Full wwPDB X-ray Structure Validation Report ⓘ

Jan 15, 2024 – 09:18 pm GMT

PDB ID	:	6HTG
Title	:	Crystal structure of Schistosoma mansoni HDAC8 complexed with a benzohydroxamate inhibitor 4
Authors	:	Shaik, T.B.; Marek, M.; Romier, C.
Deposited on	:	2018-10-04
Resolution	:	1.94 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:

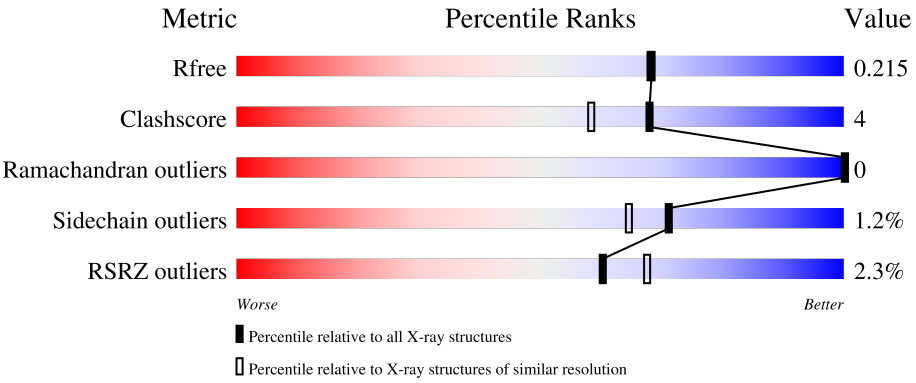
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 1.94 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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% 83% 6% 11%
1	B	447	86% 6% 8%
1	C	447	2% 85% 8% • 7%
1	D	447	3% 80% 9% • 11%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 14113 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	399	Total	C	N	O	S	0	2	0
			3205	2068	533	588	16			
1	B	412	Total	C	N	O	S	0	5	0
			3320	2140	555	608	17			
1	C	417	Total	C	N	O	S	0	7	0
			3373	2173	565	618	17			
1	D	400	Total	C	N	O	S	0	2	0
			3210	2070	534	590	16			

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

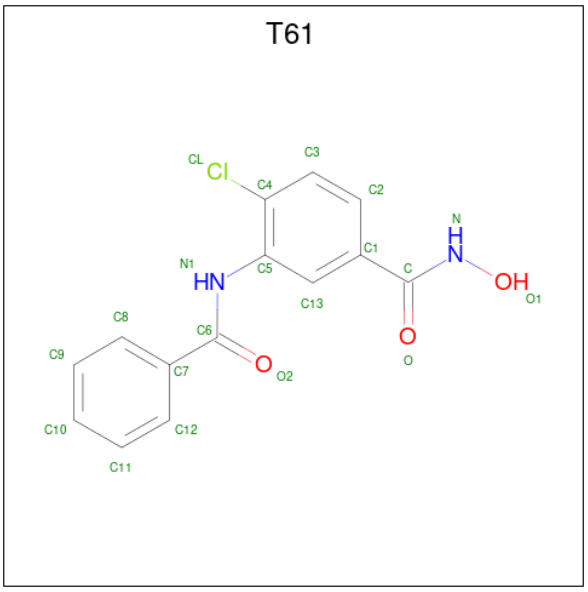
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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).

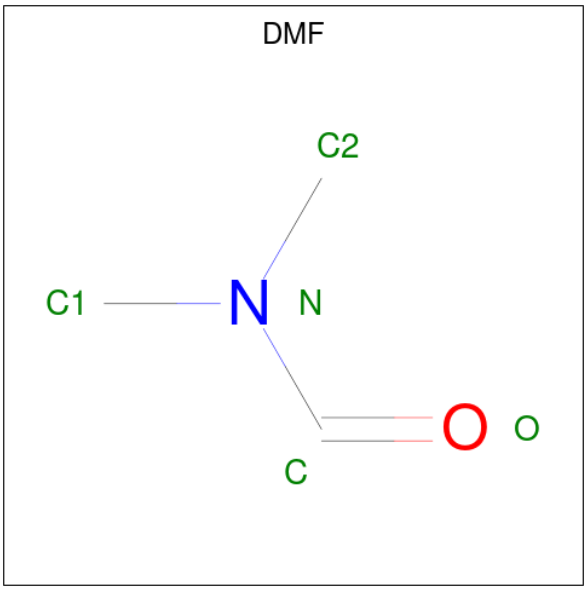
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total K 2 2	0	0
3	B	2	Total K 2 2	0	0
3	C	2	Total K 2 2	0	0
3	D	2	Total K 2 2	0	0

- Molecule 4 is 3-benzamido-4-chloranyl- {N}-oxidanyl-benzamide (three-letter code: T61) (formula: $C_{14}H_{11}ClN_2O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			20	14	1	2	3		
4	B	1	Total	C	Cl	N	O	0	0
			20	14	1	2	3		
4	C	1	Total	C	Cl	N	O	0	0
			20	14	1	2	3		
4	D	1	Total	C	Cl	N	O	0	0
			20	14	1	2	3		

- 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	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
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

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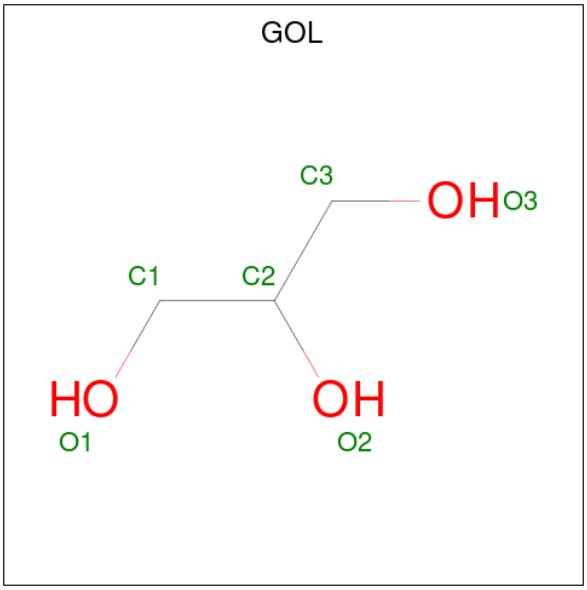
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C N O 5 3 1 1	0	0
5	D	1	Total C N O 5 3 1 1	0	0
5	D	1	Total C N O 5 3 1 1	0	0

- 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	D	1	Total C O 6 3 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	179	Total O 179 179	0	0

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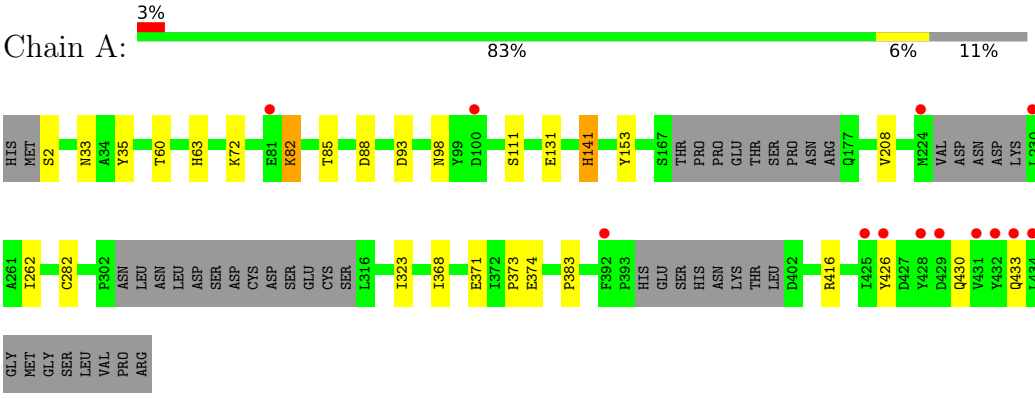
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	211	Total O 211 211	0	0
7	C	211	Total O 211 211	0	0
7	D	157	Total O 157 157	0	0

3 Residue-property plots

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.

