Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2023 – 10:56 pm GMT

PDB ID	:	4ARW
Title	:	Pseudomonas aeruginosa RmlA in complex with allosteric inhibitor
Authors	:	Alphey, M.S.; Pirrie, L.; Torrie, L.S.; Gardiner, M.; Westwood, N.J.; Gray, D.; Naismith, J.H.
Deposited on	:	2012-04-26
Resolution	:	2.20 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:

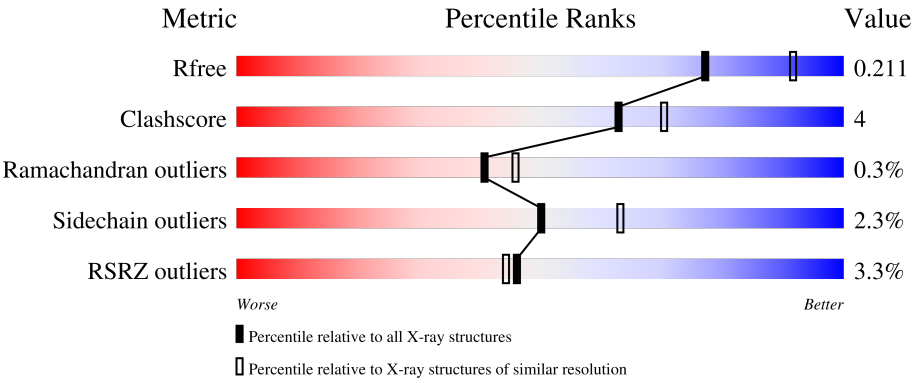
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	302	3% 88% 9% ·
1	B	302	2% 88% 8% ·
1	C	302	5% 84% 11% · ·
1	D	302	3% 87% 10% ·

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9848 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 GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	1	0
			2312	1478	393	437	4			
1	B	290	Total	C	N	O	S	0	1	0
			2273	1455	381	433	4			
1	C	289	Total	C	N	O	S	0	1	0
			2264	1449	379	432	4			
1	D	292	Total	C	N	O	S	0	1	0
			2291	1466	386	435	4			

There are 36 discrepancies between the modelled and reference sequences:

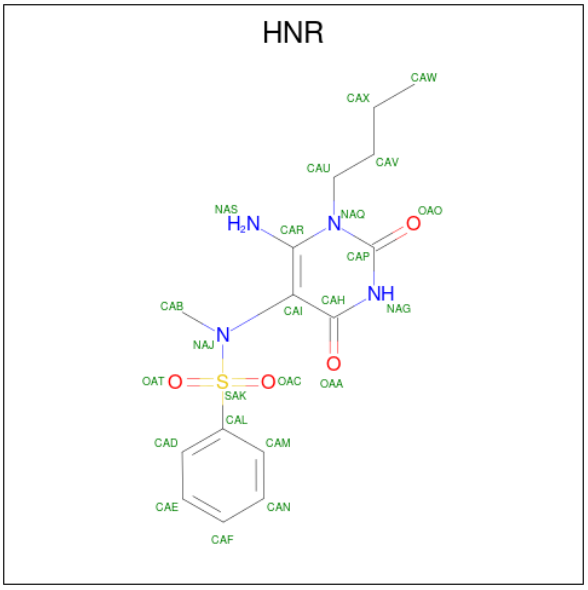
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	HIS	-	expression tag	UNP G3XCK4
A	-7	HIS	-	expression tag	UNP G3XCK4
A	-6	HIS	-	expression tag	UNP G3XCK4
A	-5	HIS	-	expression tag	UNP G3XCK4
A	-4	HIS	-	expression tag	UNP G3XCK4
A	-3	HIS	-	expression tag	UNP G3XCK4
A	-2	GLY	-	expression tag	UNP G3XCK4
A	-1	SER	-	expression tag	UNP G3XCK4
A	0	ALA	-	expression tag	UNP G3XCK4
B	-8	HIS	-	expression tag	UNP G3XCK4
B	-7	HIS	-	expression tag	UNP G3XCK4
B	-6	HIS	-	expression tag	UNP G3XCK4
B	-5	HIS	-	expression tag	UNP G3XCK4
B	-4	HIS	-	expression tag	UNP G3XCK4
B	-3	HIS	-	expression tag	UNP G3XCK4
B	-2	GLY	-	expression tag	UNP G3XCK4
B	-1	SER	-	expression tag	UNP G3XCK4
B	0	ALA	-	expression tag	UNP G3XCK4
C	-8	HIS	-	expression tag	UNP G3XCK4
C	-7	HIS	-	expression tag	UNP G3XCK4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	HIS	-	expression tag	UNP G3XCK4
C	-5	HIS	-	expression tag	UNP G3XCK4
C	-4	HIS	-	expression tag	UNP G3XCK4
C	-3	HIS	-	expression tag	UNP G3XCK4
C	-2	GLY	-	expression tag	UNP G3XCK4
C	-1	SER	-	expression tag	UNP G3XCK4
C	0	ALA	-	expression tag	UNP G3XCK4
D	-8	HIS	-	expression tag	UNP G3XCK4
D	-7	HIS	-	expression tag	UNP G3XCK4
D	-6	HIS	-	expression tag	UNP G3XCK4
D	-5	HIS	-	expression tag	UNP G3XCK4
D	-4	HIS	-	expression tag	UNP G3XCK4
D	-3	HIS	-	expression tag	UNP G3XCK4
D	-2	GLY	-	expression tag	UNP G3XCK4
D	-1	SER	-	expression tag	UNP G3XCK4
D	0	ALA	-	expression tag	UNP G3XCK4

- Molecule 2 is N-(6-AMINO-1-BUTYL-2,4-DIOXO-1,2,3,4-TETRAHYDROPYRIMIDIN-5-YL)-N-METHYL-BENZENESULFONAMIDE (three-letter code: HNR) (formula: $C_{15}H_{20}N_4O_4S$).



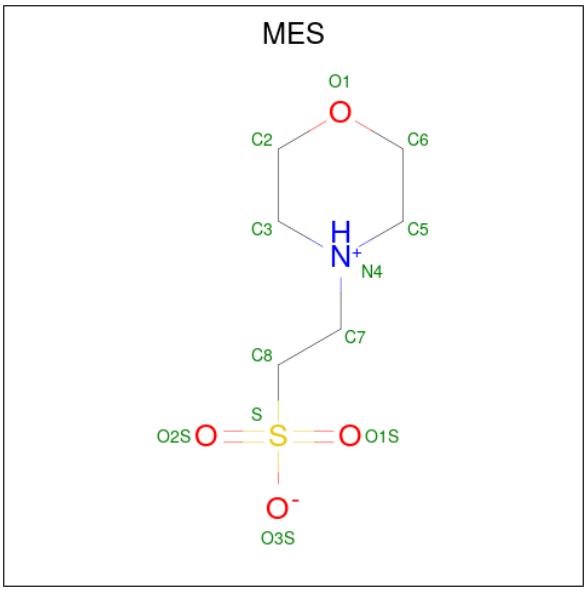
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			24	15	4	4	1		
2	B	1	Total	C	N	O	S	0	0
			24	15	4	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O S 24 15 4 4 1	0	0
2	D	1	Total C N O S 24 15 4 4 1	0	0

