



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:42 PM UTC

PDB ID : 8GDV / pdb_00008gdv
Title : Structure of M66I mutant of disulfide stabilized HIV-1 CA hexamer in complex with CPSF6 peptide and IP6
Authors : Briganti, L.; Schope, L.; Kvaratskhelia, M.
Deposited on : 2023-03-06
Resolution : 3.30 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 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

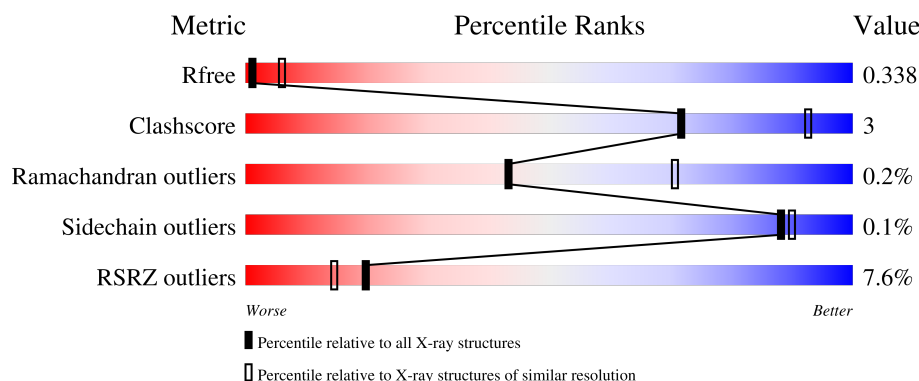
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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 $\leq 5\%$. 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	231	6% 79% 6% 14%
1	B	231	4% 77% 6% 17%
1	C	231	8% 77% 8% 15%
1	D	231	7% 80% 10% 10%
1	E	231	7% 84% 7% 9%

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Mol	Chain	Length	Quality of chain
1	F	231	
2	M	15	
2	N	15	
2	O	15	
2	P	15	
2	Q	15	
2	R	15	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9980 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 Gag polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	1	0
			1513	955	263	284	11			
1	B	192	Total	C	N	O	S	0	1	0
			1464	927	255	271	11			
1	C	197	Total	C	N	O	S	0	2	0
			1532	967	269	285	11			
1	D	209	Total	C	N	O	S	0	3	0
			1607	1014	277	304	12			
1	E	210	Total	C	N	O	S	0	1	0
			1617	1018	281	305	13			
1	F	208	Total	C	N	O	S	0	1	0
			1588	1002	273	301	12			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	CYS	ALA	engineered mutation	UNP D2ECD8
A	45	CYS	GLU	engineered mutation	UNP D2ECD8
A	66	ILE	MET	engineered mutation	UNP D2ECD8
A	184	ALA	TRP	engineered mutation	UNP D2ECD8
A	185	ALA	MET	engineered mutation	UNP D2ECD8
B	14	CYS	ALA	engineered mutation	UNP D2ECD8
B	45	CYS	GLU	engineered mutation	UNP D2ECD8
B	66	ILE	MET	engineered mutation	UNP D2ECD8
B	184	ALA	TRP	engineered mutation	UNP D2ECD8
B	185	ALA	MET	engineered mutation	UNP D2ECD8
C	14	CYS	ALA	engineered mutation	UNP D2ECD8
C	45	CYS	GLU	engineered mutation	UNP D2ECD8
C	66	ILE	MET	engineered mutation	UNP D2ECD8
C	184	ALA	TRP	engineered mutation	UNP D2ECD8
C	185	ALA	MET	engineered mutation	UNP D2ECD8
D	14	CYS	ALA	engineered mutation	UNP D2ECD8
D	45	CYS	GLU	engineered mutation	UNP D2ECD8

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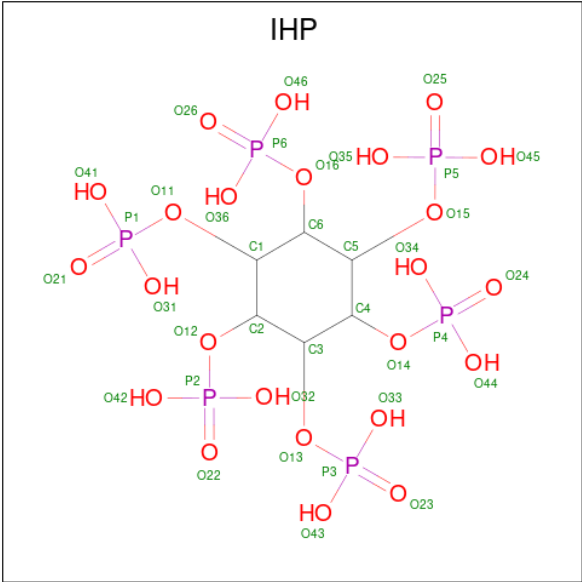
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Chain	Residue	Modelled	Actual	Comment	Reference
D	66	ILE	MET	engineered mutation	UNP D2ECD8
D	184	ALA	TRP	engineered mutation	UNP D2ECD8
D	185	ALA	MET	engineered mutation	UNP D2ECD8
E	14	CYS	ALA	engineered mutation	UNP D2ECD8
E	45	CYS	GLU	engineered mutation	UNP D2ECD8
E	66	ILE	MET	engineered mutation	UNP D2ECD8
E	184	ALA	TRP	engineered mutation	UNP D2ECD8
E	185	ALA	MET	engineered mutation	UNP D2ECD8
F	14	CYS	ALA	engineered mutation	UNP D2ECD8
F	45	CYS	GLU	engineered mutation	UNP D2ECD8
F	66	ILE	MET	engineered mutation	UNP D2ECD8
F	184	ALA	TRP	engineered mutation	UNP D2ECD8
F	185	ALA	MET	engineered mutation	UNP D2ECD8