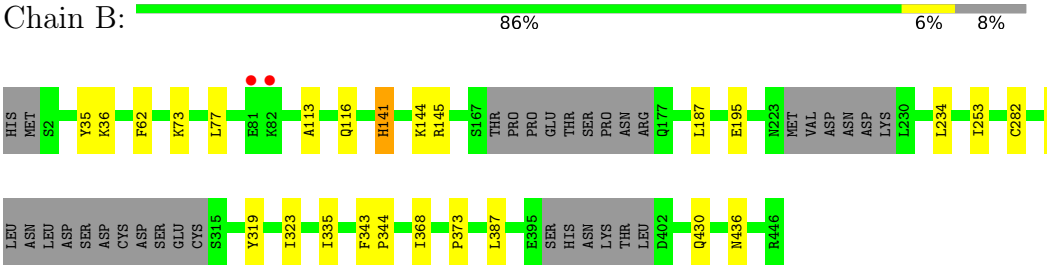
• Molecule 1: Histone deacetylase

Chain A:



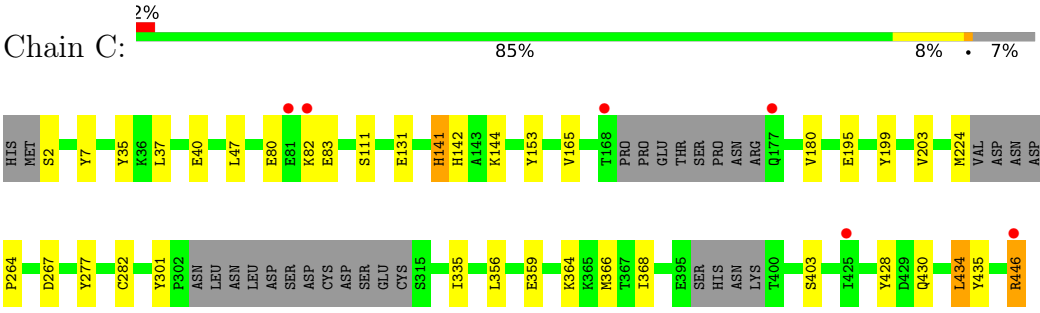
• Molecule 1: Histone deacetylase

Chain B:



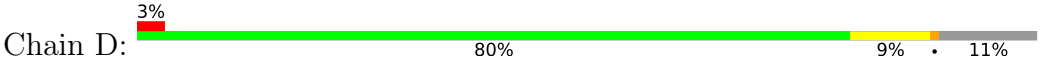
• Molecule 1: Histone deacetylase

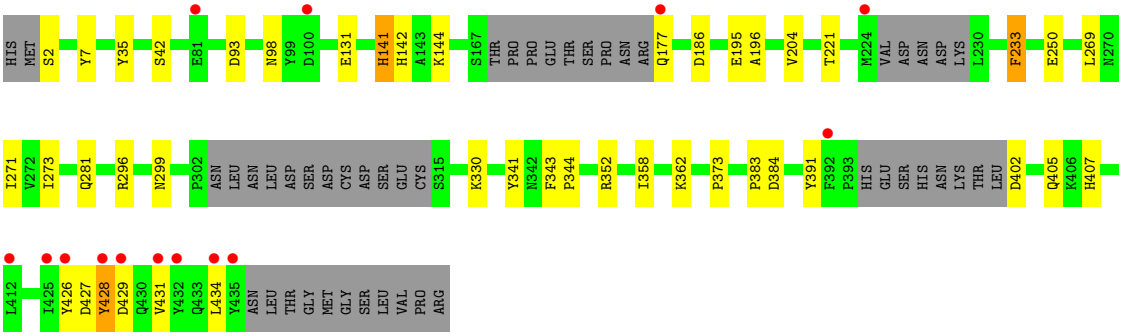
Chain C:



• Molecule 1: Histone deacetylase

Chain D:




HIS MET S2 Y7 Y35 S42 E81 D93 N98 Y99 D100 E131 H141 H142 A143 K144 S167 THR PRO PRO GLU THR SER PRO ASN ARG Q177 D186 E195 A196 V204 T221 M224 VAL ASP ASN ASP LYS L230 F233 E250 L269 N270
I271 V272 I273 Q281 R296 N299 P302 ASN LEU ASN LEU ASP SER ASP CYS ASP SER GLU CYS S315 K330 Y341 N342 F343 P344 R352 I358 K362 P373 P383 D384 Y391 F392 P393 HIS GLU SER HIS ASN LYS THR LEU D402 Q405 K406 H407
L412 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	70.66Å 70.64Å 98.33Å 77.73° 75.86° 85.63°	Depositor
Resolution (Å)	49.25 – 1.94 49.25 – 1.94	Depositor EDS
% Data completeness (in resolution range)	95.1 (49.25-1.94) 95.1 (49.25-1.94)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.08 (at 1.94Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.169 , 0.215 0.169 , 0.215	Depositor DCC
R_{free} test set	6351 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	23.3	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.118 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14113	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% 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: DMF, GOL, ZN, T61, K

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	0.47	0/3298	0.60	0/4486
1	B	0.50	0/3425	0.61	0/4658
1	C	0.48	0/3481	0.61	1/4731 (0.0%)
1	D	0.46	0/3303	0.58	0/4491
All	All	0.48	0/13507	0.60	1/18366 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	434	LEU	CA-CB-CG	5.81	128.66	115.30

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	3205	0	3100	23	1
1	B	3320	0	3219	21	0
1	C	3373	0	3283	29	1
1	D	3210	0	3100	27	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	20	0	0	0	0
4	B	20	0	0	0	0
4	C	20	0	0	1	0
4	D	20	0	0	2	0
5	A	30	0	42	3	0
5	B	40	0	56	0	0
5	C	30	0	42	5	0
5	D	25	0	35	6	0
6	A	6	0	8	0	0
6	B	12	0	16	2	0
6	C	6	0	8	0	0
6	D	6	0	8	0	0
7	A	179	0	0	5	0
7	B	211	0	0	4	0
7	C	211	0	0	0	0
7	D	157	0	0	0	0
All	All	14113	0	12917	100	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 4.

