Full wwPDB X-ray Structure Validation Report (i)

Mar 9, 2026 – 02:29 AM UTC

PDB ID	:	7L26 / pdb_00007l26
Title	:	HPK1 IN COMPLEX WITH COMPOUND 38
Authors	:	Lesburg, C.A.
Deposited on	:	2020-12-16
Resolution	:	2.30 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:

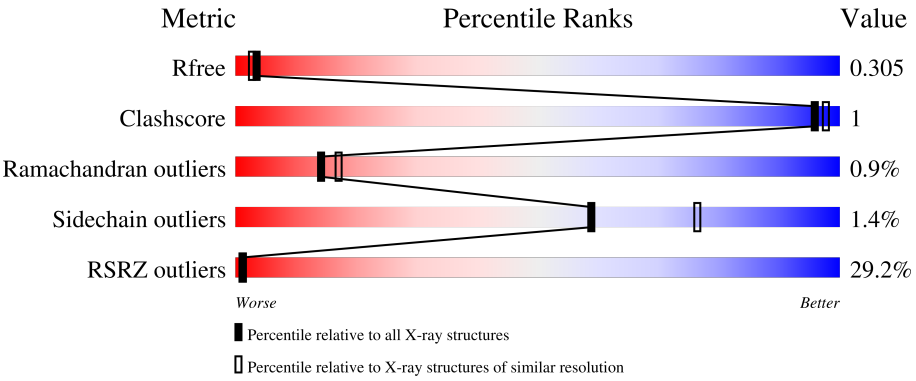
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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

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

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	287	25% 94%
1	B	287	28% 89% 7%
1	C	287	30% 92% 5%
1	D	287	29% 90% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9198 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.

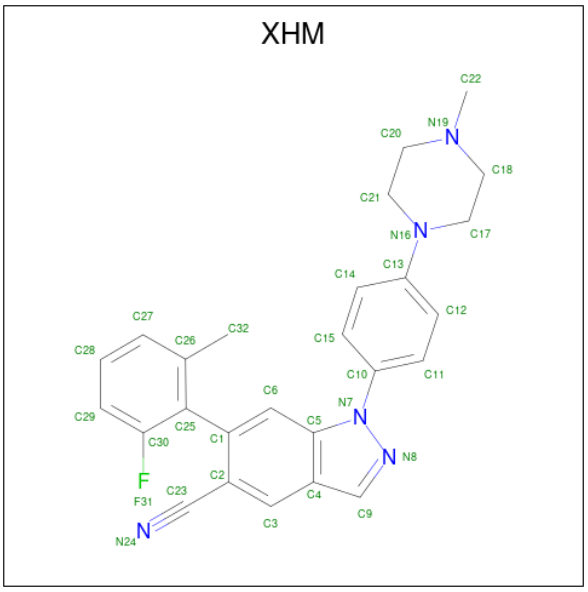
- Molecule 1 is a protein called Mitogen-activated protein kinase kinase kinase kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	77	2	0
			2234	1441	388	393	12			
1	B	275	Total	C	N	O	S	102	1	0
			2184	1409	376	388	11			
1	C	280	Total	C	N	O	S	82	1	0
			2228	1438	387	392	11			
1	D	275	Total	C	N	O	S	78	1	0
			2194	1417	379	387	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	ALA	SER	engineered mutation	UNP Q92918
A	191	CYS	GLY	engineered mutation	UNP Q92918
B	171	ALA	SER	engineered mutation	UNP Q92918
B	191	CYS	GLY	engineered mutation	UNP Q92918
C	171	ALA	SER	engineered mutation	UNP Q92918
C	191	CYS	GLY	engineered mutation	UNP Q92918
D	171	ALA	SER	engineered mutation	UNP Q92918
D	191	CYS	GLY	engineered mutation	UNP Q92918

- Molecule 2 is 6-(2-fluoro-6-methylphenyl)-1-[4-(4-methylpiperazin-1-yl)phenyl]-1H-indazole -5-carbonitrile (CCD ID: XHM) (formula: $C_{26}H_{24}FN_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C F N 32 26 1 5	0	0
2	B	1	Total C F N 32 26 1 5	0	0
2	C	1	Total C F N 32 26 1 5	0	0
2	D	1	Total C F N 32 26 1 5	0	0

- Molecule 3 is water.

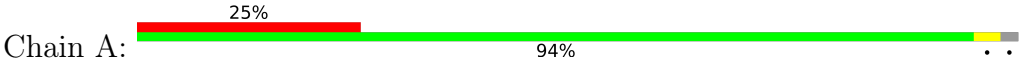
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	63	Total O 63 63	0	0
3	B	64	Total O 64 64	0	0
3	C	57	Total O 57 57	0	0
3	D	46	Total O 46 46	0	0

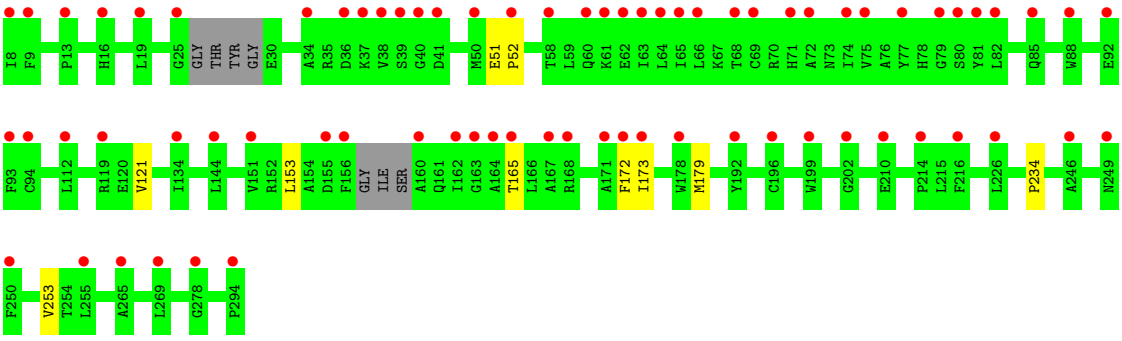
3 Residue-property plots (i)

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: Mitogen-activated protein kinase kinase kinase kinase 1

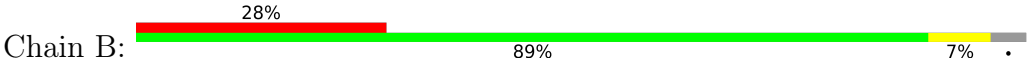
Chain A:

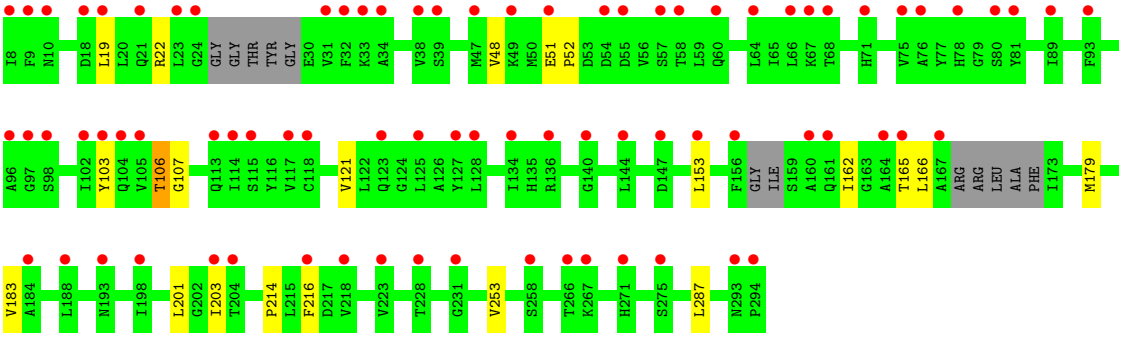




• Molecule 1: Mitogen-activated protein kinase kinase kinase kinase 1

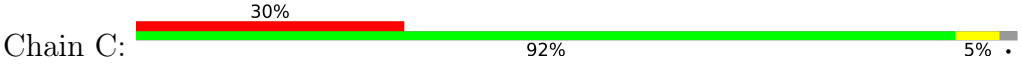
Chain B:

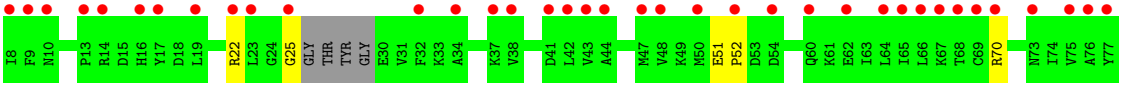


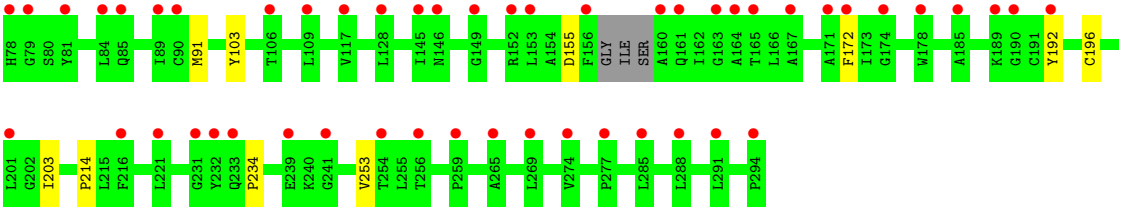


• Molecule 1: Mitogen-activated protein kinase kinase kinase kinase 1

Chain C:

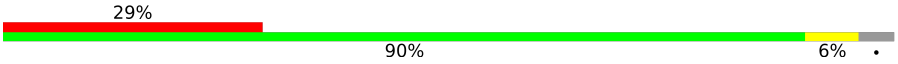


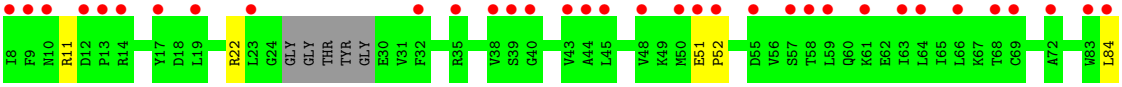


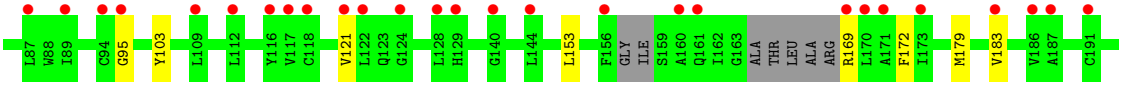


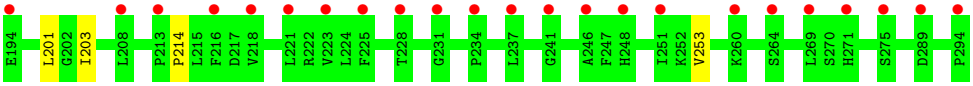
• Molecule 1: Mitogen-activated protein kinase kinase kinase kinase 1

Chain D:









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	58.14Å 58.17Å 98.95Å 89.84° 90.13° 97.60°	Depositor
Resolution (Å)	98.95 – 2.30 98.95 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.1 (98.95-2.30) 94.3 (98.95-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.262 , 0.298 0.266 , 0.305	Depositor DCC
R_{free} test set	1155 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å^2)	37.5	Xtriage
Anisotropy	0.824	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 79.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.377 for -h,-k,l 0.367 for -k,-h,-l 0.430 for k,h,-l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	9198	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.32% 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: XHM

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	0.90	2/2281 (0.1%)	1.12	0/3081
1	B	0.95	3/2229 (0.1%)	1.13	1/3011 (0.0%)
1	C	0.91	3/2275 (0.1%)	1.13	1/3073 (0.0%)
1	D	0.92	2/2240 (0.1%)	1.14	4/3024 (0.1%)
All	All	0.92	10/9025 (0.1%)	1.13	6/12189 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	22	ARG	NE-CZ	11.09	1.45	1.33
1	A	165	THR	CB-OG1	-8.04	1.30	1.43
1	D	22	ARG	NE-CZ	7.77	1.41	1.33
1	B	165	THR	CB-OG1	-7.37	1.31	1.43
1	B	162	ILE	CB-CG1	6.80	1.67	1.53
1	C	25	GLY	C-O	6.65	1.36	1.23
1	C	22	ARG	NE-CZ	5.75	1.39	1.33
1	D	11	ARG	NE-CZ	5.64	1.39	1.33
1	A	234	PRO	CA-C	5.39	1.54	1.51
1	C	70	ARG	NE-CZ	5.33	1.39	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	172	PHE	N-CA-C	6.88	119.40	110.53
1	B	162	ILE	CA-CB-CG2	6.53	121.60	110.50
1	D	172	PHE	CA-C-N	5.54	128.04	120.46
1	D	172	PHE	C-N-CA	5.54	128.04	120.46
1	C	234	PRO	O-C-N	5.44	123.81	121.31
1	D	95	GLY	N-CA-C	5.22	120.42	114.67