- Molecule 2 is a protein called Cleavage and polyadenylation specificity factor subunit 6.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	14	Total	C	N	O	0	0	0
			103	71	16	16			
2	N	13	Total	C	N	O	0	0	0
			90	64	13	13			
2	O	14	Total	C	N	O	0	0	0
			103	71	16	16			
2	P	13	Total	C	N	O	0	0	0
			94	66	14	14			
2	Q	13	Total	C	N	O	0	0	0
			98	68	15	15			
2	R	14	Total	C	N	O	0	0	0
			99	69	15	15			

- Molecule 3 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆).

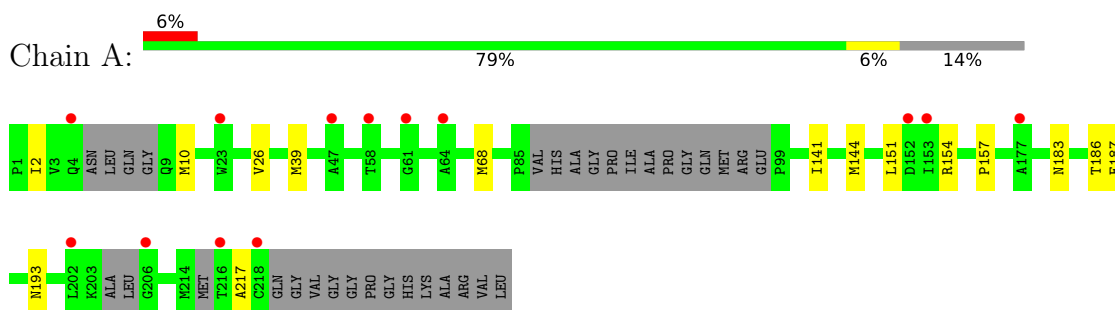


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			36	6	24	6		
3	A	1	Total	C	O	P	0	0
			36	6	24	6		

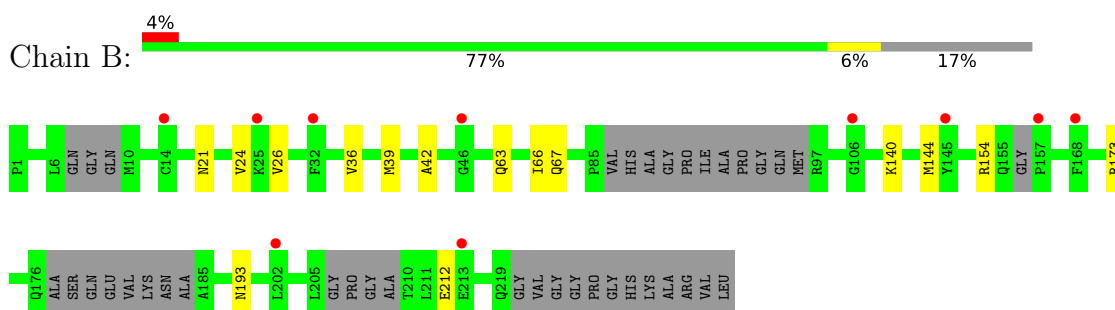
3 Residue-property plots [i](#)

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.

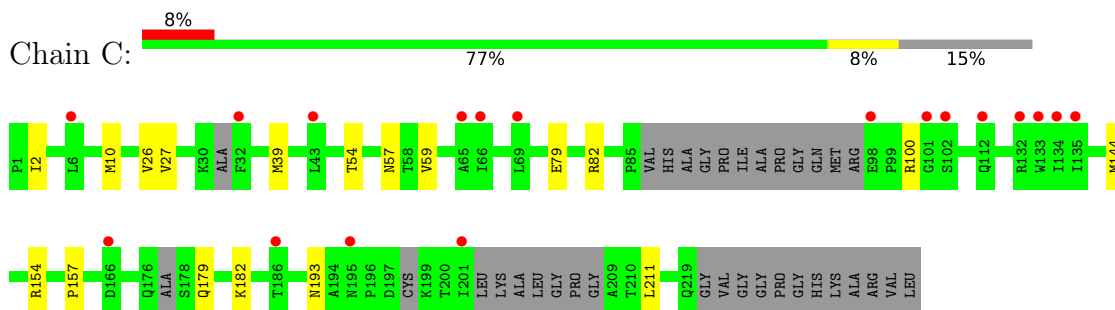
- Molecule 1: Gag polypeptide



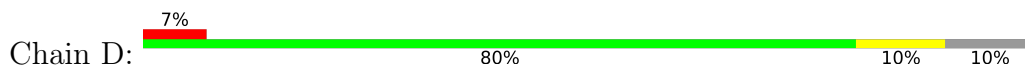
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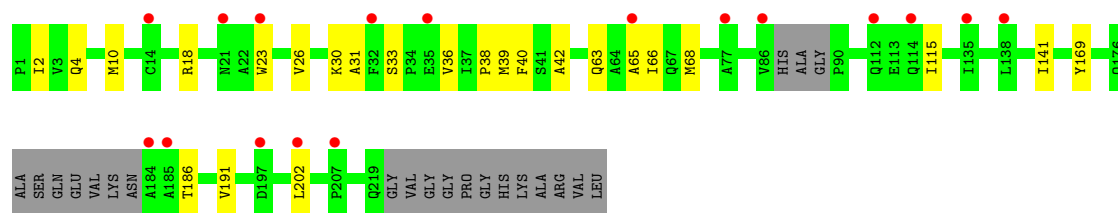