All (100) 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:D:330:LYS:HD3	5:D:505:DMF:HC	1.64	0.80
1:A:85:THR:HG23	1:A:88:ASP:H	1.51	0.75
1:C:356:LEU:HB2	5:C:506:DMF:H23	1.69	0.74
1:C:82:LYS:HE2	1:C:83:GLU:HG2	1.69	0.72
1:D:2:SER:N	1:D:131:GLU:OE1	2.24	0.70
1:B:35:TYR:CE1	1:B:368:ILE:HG23	2.32	0.65
1:D:250:GLU:OE1	5:D:508:DMF:HC	1.96	0.65
1:A:88:ASP:OD2	7:A:601:HOH:O	2.14	0.64
1:B:234:LEU:HB2	6:B:613:GOL:H12	1.80	0.64
1:A:82:LYS:HD2	7:A:707:HOH:O	1.98	0.63
1:C:2:SER:N	1:C:131:GLU:OE1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:ILE:HG21	1:B:387:LEU:HD22	1.84	0.60
1:C:165:VAL:HG11	1:C:203:VAL:HG22	1.84	0.59
1:C:40:GLU:HG3	1:C:366:MET:HE1	1.86	0.58
1:B:187:LEU:HD21	1:B:294:ILE:HD12	1.87	0.56
1:C:7[B]:TYR:CZ	5:C:505:DMF:HC	2.40	0.56
1:C:37:LEU:CD2	1:C:366:MET:HE3	2.36	0.56
1:A:85:THR:HG21	7:A:769:HOH:O	2.06	0.55
1:C:7[A]:TYR:CE1	5:C:505:DMF:H23	2.41	0.55
1:A:33:ASN:HB2	5:A:507:DMF:HC	1.89	0.55
1:B:116:GLN:NE2	7:B:706:HOH:O	2.40	0.54
1:D:358:ILE:HG23	1:D:362:LYS:HD3	1.89	0.54
1:B:116:GLN:OE1	6:B:612:GOL:H31	2.07	0.54
1:D:426:TYR:HE2	1:D:431:VAL:HG11	1.74	0.53
1:D:402:ASP:N	1:D:405:GLN:OE1	2.42	0.53
1:B:113:ALA:HA	1:B:116:GLN:HE21	1.74	0.52
1:A:85:THR:CG2	1:A:88:ASP:H	2.21	0.51
1:A:35:TYR:CE1	1:A:368:ILE:HG23	2.45	0.51
1:D:271:ILE:HD12	1:D:434:LEU:HD11	1.93	0.51
1:B:62:PHE:O	1:B:145:ARG:HG3	2.11	0.51
1:C:35:TYR:CD1	1:C:368:ILE:HG23	2.46	0.51
1:A:208:VAL:HG11	1:A:262:ILE:HD12	1.92	0.50
1:C:144:LYS:HD2	1:C:195:GLU:OE1	2.12	0.50
1:A:260:ASN:OD1	5:A:509:DMF:H12	2.13	0.49
1:B:35:TYR:CD1	1:B:368:ILE:HG23	2.48	0.48
1:A:2:SER:N	1:A:131:GLU:OE2	2.45	0.48
1:B:368:ILE:CG2	1:B:387:LEU:HD22	2.44	0.47
1:C:403:SER:HA	5:C:509:DMF:H23	1.97	0.47
1:A:72:LYS:NZ	7:A:607:HOH:O	2.47	0.47
1:D:221:THR:HA	1:D:233:PHE:CZ	2.50	0.46
1:C:428:TYR:CD1	1:C:446:ARG:HA	2.51	0.46
1:A:416:ARG:HG3	1:A:426:TYR:OH	2.15	0.46
1:D:343:PHE:HB2	1:D:344:PRO:HD3	1.97	0.46
1:A:374:GLU:HB3	5:A:510:DMF:H13	1.96	0.46
1:C:37:LEU:HD23	1:C:366:MET:HE3	1.97	0.46
1:A:383:PRO:HD2	7:A:641:HOH:O	2.15	0.46
1:C:35:TYR:CE1	1:C:368:ILE:HG23	2.52	0.46
1:B:141:HIS:H	1:B:141:HIS:CD2	2.33	0.45
1:C:82:LYS:HG3	1:C:83:GLU:O	2.17	0.45
1:C:142:HIS:NE2	4:C:504:T61:N	2.64	0.45
1:C:224:MET:HB3	1:C:231:PRO:HB3	1.98	0.45
1:A:430:GLN:O	1:A:433:GLN:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:HIS:H	1:A:141:HIS:CD2	2.34	0.44
1:C:165:VAL:HG11	1:C:203:VAL:CG2	2.46	0.44
1:D:299:ASN:O	1:D:352:ARG:HD2	2.17	0.44
1:A:35:TYR:CD1	1:A:368:ILE:HG23	2.53	0.44
1:C:359:GLU:HG2	1:C:364:LYS:O	2.17	0.44
1:D:407:HIS:HE2	5:D:508:DMF:H21	1.83	0.44
1:B:282[B]:CYS:SG	1:B:335:ILE:HG23	2.58	0.43
1:C:40:GLU:HG3	1:C:366:MET:CE	2.48	0.43
1:D:427:ASP:OD1	1:D:429:ASP:N	2.51	0.43
1:B:368:ILE:HG21	1:B:387:LEU:CD2	2.46	0.43
1:D:269:LEU:O	1:D:273:ILE:HG12	2.17	0.43
1:D:341:TYR:OH	4:D:504:T61:O	2.23	0.43
1:C:141:HIS:CD2	1:C:141:HIS:H	2.36	0.43
1:C:264:PRO:HB2	1:C:435:TYR:CZ	2.54	0.43
1:B:35:TYR:CZ	1:B:373:PRO:HD3	2.54	0.43
1:D:141:HIS:H	1:D:141:HIS:CD2	2.37	0.43
1:D:142:HIS:NE2	4:D:504:T61:N	2.67	0.42
1:A:111:SER:OG	1:A:153:TYR:HB2	2.18	0.42
1:C:165:VAL:HG12	1:C:180:VAL:CG2	2.49	0.42
1:D:427:ASP:O	1:D:431:VAL:HG12	2.18	0.42
1:B:253:ILE:HB	7:B:715:HOH:O	2.18	0.42
1:C:282[B]:CYS:SG	1:C:335:ILE:HG23	2.60	0.42
1:B:144:LYS:HD2	1:B:195:GLU:OE2	2.18	0.42
1:B:319:TYR:O	1:B:323:ILE:HG12	2.19	0.42
1:C:180:VAL:HG22	1:C:277:TYR:HB2	2.01	0.42
1:B:343:PHE:HB2	1:B:344:PRO:HD3	2.01	0.42
1:A:282[B]:CYS:SG	1:A:323:ILE:HD11	2.60	0.42
1:C:111[A]:SER:OG	1:C:153:TYR:HB2	2.20	0.41
1:C:165:VAL:HG12	1:C:180:VAL:HG23	2.02	0.41
1:D:186:ASP:HB2	1:D:281:GLN:OE1	2.19	0.41
1:D:204:VAL:HG21	1:D:273:ILE:HD12	2.01	0.41
1:A:60:THR:HA	1:A:63:HIS:O	2.20	0.41
1:C:267:ASP:HB3	1:C:434:LEU:HD11	2.02	0.41
1:D:195:GLU:HG3	5:D:509:DMF:H12	2.03	0.41
1:D:296:ARG:HD3	1:D:391:TYR:OH	2.20	0.41
1:D:196:ALA:O	5:D:507:DMF:H12	2.20	0.41
1:B:36:LYS:HA	7:B:793:HOH:O	2.20	0.41
1:B:436:ASN:ND2	7:B:701:HOH:O	2.11	0.41
1:D:93:ASP:HA	1:D:98:ASN:ND2	2.36	0.41
1:A:416:ARG:HH11	1:A:416:ARG:HB3	1.86	0.41
1:B:73:LYS:O	1:B:77:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:TYR:CZ	1:D:373:PRO:HD3	2.55	0.41
1:A:93:ASP:HA	1:A:98:ASN:ND2	2.36	0.40
1:A:35:TYR:CZ	1:A:373:PRO:HD3	2.56	0.40
1:D:7:TYR:CE1	5:D:506:DMF:H23	2.57	0.40
1:D:428:TYR:HD1	1:D:428:TYR:O	2.04	0.40
1:C:301:TYR:CZ	5:C:506:DMF:H22	2.57	0.40
1:D:142:HIS:O	1:D:144:LYS:NZ	2.52	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)
1:A:371:GLU:OE2	1:C:199:TYR:OH[1_556]	2.19	0.01

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	391/447 (88%)	383 (98%)	8 (2%)	0	100	100
1	B	407/447 (91%)	400 (98%)	7 (2%)	0	100	100
1	C	414/447 (93%)	410 (99%)	4 (1%)	0	100	100
1	D	392/447 (88%)	385 (98%)	7 (2%)	0	100	100
All	All	1604/1788 (90%)	1578 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	348/392 (89%)	345 (99%)	3 (1%)	78	75
1	B	362/392 (92%)	360 (99%)	2 (1%)	86	85
1	C	369/392 (94%)	364 (99%)	5 (1%)	67	58
1	D	349/392 (89%)	342 (98%)	7 (2%)	55	42
All	All	1428/1568 (91%)	1411 (99%)	17 (1%)	71	64