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2234	0	2295	2	0
1	B	2184	0	2241	7	0
1	C	2228	0	2291	5	0
1	D	2194	0	2251	5	0
2	A	32	0	0	0	0
2	B	32	0	0	0	0
2	C	32	0	0	0	0
2	D	32	0	0	0	0
3	A	63	0	0	0	0
3	B	64	0	0	0	0
3	C	57	0	0	1	0
3	D	46	0	0	1	0
All	All	9198	0	9078	18	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 (18) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:THR:HG21	1:B:287:LEU:HD11	1.77	0.66
1:B:179:MET:HE3	1:B:183:VAL:HG12	1.83	0.60
1:D:179:MET:HE3	1:D:183:VAL:HG12	1.89	0.53
1:B:106:THR:HG22	1:B:107:GLY:O	2.09	0.51
1:B:121:VAL:HG13	1:B:153:LEU:HD21	1.92	0.51
1:C:203:ILE:HG23	1:C:214:PRO:HD2	1.94	0.49
1:D:121:VAL:HG11	1:D:201:LEU:HD13	1.94	0.48
1:D:121:VAL:HG13	1:D:153:LEU:HD21	1.97	0.47
1:C:196:CYS:HB3	3:C:403:HOH:O	2.16	0.46
1:C:196:CYS:HB2	3:D:439:HOH:O	2.16	0.45
1:C:192:TYR:CE2	1:D:183:VAL:HG13	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:ILE:HG23	1:D:214:PRO:HD2	2.00	0.44
1:A:173:ILE:HG23	1:A:179:MET:CE	2.48	0.43
1:A:121:VAL:HG13	1:A:153:LEU:HD21	2.01	0.42
1:B:121:VAL:HG11	1:B:201:LEU:HD13	2.02	0.42
1:B:216[B]:PHE:CD1	1:B:216[B]:PHE:C	2.98	0.41
1:C:91:MET:HE1	1:C:155:ASP:HB3	2.01	0.41
1:B:203:ILE:HG23	1:B:214:PRO:HD2	2.04	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	276/287 (96%)	262 (95%)	11 (4%)	3 (1%)	11	13
1	B	268/287 (93%)	258 (96%)	8 (3%)	2 (1%)	18	23
1	C	275/287 (96%)	260 (94%)	12 (4%)	3 (1%)	11	13
1	D	268/287 (93%)	259 (97%)	7 (3%)	2 (1%)	18	23
All	All	1087/1148 (95%)	1039 (96%)	38 (4%)	10 (1%)	14	17

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	PRO
1	A	172	PHE
1	B	51	GLU
1	B	52	PRO
1	C	51	GLU
1	C	52	PRO
1	C	172	PHE
1	D	51	GLU

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Mol	Chain	Res	Type
1	D	52	PRO
1	A	51	GLU

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	241/244 (99%)	240 (100%)	1 (0%)	84 92
1	B	237/244 (97%)	231 (98%)	6 (2%)	42 60
1	C	240/244 (98%)	238 (99%)	2 (1%)	73 86
1	D	238/244 (98%)	234 (98%)	4 (2%)	53 72
All	All	956/976 (98%)	943 (99%)	13 (1%)	59 76

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	VAL
1	B	19	LEU
1	B	48	VAL
1	B	103	TYR
1	B	106	THR
1	B	166	LEU
1	B	253	VAL
1	C	103	TYR
1	C	253	VAL
1	D	84	LEU
1	D	103	TYR
1	D	169	ARG
1	D	253	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN

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Mol	Chain	Res	Type
1	A	100	GLN
1	A	249	ASN
1	B	73	ASN
1	B	249	ASN
1	C	249	ASN
1	D	249	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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	XHM	D	301	-	36,36,36	1.08	3 (8%)	49,52,52	2.41	17 (34%)
2	XHM	B	301	-	36,36,36	1.08	1 (2%)	49,52,52	2.19	12 (24%)
2	XHM	A	301	-	36,36,36	1.11	1 (2%)	49,52,52	2.11	11 (22%)
2	XHM	C	301	-	36,36,36	1.07	2 (5%)	49,52,52	2.17	14 (28%)

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	XHM	D	301	-	-	2/14/24/24	0/5/5/5
2	XHM	B	301	-	-	2/14/24/24	0/5/5/5
2	XHM	A	301	-	-	2/14/24/24	0/5/5/5
2	XHM	C	301	-	-	2/14/24/24	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	XHM	C4-C9	2.72	1.45	1.42
2	A	301	XHM	C4-C9	2.36	1.45	1.42
2	D	301	XHM	C4-C9	2.34	1.45	1.42
2	C	301	XHM	N7-N8	2.29	1.40	1.38
2	C	301	XHM	C4-C9	2.20	1.44	1.42
2	D	301	XHM	N7-N8	2.16	1.40	1.38
2	D	301	XHM	C9-N8	-2.13	1.29	1.32

