2
5	B	507	GOL	O1-C1-C2-O2
4	C	504	GQE	N13-C14-C16-C21
4	C	504	GQE	O15-C14-C16-C21
6	D	506	DMF	O-C-N-C1
4	D	504	GQE	C03-C12-N13-C14
4	A	504	GQE	C11-C12-N13-C14
4	D	504	GQE	C11-C12-N13-C14
6	D	506	DMF	O-C-N-C2
4	C	504	GQE	N13-C14-C16-C17
4	C	504	GQE	O15-C14-C16-C17
4	B	504	GQE	C11-C12-N13-C14

There are no ring outliers.

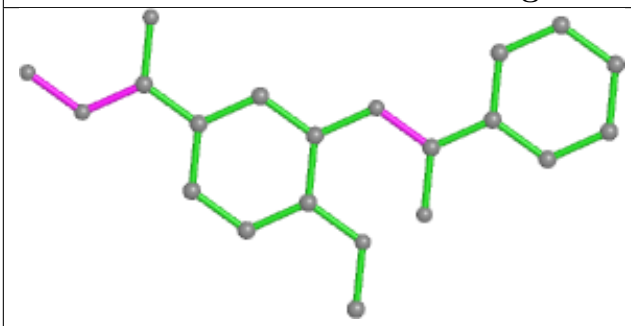
10 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	506	GOL	4	0
5	A	505	GOL	6	0
5	B	507	GOL	2	0
4	C	504	GQE	1	0
6	C	507	DMF	1	0
5	C	505	GOL	4	0
5	B	506	GOL	7	0
6	C	506	DMF	1	0
5	B	508	GOL	4	0
6	B	509	DMF	1	0

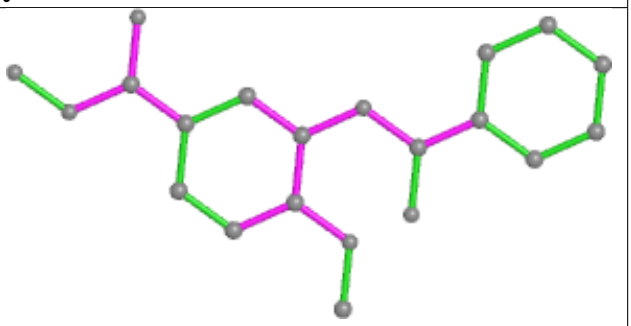
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