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	LYS
1	A	141	HIS
1	A	233	PHE
1	B	141	HIS
1	B	430	GLN
1	C	47	LEU
1	C	80	GLU
1	C	141	HIS
1	C	430	GLN
1	C	446	ARG
1	D	42	SER
1	D	141	HIS
1	D	177	GLN
1	D	233	PHE
1	D	383	PRO
1	D	384	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

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 46 ligands modelled in this entry, 12 are monoatomic - leaving 34 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	T61	C	504	2	21,21,21	0.24	0	28,28,28	1.13	2 (7%)
4	T61	A	504	2	21,21,21	0.22	0	28,28,28	0.50	0
5	DMF	C	505	-	4,4,4	0.28	0	4,4,4	0.35	0
6	GOL	B	612	-	5,5,5	0.42	0	5,5,5	0.70	0
6	GOL	D	510	-	5,5,5	0.28	0	5,5,5	0.75	0
5	DMF	D	507	-	4,4,4	0.28	0	4,4,4	0.50	0
5	DMF	B	607	-	4,4,4	0.33	0	4,4,4	0.34	0
5	DMF	B	610	-	4,4,4	0.32	0	4,4,4	0.55	0
5	DMF	B	604	-	4,4,4	0.30	0	4,4,4	0.53	0
6	GOL	A	511	-	5,5,5	0.34	0	5,5,5	0.99	1 (20%)
5	DMF	A	505	-	4,4,4	0.33	0	4,4,4	0.58	0
5	DMF	A	507	-	4,4,4	0.28	0	4,4,4	0.35	0
4	T61	D	504	2	21,21,21	0.21	0	28,28,28	1.07	2 (7%)
5	DMF	A	509	-	4,4,4	0.34	0	4,4,4	0.14	0
5	DMF	D	508	-	4,4,4	0.36	0	4,4,4	0.23	0
5	DMF	C	507	-	4,4,4	0.35	0	4,4,4	0.25	0
6	GOL	C	511	-	5,5,5	0.30	0	5,5,5	0.97	0
5	DMF	D	506	-	4,4,4	0.40	0	4,4,4	0.48	0
5	DMF	C	506	-	4,4,4	0.30	0	4,4,4	0.27	0
6	GOL	B	613	-	5,5,5	0.40	0	5,5,5	0.29	0
5	DMF	A	510	-	4,4,4	0.36	0	4,4,4	0.25	0
5	DMF	B	611	-	4,4,4	0.43	0	4,4,4	0.30	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	0.31	0	4,4,4	0.57	0
5	DMF	D	505	-	4,4,4	0.32	0	4,4,4	0.47	0
5	DMF	B	606	-	4,4,4	0.38	0	4,4,4	0.29	0
5	DMF	A	506	-	4,4,4	0.35	0	4,4,4	0.47	0
5	DMF	B	605	-	4,4,4	0.33	0	4,4,4	0.46	0
5	DMF	C	508	-	4,4,4	0.29	0	4,4,4	0.42	0
5	DMF	D	509	-	4,4,4	0.30	0	4,4,4	0.41	0
5	DMF	B	609	-	4,4,4	0.38	0	4,4,4	0.49	0
5	DMF	C	509	-	4,4,4	0.33	0	4,4,4	0.42	0
5	DMF	C	510	-	4,4,4	0.38	0	4,4,4	0.42	0
5	DMF	B	608	-	4,4,4	0.42	0	4,4,4	0.34	0
4	T61	B	603	2	21,21,21	0.19	0	28,28,28	1.04	3 (10%)

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	T61	C	504	2	-	6/14/14/14	0/2/2/2
4	T61	A	504	2	-	2/14/14/14	0/2/2/2
5	DMF	C	505	-	-	2/2/2/2	-
6	GOL	B	612	-	-	3/4/4/4	-
6	GOL	D	510	-	-	1/4/4/4	-
5	DMF	D	507	-	-	2/2/2/2	-
5	DMF	B	607	-	-	2/2/2/2	-
5	DMF	B	610	-	-	0/2/2/2	-
5	DMF	B	604	-	-	2/2/2/2	-
6	GOL	A	511	-	-	0/4/4/4	-
5	DMF	A	505	-	-	2/2/2/2	-
5	DMF	A	507	-	-	2/2/2/2	-
4	T61	D	504	2	-	6/14/14/14	0/2/2/2
5	DMF	A	509	-	-	2/2/2/2	-
5	DMF	D	508	-	-	2/2/2/2	-
5	DMF	C	507	-	-	0/2/2/2	-
6	GOL	C	511	-	-	1/4/4/4	-
5	DMF	D	506	-	-	2/2/2/2	-
5	DMF	C	506	-	-	2/2/2/2	-
6	GOL	B	613	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMF	A	510	-	-	2/2/2/2	-
5	DMF	B	611	-	-	0/2/2/2	-
5	DMF	A	508	-	-	2/2/2/2	-
5	DMF	D	505	-	-	2/2/2/2	-
5	DMF	B	606	-	-	2/2/2/2	-
5	DMF	A	506	-	-	0/2/2/2	-
5	DMF	B	605	-	-	0/2/2/2	-
5	DMF	C	508	-	-	2/2/2/2	-
5	DMF	D	509	-	-	2/2/2/2	-
5	DMF	B	609	-	-	2/2/2/2	-
5	DMF	C	509	-	-	2/2/2/2	-
5	DMF	C	510	-	-	0/2/2/2	-
5	DMF	B	608	-	-	0/2/2/2	-
4	T61	B	603	2	-	5/14/14/14	0/2/2/2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	504	T61	C5-N1-C6	4.02	137.96	126.93
4	C	504	T61	C5-N1-C6	3.93	137.69	126.93
4	B	603	T61	C5-N1-C6	3.28	135.92	126.93
4	C	504	T61	C4-C5-N1	2.97	123.94	119.24
4	D	504	T61	C4-C5-N1	2.80	123.67	119.24
4	B	603	T61	C4-C5-N1	2.47	123.16	119.24
4	B	603	T61	C13-C5-N1	-2.17	116.17	121.90
6	A	511	GOL	C3-C2-C1	-2.08	103.62	111.70

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	603	T61	C4-C5-N1-C6
4	C	504	T61	C4-C5-N1-C6
4	D	504	T61	C4-C5-N1-C6
6	B	613	GOL	O1-C1-C2-C3
4	D	504	T61	N1-C6-C7-C12
4	D	504	T61	N1-C6-C7-C8
4	D	504	T61	O2-C6-C7-C12

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Mol	Chain	Res	Type	Atoms
5	C	505	DMF	O-C-N-C2
4	D	504	T61	O2-C6-C7-C8
5	C	509	DMF	O-C-N-C1
5	C	505	DMF	O-C-N-C1
5	C	509	DMF	O-C-N-C2
4	C	504	T61	N1-C6-C7-C8
5	B	604	DMF	O-C-N-C1
5	B	604	DMF	O-C-N-C2
5	A	505	DMF	O-C-N-C1
5	A	508	DMF	O-C-N-C2
5	B	607	DMF	O-C-N-C1
5	C	506	DMF	O-C-N-C1
5	D	505	DMF	O-C-N-C1
4	C	504	T61	N1-C6-C7-C12
5	D	506	DMF	O-C-N-C1
5	D	506	DMF	O-C-N-C2
5	D	505	DMF	O-C-N-C2
5	A	505	DMF	O-C-N-C2
5	A	509	DMF	O-C-N-C1
5	C	506	DMF	O-C-N-C2
5	B	607	DMF	O-C-N-C2
5	A	508	DMF	O-C-N-C1
4	C	504	T61	O2-C6-C7-C8
5	B	606	DMF	O-C-N-C2
4	C	504	T61	O2-C6-C7-C12
5	A	509	DMF	O-C-N-C2
5	B	609	DMF	O-C-N-C1
5	B	606	DMF	O-C-N-C1
5	D	509	DMF	O-C-N-C2
5	D	507	DMF	O-C-N-C2
5	B	609	DMF	O-C-N-C2
5	D	509	DMF	O-C-N-C1
5	D	507	DMF	O-C-N-C1
5	A	510	DMF	O-C-N-C2
6	B	612	GOL	O1-C1-C2-C3
4	B	603	T61	N1-C6-C7-C8
6	B	613	GOL	O1-C1-C2-O2
4	B	603	T61	N1-C6-C7-C12
4	A	504	T61	O2-C6-N1-C5
5	C	508	DMF	O-C-N-C1
5	A	510	DMF	O-C-N-C1
4	D	504	T61	C13-C5-N1-C6

