Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2026 – 04:39 AM UTC

PDB ID	:	5FUH / pdb_00005fuh
Title	:	Pseudomonas aeruginosa RmlA in complex with allosteric inhibitor
Authors	:	Alphey, M.S.; Tran, F.; Westwood, N.J.; Naismith, J.H.
Deposited on	:	2016-01-27
Resolution	:	1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

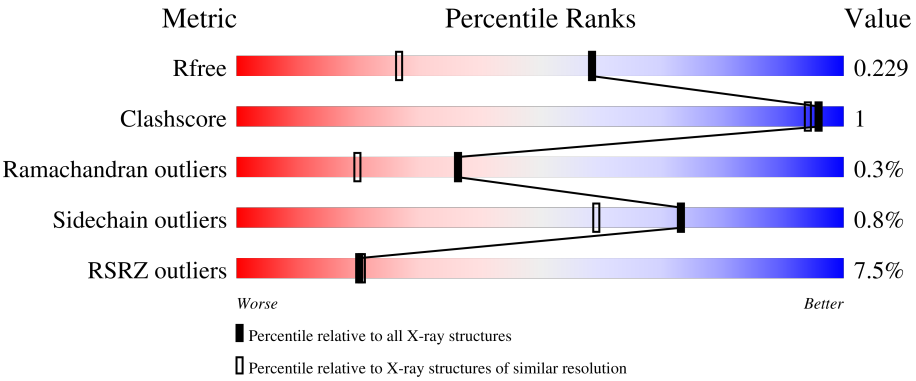
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	303	7% 95%
1	B	303	7% 94%
1	C	303	8% 96%
1	D	303	8% 95%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10103 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	298	Total	C	N	O	S	0	5	0
			2371	1519	404	443	5			
1	B	293	Total	C	N	O	S	0	3	0
			2309	1481	387	436	5			
1	C	299	Total	C	N	O	S	0	4	0
			2367	1518	401	442	6			
1	D	292	Total	C	N	O	S	0	2	0
			2296	1471	386	435	4			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	HIS	-	expression tag	UNP Q9HU22
A	-8	HIS	-	expression tag	UNP Q9HU22
A	-7	HIS	-	expression tag	UNP Q9HU22
A	-6	HIS	-	expression tag	UNP Q9HU22
A	-5	HIS	-	expression tag	UNP Q9HU22
A	-4	HIS	-	expression tag	UNP Q9HU22
A	-3	GLY	-	expression tag	UNP Q9HU22
A	-2	SER	-	expression tag	UNP Q9HU22
A	-1	MET	-	expression tag	UNP Q9HU22
A	0	ALA	-	expression tag	UNP Q9HU22
B	-9	HIS	-	expression tag	UNP Q9HU22
B	-8	HIS	-	expression tag	UNP Q9HU22
B	-7	HIS	-	expression tag	UNP Q9HU22
B	-6	HIS	-	expression tag	UNP Q9HU22
B	-5	HIS	-	expression tag	UNP Q9HU22
B	-4	HIS	-	expression tag	UNP Q9HU22
B	-3	GLY	-	expression tag	UNP Q9HU22
B	-2	SER	-	expression tag	UNP Q9HU22
B	-1	MET	-	expression tag	UNP Q9HU22
B	0	ALA	-	expression tag	UNP Q9HU22

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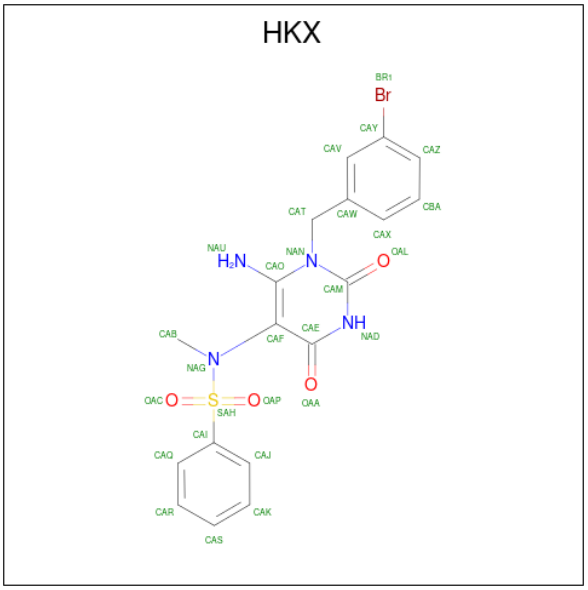
Chain	Residue	Modelled	Actual	Comment	Reference
C	-9	HIS	-	expression tag	UNP Q9HU22
C	-8	HIS	-	expression tag	UNP Q9HU22
C	-7	HIS	-	expression tag	UNP Q9HU22
C	-6	HIS	-	expression tag	UNP Q9HU22
C	-5	HIS	-	expression tag	UNP Q9HU22
C	-4	HIS	-	expression tag	UNP Q9HU22
C	-3	GLY	-	expression tag	UNP Q9HU22
C	-2	SER	-	expression tag	UNP Q9HU22
C	-1	MET	-	expression tag	UNP Q9HU22
C	0	ALA	-	expression tag	UNP Q9HU22
D	-9	HIS	-	expression tag	UNP Q9HU22
D	-8	HIS	-	expression tag	UNP Q9HU22
D	-7	HIS	-	expression tag	UNP Q9HU22
D	-6	HIS	-	expression tag	UNP Q9HU22
D	-5	HIS	-	expression tag	UNP Q9HU22
D	-4	HIS	-	expression tag	UNP Q9HU22
D	-3	GLY	-	expression tag	UNP Q9HU22
D	-2	SER	-	expression tag	UNP Q9HU22
D	-1	MET	-	expression tag	UNP Q9HU22
D	0	ALA	-	expression tag	UNP Q9HU22

- Molecule 2 is N-[6-amino-1-(3-bromobenzyl)-2,4-dioxo-1,2,3,4-tetrahydropyrimidin-5-yl]-N-methylbenzenesulfonamide (CCD ID: HKX) (formula: $C_{18}H_{17}BrN_4O_4S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	Br	C	N	O	S	0	0
			28	1	18	4	4	1		

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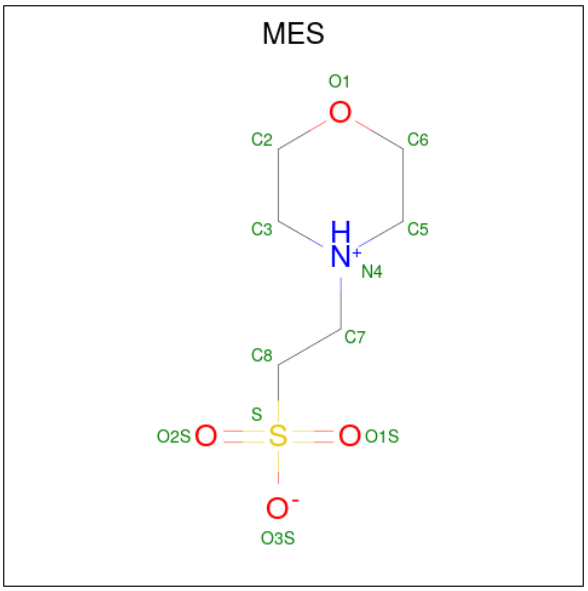
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	Br	C	N	O	S	0	0
			28	1	18	4	4	1		
2	C	1	Total	Br	C	N	O	S	0	0
			28	1	18	4	4	1		
2	D	1	Total	Br	C	N	O	S	0	0
			28	1	18	4	4	1		