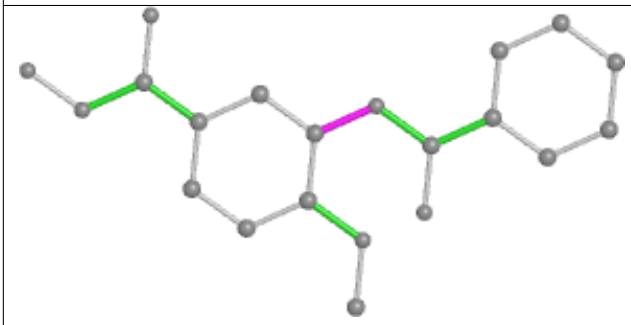
Ligand GQE A 504



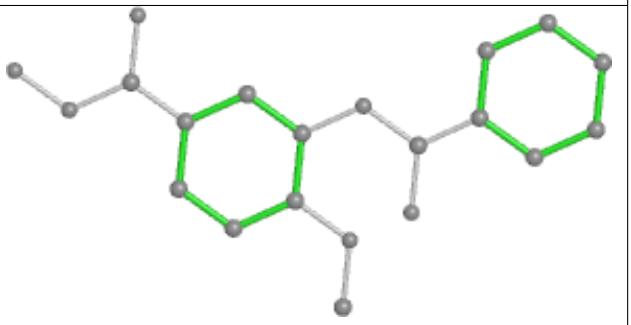
Bond lengths



Bond angles

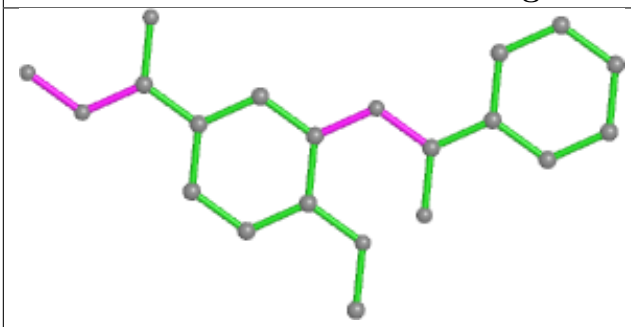


Torsions

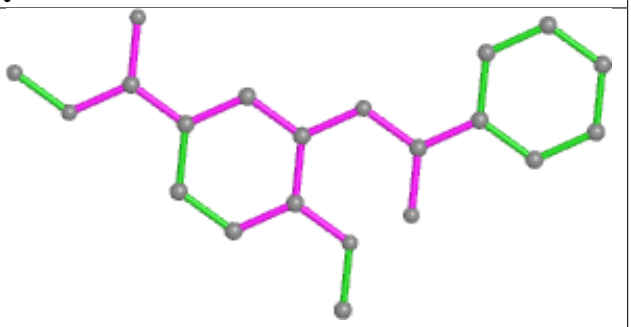


Rings

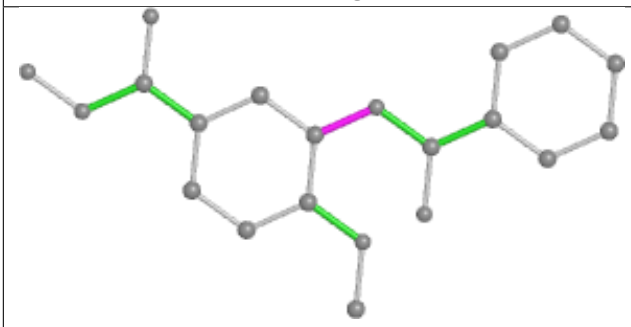
Ligand GQE B 504



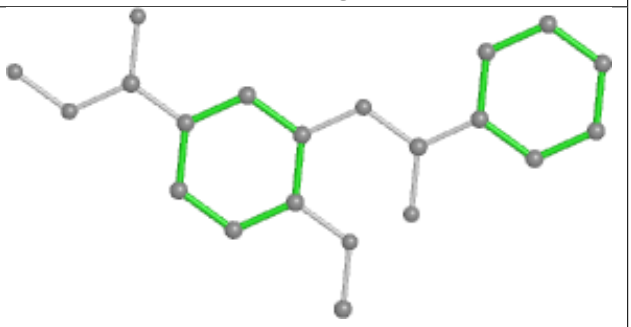
Bond lengths



Bond angles

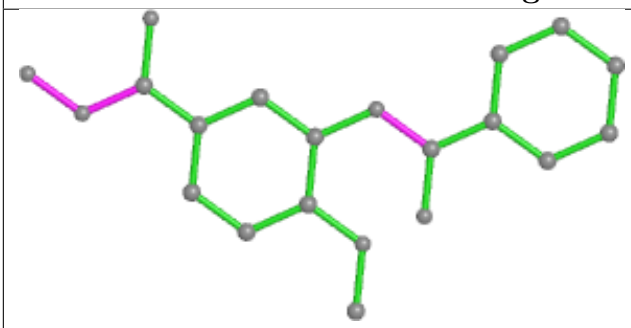


Torsions

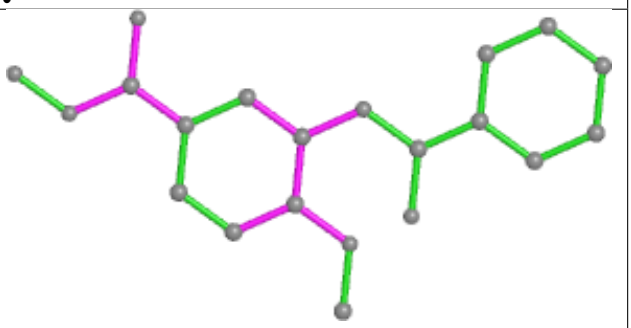


Rings

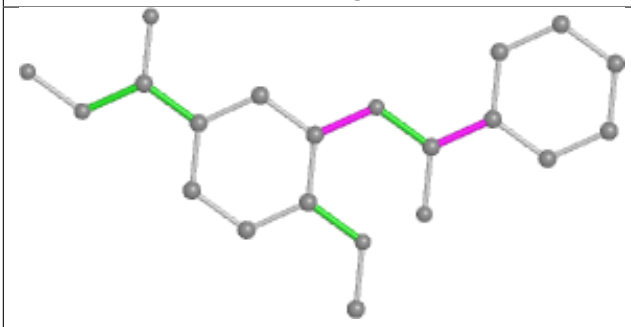
Ligand GQE C 504



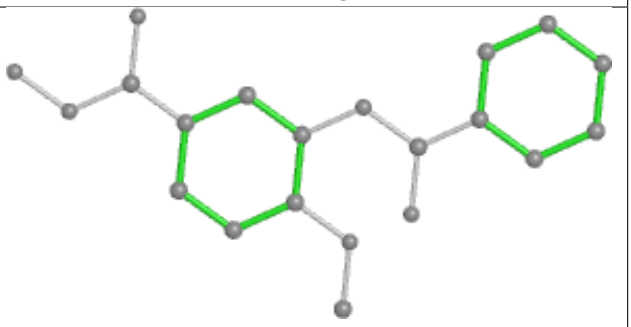
Bond lengths



Bond angles

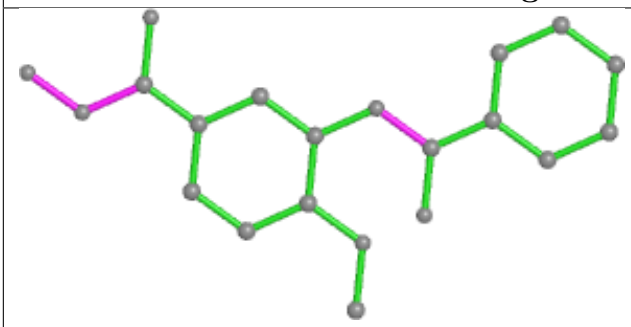


Torsions

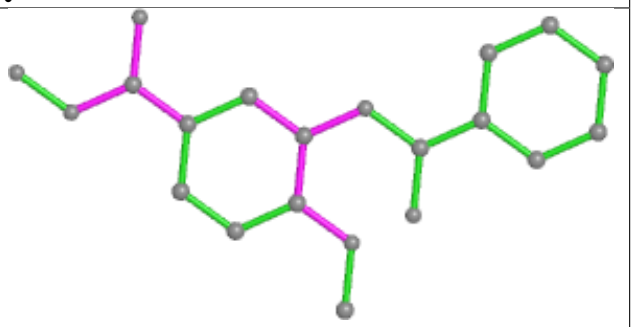


Rings

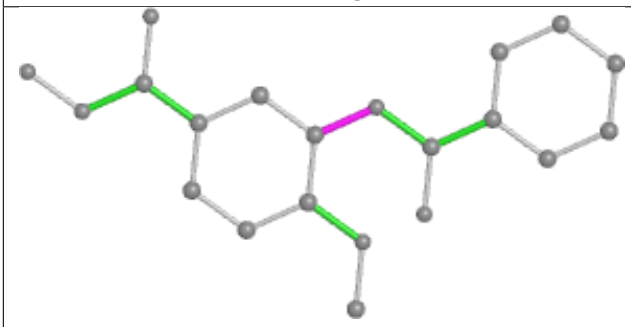
Ligand GQE D 504



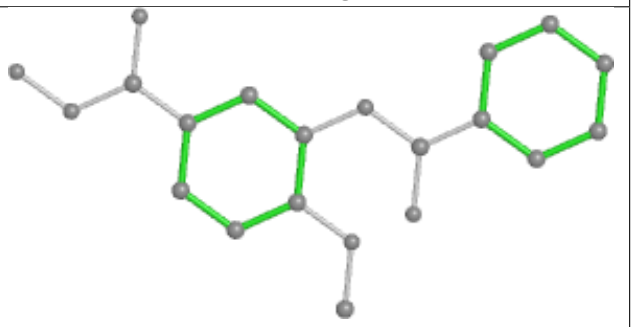
