Full wwPDB X-ray Structure Validation Report (i)

Feb 25, 2024 – 03:45 AM EST

PDB ID	:	7L26
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:

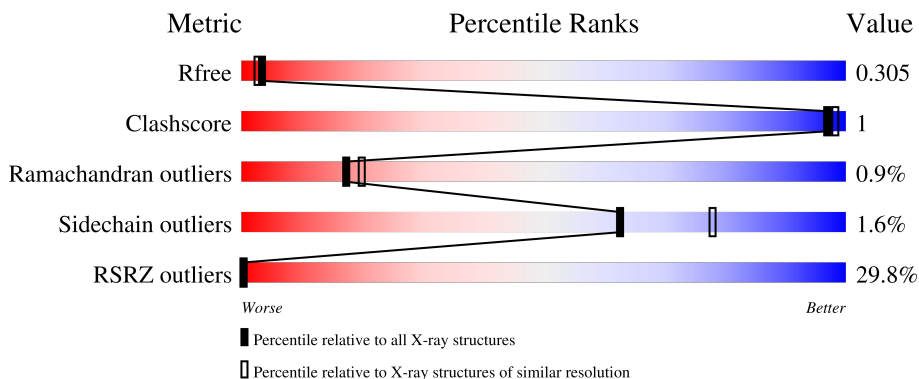|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Rfree		0.305
Clashscore		1
Ramachandran outliers		0.9%
Sidechain outliers		1.6%
RSRZ outliers		29.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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	28% / 93% / 5% ·
1	B	287	27% / 89% / 6% · ·
1	C	287	29% / 93% · ·
1	D	287	32% / 90% / 6% ·

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	XHM	B	301	-	-	-	X

2 Entry composition ⓘ

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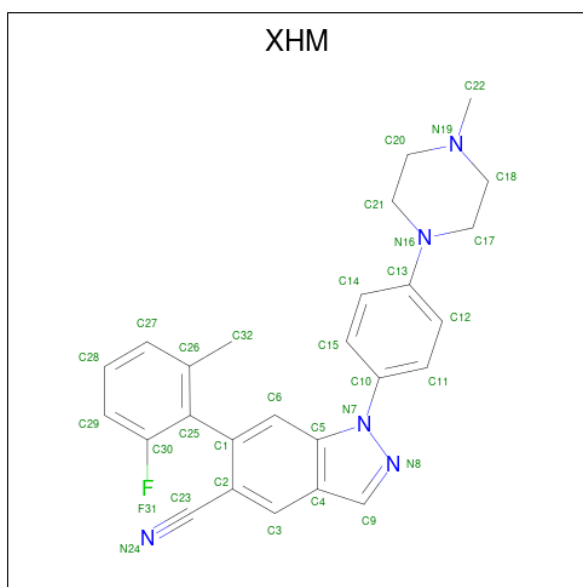
- Molecule 1 is a protein called Mitogen-activated protein kinase kinase kinase kinase 1.

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 (three-letter code: 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 32	C 26	F 1	N 5	0	0
2	B	1	Total 32	C 26	F 1	N 5	0	0
2	C	1	Total 32	C 26	F 1	N 5	0	0
2	D	1	Total 32	C 26	F 1	N 5	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	63	Total 63	O 63	0	0
3	B	64	Total 64	O 64	0	0
3	C	57	Total 57	O 57	0	0
3	D	46	Total 46	O 46	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 seq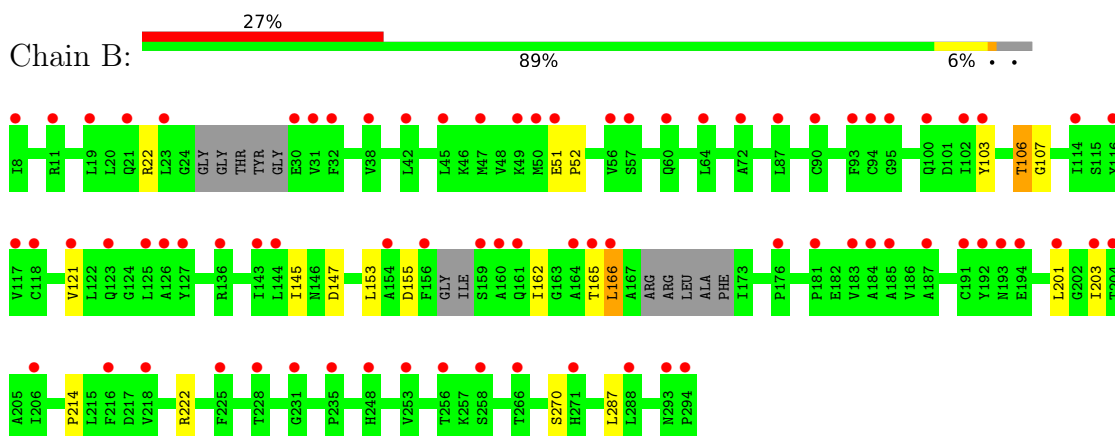uence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron 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:

L84 Q85 W88 I89 C90 M91 L99 I102 Y103 L109 Y127 L128 H129 D137 I143 N146 F156 GLY ILE SER A160 Q161 I162 G163 A164 T165 R169 F172 I173 G174 W178 A184 L188 K189 G190 C191 Y192 C196 L201 G202 I203 L211

P214 L215 L221 R222 V223 L224 Y232 Q233 P259 K260 K261 L269 V274 P277 R281 P294

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

Chain D:

32%

90%   6%   •

I8 D12 P13 R14 L19 L20 Q21 R22 L23 C24 GLY GLY THR TYR GLY E30 V31 F32 R35 V38 S39 G40 L45 K49 M50 E51 P52 V56 S57 Q60 K61 E62 I63 L64 I65 L66 K67 T68 C69 R70 H71 A72 L84 C90 G95 A96 I102 Y103

Q104 V105 L112 Q113 I114 S115 Y116 V117 C118 V121 L122 Q123 G124 L125 A126 Y127 S130 R136 G140 L153 A154 D155 F156 GLY ILE S159 A160 Q161 I162 G163 ALA THR LEU ALA ARG R169 L170 A171 F172 I173 G174 T175 P176 M179 V183 A184 A185 V186 A187 G190 C191

E194 L195 C196 L201 G202 I203 T204 L208 A209 Q212 P213 P214 L215 F216 D217 V218 R222 V223 L224 F225 T228 P235 R236 L237 A246 F247 H248 I251 K252 V253 T256 K260 P263 M268 H271 G278 L291 P294

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 49.48 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.1 (98.95-2.30) 94.3 (49.48-2.30)	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 (2.13%)	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)	0.31 , 35.2	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	0.94	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.*

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[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	0.67	1/2281 (0.0%)	0.85	4/3081 (0.1%)
1	B	0.72	2/2229 (0.1%)	0.87	7/3011 (0.2%)
1	C	0.68	1/2275 (0.0%)	0.86	2/3073 (0.1%)
1	D	0.68	1/2240 (0.0%)	0.86	3/3024 (0.1%)
All	All	0.69	5/9025 (0.1%)	0.86	16/12189 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	22	ARG	NE-CZ	9.38	1.45	1.33
1	C	25	GLY	C-O	8.25	1.36	1.23
1	D	22	ARG	NE-CZ	6.57	1.41	1.33
1	A	165	THR	CB-OG1	-6.18	1.30	1.43
1	B	165	THR	CB-OG1	-5.64	1.31	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	22	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	D	22	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	A	222	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	D	155	ASP	CB-CG-OD1	6.55	124.19	118.30
1	B	166	LEU	CB-CG-CD1	6.51	122.07	111.00
1	C	222	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	D	222	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	B	222	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	281	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	C	281	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	B	22	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	A	247	PHE	CB-CG-CD1	5.61	124.73	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	155	ASP	CB-CG-OD1	5.46	123.22	118.30
1	B	145	ILE	CG1-CB-CG2	-5.40	99.53	111.40
1	B	162	ILE	CA-CB-CG2	5.35	121.60	110.90
1	A	222	ARG	NE-CZ-NH2	-5.29	117.66	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2234	0	2295	2	0
1	B	2184	0	2241	5	0
1	C	2228	0	2291	4	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	15	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 (15) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:MET:HE3	1:D:183:VAL:HG12	1.94	0.48
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
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:203:ILE:HG23	1:B:214:PRO:HD2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	14	15
1	B	268/287 (93%)	258 (96%)	8 (3%)	2 (1%)	22	26
1	C	275/287 (96%)	260 (94%)	12 (4%)	3 (1%)	14	15
1	D	268/287 (93%)	259 (97%)	7 (3%)	2 (1%)	22	26
All	All	1087/1148 (95%)	1039 (96%)	38 (4%)	10 (1%)	17	20