- Molecule 1: Gag polypeptide

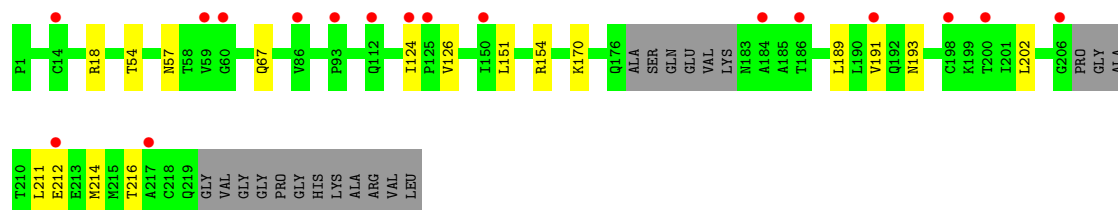
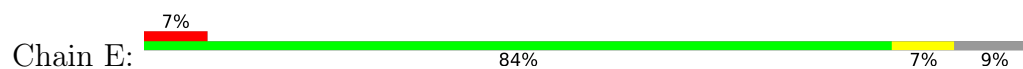


- Molecule 1: Gag polypeptide

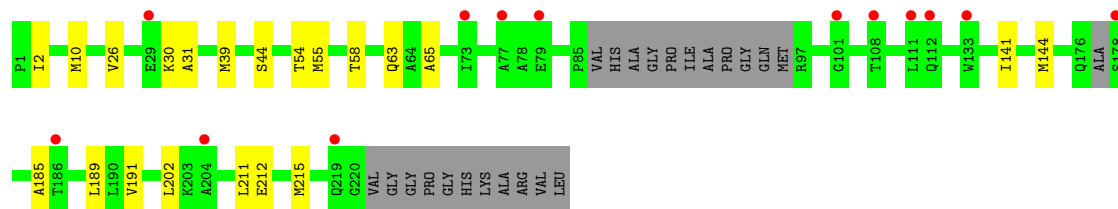
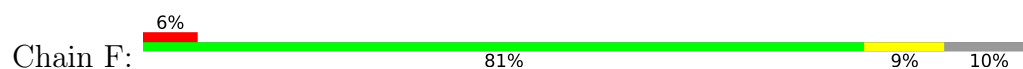




• Molecule 1: Gag polypeptide



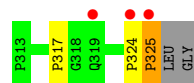
• Molecule 1: Gag polypeptide



• Molecule 2: Cleavage and polyadenylation specificity factor subunit 6



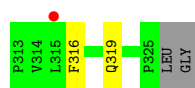
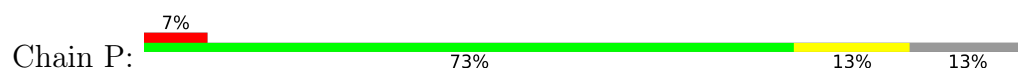
• Molecule 2: Cleavage and polyadenylation specificity factor subunit 6



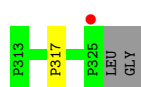
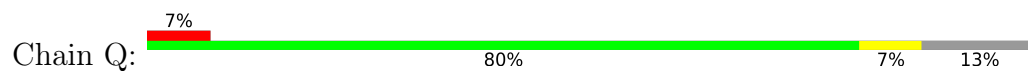
• Molecule 2: Cleavage and polyadenylation specificity factor subunit 6



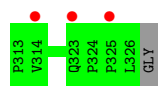
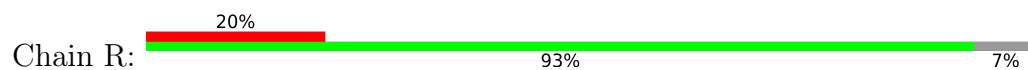
- Molecule 2: Cleavage and polyadenylation specificity factor subunit 6



- Molecule 2: Cleavage and polyadenylation specificity factor subunit 6



- Molecule 2: Cleavage and polyadenylation specificity factor subunit 6



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	133.17Å 133.17Å 205.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.88 – 3.30 47.88 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.4 (47.88-3.30) 96.0 (47.88-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.307 , 0.347 0.303 , 0.338	Depositor DCC
R_{free} test set	1365 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	68.6	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	9980	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IHP

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	0.20	0/1543	0.39	0/2097
1	B	0.12	0/1492	0.27	0/2026
1	C	0.13	0/1563	0.29	0/2121
1	D	0.11	0/1641	0.26	0/2235
1	E	0.10	0/1651	0.27	0/2247
1	F	0.11	0/1620	0.28	0/2204
2	M	0.14	0/109	0.28	0/150
2	N	0.20	0/96	0.46	0/133
2	O	0.41	0/109	0.69	0/150
2	P	0.26	0/100	0.50	0/138
2	Q	0.13	0/104	0.25	0/143
2	R	0.44	0/105	0.58	0/145
All	All	0.15	0/10133	0.31	0/13789

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	1513	0	1468	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1464	0	1407	10	0
1	C	1532	0	1504	13	0
1	D	1607	0	1559	16	0
1	E	1617	0	1580	12	0
1	F	1588	0	1550	13	0
2	M	103	0	97	0	0
2	N	90	0	83	2	0
2	O	103	0	97	0	0
2	P	94	0	89	1	0
2	Q	98	0	95	1	0
2	R	99	0	91	0	0
3	A	72	0	12	2	0
All	All	9980	0	9632	64	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 3.