Bond lengths



Bond angles



Torsions



Rings

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	398/447 (89%)	-0.02	12 (3%) 50 53	12, 26, 60, 104	0
1	B	414/447 (92%)	-0.22	6 (1%) 75 77	10, 22, 46, 110	0
1	C	411/447 (91%)	-0.21	2 (0%) 91 91	9, 23, 47, 79	0
1	D	398/447 (89%)	-0.02	11 (2%) 53 56	12, 27, 58, 94	0
All	All	1621/1788 (90%)	-0.12	31 (1%) 66 69	9, 25, 52, 110	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	425	ILE	6.2
1	B	81	GLU	5.3
1	A	434	LEU	4.6
1	D	426	TYR	4.4
1	D	428	TYR	4.1
1	D	434	LEU	4.1
1	A	426	TYR	4.0
1	A	435	TYR	3.8
1	D	432	TYR	3.8
1	A	432	TYR	3.8
1	A	433	GLN	3.3
1	D	425	ILE	3.1
1	D	431	VAL	3.0
1	A	428	TYR	3.0
1	C	445	PRO	2.9
1	D	429	ASP	2.9
1	C	438	THR	2.9
1	D	435	TYR	2.8
1	A	429	ASP	2.6
1	B	382	GLY	2.3
1	D	433	GLN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	315	SER	2.2
1	A	392	PHE	2.2
1	D	272	VAL	2.2
1	B	168	THR	2.2
1	A	273	ILE	2.1
1	A	316	LEU	2.1
1	D	274	GLN	2.1
1	A	272	VAL	2.1
1	B	421	LEU	2.0
1	B	420	ASP	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
5	GOL	B	507	6/6	0.72	0.26	50,56,65,77	0
6	DMF	A	509	5/5	0.78	0.26	46,47,49,49	0
6	DMF	B	510	5/5	0.82	0.34	24,39,65,86	0
6	DMF	C	506	5/5	0.84	0.17	34,37,49,50	0
5	GOL	A	506	6/6	0.85	0.30	44,52,55,57	0
6	DMF	B	509	5/5	0.86	0.23	36,36,56,63	0
6	DMF	D	505	5/5	0.88	0.21	60,62,65,66	0
4	GQE	A	504	21/21	0.89	0.24	33,48,56,59	0
5	GOL	C	505	6/6	0.91	0.26	24,43,47,52	0
5	GOL	B	508	6/6	0.91	0.43	32,43,50,52	0
6	DMF	A	508	5/5	0.92	0.18	52,54,57,58	0
4	GQE	B	504	21/21	0.92	0.24	28,39,45,54	0
4	GQE	D	504	21/21	0.92	0.24	31,45,55,58	0

Continued on next page...