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



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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

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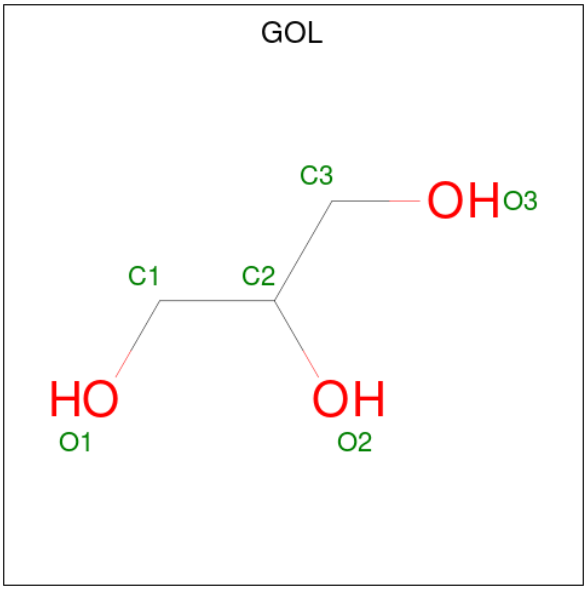
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	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	179	Total O 179 179	0	0
6	B	142	Total O 142 142	0	0
6	C	152	Total O 152 152	0	0

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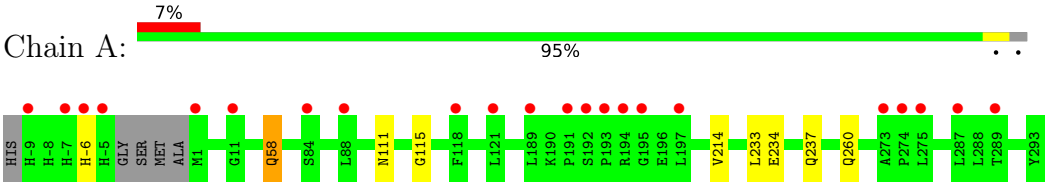
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	99	Total O 99 99	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

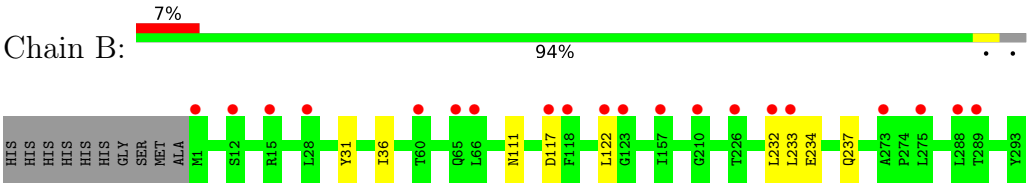
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain A:



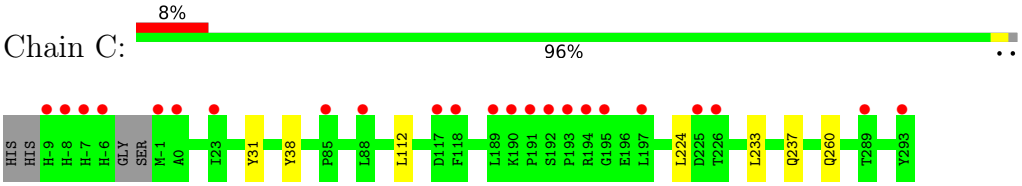
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain B:



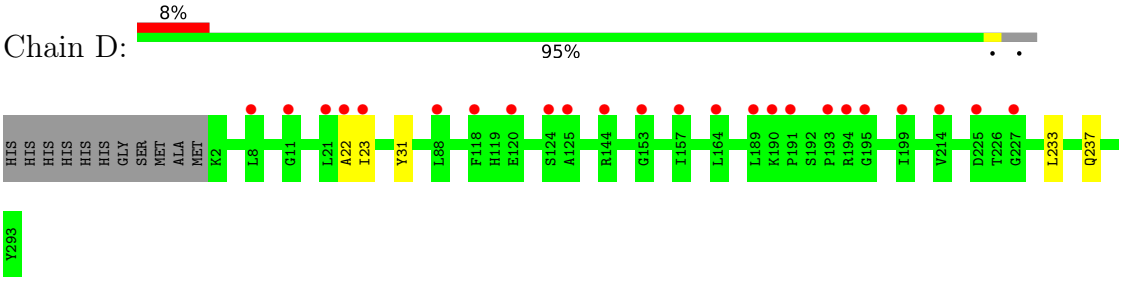
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain C:



• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	64.46Å 155.26Å 134.83Å 90.00° 92.53° 90.00°	Depositor
Resolution (Å)	67.35 – 1.60 67.35 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (67.35-1.60) 99.2 (67.35-1.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 1.59Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.202 , 0.227 0.207 , 0.229	Depositor DCC
R_{free} test set	8733 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	24.0	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 27.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.054 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10103	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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: HKX, GOL, MES, CL

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	0.59	0/2440	0.77	1/3308 (0.0%)
1	B	0.56	0/2368	0.78	0/3212
1	C	0.60	0/2432	0.76	0/3297
1	D	0.55	0/2352	0.72	0/3191
All	All	0.58	0/9592	0.76	1/13008 (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	A	115	GLY	N-CA-C	5.76	118.40	110.56

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	2371	0	2367	9	0
1	B	2309	0	2314	5	0
1	C	2367	0	2369	9	0
1	D	2296	0	2291	3	0
2	A	28	0	0	1	0
2	B	28	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	28	0	0	1	0
2	D	28	0	0	0	0
3	A	12	0	13	1	0
3	B	12	0	13	0	0
3	C	12	0	13	0	0
3	D	12	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	6	0	8	0	0
5	C	6	0	8	0	0
5	D	12	0	16	0	0
6	A	179	0	0	0	0
6	B	142	0	0	0	0
6	C	152	0	0	0	0
6	D	99	0	0	0	0
All	All	10103	0	9425	20	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 1.