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 12 6 1 4 1	0	0
3	B	1	Total C N O S 12 6 1 4 1	0	0
3	C	1	Total C N O S 12 6 1 4 1	0	0
3	D	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

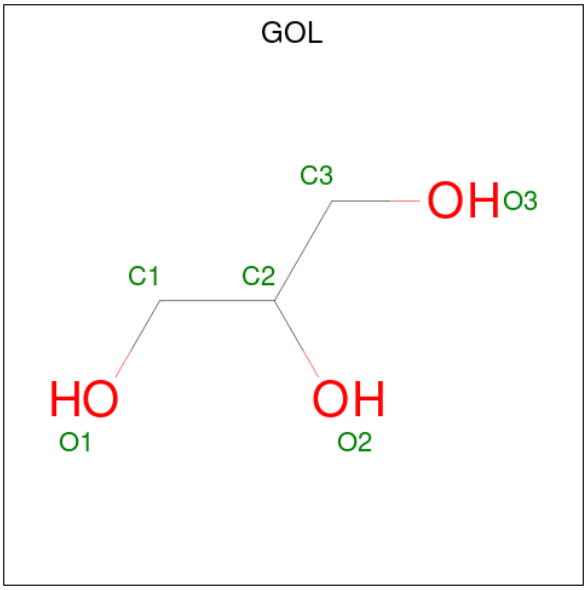
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0
4	C	2	Total Cl 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Cl 1 1	0	0

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



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

- Molecule 6 is water.

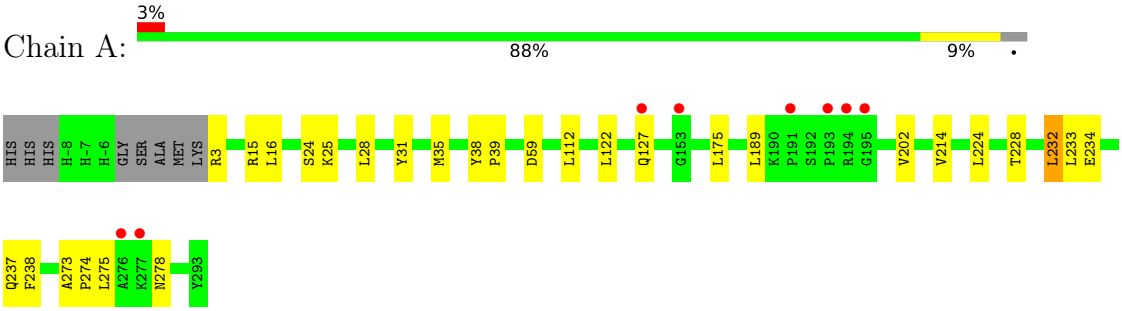
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	152	Total O 152 152	0	0
6	B	127	Total O 127 127	0	0
6	C	132	Total O 132 132	0	0
6	D	136	Total O 136 136	0	0

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.

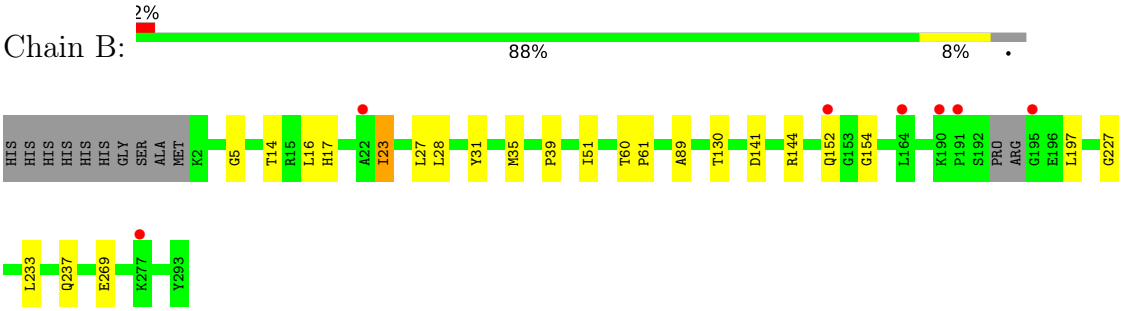
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain A:



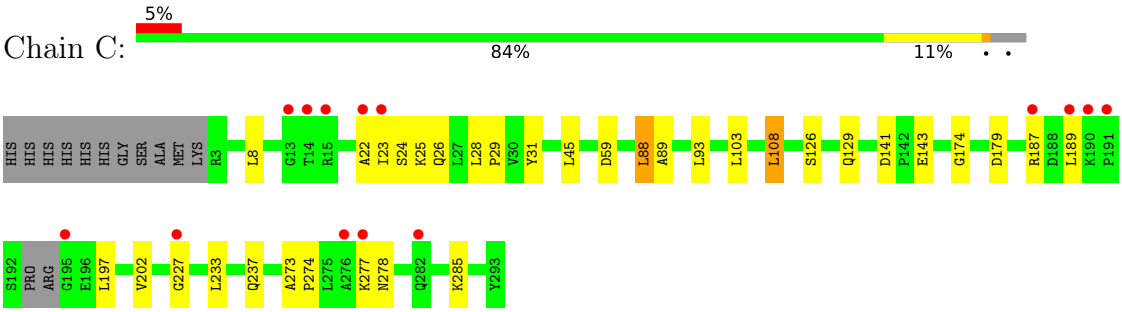
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain B:



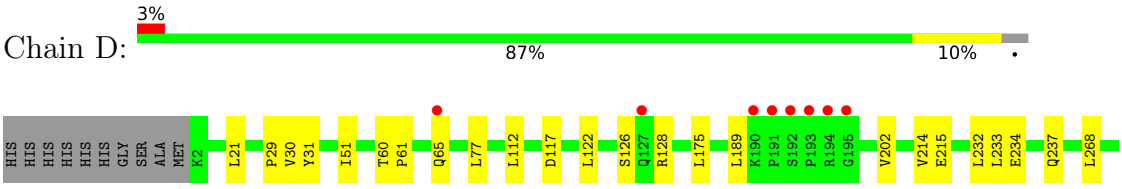
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

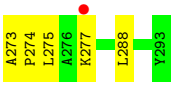
Chain C:



• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain D:




A273
P274
L275
A276
K277
L288
Y293

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	63.99Å 153.76Å 134.65Å 90.00° 92.32° 90.00°	Depositor
Resolution (Å)	30.82 – 2.20 30.81 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.1 (30.82-2.20) 96.2 (30.81-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.175 , 0.208 0.181 , 0.211	Depositor DCC
R_{free} test set	3192 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	25.3	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.084 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9848	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: GOL, HNR, CL, MES

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	0.52	0/2367	0.62	0/3211
1	B	0.48	0/2324	0.59	0/3151
1	C	0.51	0/2315	0.65	0/3140
1	D	0.50	0/2344	0.61	0/3180
All	All	0.50	0/9350	0.62	0/12682

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2312	0	2290	21	0
1	B	2273	0	2258	23	0
1	C	2264	0	2245	32	0
1	D	2291	0	2280	23	0
2	A	24	0	20	0	0
2	B	24	0	20	0	0
2	C	24	0	20	2	0
2	D	24	0	20	0	0
3	A	12	0	13	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	13	1	0
3	C	12	0	13	0	0
3	D	12	0	13	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
5	B	6	0	8	0	0
5	D	6	0	8	0	0
6	A	152	0	0	2	0
6	B	127	0	0	1	0
6	C	132	0	0	1	0
6	D	136	0	0	1	0
All	All	9848	0	9221	79	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 4.