All (64) 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:212:GLU:HG3	1:C:144:MET:HE1	1.65	0.77
1:A:144:MET:HE1	1:F:212:GLU:HG3	1.77	0.67
2:N:324:PRO:O	2:N:325:PRO:C	2.43	0.61
1:E:216:THR:HG23	1:F:144:MET:HE2	1.83	0.61
1:A:26:VAL:HG21	1:A:39:MET:HG2	1.83	0.61
1:C:79:GLU:OE1	1:C:82:ARG:NH1	2.34	0.60
1:E:151:LEU:HD23	1:E:189:LEU:HD11	1.85	0.58
1:C:2:ILE:HG22	1:C:10:MET:HE3	1.86	0.58
3:A:302:IHP:O24	1:E:18:ARG:NH1	2.37	0.57
1:F:54:THR:O	1:F:58:THR:OG1	2.26	0.53
1:D:186:THR:HG21	2:Q:317:PRO:HB2	1.91	0.53
1:F:2:ILE:HG22	1:F:10:MET:HE3	1.91	0.52
1:A:2:ILE:HG22	1:A:10:MET:HE3	1.92	0.52
1:B:26:VAL:HG12	1:B:36:VAL:HG23	1.93	0.51
1:B:42:ALA:HB2	1:C:54:THR:HG21	1.91	0.51
1:D:33:SER:O	1:D:36:VAL:HG22	2.11	0.50
1:F:44:SER:HA	1:F:55:MET:HE1	1.93	0.50
1:D:2:ILE:HD11	1:D:115:ILE:HG12	1.94	0.50
1:D:63:GLN:HA	1:D:66:ILE:HB	1.95	0.49
1:B:154:ARG:HA	1:B:193:ASN:HB3	1.96	0.48
1:C:179:GLN:HE21	1:C:182:LYS:HD2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:GLN:NE2	1:C:182:LYS:HD2	2.28	0.48
1:D:2:ILE:HG22	1:D:10:MET:HE3	1.96	0.48
1:C:144:MET:HE3	1:C:144:MET:HB2	1.68	0.47
1:E:191:VAL:HG12	1:E:202:LEU:HD13	1.96	0.47
1:D:38:PRO:HG3	1:E:57:ASN:HB3	1.96	0.47
1:E:212:GLU:HG3	1:F:144:MET:HE1	1.96	0.47
1:B:140:LYS:O	1:B:144:MET:HG2	2.15	0.46
1:A:183:ASN:O	1:A:187:GLU:HG2	2.14	0.46
1:F:185:ALA:O	1:F:189:LEU:HB2	2.16	0.46
1:B:26:VAL:HG11	1:B:39:MET:HG2	1.97	0.46
1:E:124:ILE:O	1:E:126:VAL:N	2.50	0.45
1:D:42:ALA:HB2	1:E:54:THR:HG21	1.99	0.44
1:E:154:ARG:HA	1:E:193:ASN:HB3	1.99	0.44
1:D:191:VAL:HG12	1:D:202:LEU:HD13	1.98	0.44
1:B:21:ASN:HA	1:B:24:VAL:HG12	2.00	0.44
1:C:211:LEU:HD23	1:D:68:MET:HG3	2.00	0.44
1:D:30:LYS:O	1:D:31:ALA:C	2.61	0.43
1:B:63:GLN:HA	1:B:66:ILE:HB	2.00	0.43
2:P:316:PHE:HB2	2:P:319:GLN:OE1	2.19	0.43
1:A:183:ASN:O	1:A:186:THR:OG1	2.34	0.43
1:C:154:ARG:HA	1:C:193:ASN:HB3	2.01	0.43
1:B:67:GLN:OE1	2:N:317:PRO:HA	2.18	0.42
1:E:211:LEU:HA	1:E:214:MET:HE3	2.00	0.42
1:F:65:ALA:HB1	1:F:141:ILE:HD13	2.01	0.42
1:A:68:MET:HE3	1:A:141:ILE:HG12	2.02	0.42
1:E:170:LYS:HA	1:F:63:GLN:HG3	2.01	0.42
1:A:144:MET:HB2	1:A:144:MET:HE3	1.67	0.42
1:F:191:VAL:HG13	1:F:202:LEU:HB2	2.00	0.42
1:C:26:VAL:HG21	1:C:39:MET:HG2	2.03	0.41
1:D:23:TRP:CZ3	1:D:40:PHE:HB2	2.55	0.41
1:F:211:LEU:HG	1:F:215:MET:HE2	2.03	0.41
3:A:301:IHP:O43	1:D:18:ARG:NH2	2.54	0.41
1:F:26:VAL:HG21	1:F:39:MET:HG2	2.01	0.41
1:B:173:ARG:NH2	1:C:57:ASN:O	2.45	0.41
1:C:27:VAL:HG11	1:C:59:VAL:HG13	2.02	0.41
1:D:65:ALA:HB1	1:D:141:ILE:HD13	2.02	0.41
1:D:169:TYR:CZ	1:E:67:GLN:HG2	2.56	0.41
1:C:100:ARG:HH11	1:C:100:ARG:HG2	1.85	0.41
1:D:26:VAL:HG21	1:D:39:MET:HG2	2.03	0.41
1:F:30:LYS:O	1:F:31:ALA:C	2.64	0.40
1:A:154:ARG:HA	1:A:193:ASN:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:GLN:HB2	1:D:10:MET:SD	2.61	0.40
1:A:151:LEU:HD12	1:A:151:LEU:H	1.85	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	189/231 (82%)	183 (97%)	4 (2%)	2 (1%)	11	39
1	B	181/231 (78%)	178 (98%)	3 (2%)	0	100	100
1	C	187/231 (81%)	181 (97%)	5 (3%)	1 (0%)	24	55
1	D	206/231 (89%)	202 (98%)	4 (2%)	0	100	100
1	E	205/231 (89%)	198 (97%)	7 (3%)	0	100	100
1	F	203/231 (88%)	199 (98%)	4 (2%)	0	100	100
2	M	12/15 (80%)	11 (92%)	1 (8%)	0	100	100
2	N	11/15 (73%)	11 (100%)	0	0	100	100
2	O	12/15 (80%)	12 (100%)	0	0	100	100
2	P	11/15 (73%)	11 (100%)	0	0	100	100
2	Q	11/15 (73%)	11 (100%)	0	0	100	100
2	R	12/15 (80%)	11 (92%)	1 (8%)	0	100	100
All	All	1240/1476 (84%)	1208 (97%)	29 (2%)	3 (0%)	43	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	ALA
1	A	157	PRO