All (20) 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:C:112[A]:LEU:HD22	1:C:224:LEU:HD12	1.74	0.68
1:A:58[A]:GLN:HE21	1:A:58[A]:GLN:HA	1.64	0.63
1:A:237[B]:GLN:HA	1:B:233[B]:LEU:HD21	1.81	0.60
1:C:237[B]:GLN:HG3	1:D:233:LEU:HD11	1.90	0.53
1:D:22:ALA:C	1:D:23:ILE:HD12	2.32	0.53
1:A:237[B]:GLN:CA	1:B:233[B]:LEU:HD21	2.39	0.51
1:B:234:GLU:HA	1:B:237[B]:GLN:HE21	1.74	0.51
1:A:234:GLU:HA	1:A:237[A]:GLN:HE21	1.76	0.50
1:C:233[A]:LEU:HD21	1:D:237[A]:GLN:HA	1.94	0.49
1:C:260:GLN:HG2	2:C:400:HKX:BR1	2.68	0.49
1:C:112[A]:LEU:HD13	1:C:224:LEU:HD12	1.96	0.48
1:A:233[A]:LEU:HD21	1:B:237[A]:GLN:HA	1.98	0.46
1:A:58[A]:GLN:HE21	1:A:58[A]:GLN:CA	2.25	0.46
1:C:112[A]:LEU:HD22	1:C:224:LEU:CD1	2.42	0.45
1:A:260:GLN:HG2	2:A:400:HKX:BR1	2.72	0.44
1:A:214:VAL:O	3:A:1294:MES:H71	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112[A]:LEU:CD2	1:C:224:LEU:HD12	2.46	0.41
1:A:237[B]:GLN:HA	1:B:233[B]:LEU:CD2	2.50	0.41
1:C:38:TYR:HB2	1:C:112[B]:LEU:HD22	2.03	0.41

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	299/303 (99%)	293 (98%)	6 (2%)	0	100	100
1	B	294/303 (97%)	290 (99%)	3 (1%)	1 (0%)	36	20
1	C	299/303 (99%)	296 (99%)	2 (1%)	1 (0%)	36	20
1	D	292/303 (96%)	289 (99%)	2 (1%)	1 (0%)	36	20
All	All	1184/1212 (98%)	1168 (99%)	13 (1%)	3 (0%)	36	20

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	31	TYR
1	C	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	250/248 (101%)	246 (98%)	4 (2%)	55 33
1	B	243/248 (98%)	238 (98%)	5 (2%)	47 23
1	C	249/248 (100%)	249 (100%)	0	100 100
1	D	241/248 (97%)	241 (100%)	0	100 100
All	All	983/992 (99%)	974 (99%)	9 (1%)	73 55

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

Mol	Chain	Res	Type
1	A	-6	HIS
1	A	58[A]	GLN
1	A	58[B]	GLN
1	A	111	ASN
1	B	36	ILE
1	B	111	ASN
1	B	117	ASP
1	B	122	LEU
1	B	232	LEU

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	78	GLN
1	A	82	GLN
1	B	82	GLN
1	B	90	GLN
1	C	82	GLN
1	C	90	GLN
1	C	181	GLN
1	C	211	GLN
1	D	65	GLN
1	D	181	GLN
1	D	211	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	HKX	C	400	-	30,30,30	2.87	7 (23%)	39,44,44	2.26	16 (41%)
3	MES	B	1294	-	12,12,12	2.27	1 (8%)	15,16,16	1.73	3 (20%)
3	MES	D	1294	-	12,12,12	2.13	1 (8%)	15,16,16	1.82	2 (13%)
3	MES	A	1294	-	12,12,12	2.25	1 (8%)	15,16,16	1.28	2 (13%)
5	GOL	D	1297	-	5,5,5	0.22	0	5,5,5	0.29	0
5	GOL	D	1296	-	5,5,5	0.29	0	5,5,5	0.36	0
5	GOL	A	1296	-	5,5,5	0.27	0	5,5,5	0.32	0
2	HKX	B	400	-	30,30,30	2.85	8 (26%)	39,44,44	2.19	12 (30%)
3	MES	C	1294	-	12,12,12	2.30	1 (8%)	15,16,16	1.56	2 (13%)
2	HKX	D	400	-	30,30,30	2.91	7 (23%)	39,44,44	2.29	16 (41%)
2	HKX	A	400	-	30,30,30	2.85	6 (20%)	39,44,44	2.49	16 (41%)
5	GOL	C	1296	-	5,5,5	0.28	0	5,5,5	0.37	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
2	HKX	C	400	-	-	5/16/20/20	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MES	B	1294	-	-	4/6/14/14	0/1/1/1
3	MES	D	1294	-	-	3/6/14/14	0/1/1/1
3	MES	A	1294	-	-	0/6/14/14	0/1/1/1
5	GOL	D	1297	-	-	0/4/4/4	-
5	GOL	D	1296	-	-	2/4/4/4	-
5	GOL	A	1296	-	-	2/4/4/4	-
2	HKX	B	400	-	-	5/16/20/20	0/3/3/3
3	MES	C	1294	-	-	5/6/14/14	0/1/1/1
2	HKX	D	400	-	-	5/16/20/20	0/3/3/3
2	HKX	A	400	-	-	5/16/20/20	0/3/3/3
5	GOL	C	1296	-	-	0/4/4/4	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	HKX	OAP-SAH	9.42	1.53	1.43
2	C	400	HKX	OAP-SAH	9.30	1.53	1.43
2	C	400	HKX	OAC-SAH	9.26	1.53	1.43
2	D	400	HKX	OAP-SAH	9.24	1.53	1.43
2	A	400	HKX	OAC-SAH	9.04	1.53	1.43
2	B	400	HKX	OAP-SAH	8.90	1.53	1.43
2	D	400	HKX	OAC-SAH	8.86	1.53	1.43
2	B	400	HKX	OAC-SAH	8.72	1.52	1.43
3	A	1294	MES	C8-S	-7.42	1.67	1.77
3	C	1294	MES	C8-S	-7.31	1.67	1.77
3	B	1294	MES	C8-S	-7.29	1.67	1.77
3	D	1294	MES	C8-S	-7.03	1.67	1.77
2	B	400	HKX	CAT-CAW	-6.66	1.39	1.51
2	D	400	HKX	CAT-CAW	-6.25	1.40	1.51
2	A	400	HKX	CAT-CAW	-6.08	1.40	1.51
2	C	400	HKX	CAT-CAW	-6.00	1.40	1.51
2	D	400	HKX	CAI-SAH	3.99	1.81	1.76
2	A	400	HKX	SAH-NAG	3.35	1.73	1.65
2	D	400	HKX	CAM-NAN	-3.15	1.34	1.39
2	B	400	HKX	CAM-NAN	-3.05	1.34	1.39
2	C	400	HKX	BR1-CAY	-2.98	1.84	1.90
2	B	400	HKX	CAI-SAH	-2.81	1.72	1.76
2	B	400	HKX	CAF-NAG	-2.73	1.34	1.40
2	C	400	HKX	CAM-NAN	-2.72	1.35	1.39
2	B	400	HKX	BR1-CAY	-2.58	1.85	1.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	HKX	CAM-NAN	-2.31	1.35	1.39
2	C	400	HKX	CAF-NAG	-2.26	1.35	1.40
2	A	400	HKX	BR1-CAY	-2.23	1.85	1.90
2	D	400	HKX	CAF-NAG	-2.14	1.35	1.40
2	D	400	HKX	SAH-NAG	2.13	1.70	1.65
2	B	400	HKX	CAO-NAN	-2.06	1.35	1.39
2	C	400	HKX	CAF-CAE	-2.01	1.38	1.43