All (79) 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:60:THR:HG23	1:D:61:PRO:HD3	1.37	1.03
1:B:23:ILE:HD12	1:C:23:ILE:HG12	1.50	0.94
1:D:60:THR:CG2	1:D:61:PRO:HD3	2.16	0.75
1:B:89:ALA:HB3	1:B:197:LEU:HB3	1.72	0.71
1:A:233:LEU:HD11	1:D:237[B]:GLN:HG3	1.72	0.70
1:A:234:GLU:HA	1:A:237[A]:GLN:HE21	1.55	0.68
1:C:8:LEU:HD23	1:C:88:LEU:HD12	1.78	0.65
1:D:60:THR:HG23	1:D:61:PRO:CD	2.21	0.65
1:B:23:ILE:HD12	1:C:23:ILE:CG1	2.25	0.63
1:B:23:ILE:HB	1:C:23:ILE:HD13	1.83	0.61
1:A:15:ARG:NH1	6:A:2009:HOH:O	2.35	0.59
1:A:275:LEU:HD22	1:A:278:ASN:HD21	1.67	0.58
1:B:154:GLY:O	3:B:450:MES:H82	2.04	0.58
1:C:273:ALA:HB3	1:C:274:PRO:HD3	1.86	0.58
1:D:268:LEU:HD23	1:D:288:LEU:HD23	1.86	0.57
1:B:16:LEU:HD21	1:B:227:GLY:O	2.05	0.56
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.88	0.55
1:B:27:LEU:HB3	1:C:22:ALA:HB1	1.89	0.55
1:D:189:LEU:HD11	1:D:202:VAL:HG23	1.91	0.53
1:D:234:GLU:HA	1:D:237[B]:GLN:HE21	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:ASP:HB3	6:C:2056:HOH:O	2.09	0.53
1:D:122:LEU:CD2	1:D:175:LEU:HD21	2.39	0.53
1:C:24:SER:HB2	1:C:59:ASP:OD2	2.09	0.52
1:A:237[B]:GLN:HA	1:D:233:LEU:HD21	1.91	0.52
1:C:8:LEU:CD2	1:C:88:LEU:HD12	2.39	0.52
1:A:38:TYR:CB	1:A:112:LEU:HD22	2.40	0.51
1:C:103:LEU:HD23	1:C:179:ASP:HA	1.92	0.51
1:A:237[A]:GLN:HA	1:D:233:LEU:HD21	1.93	0.51
1:B:23:ILE:CG2	1:C:23:ILE:HD13	2.42	0.50
1:A:228:THR:O	1:A:232:LEU:HD12	2.13	0.49
1:A:233:LEU:HD21	1:D:237[B]:GLN:CG	2.43	0.49
1:A:28:LEU:HD22	1:D:29:PRO:HD2	1.95	0.48
1:D:60:THR:CG2	1:D:61:PRO:CD	2.88	0.48
1:A:35:MET:O	1:A:39:PRO:HD2	2.13	0.48
1:B:14:THR:O	1:C:278:ASN:ND2	2.46	0.48
1:B:23:ILE:CB	1:C:23:ILE:HD13	2.43	0.47
1:D:214:VAL:O	3:D:450:MES:H81	2.14	0.47
1:C:25:LYS:HZ1	1:C:227:GLY:HA2	1.80	0.47
1:D:30:VAL:HG11	1:D:112:LEU:HD21	1.96	0.47
1:D:275:LEU:HD11	6:D:2013:HOH:O	2.13	0.47
1:D:51:ILE:HB	1:D:77:LEU:HD23	1.96	0.47
1:B:233:LEU:HD21	1:C:237[A]:GLN:HA	1.96	0.47
1:B:141:ASP:OD2	1:B:144:ARG:HD3	2.15	0.47
1:A:214:VAL:O	3:A:450:MES:H71	2.15	0.46
1:B:35:MET:O	1:B:39:PRO:HD2	2.16	0.46
1:C:45:LEU:HD22	2:C:400:HNR:CAM	2.45	0.46
1:C:187:ARG:HG2	1:C:187:ARG:HH11	1.81	0.46
1:D:122:LEU:HD21	1:D:175:LEU:HD21	1.97	0.46
1:A:233:LEU:HD21	1:D:237[B]:GLN:HG2	1.97	0.45
1:B:233:LEU:HD21	1:C:237[B]:GLN:HA	1.98	0.45
1:D:273:ALA:HB3	1:D:274:PRO:CD	2.47	0.45
1:D:273:ALA:HB3	1:D:274:PRO:HD3	1.98	0.45
1:C:45:LEU:HD22	2:C:400:HNR:HAM	1.99	0.45
1:C:189:LEU:HD11	1:C:202:VAL:HG23	1.99	0.45
3:D:450:MES:H82	3:D:450:MES:H51	1.64	0.45
1:A:189:LEU:HD11	1:A:202:VAL:CG2	2.48	0.44
1:B:237[B]:GLN:HE22	1:C:237[B]:GLN:HG2	1.57	0.44
1:C:23:ILE:HD11	1:C:28:LEU:HD23	1.99	0.44
1:D:128:ARG:HG3	1:D:128:ARG:HH11	1.83	0.44
1:A:24:SER:OG	1:A:59:ASP:OD2	2.25	0.44
1:B:23:ILE:HD12	1:C:23:ILE:CD1	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:GLN:HG3	6:B:2074:HOH:O	2.18	0.44
1:B:237[A]:GLN:HA	1:C:233:LEU:HD21	2.00	0.44
1:C:273:ALA:HB3	1:C:274:PRO:CD	2.45	0.44
1:A:38:TYR:HB2	1:A:112:LEU:HD22	2.00	0.44
1:C:108:LEU:HD22	1:C:174:GLY:HA3	2.00	0.43
1:C:103:LEU:CD2	1:C:179:ASP:HA	2.48	0.43
1:B:28:LEU:HD22	1:C:29:PRO:HG3	2.00	0.43
1:A:122:LEU:CD2	1:A:175:LEU:HD21	2.48	0.43
1:B:237[B]:GLN:HA	1:C:233:LEU:HD21	2.01	0.43
1:C:25:LYS:NZ	1:C:227:GLY:HA2	2.34	0.42
1:C:89:ALA:HB3	1:C:197:LEU:HB3	2.02	0.42
1:D:268:LEU:HD23	1:D:288:LEU:CD2	2.49	0.42
1:B:60:THR:HB	1:B:61:PRO:HD3	2.02	0.41
1:A:3:ARG:N	6:A:2001:HOH:O	2.53	0.41
1:B:5:GLY:O	1:B:51:ILE:HA	2.21	0.41
1:A:224:LEU:HD11	1:A:238:PHE:CD2	2.56	0.41
1:A:16:LEU:CD1	1:A:25:LYS:HD3	2.52	0.40
1:B:23:ILE:HG21	1:C:23:ILE:CD1	2.52	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	291/302 (96%)	286 (98%)	4 (1%)	1 (0%)	41	46
1	B	287/302 (95%)	282 (98%)	4 (1%)	1 (0%)	41	46
1	C	286/302 (95%)	281 (98%)	4 (1%)	1 (0%)	41	46
1	D	291/302 (96%)	287 (99%)	3 (1%)	1 (0%)	41	46
All	All	1155/1208 (96%)	1136 (98%)	15 (1%)	4 (0%)	41	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	31	TYR
1	C	31	TYR
1	A	31	TYR
1	D	31	TYR