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Mol	Chain	Res	Type
1	C	157	PRO

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	159/193 (82%)	159 (100%)	0	100	100
1	B	151/193 (78%)	151 (100%)	0	100	100
1	C	164/193 (85%)	164 (100%)	0	100	100
1	D	170/193 (88%)	170 (100%)	0	100	100
1	E	173/193 (90%)	173 (100%)	0	100	100
1	F	169/193 (88%)	169 (100%)	0	100	100
2	M	11/12 (92%)	11 (100%)	0	100	100
2	N	9/12 (75%)	8 (89%)	1 (11%)	6	22
2	O	11/12 (92%)	11 (100%)	0	100	100
2	P	10/12 (83%)	10 (100%)	0	100	100
2	Q	11/12 (92%)	11 (100%)	0	100	100
2	R	10/12 (83%)	10 (100%)	0	100	100
All	All	1048/1230 (85%)	1047 (100%)	1 (0%)	88	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	325	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	GLN
1	A	179	GLN
1	B	21	ASN

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Mol	Chain	Res	Type
1	C	4	GLN
1	C	121	ASN
1	C	139	ASN
1	C	179	GLN
1	E	193	ASN
1	F	12	HIS
1	F	179	GLN
2	M	319	GLN
2	Q	319	GLN

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](#)

2 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	$\# Z > 2$
3	IHP	A	301	-	36,36,36	1.72	6 (16%)	60,60,60	1.13	6 (10%)
3	IHP	A	302	-	36,36,36	1.66	6 (16%)	60,60,60	1.05	3 (5%)

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
3	IHP	A	301	-	-	11/30/54/54	0/1/1/1
3	IHP	A	302	-	-	11/30/54/54	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	IHP	P4-O14	4.13	1.66	1.59
3	A	302	IHP	P4-O14	4.00	1.66	1.59
3	A	301	IHP	P5-O15	3.87	1.66	1.59
3	A	301	IHP	P2-O12	3.85	1.66	1.59
3	A	302	IHP	P3-O13	3.63	1.65	1.59
3	A	302	IHP	P5-O15	3.62	1.65	1.59
3	A	301	IHP	P1-O11	3.57	1.65	1.59
3	A	301	IHP	P3-O13	3.49	1.65	1.59
3	A	302	IHP	P1-O11	3.46	1.65	1.59
3	A	302	IHP	P6-O16	3.37	1.65	1.59
3	A	301	IHP	P6-O16	3.37	1.65	1.59
3	A	302	IHP	P2-O12	3.37	1.65	1.59

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	IHP	O14-C4-C3	4.28	117.86	108.76
3	A	301	IHP	O14-C4-C3	2.75	114.61	108.76
3	A	301	IHP	P4-O14-C4	2.72	130.69	123.43
3	A	301	IHP	O14-C4-C5	2.64	114.38	108.76
3	A	301	IHP	C5-C6-C1	2.56	116.03	110.43
3	A	302	IHP	O12-C2-C3	2.52	114.13	108.76
3	A	301	IHP	C6-C1-C2	2.40	115.70	110.43
3	A	302	IHP	P4-O14-C4	2.30	129.57	123.43
3	A	301	IHP	O13-C3-C4	2.25	113.54	108.76

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	IHP	C3-C2-O12-P2
3	A	301	IHP	C4-C3-O13-P3