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Mol	Chain	Res	Type	Atoms
4	C	504	T61	C13-C5-N1-C6
5	A	507	DMF	O-C-N-C1
5	C	508	DMF	O-C-N-C2
5	A	507	DMF	O-C-N-C2
5	D	508	DMF	O-C-N-C1
6	B	612	GOL	O1-C1-C2-O2
4	B	603	T61	O2-C6-C7-C8
5	D	508	DMF	O-C-N-C2
4	B	603	T61	O2-C6-C7-C12
4	A	504	T61	C7-C6-N1-C5
6	D	510	GOL	C1-C2-C3-O3
6	B	612	GOL	O2-C2-C3-O3
6	C	511	GOL	O2-C2-C3-O3

There are no ring outliers.

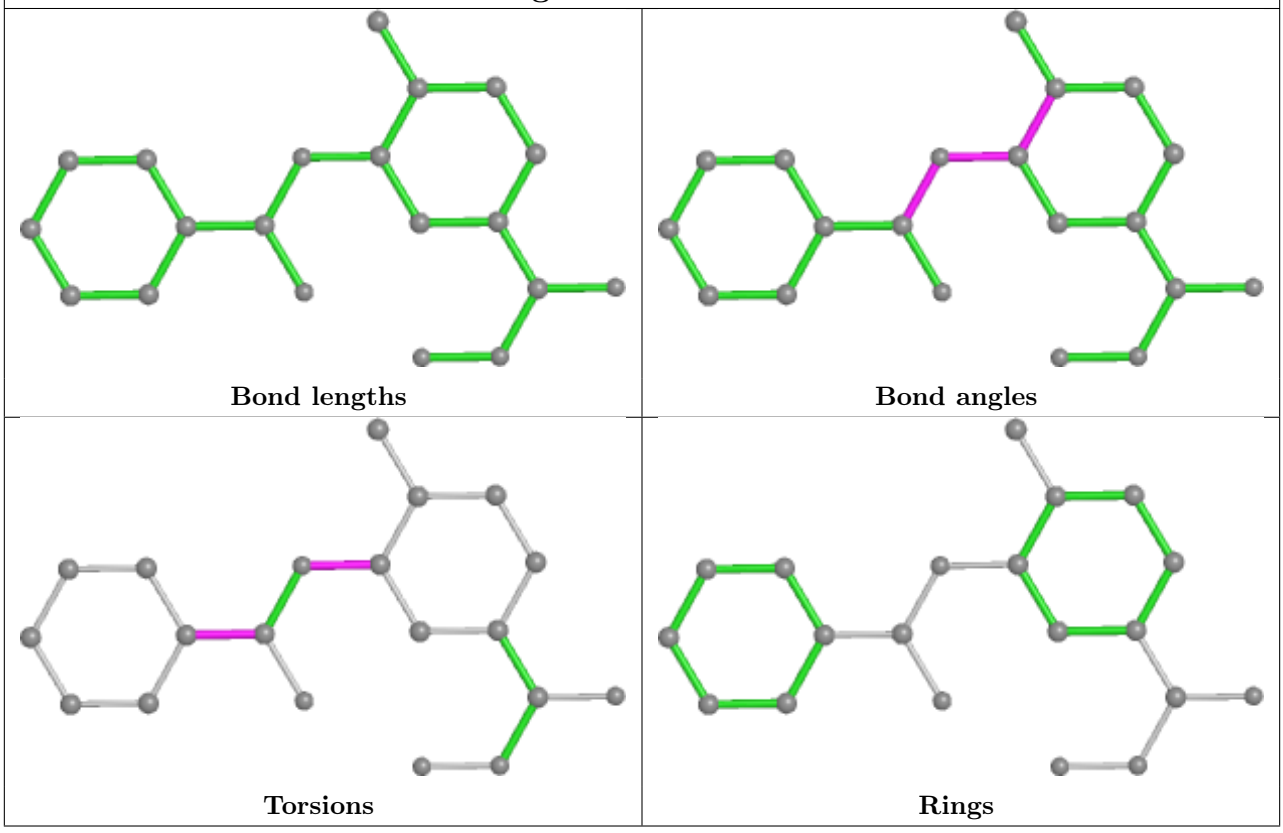
15 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	504	T61	1	0
5	C	505	DMF	2	0
6	B	612	GOL	1	0
5	D	507	DMF	1	0
5	A	507	DMF	1	0
4	D	504	T61	2	0
5	A	509	DMF	1	0
5	D	508	DMF	2	0
5	D	506	DMF	1	0
5	C	506	DMF	2	0
6	B	613	GOL	1	0
5	A	510	DMF	1	0
5	D	505	DMF	1	0
5	D	509	DMF	1	0
5	C	509	DMF	1	0

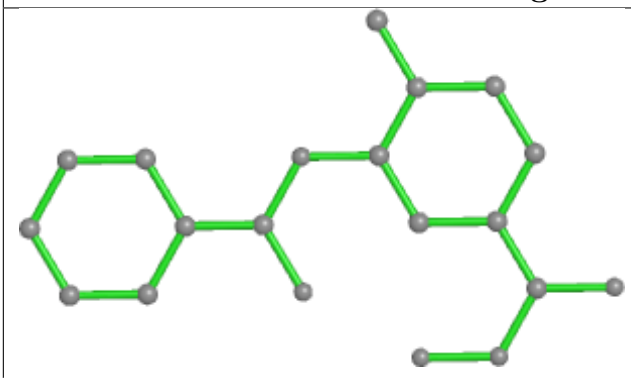
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