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	242/247 (98%)	240 (99%)	2 (1%)	81 90
1	B	238/247 (96%)	234 (98%)	4 (2%)	60 74
1	C	237/247 (96%)	228 (96%)	9 (4%)	33 42
1	D	240/247 (97%)	233 (97%)	7 (3%)	42 54
All	All	957/988 (97%)	935 (98%)	22 (2%)	50 63

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	232	LEU
1	B	17	HIS
1	B	23	ILE
1	B	130	THR
1	B	269	GLU
1	C	26	GLN
1	C	88	LEU
1	C	93	LEU
1	C	108	LEU
1	C	126	SER
1	C	129	GLN
1	C	143	GLU
1	C	277	LYS
1	C	285	LYS
1	D	21	LEU
1	D	65	GLN
1	D	117	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	126	SER
1	D	215	GLU
1	D	232	LEU
1	D	277	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	101	ASN
1	A	127	GLN
1	A	203	ASN
1	B	127	GLN
1	B	229	HIS
1	C	17	HIS
1	C	26	GLN
1	C	111	ASN
1	C	129	GLN
1	C	203	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
2	HNR	D	400	-	23,25,25	1.30	1 (4%)	30,36,36	2.20	8 (26%)
2	HNR	A	400	-	23,25,25	1.24	1 (4%)	30,36,36	2.26	8 (26%)
2	HNR	C	400	-	23,25,25	1.35	2 (8%)	30,36,36	2.33	8 (26%)
3	MES	A	450	-	12,12,12	1.67	1 (8%)	14,16,16	1.23	1 (7%)
3	MES	C	450	-	12,12,12	1.73	2 (16%)	14,16,16	2.25	6 (42%)
3	MES	B	450	-	12,12,12	1.74	2 (16%)	14,16,16	1.37	2 (14%)
5	GOL	B	1295	-	5,5,5	0.34	0	5,5,5	0.41	0
5	GOL	D	1295	-	5,5,5	0.35	0	5,5,5	0.42	0
3	MES	D	450	-	12,12,12	1.60	1 (8%)	14,16,16	1.41	1 (7%)
2	HNR	B	400	-	23,25,25	1.53	4 (17%)	30,36,36	2.31	8 (26%)

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
2	HNR	D	400	-	-	2/16/20/20	0/2/2/2
2	HNR	A	400	-	-	2/16/20/20	0/2/2/2
2	HNR	C	400	-	-	1/16/20/20	0/2/2/2
3	MES	A	450	-	-	3/6/14/14	0/1/1/1
3	MES	C	450	-	-	0/6/14/14	0/1/1/1
3	MES	B	450	-	-	0/6/14/14	0/1/1/1
5	GOL	B	1295	-	-	2/4/4/4	-
5	GOL	D	1295	-	-	2/4/4/4	-
3	MES	D	450	-	-	4/6/14/14	0/1/1/1
2	HNR	B	400	-	-	2/16/20/20	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	HNR	OAC-SAK	5.52	1.49	1.43
2	C	400	HNR	OAC-SAK	5.51	1.49	1.43
2	B	400	HNR	OAC-SAK	5.33	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	400	HNR	OAC-SAK	5.23	1.49	1.43
3	B	450	MES	C8-S	5.07	1.84	1.77
3	A	450	MES	C8-S	4.86	1.84	1.77
3	C	450	MES	C8-S	4.67	1.84	1.77
3	D	450	MES	C8-S	4.31	1.83	1.77
2	B	400	HNR	CAR-NAQ	2.54	1.43	1.38
2	C	400	HNR	CAR-NAQ	2.49	1.43	1.38
2	B	400	HNR	OAT-SAK	-2.43	1.40	1.43
2	B	400	HNR	CAH-NAG	2.14	1.42	1.38
3	B	450	MES	O1S-S	2.13	1.51	1.45
3	C	450	MES	O1S-S	2.01	1.51	1.45

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	400	HNR	OAC-SAK-OAT	-7.37	107.58	119.52
2	C	400	HNR	CAI-CAH-NAG	6.07	121.68	110.99
2	B	400	HNR	CAH-NAG-CAP	-5.98	119.61	127.35
2	A	400	HNR	CAI-CAH-NAG	5.84	121.28	110.99
2	B	400	HNR	OAC-SAK-OAT	-5.80	110.12	119.52
2	D	400	HNR	OAC-SAK-OAT	-5.69	110.31	119.52
2	D	400	HNR	CAI-CAH-NAG	5.67	120.98	110.99
2	B	400	HNR	CAI-CAH-NAG	5.51	120.70	110.99
2	A	400	HNR	OAC-SAK-OAT	-5.39	110.79	119.52
2	A	400	HNR	CAH-NAG-CAP	-5.32	120.46	127.35
2	D	400	HNR	CAH-NAG-CAP	-5.28	120.52	127.35
2	C	400	HNR	CAH-NAG-CAP	-4.53	121.48	127.35
2	A	400	HNR	OAC-SAK-NAJ	4.30	112.47	106.57
2	C	400	HNR	OAC-SAK-NAJ	4.05	112.14	106.57
3	D	450	MES	O1S-S-C8	3.86	111.57	106.92
2	B	400	HNR	OAT-SAK-NAJ	3.80	111.78	106.57
3	C	450	MES	C7-N4-C3	-3.64	101.92	111.23
3	C	450	MES	C7-N4-C5	-3.59	102.07	111.23
3	C	450	MES	O1S-S-C8	3.57	111.21	106.92
3	B	450	MES	O1S-S-C8	3.50	111.13	106.92
3	A	450	MES	O3S-S-C8	3.29	111.09	105.77
2	B	400	HNR	OAA-CAH-CAI	-3.19	119.72	127.54
2	A	400	HNR	OAT-SAK-NAJ	3.05	110.75	106.57
2	B	400	HNR	OAO-CAP-NAQ	-2.91	118.49	122.35
2	B	400	HNR	NAG-CAP-NAQ	2.74	120.19	115.29
3	C	450	MES	C6-O1-C2	2.70	118.92	109.89
2	D	400	HNR	OAT-SAK-NAJ	2.67	110.23	106.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	450	MES	C5-N4-C3	2.67	114.83	108.83
2	B	400	HNR	OAC-SAK-NAJ	2.65	110.21	106.57
2	D	400	HNR	OAC-SAK-NAJ	2.47	109.96	106.57
2	C	400	HNR	OAA-CAH-NAG	-2.45	115.43	120.12
2	A	400	HNR	NAG-CAP-NAQ	2.38	119.56	115.29
3	B	450	MES	O3S-S-C8	2.37	109.59	105.77
2	D	400	HNR	NAG-CAP-NAQ	2.33	119.47	115.29
2	A	400	HNR	CAV-CAU-NAQ	-2.22	107.26	112.39
2	C	400	HNR	NAG-CAP-NAQ	2.13	119.11	115.29
2	C	400	HNR	OAT-SAK-NAJ	2.12	109.48	106.57
2	D	400	HNR	CAU-NAQ-CAP	2.10	119.54	117.13
2	A	400	HNR	OAA-CAH-CAI	-2.09	122.42	127.54
2	D	400	HNR	OAA-CAH-CAI	-2.09	122.42	127.54
3	C	450	MES	O1-C2-C3	2.07	116.34	111.80
2	C	400	HNR	OAT-SAK-CAL	2.02	110.61	108.05