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Mol	Chain	Res	Type	Atoms
3	A	301	IHP	C5-C4-O14-P4
3	A	301	IHP	C4-C5-O15-P5
3	A	301	IHP	C6-C5-O15-P5
3	A	302	IHP	C2-C1-O11-P1
3	A	302	IHP	C6-C1-O11-P1
3	A	302	IHP	C3-C2-O12-P2
3	A	302	IHP	C4-C3-O13-P3
3	A	302	IHP	C3-C4-O14-P4
3	A	301	IHP	C5-C6-O16-P6
3	A	302	IHP	C6-C5-O15-P5
3	A	301	IHP	C1-O11-P1-O21
3	A	301	IHP	C6-O16-P6-O26
3	A	302	IHP	C3-O13-P3-O23
3	A	302	IHP	C1-C6-O16-P6
3	A	302	IHP	C2-C3-O13-P3
3	A	301	IHP	C3-O13-P3-O43
3	A	302	IHP	C4-C5-O15-P5
3	A	301	IHP	C2-C3-O13-P3
3	A	301	IHP	C6-O16-P6-O36
3	A	302	IHP	C5-C6-O16-P6

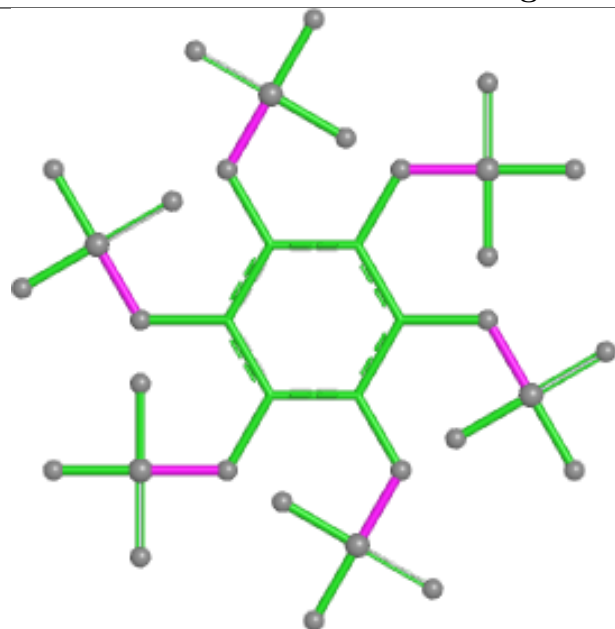
There are no ring outliers.

2 monomers are involved in 2 short contacts:

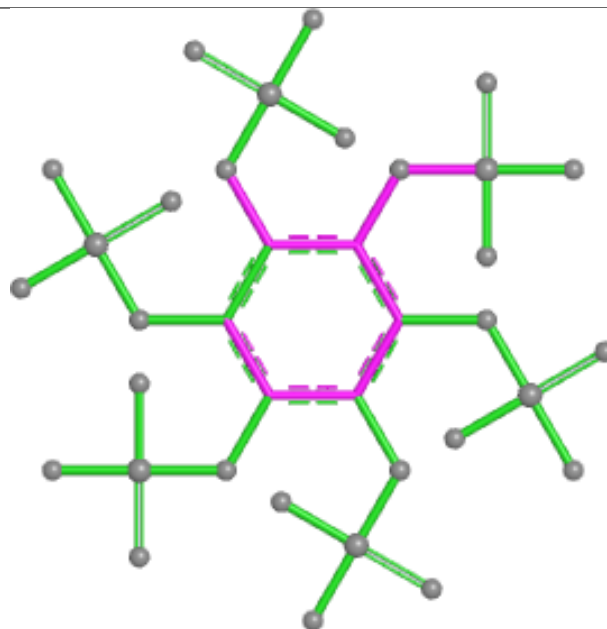
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	IHP	1	0
3	A	302	IHP	1	0

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 than 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.