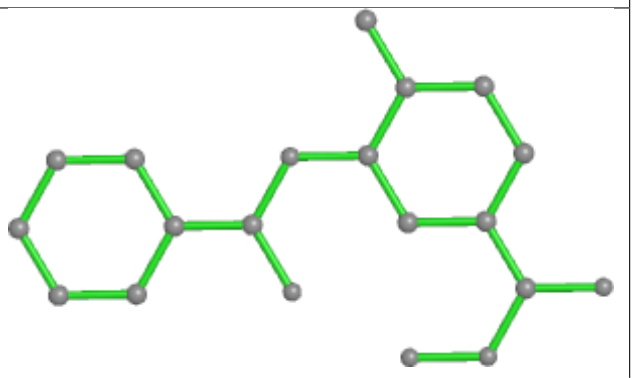
Ligand T61 C 504



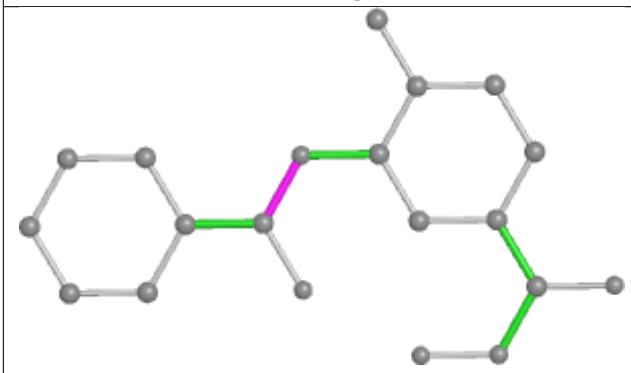
Ligand T61 A 504



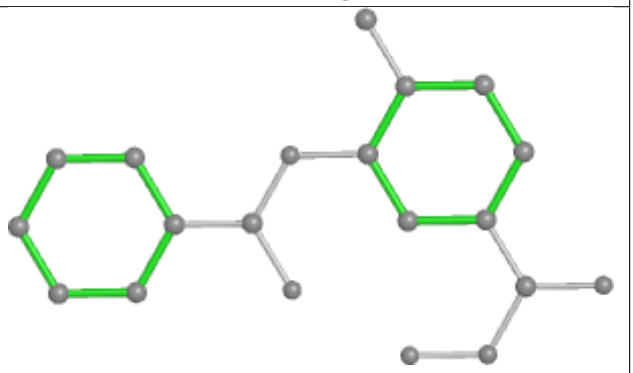
Bond lengths



Bond angles

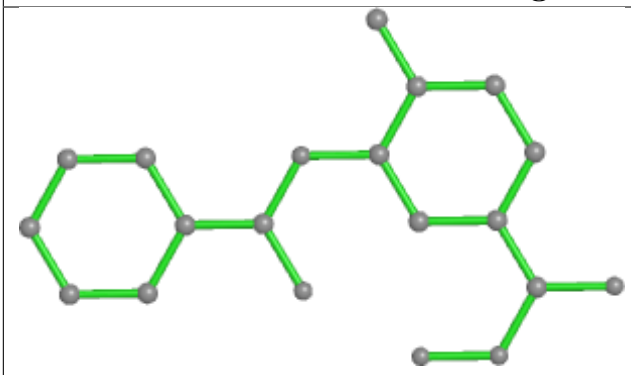


Torsions

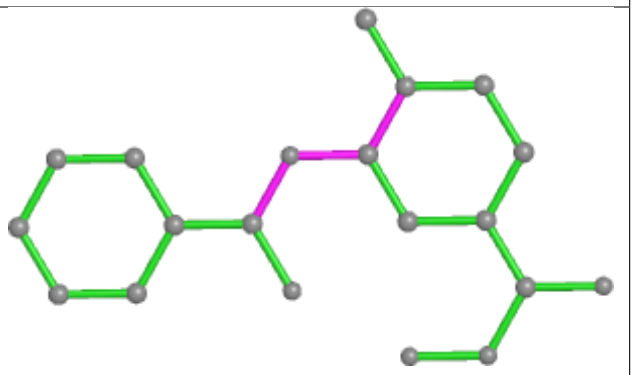


Rings

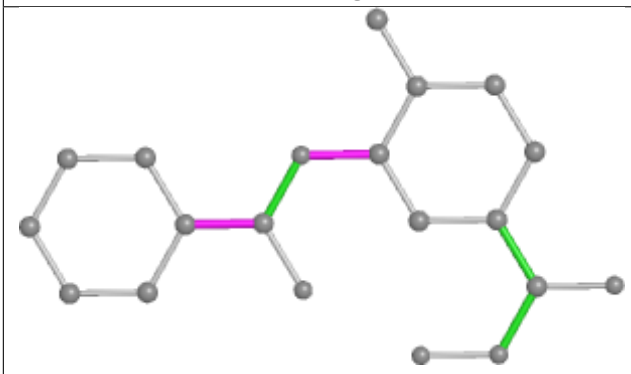
Ligand T61 D 504



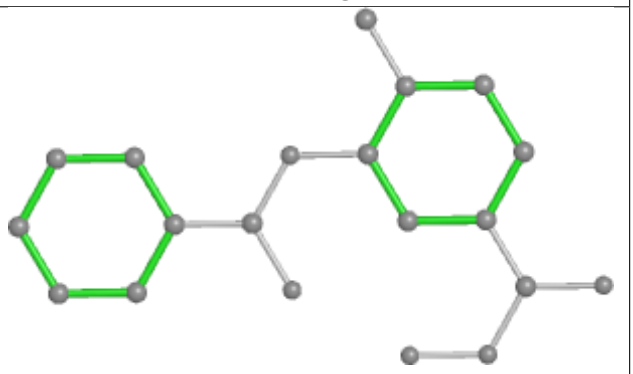
Bond lengths



Bond angles

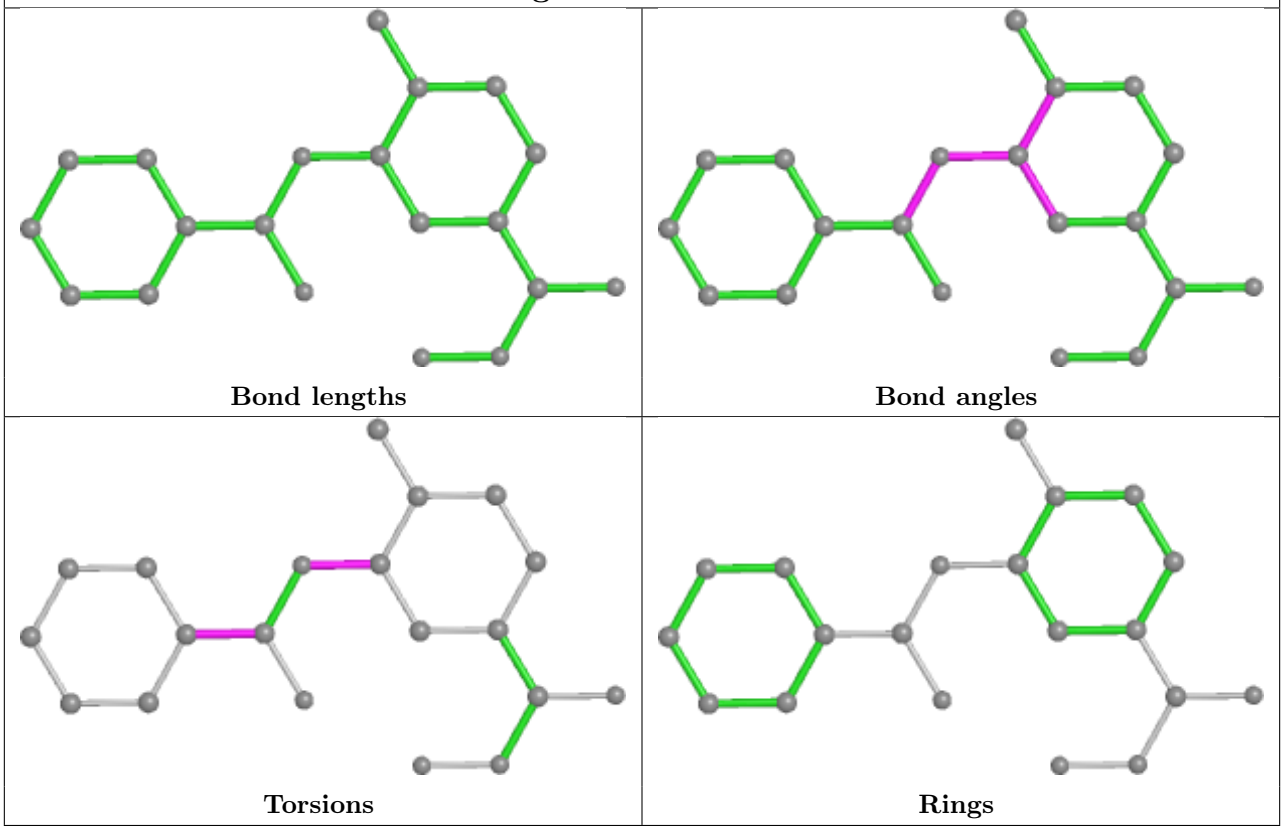


Torsions



Rings

Ligand T61 B 603



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	399/447 (89%)	-0.06	14 (3%) 44 51	15, 24, 56, 86	0
1	B	412/447 (92%)	-0.24	2 (0%) 91 93	12, 21, 42, 100	0
1	C	417/447 (93%)	-0.21	7 (1%) 70 75	13, 22, 45, 105	0
1	D	400/447 (89%)	-0.05	14 (3%) 44 51	15, 25, 58, 100	0
All	All	1628/1788 (91%)	-0.14	37 (2%) 60 67	12, 23, 51, 105	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	82	LYS	7.5
1	A	432	TYR	7.2
1	A	425	ILE	6.9
1	C	82	LYS	6.7
1	D	426	TYR	6.5
1	A	434	LEU	5.9
1	A	230	LEU	5.7
1	A	428	TYR	5.7
1	D	428	TYR	5.5
1	A	435	TYR	5.4
1	D	435	TYR	5.2
1	D	432	TYR	5.0
1	A	426	TYR	4.5
1	D	434	LEU	4.4
1	D	429	ASP	4.1
1	C	81	GLU	4.1
1	B	81	GLU	4.0
1	A	433	GLN	3.9
1	A	392	PHE	3.8
1	A	224	MET	3.6
1	A	429	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	425	ILE	3.2
1	D	431	VAL	3.2
1	D	100	ASP	3.2
1	C	230	LEU	2.9
1	D	392	PHE	2.9
1	D	412	LEU	2.7
1	D	177	GLN	2.5
1	A	431	VAL	2.4
1	A	81	GLU	2.4
1	C	168	THR	2.4
1	A	100	ASP	2.2
1	D	81	GLU	2.2
1	C	425	ILE	2.2
1	C	446	ARG	2.1
1	C	177	GLN	2.0
1	D	224	MET	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	DMF	D	506	5/5	0.74	0.28	61,62,63,63	0
5	DMF	D	508	5/5	0.76	0.21	57,58,66,68	0
5	DMF	C	510	5/5	0.79	0.20	48,49,53,58	0
5	DMF	B	608	5/5	0.80	0.15	37,41,48,52	0
5	DMF	A	506	5/5	0.81	0.20	49,53,57,57	0
5	DMF	B	607	5/5	0.82	0.20	52,55,57,59	0
4	T61	D	504	20/20	0.83	0.20	35,46,66,68	0