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	450	MES	C7-C8-S-O2S
3	A	450	MES	C7-C8-S-O3S
3	D	450	MES	C8-C7-N4-C5
3	D	450	MES	C7-C8-S-O1S
3	D	450	MES	C7-C8-S-O3S
5	D	1295	GOL	O1-C1-C2-C3
2	A	400	HNR	NAQ-CAU-CAV-CAX
2	D	400	HNR	NAQ-CAU-CAV-CAX
5	B	1295	GOL	O1-C1-C2-C3
5	D	1295	GOL	O1-C1-C2-O2
5	B	1295	GOL	O1-C1-C2-O2
3	A	450	MES	C7-C8-S-O1S
3	D	450	MES	C7-C8-S-O2S
2	B	400	HNR	NAQ-CAU-CAV-CAX
2	C	400	HNR	CAB-NAJ-SAK-OAT
2	A	400	HNR	CAB-NAJ-SAK-OAT
2	B	400	HNR	CAB-NAJ-SAK-OAT
2	D	400	HNR	CAB-NAJ-SAK-OAT

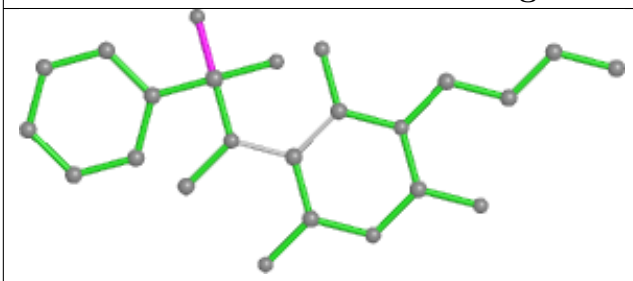
There are no ring outliers.

4 monomers are involved in 6 short contacts:

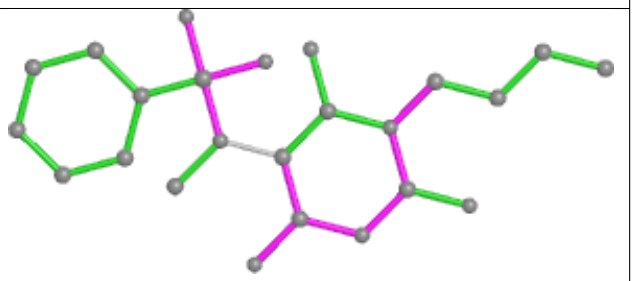
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	400	HNR	2	0
3	A	450	MES	1	0
3	B	450	MES	1	0
3	D	450	MES	2	0