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

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

5.3.2 Protein sidechains ⓘ

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%)	238 (99%)	3 (1%)	71	84
1	B	237/244 (97%)	232 (98%)	5 (2%)	53	70
1	C	240/244 (98%)	238 (99%)	2 (1%)	81	91
1	D	238/244 (98%)	233 (98%)	5 (2%)	53	70
All	All	956/976 (98%)	941 (98%)	15 (2%)	62	78

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	TYR
1	A	147	ASP
1	A	253	VAL
1	B	103	TYR
1	B	106	THR
1	B	147	ASP
1	B	166	LEU
1	B	270	SER
1	C	41	ASP
1	C	103	TYR
1	D	84	LEU
1	D	103	TYR
1	D	169	ARG
1	D	170	LEU
1	D	253	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	249	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 ⓘ

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	B	301	-	35,36,36	1.01	1 (2%)	46,52,52	1.78	10 (21%)
2	XHM	C	301	-	35,36,36	0.98	0	46,52,52	1.70	9 (19%)
2	XHM	D	301	-	35,36,36	1.01	0	46,52,52	1.95	11 (23%)
2	XHM	A	301	-	35,36,36	1.06	1 (2%)	46,52,52	1.65	8 (17%)

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	B	301	-	-	4/14/24/24	0/5/5/5
2	XHM	C	301	-	-	4/14/24/24	0/5/5/5
2	XHM	D	301	-	-	4/14/24/24	0/5/5/5
2	XHM	A	301	-	-	3/14/24/24	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	XHM	C9-C4	2.14	1.45	1.40
2	A	301	XHM	C6-C1	2.08	1.41	1.37

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	XHM	C9-N8-N7	5.78	111.50	103.93
2	B	301	XHM	C1-C25-C30	-5.72	116.88	122.64
2	C	301	XHM	C9-N8-N7	5.34	110.93	103.93
2	A	301	XHM	C9-N8-N7	5.32	110.90	103.93
2	B	301	XHM	C9-N8-N7	5.29	110.86	103.93
2	D	301	XHM	C1-C25-C30	-5.27	117.32	122.64
2	A	301	XHM	C6-C5-N7	4.53	136.57	131.99
2	C	301	XHM	C6-C5-N7	4.49	136.53	131.99
2	D	301	XHM	C6-C5-N7	4.15	136.19	131.99
2	B	301	XHM	C6-C5-N7	3.75	135.78	131.99
2	C	301	XHM	C1-C25-C30	-3.51	119.10	122.64
2	A	301	XHM	C1-C25-C30	-3.19	119.42	122.64
2	D	301	XHM	C29-C30-C25	-3.12	120.13	123.94
2	D	301	XHM	C6-C1-C2	3.06	120.27	117.60
2	D	301	XHM	C22-N19-C20	3.04	115.21	110.66
2	B	301	XHM	C29-C30-C25	-3.00	120.28	123.94
2	D	301	XHM	C6-C5-C4	-2.92	117.31	121.37
2	C	301	XHM	C29-C30-C25	-2.91	120.39	123.94
2	B	301	XHM	C1-C25-C26	2.88	123.63	120.00
2	A	301	XHM	C6-C5-C4	-2.83	117.42	121.37
2	C	301	XHM	C6-C5-C4	-2.78	117.50	121.37
2	C	301	XHM	C6-C1-C2	2.70	119.96	117.60
2	A	301	XHM	C15-C10-C11	-2.63	117.43	121.33
2	A	301	XHM	C29-C30-C25	-2.61	120.76	123.94
2	B	301	XHM	C20-N19-C18	2.56	113.10	109.52
2	D	301	XHM	C12-C13-N16	-2.55	117.86	121.38
2	D	301	XHM	C15-C10-C11	-2.53	117.58	121.33
2	C	301	XHM	C15-C10-C11	-2.51	117.61	121.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	XHM	C6-C5-C4	-2.40	118.03	121.37
2	A	301	XHM	C6-C1-C2	2.37	119.67	117.60
2	B	301	XHM	C22-N19-C20	2.36	114.20	110.66
2	B	301	XHM	C6-C1-C2	2.35	119.66	117.60
2	A	301	XHM	C22-N19-C20	2.33	114.14	110.66
2	D	301	XHM	C14-C13-N16	2.22	124.44	121.38
2	D	301	XHM	C1-C25-C26	2.13	122.69	120.00
2	B	301	XHM	C15-C10-C11	-2.13	118.17	121.33
2	C	301	XHM	C14-C13-N16	2.12	124.31	121.38
2	C	301	XHM	C22-N19-C20	2.03	113.70	110.66