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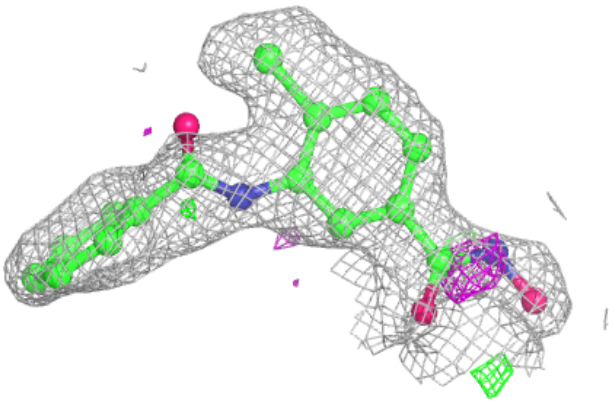
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DMF	B	611	5/5	0.84	0.19	35,51,57,60	0
5	DMF	A	510	5/5	0.84	0.14	39,53,65,67	0
4	T61	C	504	20/20	0.85	0.17	31,42,63,64	0
5	DMF	A	509	5/5	0.86	0.29	46,48,52,53	0
6	GOL	B	612	6/6	0.86	0.17	38,46,50,57	0
5	DMF	D	509	5/5	0.88	0.16	52,53,53,54	0
4	T61	B	603	20/20	0.89	0.15	25,37,45,53	0
4	T61	A	504	20/20	0.89	0.17	35,46,59,60	0
5	DMF	C	509	5/5	0.90	0.15	56,58,62,66	0
5	DMF	B	610	5/5	0.91	0.13	53,54,55,57	0
5	DMF	C	507	5/5	0.91	0.18	33,38,38,40	0
5	DMF	D	507	5/5	0.92	0.12	48,55,62,63	0
5	DMF	C	506	5/5	0.92	0.13	36,38,44,46	0
6	GOL	B	613	6/6	0.92	0.16	24,32,37,46	0
5	DMF	A	505	5/5	0.93	0.22	36,39,41,43	0
5	DMF	A	507	5/5	0.93	0.16	48,51,57,58	0
6	GOL	C	511	6/6	0.93	0.11	30,33,36,41	0
5	DMF	B	609	5/5	0.94	0.12	44,52,55,59	0
5	DMF	B	606	5/5	0.94	0.10	24,30,41,42	0
6	GOL	A	511	6/6	0.94	0.12	26,35,36,39	0
5	DMF	B	604	5/5	0.94	0.19	38,45,52,60	0
5	DMF	C	505	5/5	0.94	0.16	46,48,50,50	0
5	DMF	B	605	5/5	0.94	0.08	22,29,49,53	0
5	DMF	D	505	5/5	0.95	0.14	44,48,49,52	0
5	DMF	A	508	5/5	0.95	0.12	35,39,45,51	0
5	DMF	C	508	5/5	0.95	0.13	47,47,49,51	0
6	GOL	D	510	6/6	0.95	0.10	19,31,34,37	0
3	K	A	503	1/1	0.99	0.08	20,20,20,20	0
2	ZN	C	501	1/1	1.00	0.06	21,21,21,21	0
2	ZN	D	501	1/1	1.00	0.08	24,24,24,24	0
3	K	A	502	1/1	1.00	0.06	19,19,19,19	0
2	ZN	A	501	1/1	1.00	0.08	22,22,22,22	0
3	K	B	601	1/1	1.00	0.06	18,18,18,18	0
3	K	B	602	1/1	1.00	0.07	19,19,19,19	0
3	K	C	502	1/1	1.00	0.06	19,19,19,19	0
3	K	C	503	1/1	1.00	0.06	20,20,20,20	0
3	K	D	502	1/1	1.00	0.07	21,21,21,21	0
3	K	D	503	1/1	1.00	0.07	21,21,21,21	0
2	ZN	B	614	1/1	1.00	0.06	20,20,20,20	0

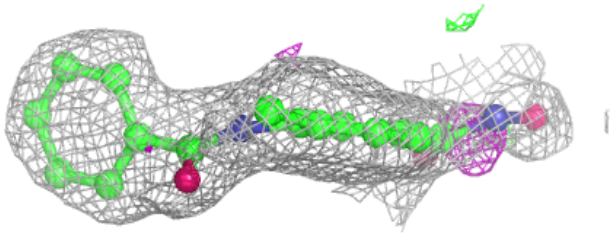
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

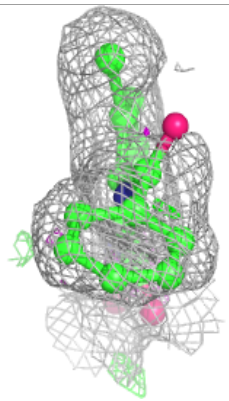
orientation to approximate a three-dimensional view.