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

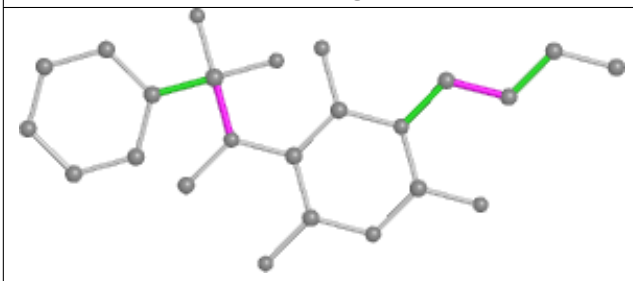
Ligand HNR D 400



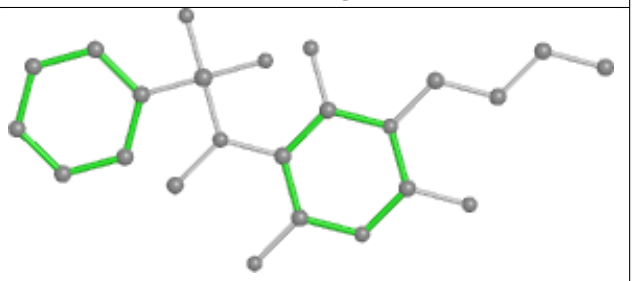
Bond lengths



Bond angles

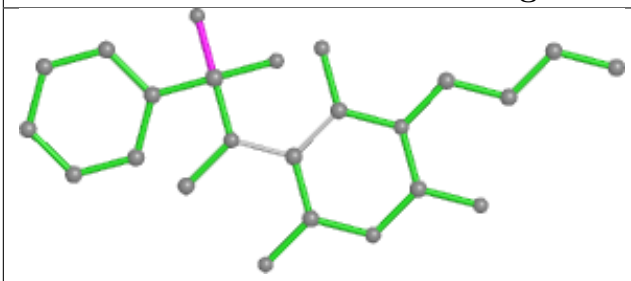


Torsions

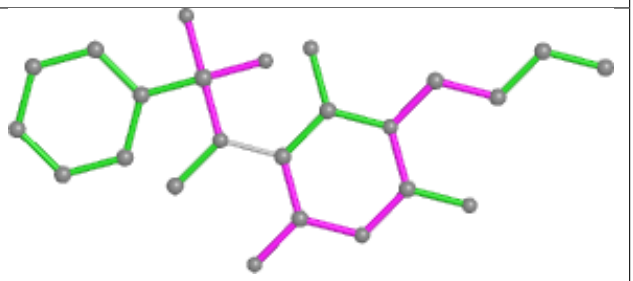


Rings

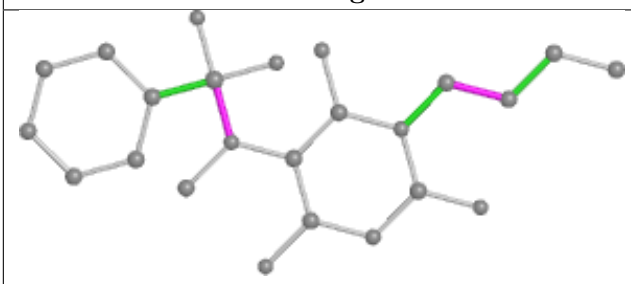
Ligand HNR A 400



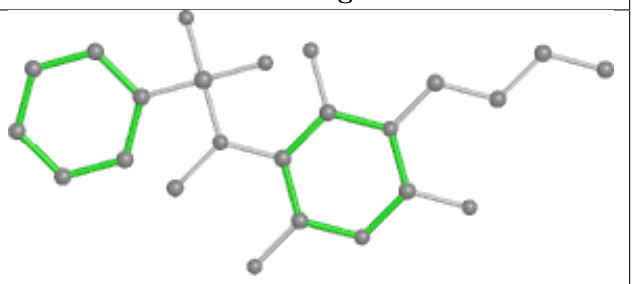
Bond lengths



Bond angles

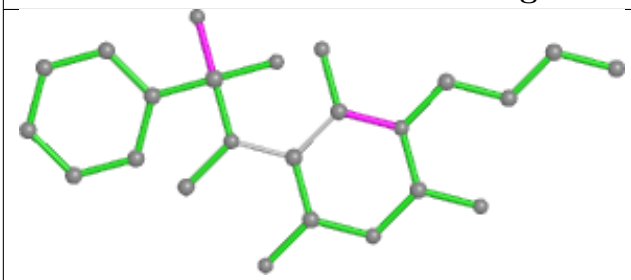


Torsions

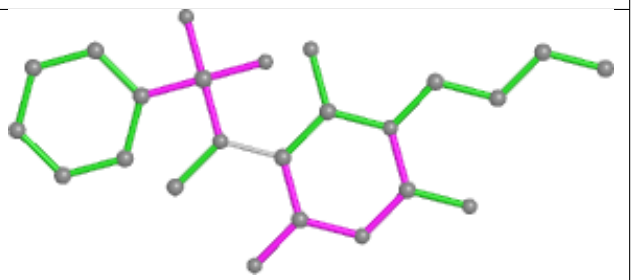


Rings

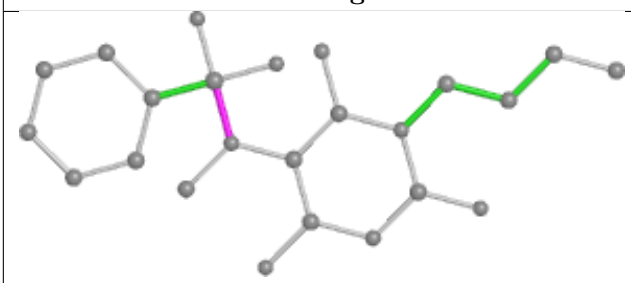
Ligand HNR C 400



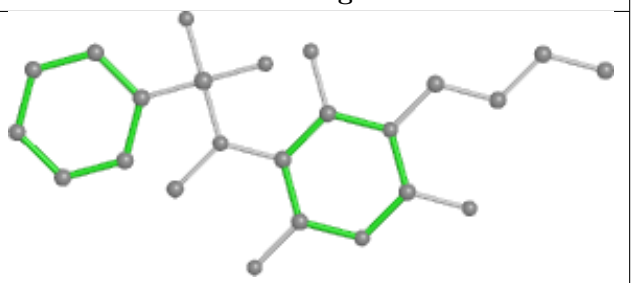
Bond lengths



Bond angles

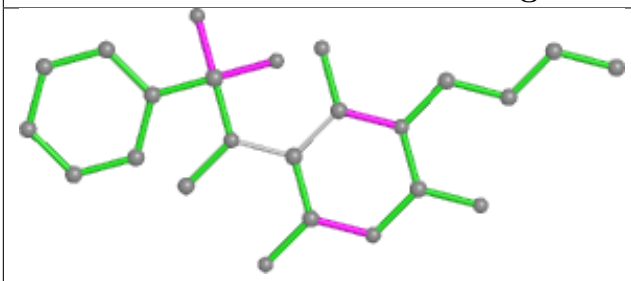


Torsions

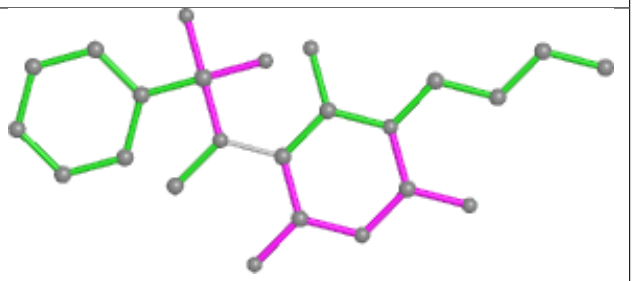


Rings

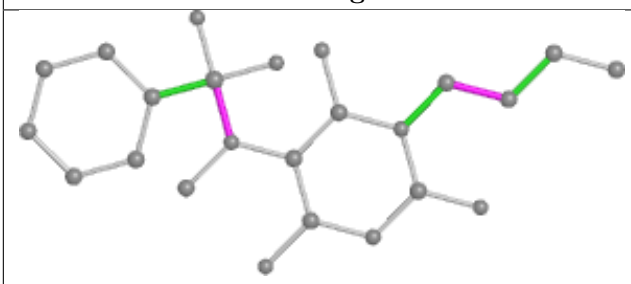
Ligand HNR B 400



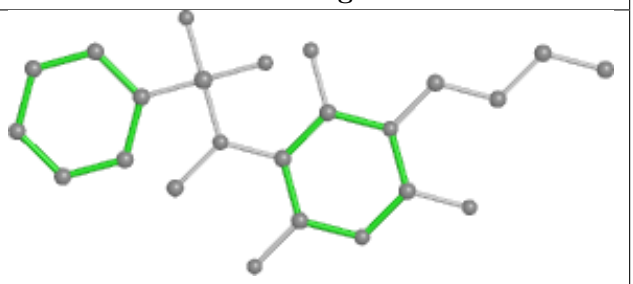
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	294/302 (97%)	-0.27	8 (2%)	54	52	25, 36, 58, 93	0
1	B	290/302 (96%)	-0.13	7 (2%)	59	56	27, 41, 61, 79	0
1	C	289/302 (95%)	-0.12	14 (4%)	30	29	23, 36, 69, 97	0
1	D	292/302 (96%)	-0.08	9 (3%)	49	47	30, 40, 60, 83	0
All	All	1165/1208 (96%)	-0.15	38 (3%)	46	44	23, 38, 62, 97	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	190	LYS	4.4
1	C	14	THR	4.1
1	D	193	PRO	3.9
1	A	127	GLN	3.8
1	C	191	PRO	3.8
1	C	277	LYS	3.2
1	D	194	ARG	3.2
1	C	187	ARG	3.1
1	C	15	ARG	3.1
1	D	195	GLY	3.0
1	B	22	ALA	2.9
1	C	189	LEU	2.7
1	C	195	GLY	2.6
1	D	65	GLN	2.5
1	D	190	LYS	2.5
1	D	277	LYS	2.5
1	C	276	ALA	2.5
1	C	13	GLY	2.5
1	A	276	ALA	2.5
1	B	152	GLN	2.5
1	A	153	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	191	PRO	2.4
1	C	23	ILE	2.4
1	A	194	ARG	2.4
1	A	195	GLY	2.3
1	D	192	SER	2.3
1	B	277	LYS	2.3
1	A	193	PRO	2.3
1	D	127	GLN	2.3
1	C	22	ALA	2.2
1	B	164	LEU	2.2
1	B	195	GLY	2.2
1	C	190	LYS	2.2
1	A	191	PRO	2.2
1	B	191	PRO	2.2
1	A	277	LYS	2.1
1	C	282	GLN	2.1
1	C	227	GLY	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	1295	6/6	0.80	0.15	57,59,61,63	0
3	MES	D	450	12/12	0.91	0.21	57,59,65,72	0
3	MES	B	450	12/12	0.93	0.17	57,60,63,66	0
3	MES	C	450	12/12	0.93	0.20	46,47,49,51	0
5	GOL	D	1295	6/6	0.93	0.12	51,52,54,54	0
3	MES	A	450	12/12	0.94	0.23	50,55,61,61	0

Continued on next page...