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	301	XHM	C9-N8-N7	8.43	111.50	106.14
2	C	301	XHM	C9-N8-N7	7.54	110.93	106.14
2	A	301	XHM	C9-N8-N7	7.49	110.90	106.14
2	B	301	XHM	C9-N8-N7	7.43	110.86	106.14
2	D	301	XHM	C6-C5-C4	-6.03	117.31	122.29
2	A	301	XHM	C6-C5-C4	-5.89	117.42	122.29
2	C	301	XHM	C6-C5-C4	-5.79	117.50	122.29
2	B	301	XHM	C1-C25-C30	-5.72	116.88	122.64
2	D	301	XHM	C1-C25-C30	-5.27	117.32	122.64
2	B	301	XHM	C6-C5-C4	-5.16	118.03	122.29
2	D	301	XHM	C4-C9-N8	-5.11	108.19	112.05
2	C	301	XHM	C4-C9-N8	-4.83	108.40	112.05
2	B	301	XHM	C4-C9-N8	-4.81	108.42	112.05
2	A	301	XHM	C4-C9-N8	-4.72	108.49	112.05
2	D	301	XHM	C5-N7-N8	-4.70	107.57	111.33
2	C	301	XHM	C5-N7-N8	-4.03	108.10	111.33
2	A	301	XHM	C5-N7-N8	-3.90	108.20	111.33
2	B	301	XHM	C10-N7-N8	3.78	122.32	119.15
2	B	301	XHM	C5-N7-N8	-3.75	108.33	111.33
2	C	301	XHM	C5-C4-C9	3.74	106.61	104.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	301	XHM	C10-N7-N8	3.66	122.22	119.15
2	C	301	XHM	C1-C25-C30	-3.51	119.10	122.64
2	C	301	XHM	C10-N7-N8	3.43	122.03	119.15
2	A	301	XHM	C5-C4-C9	3.37	106.39	104.48
2	A	301	XHM	C10-N7-N8	3.25	121.88	119.15
2	A	301	XHM	C1-C25-C30	-3.19	119.42	122.64
2	D	301	XHM	C5-C4-C9	3.07	106.22	104.48
2	B	301	XHM	C5-C4-C9	3.02	106.19	104.48
2	D	301	XHM	C4-C3-C2	-2.88	119.83	122.09
2	B	301	XHM	C1-C25-C26	2.87	123.63	120.00
2	C	301	XHM	C4-C3-C2	-2.68	119.99	122.09
2	B	301	XHM	C4-C3-C2	-2.62	120.04	122.09
2	A	301	XHM	C6-C5-N7	2.54	136.57	131.86
2	D	301	XHM	C12-C13-N16	-2.54	117.86	121.39
2	D	301	XHM	C29-C30-C25	-2.53	120.13	123.73
2	C	301	XHM	C6-C5-N7	2.52	136.53	131.86
2	C	301	XHM	C3-C4-C9	-2.51	131.79	135.46
2	B	301	XHM	C29-C30-C25	-2.43	120.28	123.73
2	D	301	XHM	C22-N19-C20	2.40	115.21	110.63
2	D	301	XHM	C3-C4-C9	-2.35	132.02	135.46
2	C	301	XHM	C29-C30-C25	-2.35	120.39	123.73
2	D	301	XHM	C6-C5-N7	2.33	136.19	131.86
2	A	301	XHM	C3-C4-C9	-2.30	132.10	135.46
2	A	301	XHM	C4-C3-C2	-2.29	120.29	122.09
2	D	301	XHM	C15-C10-N7	2.29	122.38	119.93
2	B	301	XHM	C20-N19-C18	2.23	113.10	109.54
2	D	301	XHM	C14-C13-N16	2.20	124.44	121.39
2	D	301	XHM	C3-C4-C5	2.17	121.75	119.56
2	C	301	XHM	C15-C10-N7	2.15	122.23	119.93
2	D	301	XHM	C1-C25-C26	2.13	122.69	120.00
2	B	301	XHM	C6-C5-N7	2.12	135.78	131.86
2	C	301	XHM	C14-C13-N16	2.10	124.31	121.39
2	A	301	XHM	C29-C30-C25	-2.09	120.76	123.73
2	C	301	XHM	C3-C4-C5	2.02	121.61	119.56

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	XHM	C12-C13-N16-C21
2	B	301	XHM	C14-C13-N16-C21
2	D	301	XHM	C14-C13-N16-C21

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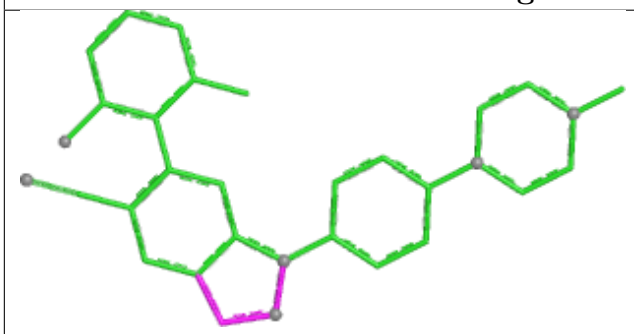
Mol	Chain	Res	Type	Atoms
2	D	301	XHM	C12-C13-N16-C21
2	C	301	XHM	C14-C13-N16-C21
2	C	301	XHM	C12-C13-N16-C21
2	A	301	XHM	C14-C13-N16-C21
2	A	301	XHM	C1-C2-C23-N24

There are no ring outliers.

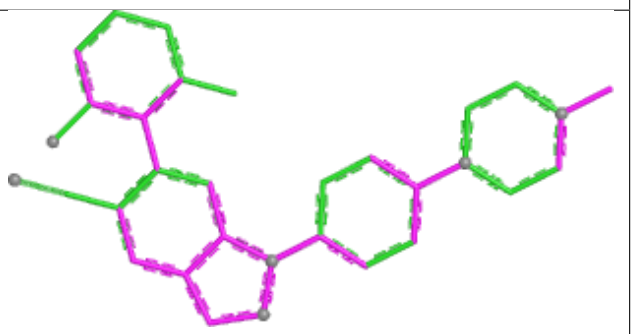
No monomer is involved in short contacts.

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.