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	400	HKX	OAP-SAH-OAC	-7.19	108.37	119.59
2	D	400	HKX	OAP-SAH-OAC	-6.66	109.20	119.59
2	C	400	HKX	OAP-SAH-OAC	-6.30	109.75	119.59
2	B	400	HKX	OAP-SAH-OAC	-6.28	109.79	119.59
2	B	400	HKX	CAE-NAD-CAM	-5.97	119.51	127.34
2	D	400	HKX	CAE-NAD-CAM	-5.48	120.16	127.34
3	D	1294	MES	O1S-S-C8	5.40	114.89	106.73
2	A	400	HKX	OAP-SAH-CAI	-5.14	101.71	108.10
2	A	400	HKX	CAE-NAD-CAM	-5.07	120.70	127.34
2	C	400	HKX	CAE-NAD-CAM	-4.82	121.02	127.34
2	A	400	HKX	OAC-SAH-NAG	4.54	112.90	106.59
2	A	400	HKX	CAF-CAE-NAD	4.38	118.65	110.94
2	B	400	HKX	CAF-CAE-NAD	4.01	117.99	110.94
2	D	400	HKX	CAF-CAE-NAD	3.98	117.95	110.94
2	C	400	HKX	OAP-SAH-CAI	-3.92	103.23	108.10
2	C	400	HKX	CAF-CAE-NAD	3.71	117.47	110.94
2	D	400	HKX	CAQ-CAI-SAH	3.58	123.29	119.73
3	C	1294	MES	O2S-S-C8	3.48	111.99	106.73
2	C	400	HKX	CAQ-CAI-SAH	3.38	123.09	119.73
2	D	400	HKX	OAC-SAH-NAG	3.26	111.12	106.59
3	B	1294	MES	C2-C3-N4	3.23	115.03	110.12
2	D	400	HKX	CAI-SAH-NAG	3.22	112.85	106.66
2	C	400	HKX	CAI-SAH-NAG	3.20	112.83	106.66
3	B	1294	MES	C6-C5-N4	3.08	114.80	110.12
2	B	400	HKX	NAU-CAO-NAN	3.06	122.28	116.29
2	C	400	HKX	OAC-SAH-NAG	3.06	110.84	106.59
2	C	400	HKX	OAC-SAH-CAI	3.06	111.90	108.10
3	D	1294	MES	C2-C3-N4	2.99	114.66	110.12
2	B	400	HKX	NAD-CAM-NAN	2.94	120.73	115.45
2	B	400	HKX	CAF-CAO-NAU	-2.92	117.23	123.38
2	A	400	HKX	OAC-SAH-CAI	2.92	111.73	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	400	HKX	OAA-CAE-CAF	-2.91	120.47	127.62
2	A	400	HKX	OAA-CAE-CAF	-2.88	120.55	127.62
2	B	400	HKX	OAP-SAH-NAG	2.88	110.58	106.59
2	D	400	HKX	CAF-CAO-NAU	-2.87	117.32	123.38
2	D	400	HKX	NAU-CAO-NAN	2.87	121.91	116.29
2	A	400	HKX	CAQ-CAI-SAH	2.84	122.55	119.73
3	C	1294	MES	C2-C3-N4	2.82	114.41	110.12
2	D	400	HKX	NAD-CAM-NAN	2.81	120.50	115.45
3	B	1294	MES	O3S-S-C8	2.81	111.51	106.00
2	B	400	HKX	OAA-CAE-CAF	-2.79	120.77	127.62
2	A	400	HKX	CAF-CAO-NAN	2.79	121.06	119.01
2	C	400	HKX	OAA-CAE-CAF	-2.75	120.87	127.62
2	C	400	HKX	NAD-CAM-NAN	2.75	120.39	115.45
2	A	400	HKX	CAF-CAO-NAU	-2.71	117.67	123.38
2	C	400	HKX	CAB-NAG-CAF	-2.71	115.95	121.14
3	A	1294	MES	O1S-S-C8	2.66	110.74	106.73
3	A	1294	MES	O3S-S-C8	2.58	111.05	106.00
2	A	400	HKX	CAI-SAH-NAG	2.55	111.57	106.66
2	A	400	HKX	NAU-CAO-NAN	2.54	121.25	116.29
2	A	400	HKX	CAB-NAG-CAF	-2.50	116.35	121.14
2	A	400	HKX	NAD-CAM-NAN	2.44	119.83	115.45
2	B	400	HKX	OAP-SAH-CAI	-2.41	105.11	108.10
2	A	400	HKX	OAP-SAH-NAG	2.41	109.93	106.59
2	D	400	HKX	OAP-SAH-CAI	-2.40	105.12	108.10
2	A	400	HKX	CAF-NAG-SAH	2.38	123.98	120.72
2	D	400	HKX	CAF-CAO-NAN	2.38	120.76	119.01
2	B	400	HKX	CAI-SAH-NAG	2.38	111.24	106.66
2	C	400	HKX	CAF-CAO-NAN	2.35	120.74	119.01
2	C	400	HKX	CAF-CAO-NAU	-2.32	118.50	123.38
2	C	400	HKX	NAU-CAO-NAN	2.27	120.72	116.29
2	D	400	HKX	CAK-CAJ-CAI	2.25	121.25	118.95
2	C	400	HKX	CAJ-CAI-SAH	-2.23	117.52	119.73
2	D	400	HKX	CAB-NAG-CAF	-2.22	116.88	121.14
2	B	400	HKX	OAC-SAH-NAG	2.21	109.66	106.59
2	D	400	HKX	CAJ-CAI-SAH	-2.15	117.60	119.73
2	B	400	HKX	OAL-CAM-NAN	-2.14	119.52	122.32
2	D	400	HKX	OAL-CAM-NAN	-2.05	119.65	122.32
2	C	400	HKX	CAK-CAJ-CAI	2.02	121.01	118.95

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1294	MES	C8-C7-N4-C5
3	B	1294	MES	C7-C8-S-O2S
3	C	1294	MES	C8-C7-N4-C5
3	D	1294	MES	C7-C8-S-O2S
3	D	1294	MES	C7-C8-S-O3S
2	D	400	HKX	CAQ-CAI-SAH-NAG
2	D	400	HKX	CAJ-CAI-SAH-NAG
2	C	400	HKX	CAQ-CAI-SAH-NAG
2	A	400	HKX	CAQ-CAI-SAH-NAG
2	C	400	HKX	CAJ-CAI-SAH-NAG
5	D	1296	GOL	O1-C1-C2-O2
2	A	400	HKX	CAJ-CAI-SAH-NAG
3	B	1294	MES	C7-C8-S-O3S
2	B	400	HKX	CAQ-CAI-SAH-NAG
2	B	400	HKX	CAJ-CAI-SAH-NAG
5	A	1296	GOL	O1-C1-C2-C3
5	D	1296	GOL	O1-C1-C2-C3
2	B	400	HKX	CAJ-CAI-SAH-OAC
2	B	400	HKX	CAQ-CAI-SAH-OAC
2	A	400	HKX	CAJ-CAI-SAH-OAC
2	C	400	HKX	CAJ-CAI-SAH-OAC
2	A	400	HKX	CAQ-CAI-SAH-OAC
2	C	400	HKX	CAQ-CAI-SAH-OAC
2	D	400	HKX	CAJ-CAI-SAH-OAC
2	D	400	HKX	CAQ-CAI-SAH-OAC
3	C	1294	MES	C7-C8-S-O3S
3	B	1294	MES	C7-C8-S-O1S
3	C	1294	MES	C7-C8-S-O1S
3	C	1294	MES	C7-C8-S-O2S
3	D	1294	MES	C7-C8-S-O1S
3	C	1294	MES	C8-C7-N4-C3
5	A	1296	GOL	O1-C1-C2-O2
2	A	400	HKX	CAB-NAG-SAH-OAC
2	D	400	HKX	CAB-NAG-SAH-OAC
2	C	400	HKX	CAB-NAG-SAH-OAC
2	B	400	HKX	CAB-NAG-SAH-OAC