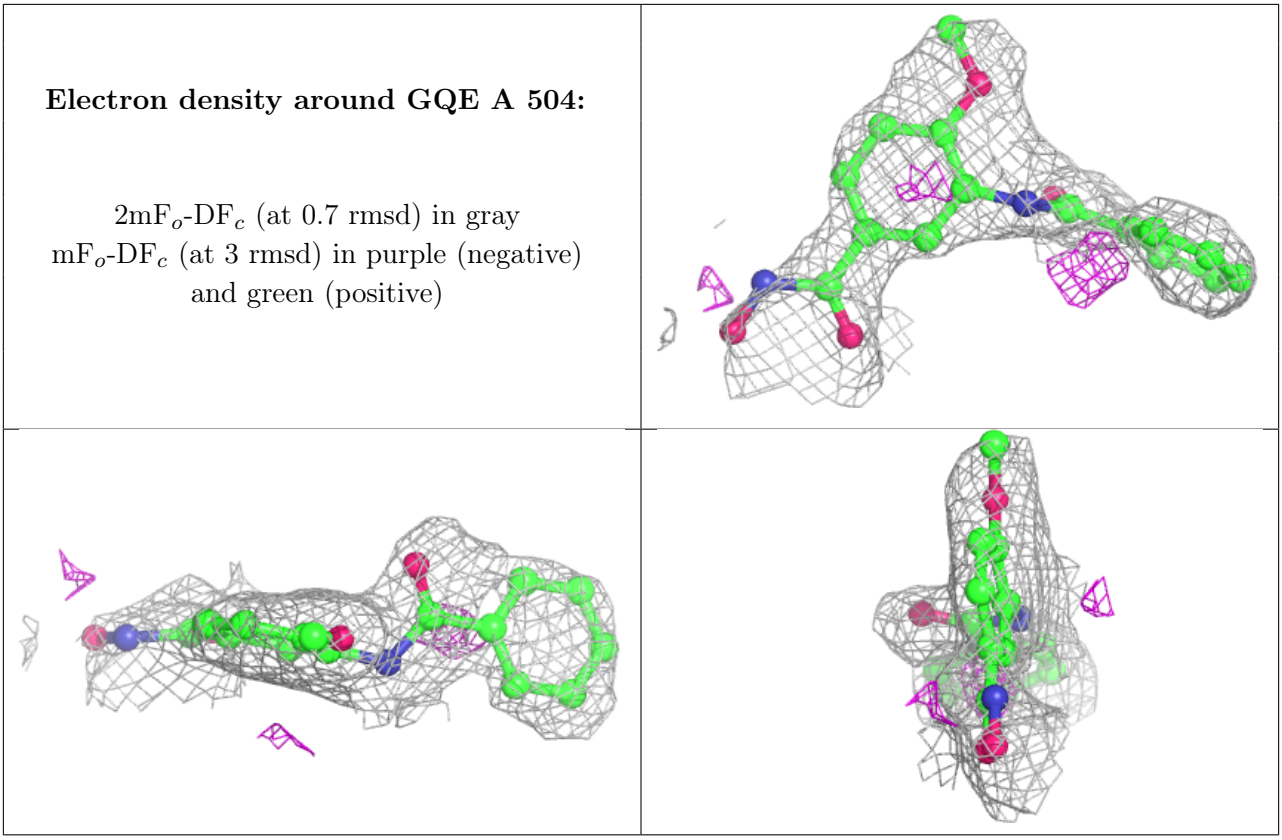
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GQE	C	504	21/21	0.93	0.19	26,34,44,50	0
5	GOL	B	506	6/6	0.94	0.32	25,44,51,53	0
6	DMF	C	507	5/5	0.94	0.19	41,42,49,51	0
5	GOL	B	505	6/6	0.94	0.13	22,26,32,35	0
6	DMF	D	506	5/5	0.94	0.17	51,57,59,61	0
5	GOL	A	507	6/6	0.95	0.18	33,39,41,43	0
5	GOL	A	505	6/6	0.95	0.26	12,23,33,34	0
3	K	B	502	1/1	0.97	0.11	21,21,21,21	0
3	K	C	502	1/1	0.97	0.10	20,20,20,20	0
3	K	A	503	1/1	0.99	0.06	25,25,25,25	0
2	ZN	A	501	1/1	0.99	0.07	28,28,28,28	0
3	K	B	503	1/1	0.99	0.09	18,18,18,18	0
3	K	A	502	1/1	0.99	0.09	25,25,25,25	0
3	K	D	502	1/1	0.99	0.10	21,21,21,21	0
2	ZN	B	501	1/1	1.00	0.06	26,26,26,26	0
2	ZN	C	501	1/1	1.00	0.07	23,23,23,23	0
3	K	C	503	1/1	1.00	0.10	21,21,21,21	0
2	ZN	D	501	1/1	1.00	0.06	26,26,26,26	0
3	K	D	503	1/1	1.00	0.07	23,23,23,23	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.