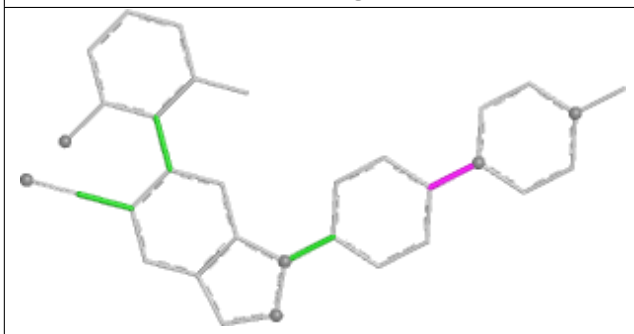
Ligand XHM D 301



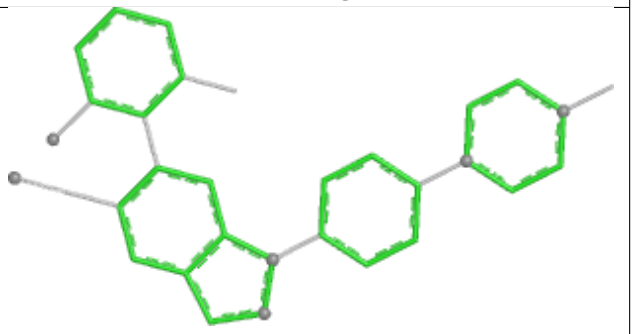
Bond lengths



Bond angles

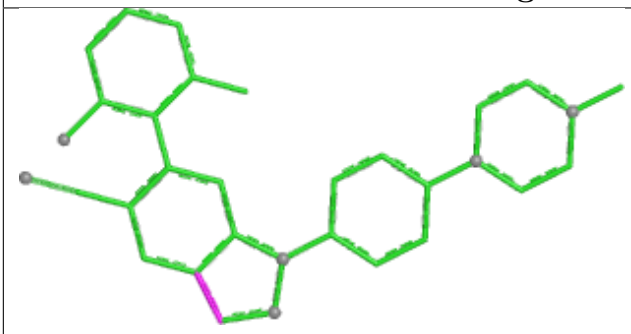


Torsions

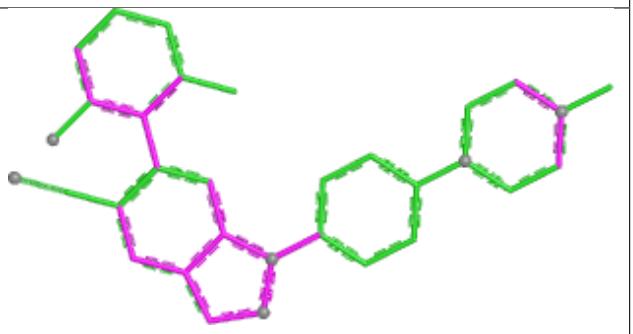


Rings

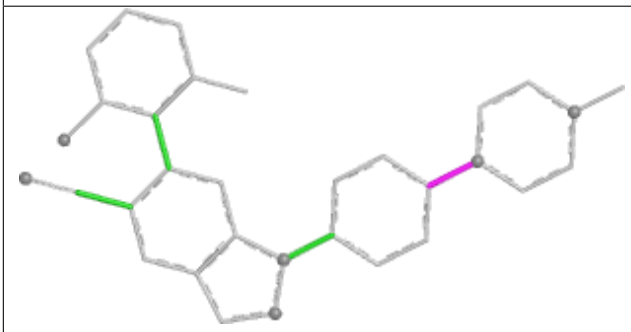
Ligand XHM B 301



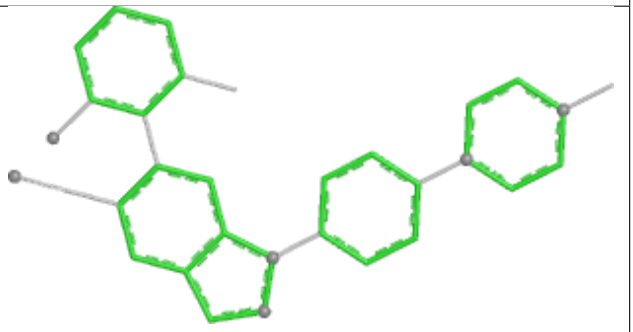
Bond lengths



Bond angles

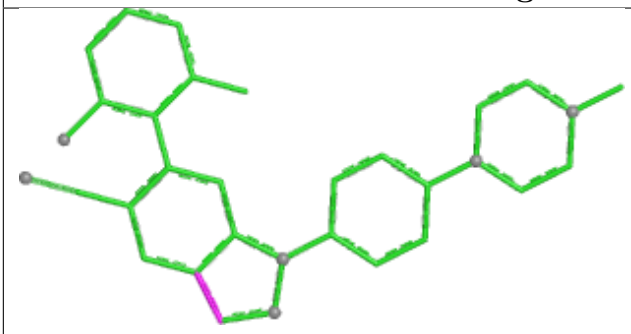


Torsions

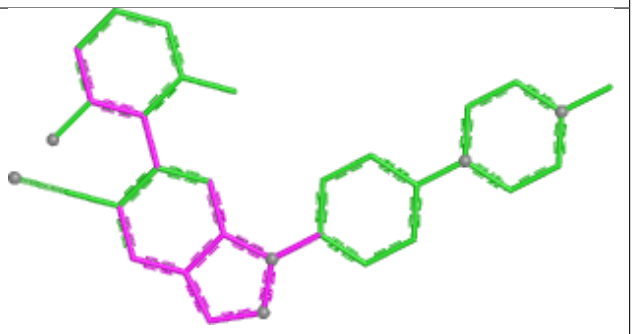


Rings

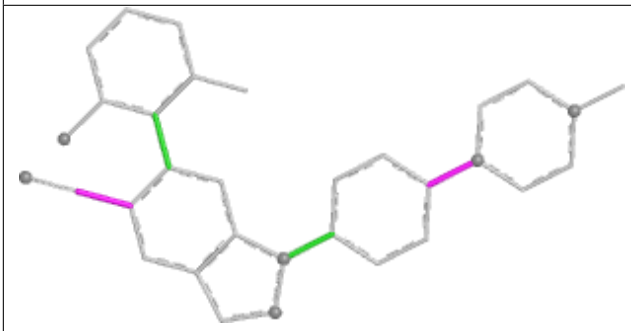
Ligand XHM A 301



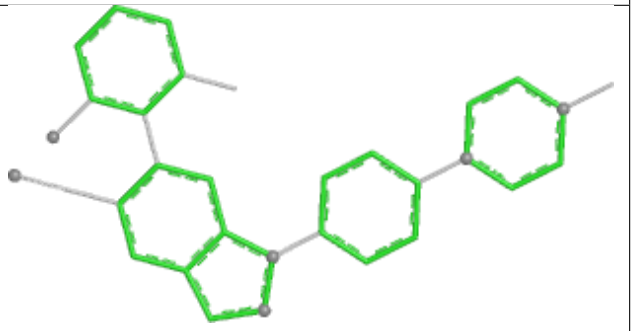
Bond lengths



Bond angles

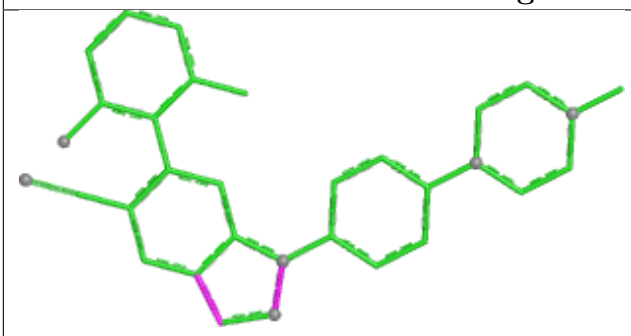


Torsions

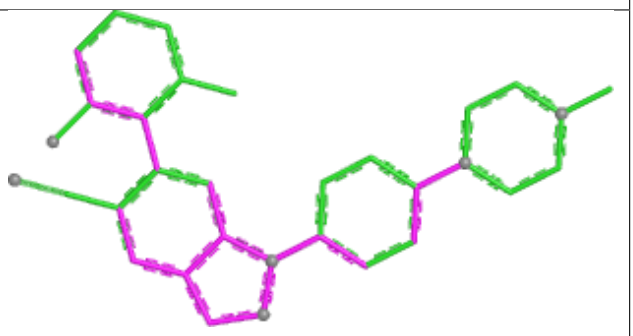


Rings

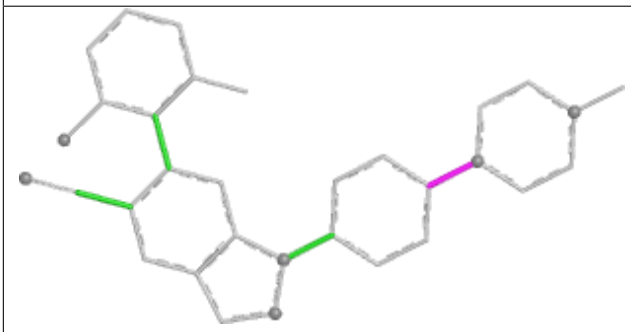
Ligand XHM C 301



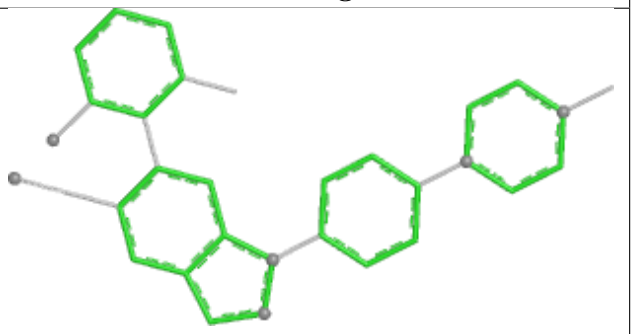
Bond lengths



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, 95th 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	280/287 (97%)	1.53	73 (26%)	1 2	22, 56, 101, 133	33 (11%)
1	B	275/287 (95%)	1.57	80 (29%)	1 1	24, 57, 94, 121	40 (14%)
1	C	280/287 (97%)	1.64	87 (31%)	1 1	22, 56, 99, 127	34 (12%)
1	D	275/287 (95%)	1.57	84 (30%)	1 1	23, 56, 100, 120	31 (11%)
All	All	1110/1148 (96%)	1.58	324 (29%)	1 1	22, 56, 99, 133	138 (12%)