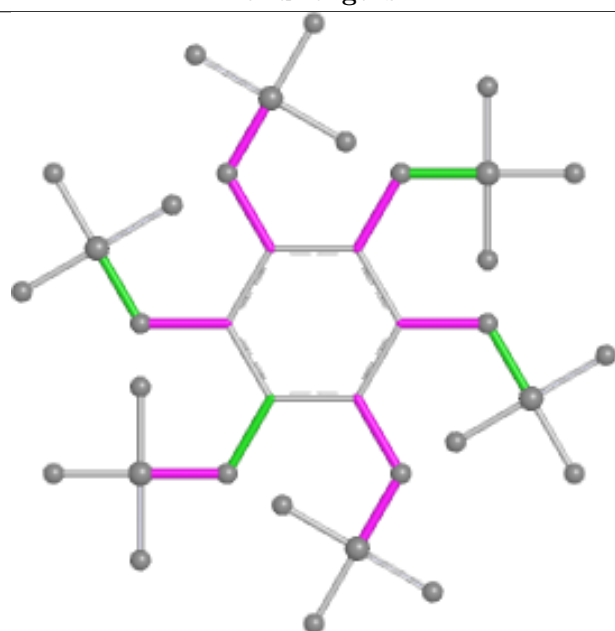
Ligand IHP A 301



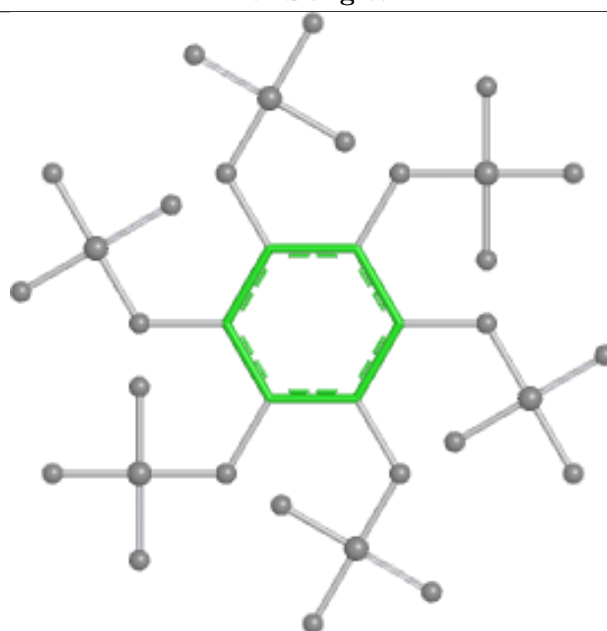
Bond lengths



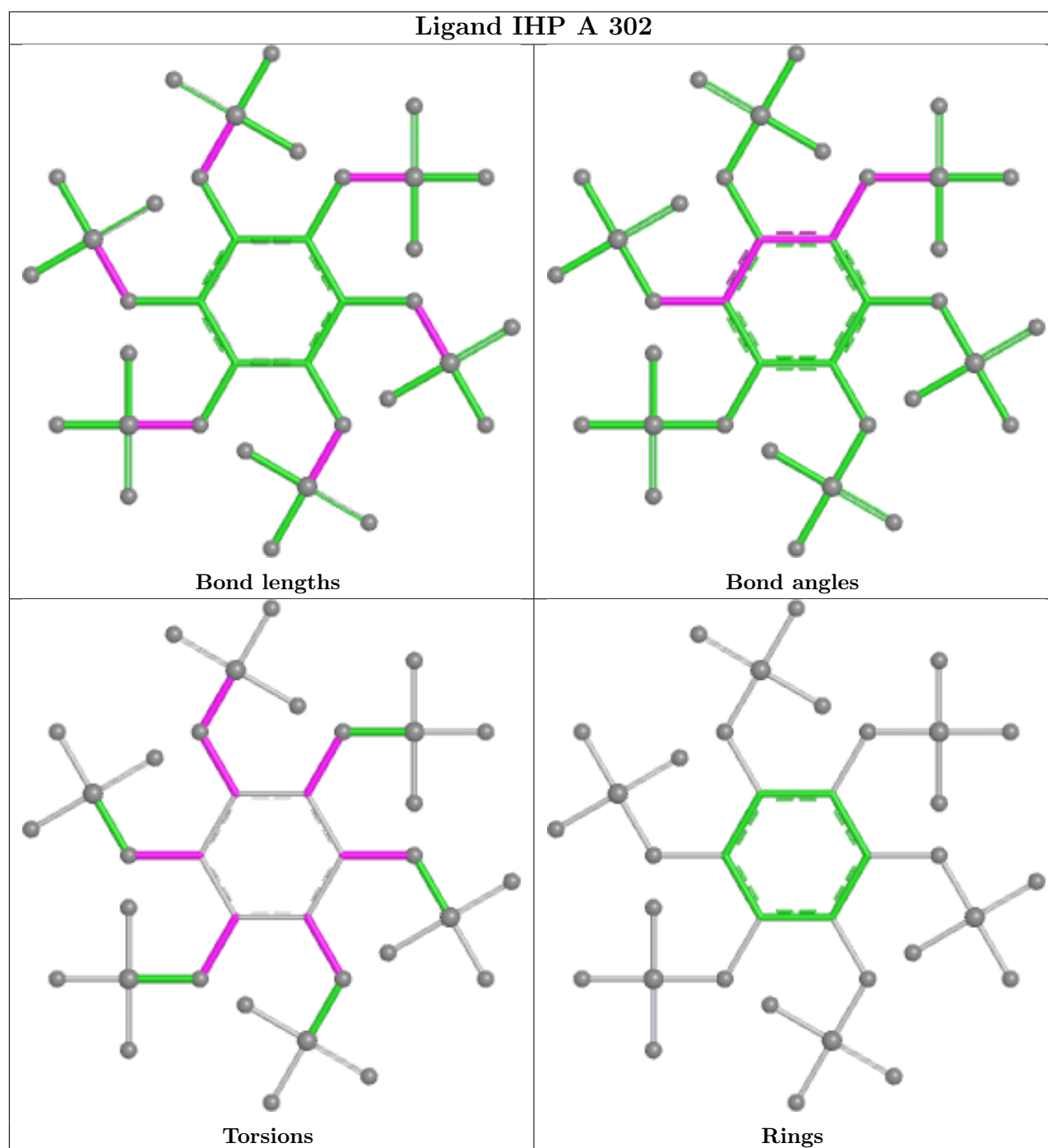
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	198/231 (85%)	0.72	13 (6%)	24 16	30, 67, 90, 100	1 (0%)
1	B	192/231 (83%)	0.74	10 (5%)	33 22	30, 71, 122, 134	1 (0%)
1	C	197/231 (85%)	0.89	18 (9%)	15 11	40, 84, 120, 135	2 (1%)
1	D	209/231 (90%)	0.77	17 (8%)	18 13	33, 86, 128, 139	3 (1%)
1	E	210/231 (90%)	0.92	17 (8%)	18 13	39, 92, 130, 138	1 (0%)
1	F	208/231 (90%)	0.74	13 (6%)	26 17	39, 79, 99, 109	1 (0%)
2	M	14/15 (93%)	0.58	0	100 100	60, 68, 75, 85	0
2	N	13/15 (86%)	1.39	3 (23%)	2 2	67, 74, 91, 99	0
2	O	14/15 (93%)	1.37	3 (21%)	2 2	75, 85, 94, 96	0
2	P	13/15 (86%)	1.23	1 (7%)	19 14	79, 92, 100, 100	0
2	Q	13/15 (86%)	0.89	1 (7%)	19 14	82, 94, 101, 102	0
2	R	14/15 (93%)	1.31	3 (21%)	2 2	80, 99, 106, 117	0
All	All	1295/1476 (87%)	0.82	99 (7%)	20 14	30, 80, 122, 139	9 (0%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	321	PHE	4.9
1	D	21[A]	ASN	4.5
1	A	153	ILE	4.4
1	C	101	GLY	4.4
1	E	14	CYS	4.2
1	A	216	THR	3.8
1	C	133	TRP	3.5
1	E	212	GLU	3.4
1	C	186	THR	3.4
1	E	124	ILE	3.4
1	E	112[A]	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	125	PRO	3.3
2	Q	325	PRO	3.3
1	A	218	CYS	3.2
1	D	197	ASP	3.2
1	E	198	CYS	3.2
1	E	186	THR	3.2
1	D	32	PHE	3.1
1	C	32	PHE	3.0
1	A	4	GLN	3.0
1	B	157	PRO	3.0
1	D	114	GLN	2.9