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	XHM	C11-C10-N7-C5
2	B	301	XHM	C12-C13-N16-C21
2	B	301	XHM	C14-C13-N16-C21
2	D	301	XHM	C14-C13-N16-C21
2	D	301	XHM	C12-C13-N16-C21
2	A	301	XHM	C11-C10-N7-C5
2	A	301	XHM	C15-C10-N7-C5
2	B	301	XHM	C11-C10-N7-C5
2	B	301	XHM	C15-C10-N7-C5
2	C	301	XHM	C15-C10-N7-C5
2	D	301	XHM	C11-C10-N7-C5
2	D	301	XHM	C15-C10-N7-C5
2	C	301	XHM	C14-C13-N16-C21
2	C	301	XHM	C12-C13-N16-C21
2	A	301	XHM	C14-C13-N16-C21

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 B 301

Bond lengths

Bond angles

Torsions

Rings

Ligand XHM C 301

Bond lengths

Bond angles

Torsions

Rings

Ligand XHM D 301

Bond lengths

Bond angles

Torsions

Rings

Ligand XHM A 301

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

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, 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%)	1.58	80 (28%)	0	0	36, 58, 106, 133	31 (11%)
1	B	275/287 (95%)	1.53	77 (28%)	0	0	31, 60, 99, 128	39 (14%)
1	C	280/287 (97%)	1.67	82 (29%)	0	0	36, 58, 107, 127	33 (11%)
1	D	275/287 (95%)	1.71	92 (33%)	0	0	32, 58, 101, 132	30 (10%)
All	All	1110/1148 (96%)	1.62	331 (29%)	0	0	31, 58, 103, 133	133 (11%)

All (331) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	65	ILE	12.3
1	A	64	LEU	10.7
1	C	190	GLY	9.0
1	C	191	CYS	8.4
1	C	38	VAL	8.2
1	C	84	LEU	7.9
1	A	38	VAL	7.9
1	A	63	ILE	7.9
1	C	64	LEU	7.7
1	D	260	LYS	7.6
1	A	60	GLN	7.5
1	A	65	ILE	7.3
1	A	40	GLY	7.2
1	D	191	CYS	7.1
1	A	79	GLY	7.0
1	A	190	GLY	6.9
1	C	189	LYS	6.8
1	D	72	ALA	6.7
1	C	60	GLN	6.6
1	D	69	CYS	6.6
1	C	109	LEU	6.6