All (324) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	38	VAL	7.6
1	A	79	GLY	7.4
1	C	277	PRO	6.7
1	B	64	LEU	6.7
1	B	118	CYS	6.2
1	D	118	CYS	5.8
1	C	38	VAL	5.7
1	A	165	THR	5.7
1	C	109	LEU	5.7
1	B	114	ILE	5.5
1	B	156	PHE	5.3
1	C	221	LEU	5.3
1	B	218	VAL	5.1
1	A	63	ILE	5.0
1	D	58	THR	5.0
1	A	62	GLU	5.0
1	C	75	VAL	4.9
1	D	32	PHE	4.8
1	C	216[A]	PHE	4.7
1	B	140	GLY	4.6
1	B	68	THR	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	65	ILE	4.6
1	B	147	ASP	4.5
1	D	121	VAL	4.5
1	C	156	PHE	4.4
1	B	125	LEU	4.4
1	A	60	GLN	4.3
1	C	10	ASN	4.3
1	D	112	LEU	4.3
1	C	160	ALA	4.3
1	C	90	CYS	4.2
1	A	39	SER	4.2
1	C	77	TYR	4.2
1	B	31	VAL	4.2
1	B	134	ILE	4.1
1	A	250	PHE	4.1
1	B	228	THR	4.1
1	D	69	CYS	4.1
1	D	171	ALA	4.1
1	A	65	ILE	4.1
1	D	271	HIS	3.9
1	A	160	ALA	3.9
1	B	103	TYR	3.9
1	A	151	VAL	3.9
1	D	38	VAL	3.9
1	C	165	THR	3.9
1	B	216[A]	PHE	3.9
1	A	164	ALA	3.9
1	A	36	ASP	3.8
1	A	93	PHE	3.8
1	B	161	GLN	3.8
1	D	116	TYR	3.8
1	C	9	PHE	3.8
1	C	43	VAL	3.8
1	A	269	LEU	3.8
1	C	164	ALA	3.7
1	D	68	THR	3.7
1	B	8	ILE	3.7
1	C	13	PRO	3.6
1	C	152	ARG	3.6
1	C	241	GLY	3.6
1	C	66	LEU	3.6
1	B	51	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	233	GLN	3.5
1	B	96	ALA	3.5
1	A	202	GLY	3.4
1	B	293	ASN	3.4
1	A	16	HIS	3.4
1	D	59	LEU	3.4
1	D	264	SER	3.4
1	C	190	GLY	3.4
1	C	81	TYR	3.4
1	B	38	VAL	3.4
1	A	81	TYR	3.3
1	D	231	GLY	3.3
1	D	213	PRO	3.3
1	D	17	TYR	3.3
1	A	40	GLY	3.3
1	D	246	ALA	3.3
1	A	82	LEU	3.3
1	A	144	LEU	3.3
1	C	73	ASN	3.2
1	A	74	ILE	3.2
1	C	89	ILE	3.2
1	D	8	ILE	3.2
1	D	218	VAL	3.2
1	D	87	LEU	3.2
1	B	47	MET	3.2
1	B	164	ALA	3.2
1	D	44	ALA	3.2
1	C	265	ALA	3.2
1	C	178	TRP	3.2
1	C	76	ALA	3.1
1	D	289	ASP	3.1
1	C	42	LEU	3.1
1	C	201	LEU	3.1
1	D	13	PRO	3.1
1	B	266	THR	3.1
1	B	39	SER	3.1
1	D	140	GLY	3.1
1	C	288	LEU	3.1
1	A	58	THR	3.1
1	B	75	VAL	3.1
1	D	186	VAL	3.1
1	C	17	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	258	SER	3.0
1	C	69	CYS	3.0
1	D	40	GLY	3.0
1	A	52	PRO	3.0
1	C	44	ALA	3.0
1	C	48	VAL	3.0
1	D	35	ARG	3.0
1	B	9	PHE	3.0
1	A	196[A]	CYS	3.0
1	D	19	LEU	3.0
1	B	49	LYS	3.0
1	C	47	MET	3.0
1	A	92	GLU	3.0
1	A	69	CYS	2.9
1	C	16	HIS	2.9
1	D	48	VAL	2.9
1	C	60	GLN	2.9
1	A	25	GLY	2.9
1	A	249	ASN	2.9
1	C	163	GLY	2.9
1	A	72	ALA	2.9
1	C	161	GLN	2.9
1	D	260	LYS	2.9
1	C	171	ALA	2.9
1	D	169	ARG	2.9
1	D	51	GLU	2.9
1	C	231	GLY	2.9
1	D	294	PRO	2.9
1	A	172	PHE	2.9
1	B	21	GLN	2.9
1	D	173	ILE	2.9
1	A	214	PRO	2.8
1	C	269	LEU	2.8
1	D	66	LEU	2.8
1	A	80	SER	2.8
1	D	57	SER	2.8
1	B	271	HIS	2.8
1	A	156	PHE	2.8
1	A	216[A]	PHE	2.8
1	C	37	LYS	2.8
1	A	192	TYR	2.8
1	D	225	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	183	VAL	2.8
1	B	71	HIS	2.8
1	D	63	ILE	2.8
1	D	191	CYS	2.8
1	C	85	GLN	2.8
1	B	34	ALA	2.8
1	B	203	ILE	2.7
1	D	45	LEU	2.7
1	B	167	ALA	2.7
1	C	256	THR	2.7
1	D	61	LYS	2.7
1	B	19	LEU	2.7
1	A	167	ALA	2.7
1	D	216[A]	PHE	2.7