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	400	HKX	1	0
3	A	1294	MES	1	0

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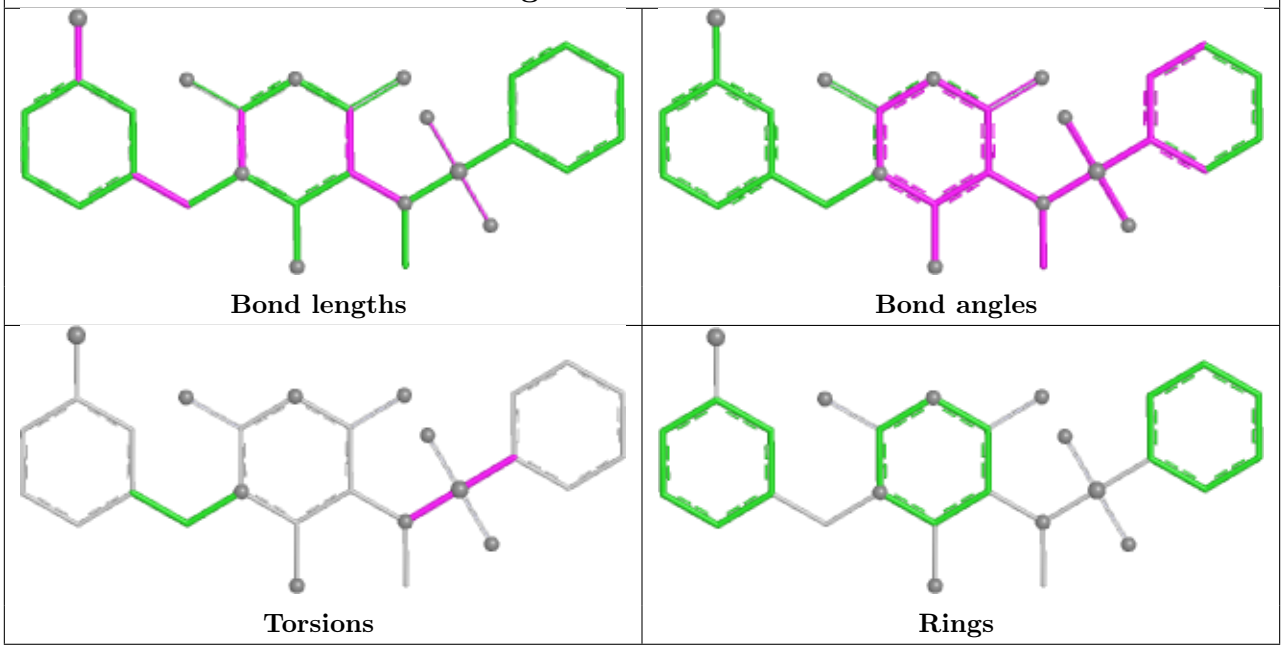
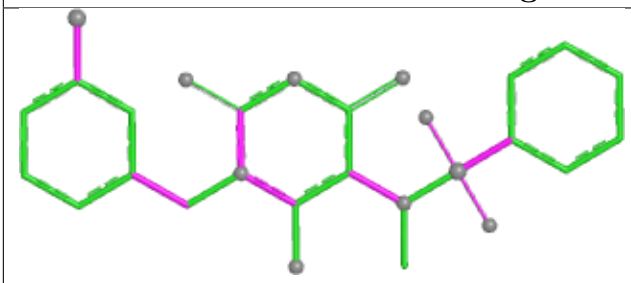
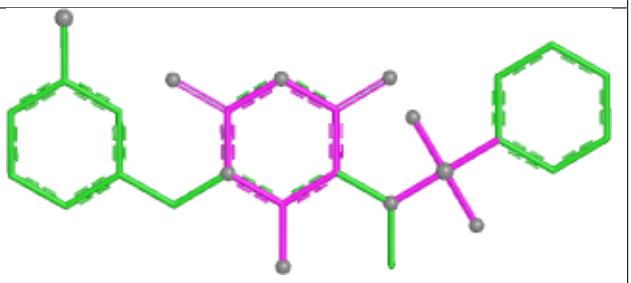
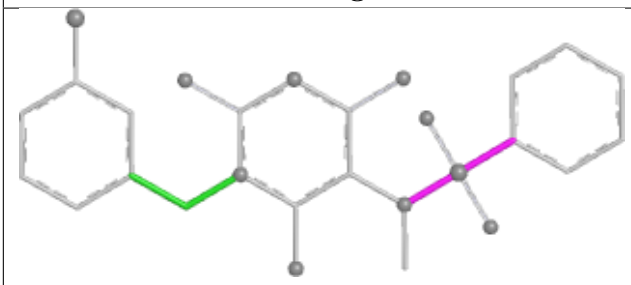
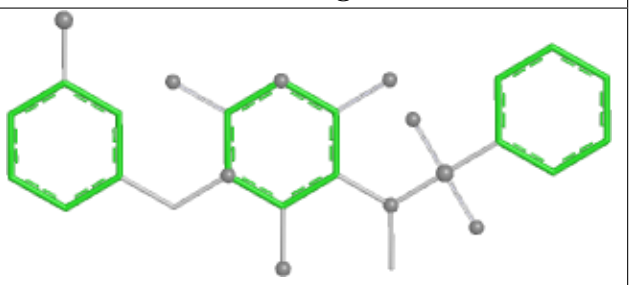
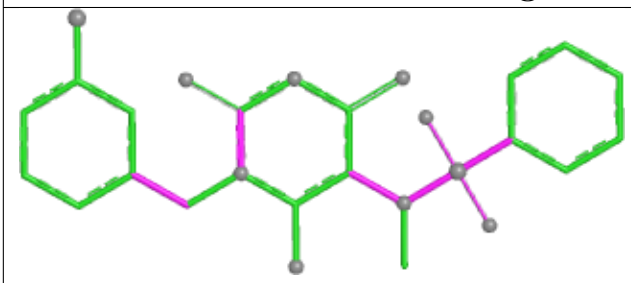
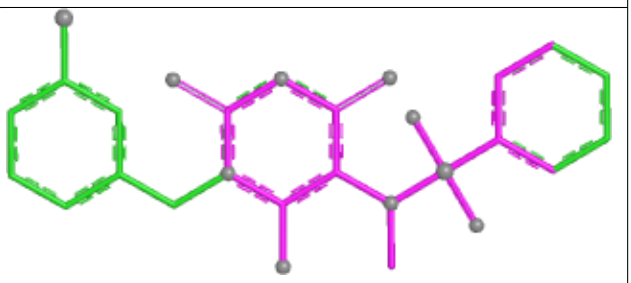
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	HKX	1	0