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Mol	Chain	Res	Type	RSRZ
1	B	118	CYS	6.5
1	D	170	LEU	6.5
1	C	9	PHE	6.4
1	D	20	LEU	6.3
1	B	114	ILE	6.3
1	D	51	GLU	6.3
1	D	156	PHE	6.1
1	A	85	GLN	6.0
1	B	125	LEU	6.0
1	B	294	PRO	5.9
1	B	64	LEU	5.9
1	D	118	CYS	5.9
1	C	160	ALA	5.9
1	D	14	ARG	5.8
1	C	42	LEU	5.8
1	D	19	LEU	5.8
1	A	169	ARG	5.7
1	A	191	CYS	5.7
1	D	248	HIS	5.7
1	B	93	PHE	5.7
1	B	102	ILE	5.6
1	D	125	LEU	5.5
1	A	160	ALA	5.5
1	C	233	GLN	5.5
1	C	63	ILE	5.5
1	C	22	ARG	5.5
1	C	34	ALA	5.4
1	B	191	CYS	5.3
1	D	38	VAL	5.3
1	B	161	GLN	5.3
1	D	68	THR	5.2
1	C	274	VAL	5.1
1	D	121	VAL	5.1
1	C	294	PRO	5.1
1	D	172	PHE	5.0
1	C	81	TYR	5.0
1	C	69	CYS	4.9
1	D	183	VAL	4.9
1	A	19	LEU	4.9
1	B	271	HIS	4.9
1	D	116	TYR	4.8
1	D	61	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	30	GLU	4.8
1	D	114	ILE	4.7
1	A	15	ASP	4.7
1	A	81	TYR	4.6
1	A	88	TRP	4.6
1	B	31	VAL	4.6
1	B	192	TYR	4.6
1	C	232	TYR	4.5
1	C	16	HIS	4.4
1	C	52	PRO	4.4
1	A	37	LYS	4.4
1	D	251	ILE	4.3
1	D	159	SER	4.3
1	B	51	GLU	4.2
1	D	218	VAL	4.2
1	D	184	ALA	4.2
1	A	39	SER	4.2
1	D	45	LEU	4.1
1	C	10	ASN	4.1
1	B	127	TYR	4.1
1	A	241	GLY	4.1
1	A	172	PHE	4.1
1	D	256	THR	4.0
1	C	161	GLN	4.0
1	C	13	PRO	4.0
1	A	80	SER	4.0
1	D	271	HIS	4.0
1	C	48	VAL	4.0
1	A	59	LEU	3.9
1	B	21	GLN	3.9
1	A	164	ALA	3.9
1	D	171	ALA	3.9
1	D	52	PRO	3.9
1	A	189	LYS	3.9
1	B	218	VAL	3.9
1	C	76	ALA	3.9
1	D	291	LEU	3.8
1	C	89	ILE	3.8
1	A	192	TYR	3.8
1	A	165	THR	3.8
1	D	122	LEU	3.7
1	C	146	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	50	MET	3.7
1	A	274	VAL	3.7
1	D	203	ILE	3.7
1	C	192	TYR	3.7
1	C	66	LEU	3.6
1	A	168	ARG	3.6
1	B	156	PHE	3.6
1	C	41	ASP	3.6
1	B	45	LEU	3.6
1	B	187	ALA	3.6
1	B	19	LEU	3.6
1	B	166	LEU	3.6
1	B	185	ALA	3.5
1	D	155	ASP	3.5
1	A	91	MET	3.5
1	D	105	VAL	3.5
1	B	103	TYR	3.5
1	D	49	LYS	3.5
1	C	77	TYR	3.5
1	B	248	HIS	3.5
1	B	201	LEU	3.5
1	D	187	ALA	3.5
1	D	127	TYR	3.4
1	C	37	LYS	3.4
1	D	225	PHE	3.4
1	C	277	PRO	3.4
1	C	129	HIS	3.4
1	D	63	ILE	3.4
1	B	47	MET	3.4
1	A	156	PHE	3.4
1	B	56	VAL	3.4
1	A	62	GLU	3.4
1	C	156	PHE	3.4
1	C	15	ASP	3.3
1	D	8	ILE	3.3
1	B	183	VAL	3.3
1	A	149	GLY	3.3
1	B	116	TYR	3.3
1	D	212	GLN	3.3
1	B	87	LEU	3.3
1	D	66	LEU	3.3
1	D	64	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	16	HIS	3.3
1	D	216[A]	PHE	3.3
1	B	57	SER	3.3
1	C	47	MET	3.3
1	D	161	GLN	3.3
1	C	75	VAL	3.3
1	B	136	ARG	3.3
1	D	140	GLY	3.2
1	B	126	ALA	3.2
1	D	31	VAL	3.2
1	A	41	ASP	3.2
1	B	121	VAL	3.2
1	B	203	ILE	3.2
1	D	32	PHE	3.2
1	D	65	ILE	3.2
1	A	269	LEU	3.2
1	D	268	MET	3.2
1	B	193	ASN	3.1
1	B	206	ILE	3.1
1	D	40	GLY	3.1
1	C	51	GLU	3.1
1	C	91	MET	3.1
1	B	32	PHE	3.1
1	A	195	LEU	3.1
1	D	12	ASP	3.0
1	D	208	LEU	3.0
1	A	46	LYS	3.0
1	D	60	GLN	3.0