1	A	75	VAL	2.7
1	B	204	THR	2.7
1	B	24	GLY	2.7
1	B	294	PRO	2.7
1	A	64	LEU	2.7
1	D	122	LEU	2.7
1	D	72	ALA	2.7
1	B	127	TYR	2.7
1	A	41	ASP	2.7
1	C	117	VAL	2.7
1	D	10	ASN	2.7
1	D	12	ASP	2.7
1	D	223	VAL	2.7
1	B	198	ILE	2.7
1	B	98	SER	2.7
1	D	275	SER	2.7
1	A	168	ARG	2.7
1	D	208	LEU	2.7
1	B	104	GLN	2.6
1	B	93	PHE	2.6
1	C	192	TYR	2.6
1	A	278	GLY	2.6
1	C	25	GLY	2.6
1	B	33	LYS	2.6
1	B	193	ASN	2.6
1	C	41	ASP	2.6
1	B	58	THR	2.6
1	B	165	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	84	LEU	2.6
1	C	67	LYS	2.6
1	A	265	ALA	2.6
1	D	9	PHE	2.6
1	D	234	PRO	2.6
1	D	241	GLY	2.6
1	A	61	LYS	2.6
1	C	153	LEU	2.6
1	A	88	TRP	2.6
1	D	83	TRP	2.5
1	A	13	PRO	2.5
1	B	115	SER	2.5
1	B	153	LEU	2.5
1	A	246	ALA	2.5
1	B	57	SER	2.5
1	B	117	VAL	2.5
1	B	223	VAL	2.5
1	B	66	LEU	2.5
1	B	144	LEU	2.5
1	D	170	LEU	2.5
1	A	94	CYS	2.5
1	C	79	GLY	2.5
1	B	60	GLN	2.5
1	B	32	PHE	2.5
1	C	32	PHE	2.5
1	A	8	ILE	2.5
1	B	102	ILE	2.5
1	C	14	ARG	2.5
1	C	232	TYR	2.5
1	C	19	LEU	2.5
1	C	54	ASP	2.5
1	B	160	ALA	2.5
1	C	52	PRO	2.5
1	C	174	GLY	2.5
1	A	66	LEU	2.4
1	A	226	LEU	2.4
1	C	189	LYS	2.4
1	D	50	MET	2.4
1	A	162	ILE	2.4
1	B	54	ASP	2.4
1	C	146	ASN	2.4
1	A	173	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	89	ILE	2.4
1	B	23	LEU	2.4
1	C	294	PRO	2.4
1	D	95	GLY	2.4
1	A	255	LEU	2.4
1	B	188	LEU	2.4
1	D	194	GLU	2.4
1	D	124	GLY	2.3
1	C	172	PHE	2.3
1	D	156	PHE	2.3
1	A	71	HIS	2.3
1	A	19	LEU	2.3
1	D	187	ALA	2.3
1	D	39	SER	2.3
1	C	274	VAL	2.3
1	C	23	LEU	2.3
1	D	128	LEU	2.3
1	B	55	ASP	2.3
1	A	178	TRP	2.3
1	A	119	ARG	2.3
1	D	43	VAL	2.3
1	D	94	CYS	2.3
1	B	18	ASP	2.3
1	C	167	ALA	2.3
1	A	163	GLY	2.2
1	A	37	LYS	2.2
1	C	128	LEU	2.2
1	A	155	ASP	2.2
1	D	52	PRO	2.2
1	A	85	GLN	2.2
1	B	123	GLN	2.2
1	A	34	ALA	2.2
1	D	160	ALA	2.2
1	B	80	SER	2.2
1	D	251	ILE	2.2
1	D	237	LEU	2.2
1	D	248	HIS	2.2
1	B	275	SER	2.2
1	B	81	TYR	2.2
1	A	112	LEU	2.2
1	D	144	LEU	2.2
1	C	259	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	231	GLY	2.2
1	C	254	THR	2.2
1	D	228	THR	2.2
1	A	77	TYR	2.1
1	C	145	ILE	2.1
1	D	221	LEU	2.1
1	B	10	ASN	2.1
1	C	34	ALA	2.1
1	C	185	ALA	2.1
1	A	50	MET	2.1
1	A	134	ILE	2.1
1	C	291	LEU	2.1
1	B	113	GLN	2.1
1	C	149	GLY	2.1
1	A	68	THR	2.1
1	A	171	ALA	2.1
1	B	267	LYS	2.1
1	C	50	MET	2.1
1	A	210	GLU	2.1
1	C	285	LEU	2.1
1	D	23	LEU	2.1
1	D	55	ASP	2.1
1	D	129	HIS	2.1
1	B	105	VAL	2.1
1	A	199	TRP	2.1
1	C	22	ARG	2.1
1	C	106	THR	2.1
1	B	184	ALA	2.1
1	C	239	GLU	2.1
1	B	128	LEU	2.1
1	C	64	LEU	2.1
1	D	64	LEU	2.1
1	D	84	LEU	2.1
1	D	109	LEU	2.1
1	A	9	PHE	2.1
1	C	70	ARG	2.1
1	B	67	LYS	2.0
1	C	68	THR	2.0
1	B	76	ALA	2.0
1	C	62	GLU	2.0
1	B	78	HIS	2.0
1	A	294	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	14	ARG	2.0
1	D	117	VAL	2.0
1	B	97	GLY	2.0
1	C	78	HIS	2.0
1	D	161	GLN	2.0
1	D	269	LEU	2.0
1	B	136	ARG	2.0
1	C	8	ILE	2.0
1	D	89	ILE	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)