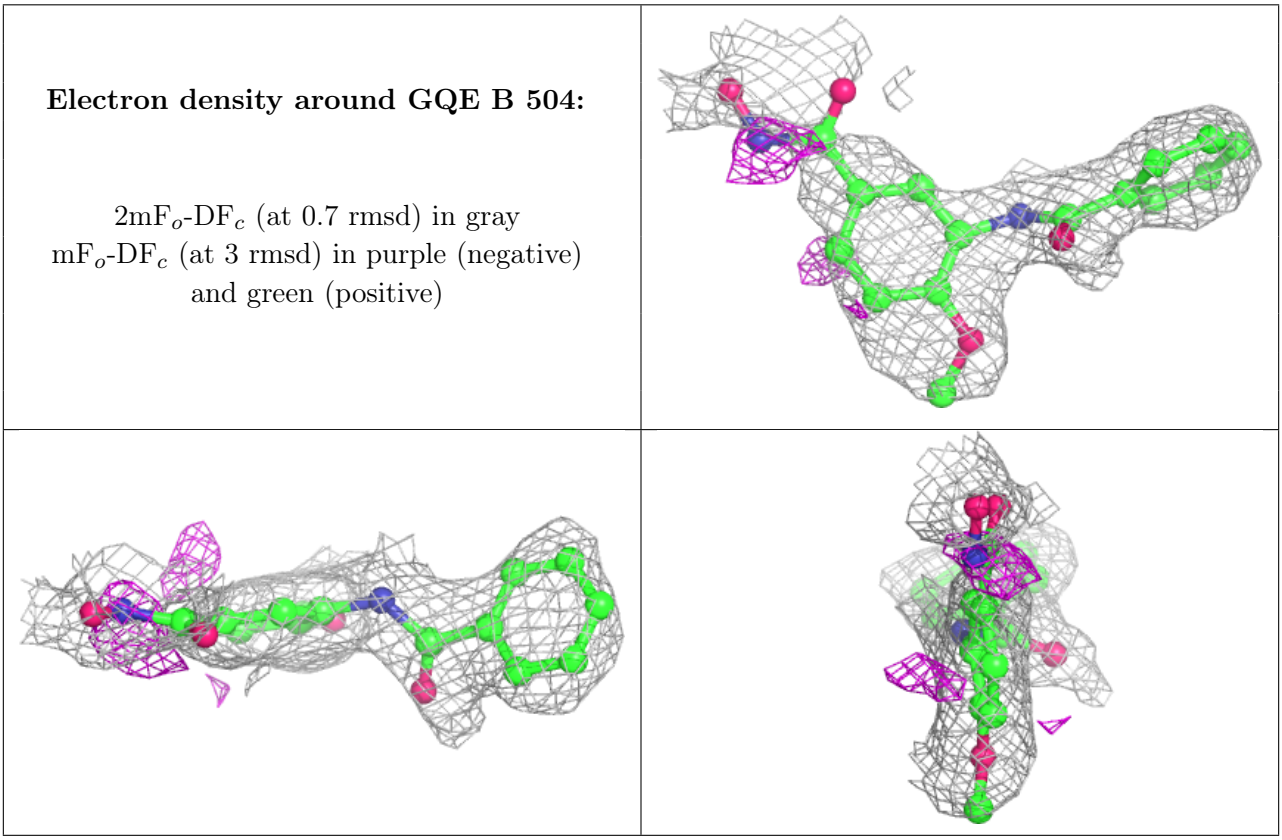
Electron density around GQE A 504:

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



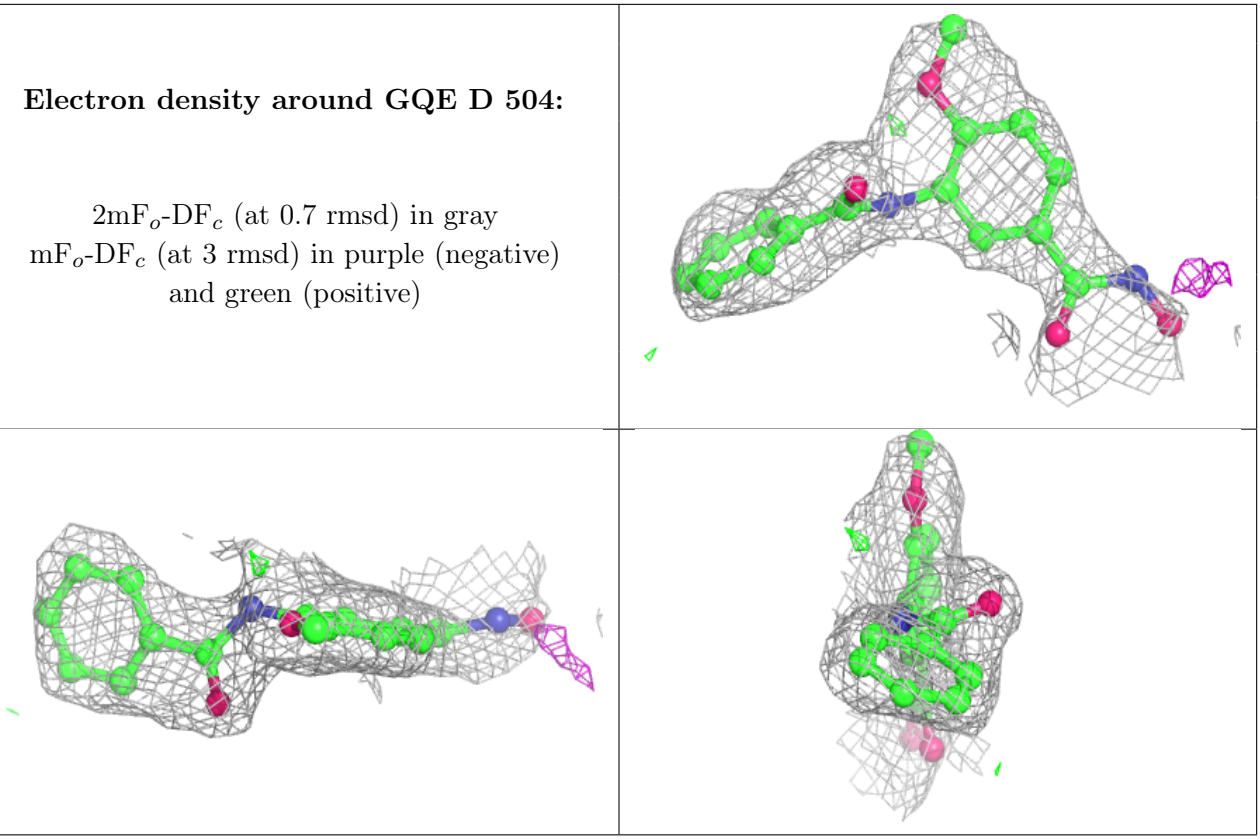
Electron density around GQE B 504:

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



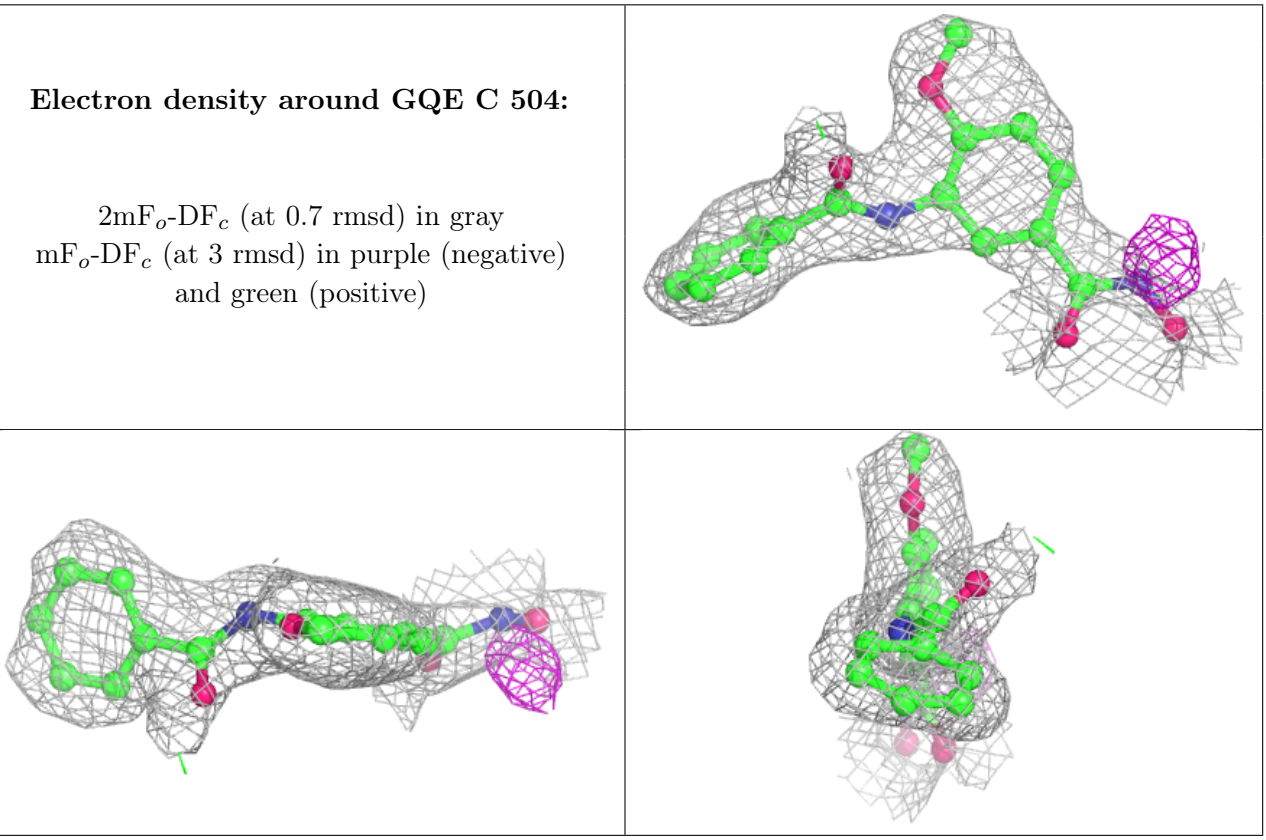
Electron density around GQE D 504:

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



Electron density around GQE C 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.