1	B	164	ALA	3.0
1	A	250	PHE	3.0
1	C	85	GLN	3.0
1	C	169	ARG	3.0
1	B	11	ARG	3.0
1	D	169	ARG	3.0
1	A	265	ALA	3.0
1	A	232	TYR	2.9
1	C	128	LEU	2.9
1	B	176	PRO	2.9
1	B	117	VAL	2.9
1	D	175	THR	2.9
1	C	221	LEU	2.9
1	C	174	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	60	GLN	2.9
1	C	67	LYS	2.9
1	C	19	LEU	2.8
1	D	253	VAL	2.8
1	C	90	CYS	2.8
1	B	165	THR	2.8
1	C	163	GLY	2.8
1	D	136	ARG	2.8
1	C	196	CYS	2.8
1	B	123	GLN	2.8
1	B	253	VAL	2.8
1	B	216[A]	PHE	2.7
1	B	204	THR	2.7
1	C	24	GLY	2.7
1	C	79	GLY	2.7
1	C	59	LEU	2.7
1	C	201	LEU	2.7
1	C	36	ASP	2.7
1	B	50	MET	2.7
1	B	143	ILE	2.7
1	B	225	PHE	2.7
1	C	172	PHE	2.7
1	C	30	GLU	2.6
1	B	95	GLY	2.6
1	A	84	LEU	2.6
1	A	210	GLU	2.6
1	B	38	VAL	2.6
1	B	258	SER	2.6
1	A	294	PRO	2.6
1	A	162	ILE	2.6
1	D	196	CYS	2.6
1	B	266	THR	2.6
1	A	188	LEU	2.6
1	D	176	PRO	2.6
1	B	72	ALA	2.6
1	D	209	ALA	2.6
1	A	69	CYS	2.6
1	A	61	LYS	2.6
1	A	138	ILE	2.6
1	C	165	THR	2.5
1	D	96	ALA	2.5
1	A	214	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	83	TRP	2.5
1	D	35	ARG	2.5
1	C	137	ASP	2.5
1	A	89	ILE	2.5
1	B	8	ILE	2.5
1	D	263	PRO	2.5
1	C	32	PHE	2.5
1	A	167	ALA	2.5
1	A	45	LEU	2.5
1	B	144	LEU	2.5
1	A	216[A]	PHE	2.5
1	C	143	ILE	2.5
1	D	102	ILE	2.5
1	C	269	LEU	2.5
1	D	57	SER	2.4
1	B	194	GLU	2.4
1	C	178	TRP	2.4
1	A	115	SER	2.4
1	B	184	ALA	2.4
1	D	185	ALA	2.4
1	C	39	SER	2.4
1	C	224	LEU	2.4
1	A	44	ALA	2.4
1	D	246	ALA	2.4
1	A	155	ASP	2.4
1	A	261	LYS	2.4
1	C	25	GLY	2.4
1	B	42	LEU	2.4
1	A	77	TYR	2.3
1	A	170	LEU	2.3
1	A	202	GLY	2.3
1	A	87	LEU	2.3
1	A	58	THR	2.3
1	B	159	SER	2.3
1	A	166	LEU	2.3
1	B	90	CYS	2.3
1	C	261	LYS	2.3
1	D	174	GLY	2.3
1	D	194	GLU	2.3
1	D	13	PRO	2.3
1	D	235	PRO	2.3
1	A	173	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	17	TYR	2.3
1	A	66	LEU	2.2
1	D	112	LEU	2.2
1	A	55	ASP	2.2
1	B	94	CYS	2.2
1	D	237	LEU	2.2
1	B	181	PRO	2.2
1	B	235	PRO	2.2
1	A	48	VAL	2.2
1	D	117	VAL	2.2
1	B	231	GLY	2.2
1	D	95	GLY	2.2
1	D	278	GLY	2.2
1	D	204	THR	2.2
1	B	49	LYS	2.2
1	C	259	PRO	2.2
1	D	223	VAL	2.2
1	D	24	GLY	2.2
1	B	293	ASN	2.2
1	D	228	THR	2.2
1	A	153	LEU	2.2
1	D	190	GLY	2.2
1	C	58	THR	2.2
1	C	184	ALA	2.2
1	D	70	ARG	2.2
1	B	288	LEU	2.2
1	C	127	TYR	2.1
1	A	78	HIS	2.1
1	C	102	ILE	2.1
1	A	13	PRO	2.1
1	A	73	ASN	2.1
1	B	154	ALA	2.1
1	A	18	ASP	2.1
1	A	86	LYS	2.1
1	C	188	LEU	2.1
1	D	201	LEU	2.1
1	C	88	TRP	2.1
1	D	90	CYS	2.1
1	D	56	VAL	2.1
1	D	130	SER	2.1
1	A	277	PRO	2.1
1	A	291	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	8	ILE	2.1
1	B	160	ALA	2.1
1	D	160	ALA	2.1
1	A	24	GLY	2.1
1	D	123	GLN	2.0
1	C	215	LEU	2.0
1	D	23	LEU	2.0
1	A	145	ILE	2.0
1	C	211	LEU	2.0
1	B	100	GLN	2.0
1	B	256	THR	2.0
1	A	32	PHE	2.0
1	C	83	TRP	2.0
1	B	23	LEU	2.0
1	C	99	LEU	2.0
1	B	228	THR	2.0