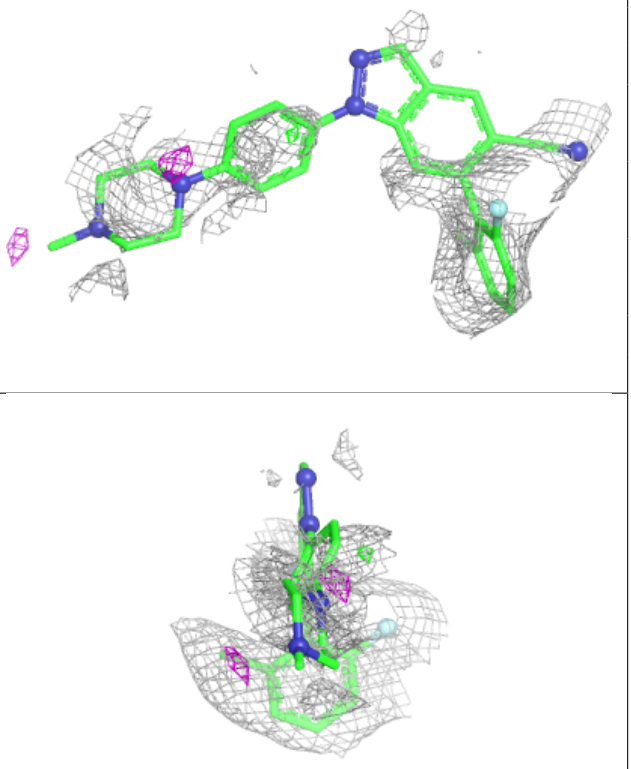
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

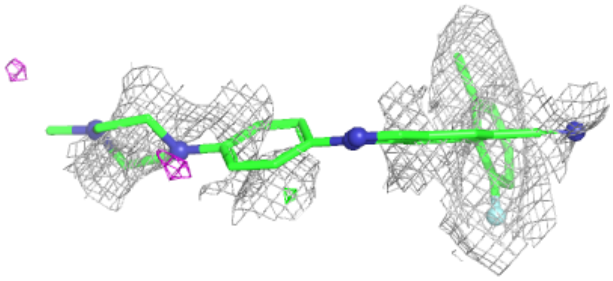
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	XHM	D	301	32/32	0.93	0.20	51,92,111,116	0
2	XHM	B	301	32/32	0.94	0.18	58,90,127,129	0
2	XHM	C	301	32/32	0.95	0.13	39,53,93,98	0
2	XHM	A	301	32/32	0.96	0.14	40,54,99,104	0

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 XHM D 301:

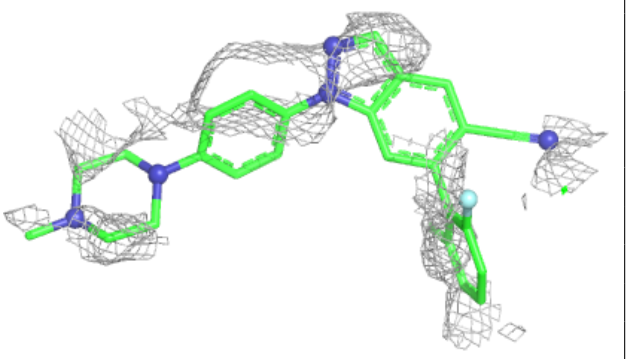
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

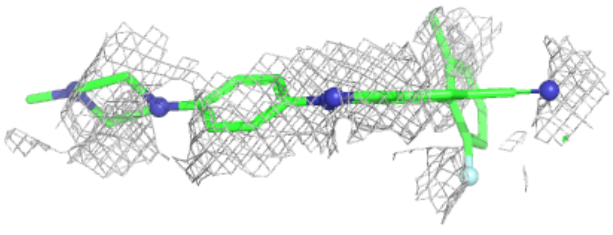


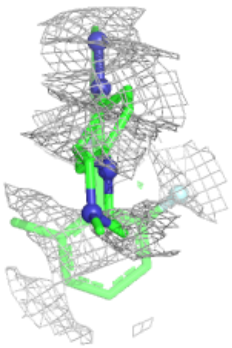


Electron density around XHM B 301:

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

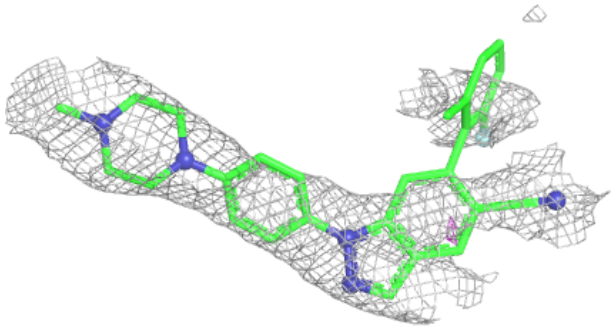


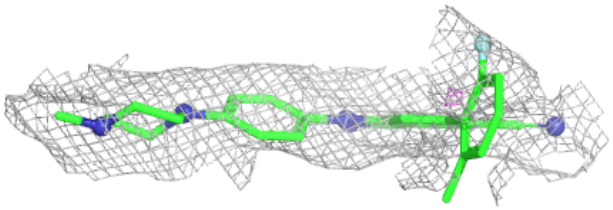


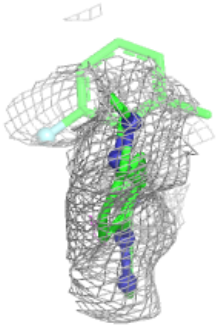


Electron density around XHM C 301:

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

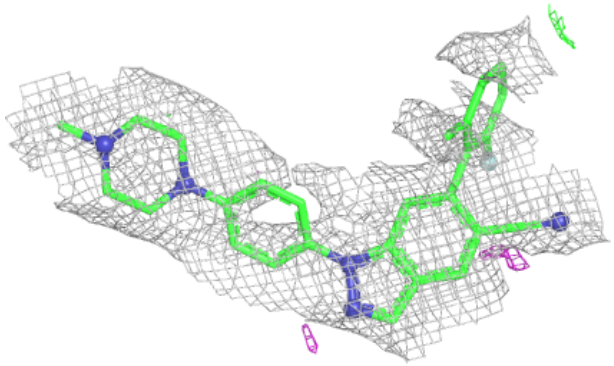


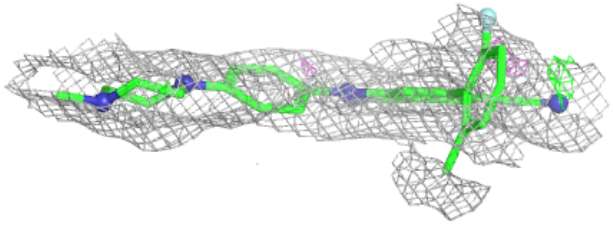


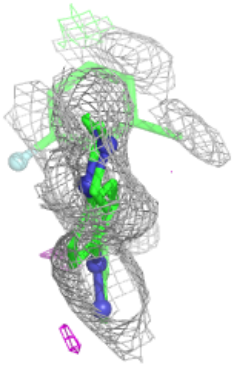


Electron density around XHM A 301:

$2mF_o$-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.