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 HKX C 400



Ligand HKX B 400	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand HKX D 400	
	
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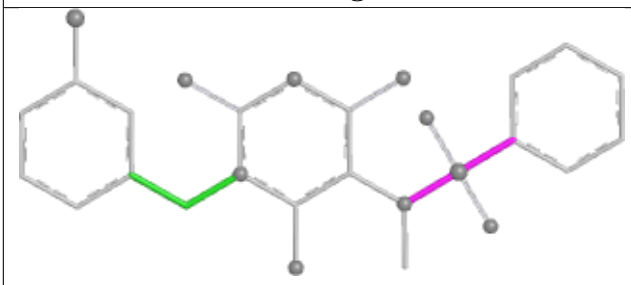
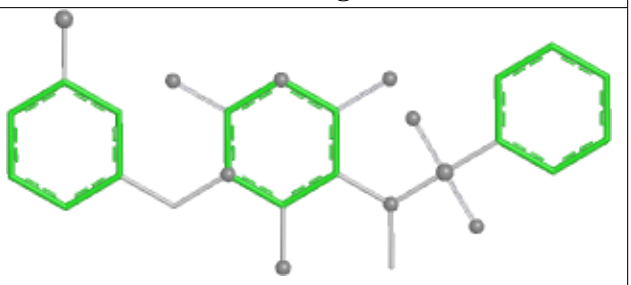
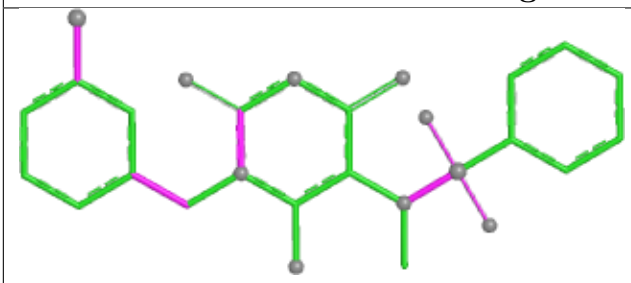
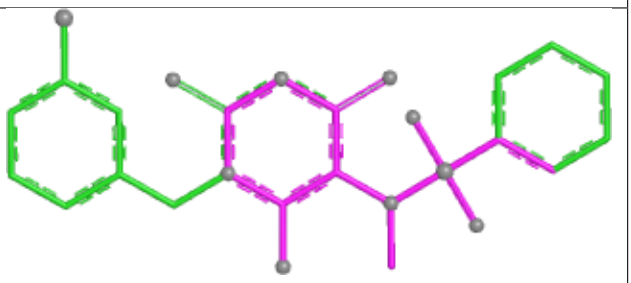
	
Torsions	Rings

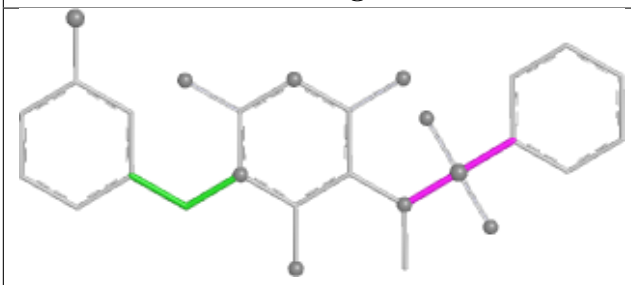
Ligand HKX A 400



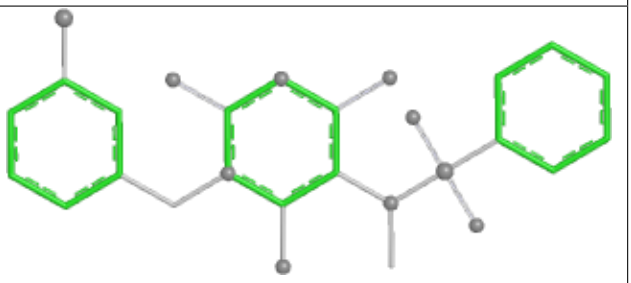
Bond lengths



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	298/303 (98%)	0.47	22 (7%)	20	21	8, 24, 43, 67	5 (1%)
1	B	293/303 (96%)	0.81	20 (6%)	23	24	13, 29, 44, 58	3 (1%)
1	C	299/303 (98%)	0.61	23 (7%)	19	20	9, 26, 51, 68	4 (1%)
1	D	292/303 (96%)	0.80	24 (8%)	17	17	11, 30, 49, 89	2 (0%)
All	All	1182/1212 (97%)	0.67	89 (7%)	20	20	8, 27, 47, 89	14 (1%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	22	ALA	5.5
1	C	23	ILE	5.0
1	D	23	ILE	4.8
1	C	88	LEU	4.2
1	A	-5	HIS	4.0
1	B	122	LEU	3.5
1	C	193	PRO	3.5
1	A	194	ARG	3.4
1	D	195	GLY	3.4
1	C	189	LEU	3.3
1	B	118	PHE	3.3
1	C	192	SER	3.3
1	C	225	ASP	3.2
1	A	11	GLY	3.2
1	D	118	PHE	3.2
1	D	191	PRO	3.1
1	C	-6	HIS	3.1
1	B	15	ARG	3.0
1	D	189	LEU	3.0
1	A	192	SER	3.0
1	D	194	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	191	PRO	3.0
1	B	117	ASP	2.9
1	A	273	ALA	2.9
1	D	11	GLY	2.9
1	A	193	PRO	2.9
1	C	-7	HIS	2.9
1	D	157	ILE	2.8
1	C	-9	HIS	2.8
1	C	0	ALA	2.7
1	A	118	PHE	2.7
1	B	123	GLY	2.7
1	D	153	GLY	2.7
1	A	1	MET	2.7
1	D	225	ASP	2.7
1	C	190	LYS	2.6
1	C	117	ASP	2.6
1	C	-1	MET	2.6
1	B	210	GLY	2.6
1	A	197	LEU	2.6
1	B	233[A]	LEU	2.6
1	D	199	ILE	2.6
1	D	125	ALA	2.6
1	B	12	SER	2.6
1	A	191	PRO	2.5
1	A	-6	HIS	2.5
1	C	194	ARG	2.5
1	D	164	LEU	2.5
1	B	60	THR	2.5
1	A	289	THR	2.5
1	A	274	PRO	2.4
1	A	275	LEU	2.4
1	A	84	SER	2.4
1	C	289	THR	2.4
1	C	85	PRO	2.4
1	A	189	LEU	2.4
1	C	226	THR	2.4
1	B	289	THR	2.3
1	B	157	ILE	2.3
1	D	193	PRO	2.3
1	B	232	LEU	2.3
1	D	8	LEU	2.3
1	D	214	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	21	LEU	2.2
1	A	195	GLY	2.2
1	B	1	MET	2.2
1	A	-7	HIS	2.2
1	D	144	ARG	2.2
1	A	88	LEU	2.2
1	A	121	LEU	2.2
1	D	227	GLY	2.2
1	A	-9	HIS	2.1
1	B	288	LEU	2.1
1	C	118	PHE	2.1
1	C	293	TYR	2.1
1	B	273	ALA	2.1
1	C	-8	HIS	2.1
1	D	190	LYS	2.1
1	B	28	LEU	2.1
1	B	66	LEU	2.1
1	B	65	GLN	2.1
1	B	226	THR	2.1
1	C	195	GLY	2.1
1	D	124	SER	2.1
1	A	287	LEU	2.1
1	B	275	LEU	2.1
1	D	88	LEU	2.1
1	C	197	LEU	2.0
1	D	120	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