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

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

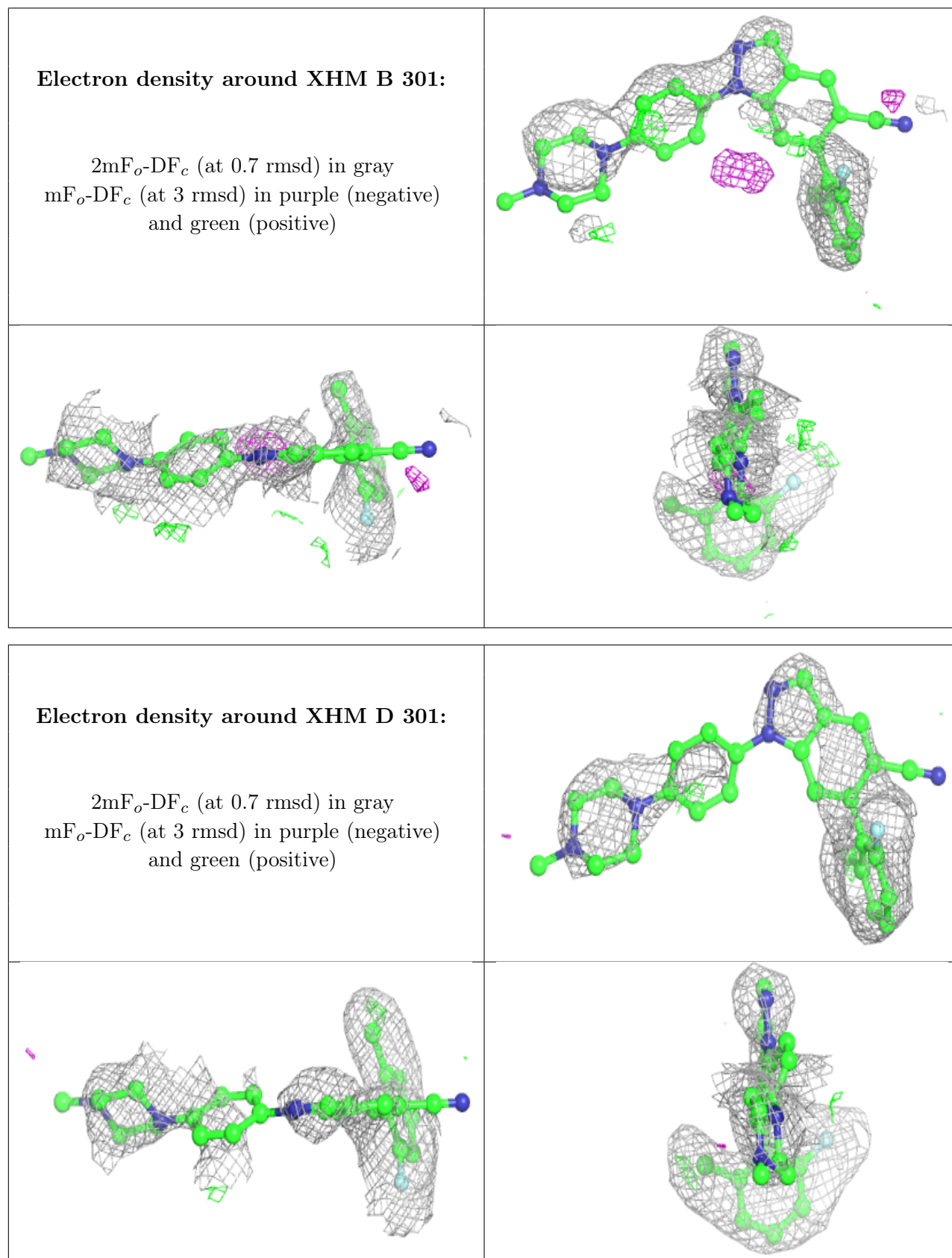## 6.3 Carbohydrates ⓘ

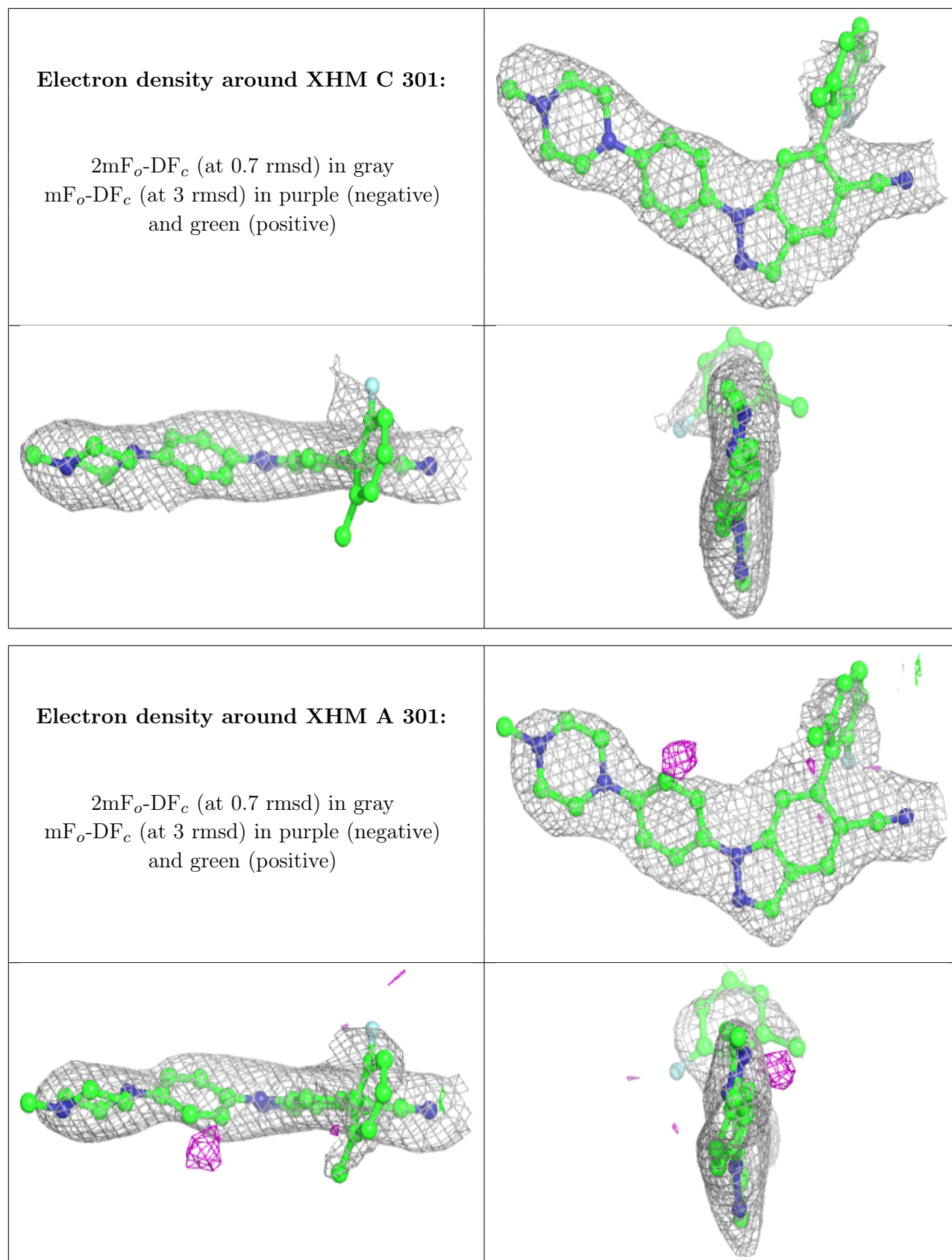There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	B	301	32/32	0.45	0.44	58,90,127,129	0
2	XHM	D	301	32/32	0.74	0.38	51,92,111,116	0
2	XHM	C	301	32/32	0.85	0.23	39,53,93,98	0
2	XHM	A	301	32/32	0.87	0.26	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 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 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 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 ⓘ

There are no such residues in this entry.