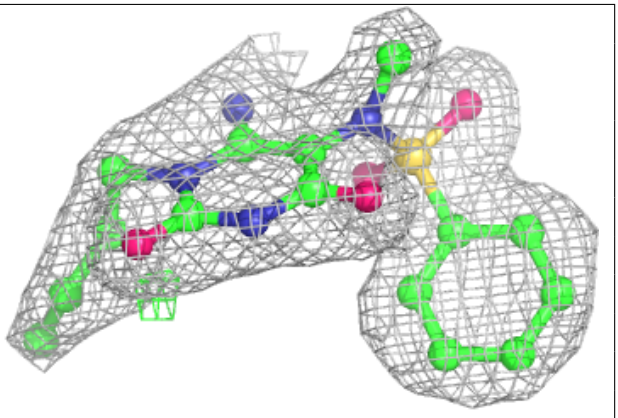
Continued from previous page...

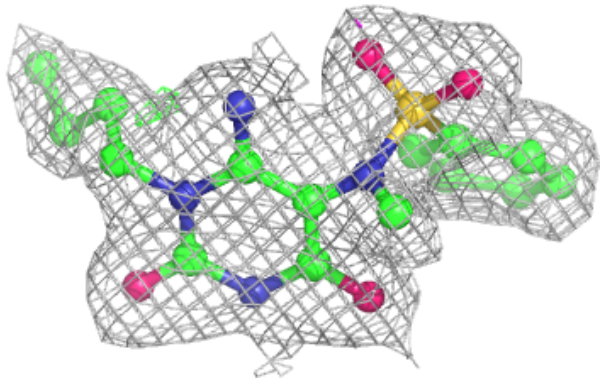
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HNR	D	400	24/24	0.96	0.11	33,38,50,54	0
2	HNR	B	400	24/24	0.97	0.11	31,35,42,44	0
2	HNR	C	400	24/24	0.97	0.13	26,30,33,35	0
2	HNR	A	400	24/24	0.97	0.13	27,29,34,40	0
4	CL	C	1294	1/1	0.98	0.16	29,29,29,29	0
4	CL	B	1294	1/1	0.99	0.14	30,30,30,30	0
4	CL	C	1295	1/1	0.99	0.06	42,42,42,42	0
4	CL	A	1294	1/1	1.00	0.20	28,28,28,28	0
4	CL	D	1294	1/1	1.00	0.13	35,35,35,35	0

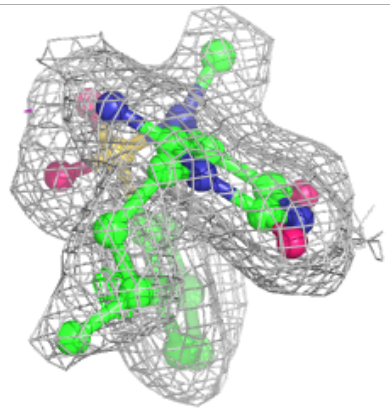
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HNR D 400:

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

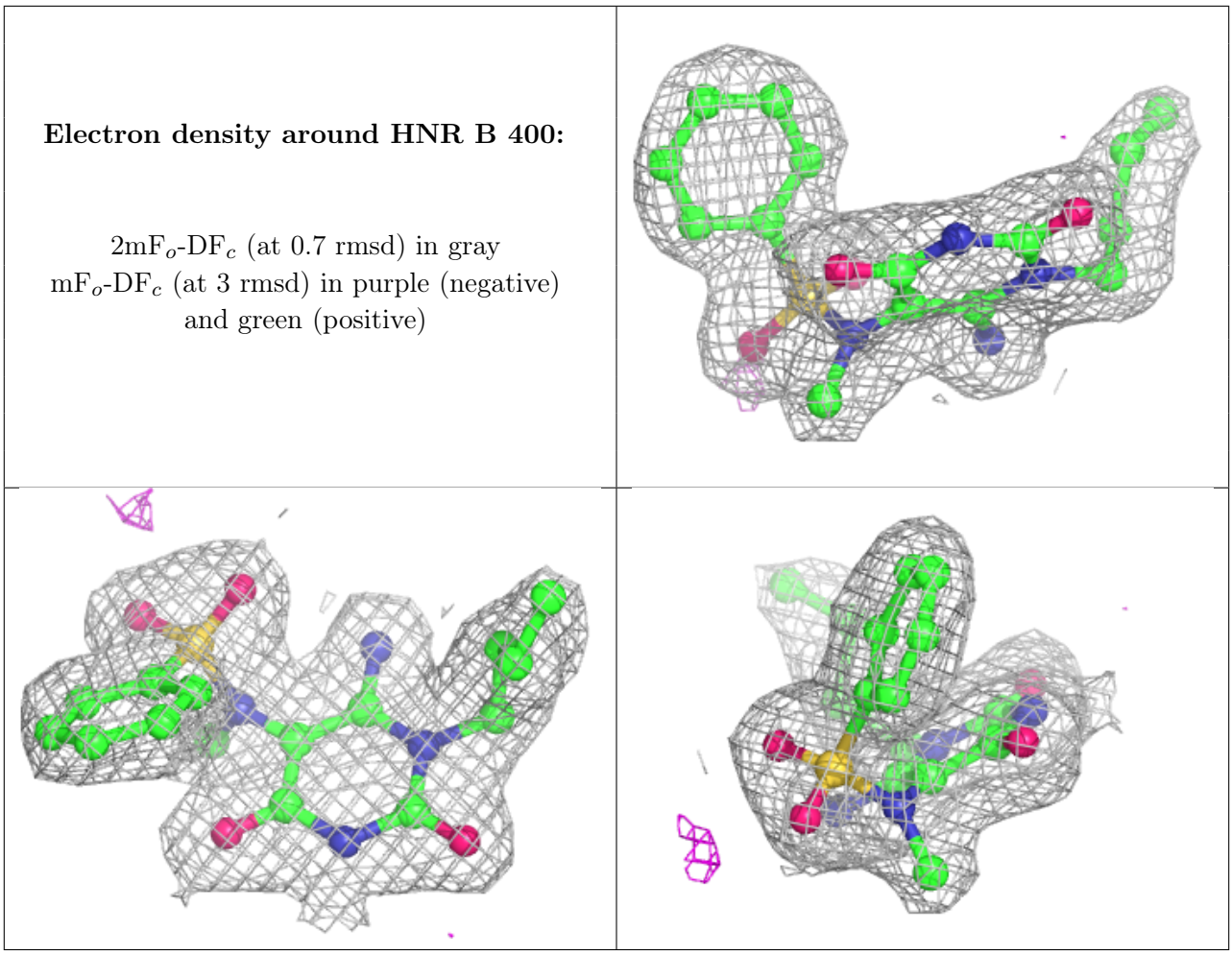






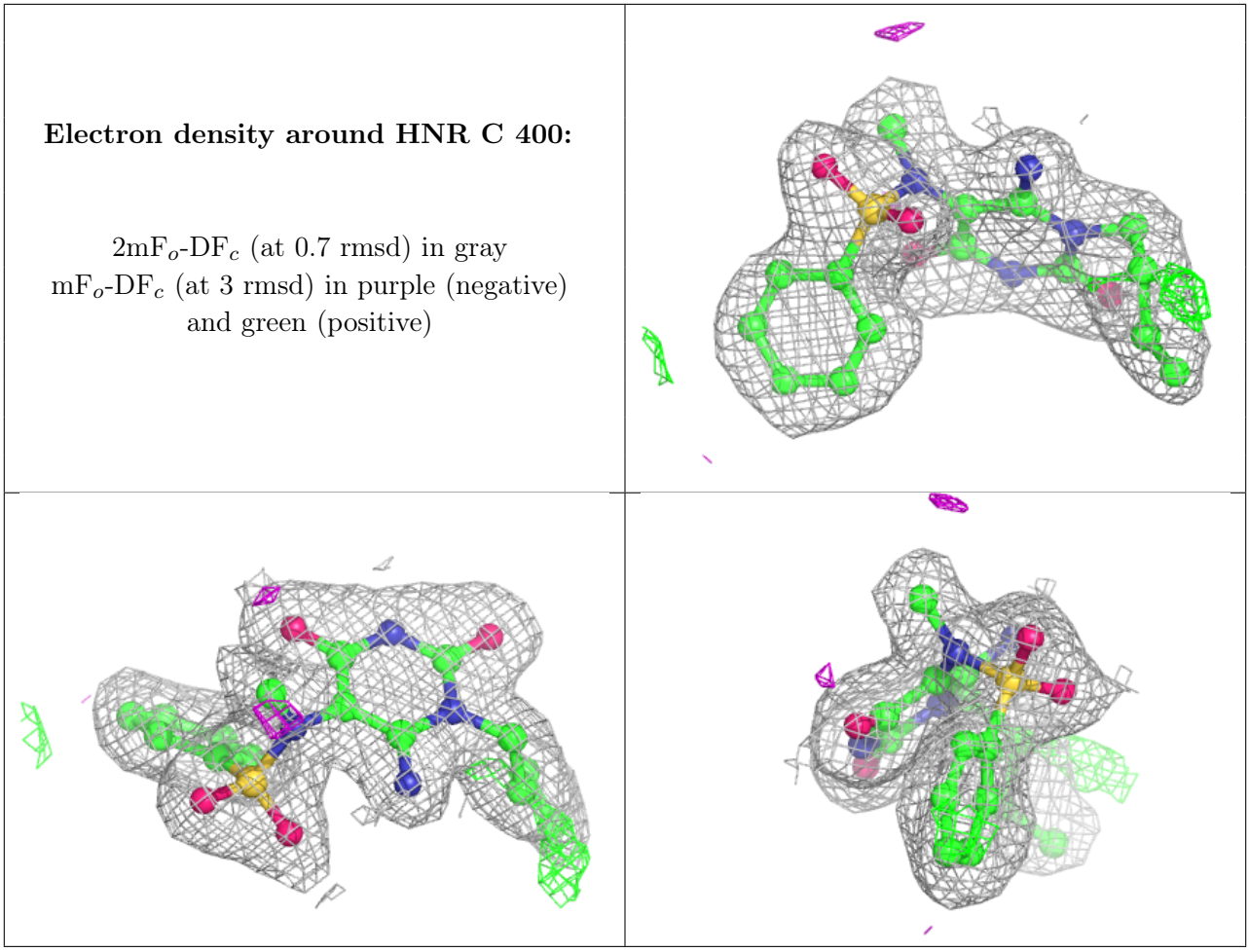
Electron density around HNR B 400:

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



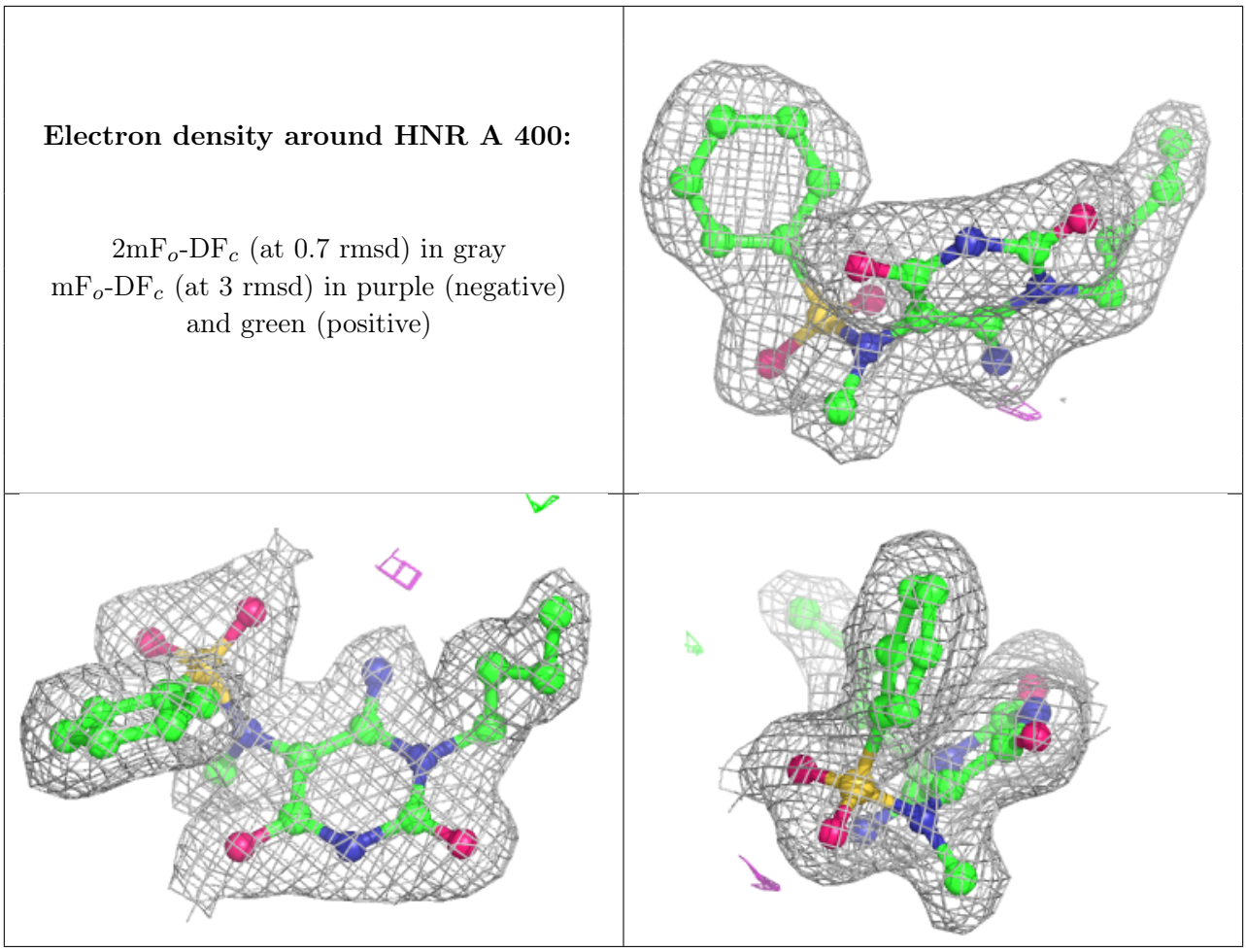
Electron density around HNR C 400:

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



Electron density around HNR A 400:

$2mF_o$-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.