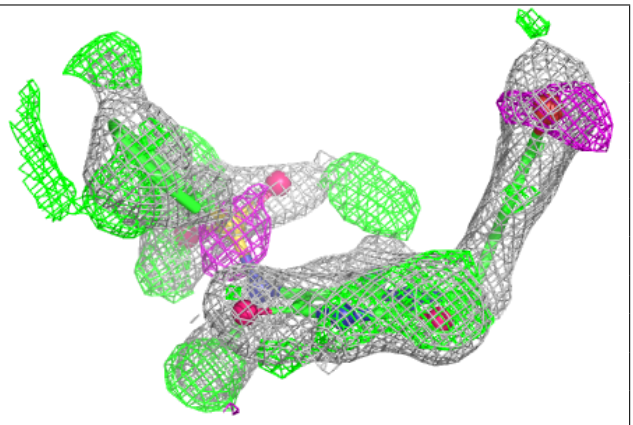
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

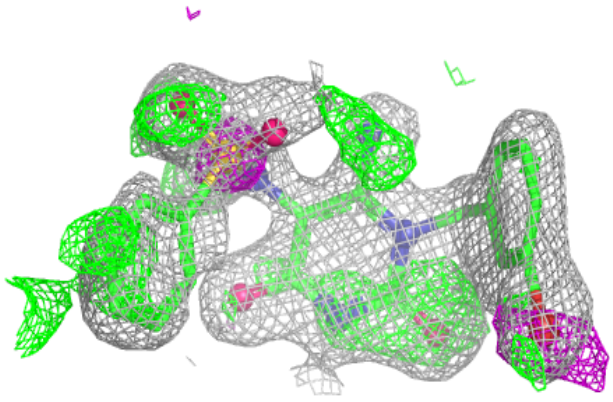
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MES	B	1294	12/12	0.73	0.24	44,47,48,49	12
5	GOL	C	1296	6/6	0.75	0.17	44,47,48,50	0
2	HKX	C	400	28/28	0.76	0.26	22,27,33,34	28
2	HKX	B	400	28/28	0.77	0.27	32,38,42,42	28
5	GOL	A	1296	6/6	0.77	0.18	37,43,44,46	0
2	HKX	D	400	28/28	0.77	0.27	31,36,40,43	28
2	HKX	A	400	28/28	0.78	0.26	22,29,33,35	28
5	GOL	D	1297	6/6	0.78	0.15	52,53,53,54	0
5	GOL	D	1296	6/6	0.82	0.16	49,51,52,53	0
3	MES	A	1294	12/12	0.82	0.19	36,40,40,42	12
3	MES	D	1294	12/12	0.85	0.19	44,51,54,54	12
3	MES	C	1294	12/12	0.88	0.17	30,36,38,38	12
4	CL	A	1295	1/1	0.96	0.08	26,26,26,26	1
4	CL	C	1295	1/1	0.97	0.09	29,29,29,29	1
4	CL	D	1295	1/1	0.97	0.13	38,38,38,38	1
4	CL	B	1295	1/1	0.98	0.15	32,32,32,32	1

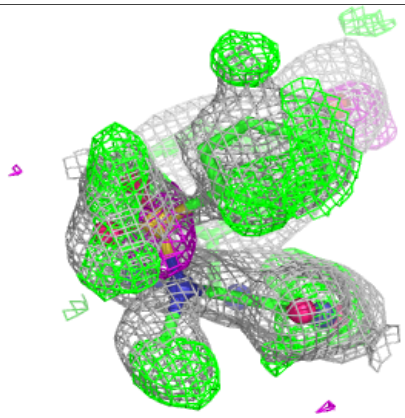
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HKX 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)

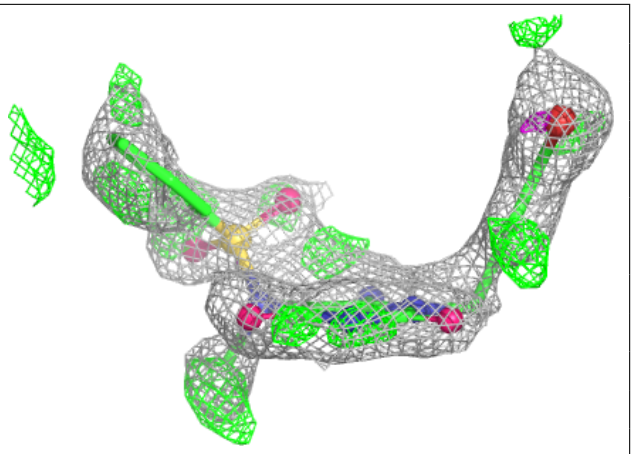


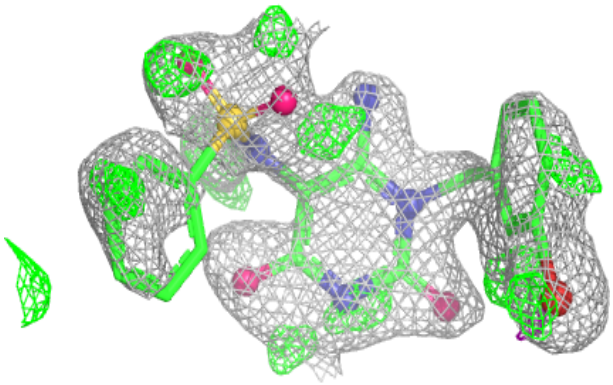


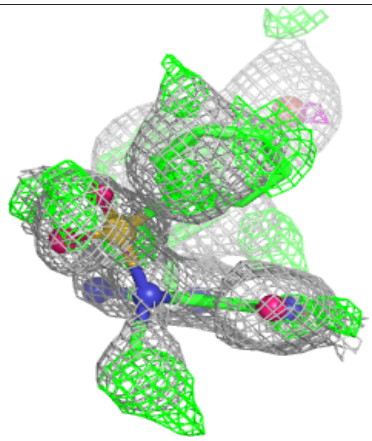


Electron density around HKX B 400:

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

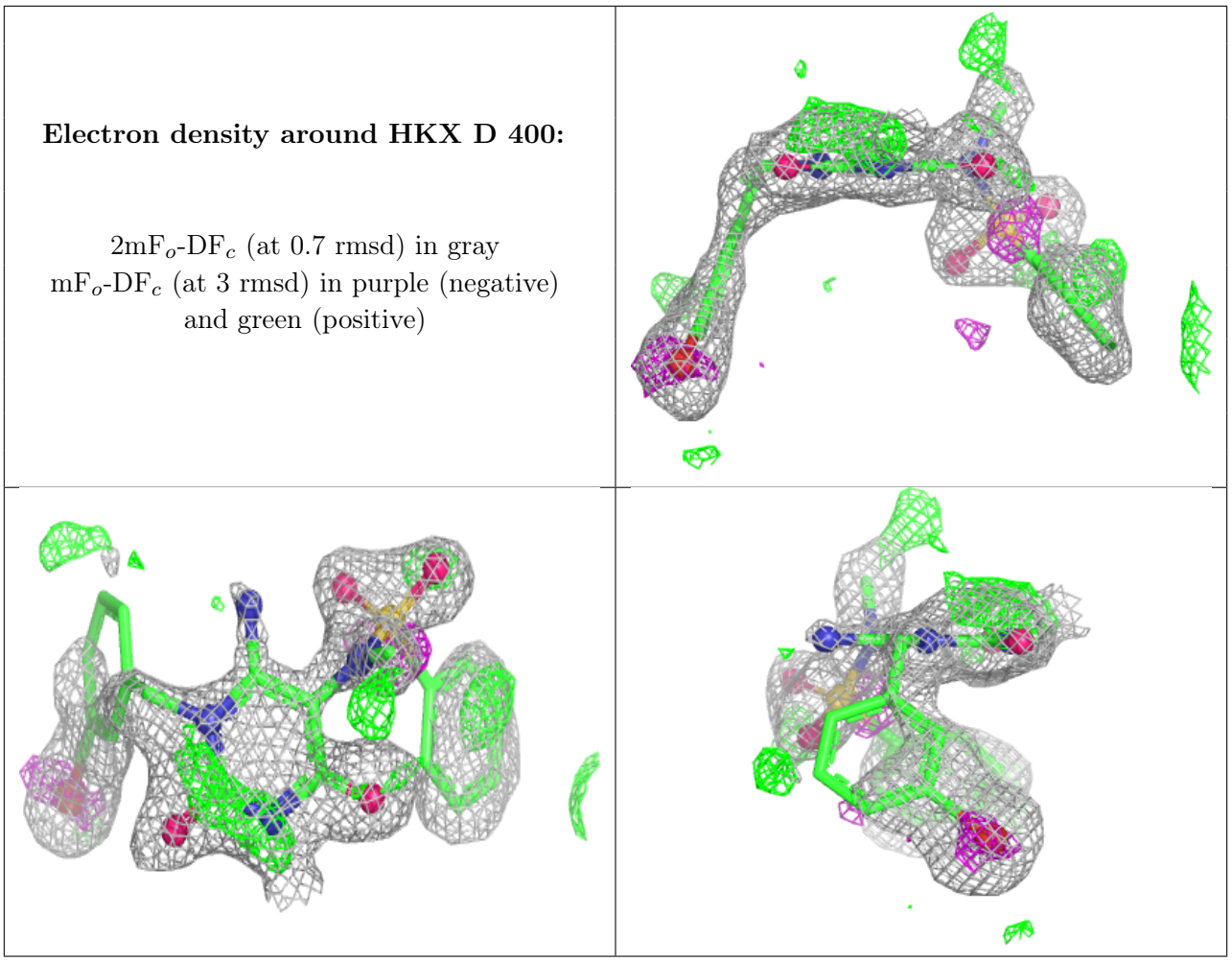






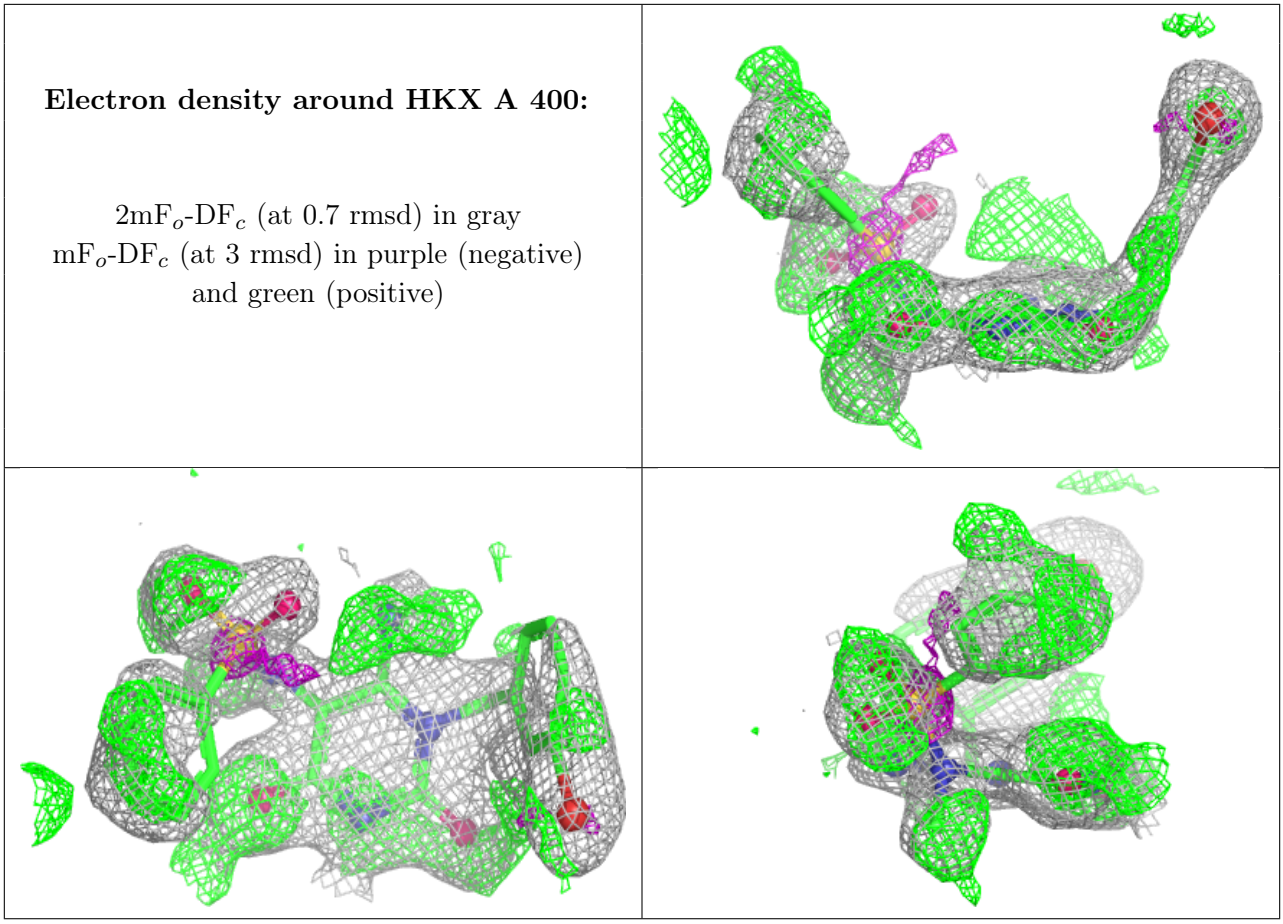
Electron density around HKX D 400:

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



Electron density around HKX 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.