Electron density around T61 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)

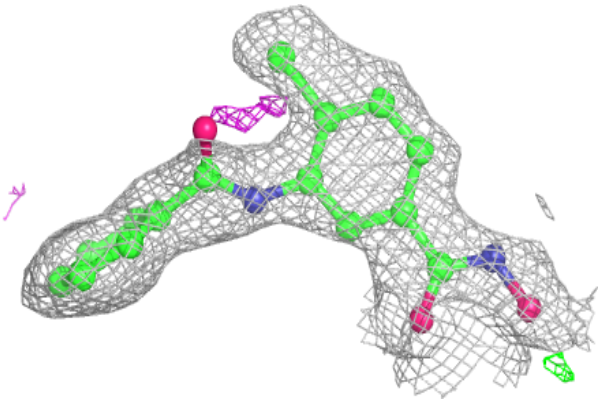


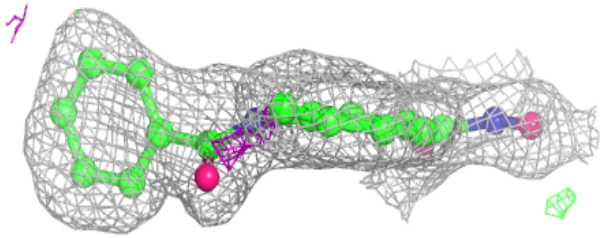


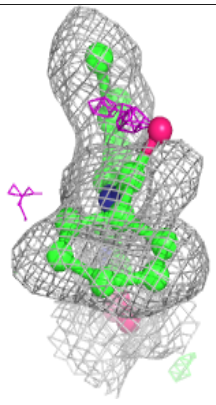


Electron density around T61 C 504:

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

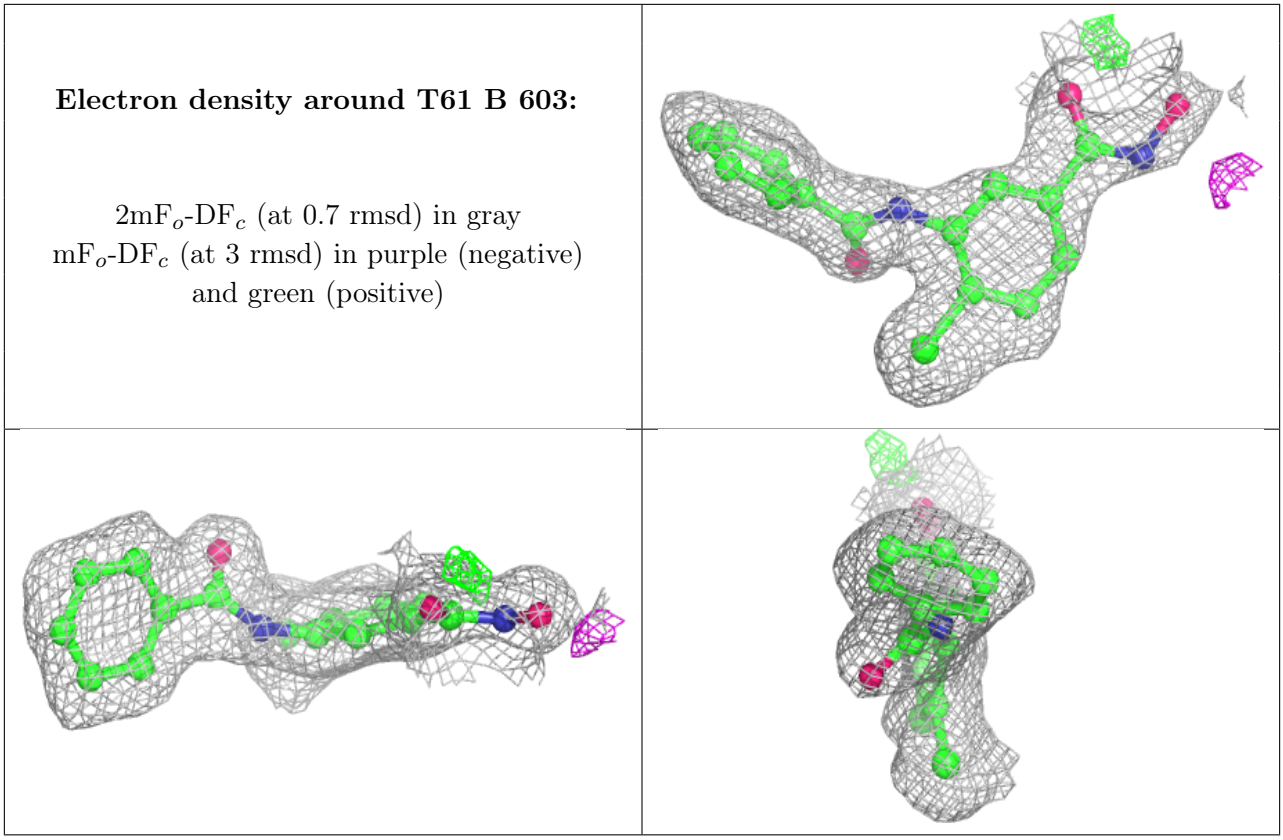






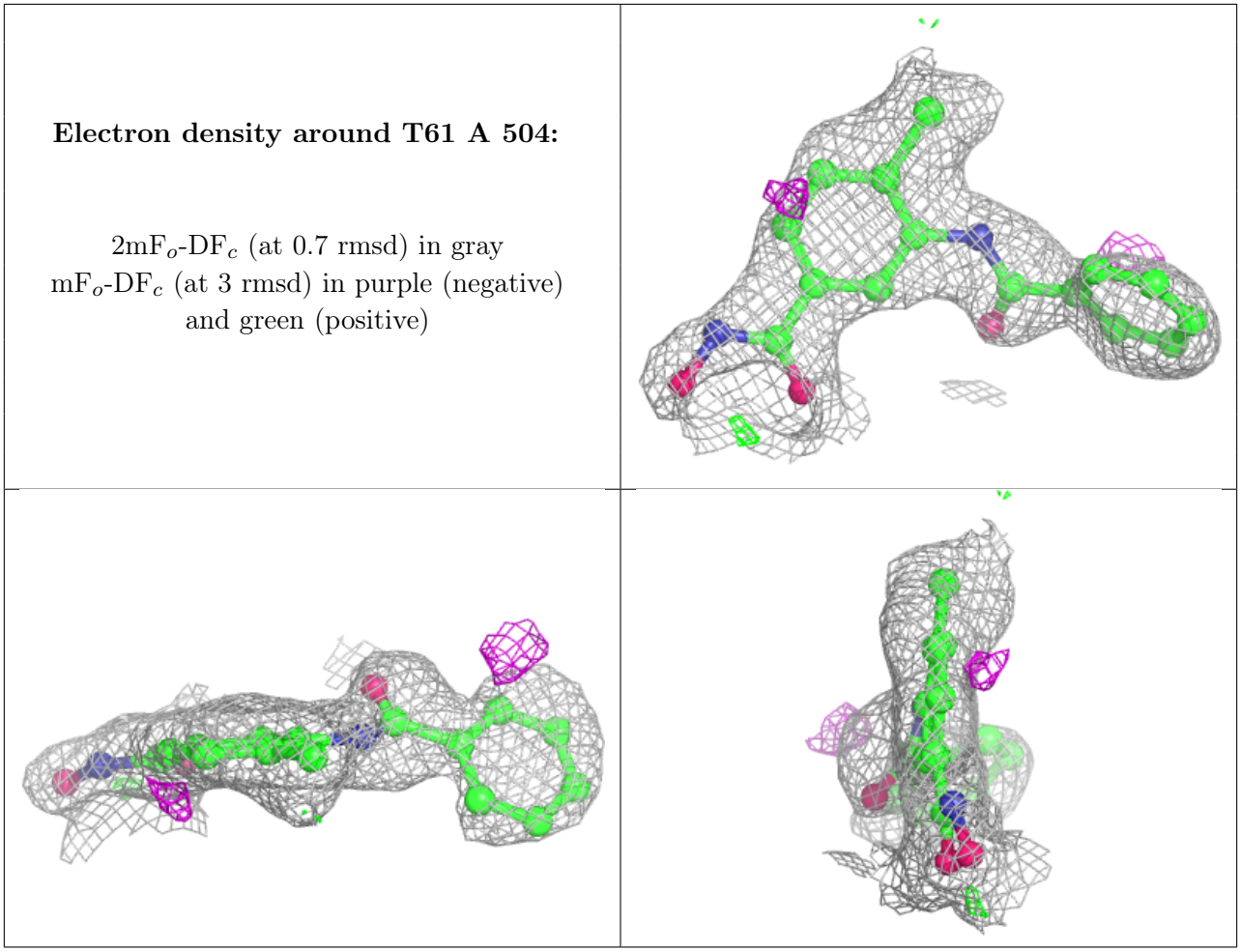
Electron density around T61 B 603:

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



Electron density around T61 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)



6.5 Other polymers (i)

There are no such residues in this entry.