1	D	138	LEU	2.9
1	C	66	ILE	2.8
1	C	135	ILE	2.7
1	F	79	GLU	2.7
1	C	102	SER	2.7
1	F	133	TRP	2.7
1	A	202	LEU	2.7
1	C	134	ILE	2.7
1	B	14	CYS	2.7
1	F	186	THR	2.6
1	C	166	ASP	2.6
1	C	195	ASN	2.6
2	N	319	GLN	2.6
1	C	43	LEU	2.6
1	F	204	ALA	2.6
1	E	217	ALA	2.6
1	E	93	PRO	2.5
1	A	177	ALA	2.5
1	F	73	ILE	2.5
1	B	106	GLY	2.5
2	R	323	GLN	2.5
1	D	184	ALA	2.5
1	A	61	GLY	2.5
1	A	64	ALA	2.5
1	E	59	VAL	2.5
1	A	58	THR	2.5
1	F	101	GLY	2.5
1	F	29	GLU	2.4
2	N	324	PRO	2.4
1	A	23	TRP	2.4
1	F	108	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	206	GLY	2.4
1	B	213	GLU	2.4
1	D	14	CYS	2.4
1	D	77	ALA	2.3
1	B	25[A]	LYS	2.3
1	D	135	ILE	2.3
1	D	202	LEU	2.3
1	F	219	GLN	2.3
1	D	65	ALA	2.3
1	C	112	GLN	2.3
2	R	314	VAL	2.3
1	C	6	LEU	2.2
1	B	168	PHE	2.2
1	D	112	GLN	2.2
1	D	35	GLU	2.2
1	F	111	LEU	2.2
1	F	112	GLN	2.2
2	N	325	PRO	2.2
2	R	325	PRO	2.2
1	B	32	PHE	2.2
1	E	191	VAL	2.1
1	C	69	LEU	2.1
1	D	185	ALA	2.1
1	A	152	ASP	2.1
1	B	145	TYR	2.1
2	O	326	LEU	2.1
1	C	132[A]	ARG	2.1
2	O	314	VAL	2.1
1	A	206	GLY	2.1
1	D	207	PRO	2.1
1	E	200	THR	2.1
1	E	184	ALA	2.1
1	D	86	VAL	2.1
1	E	150	ILE	2.1
1	E	60	GLY	2.1
1	F	178	SER	2.0
2	P	315	LEU	2.0
1	D	23	TRP	2.0
1	A	47	ALA	2.0
1	F	77	ALA	2.0
1	E	86	VAL	2.0
1	C	65	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	46	GLY	2.0
1	C	98	GLU	2.0
1	B	202	LEU	2.0
1	C	201	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](#)

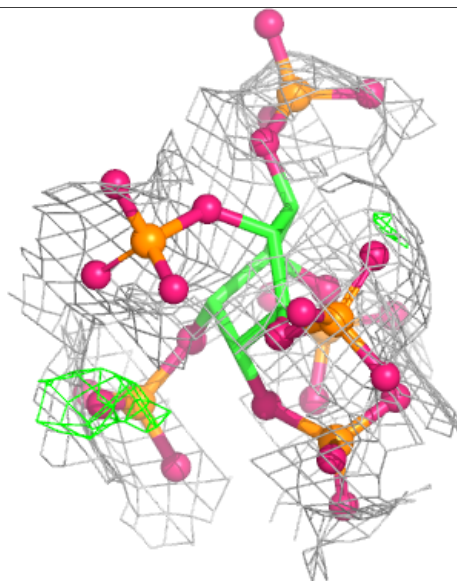
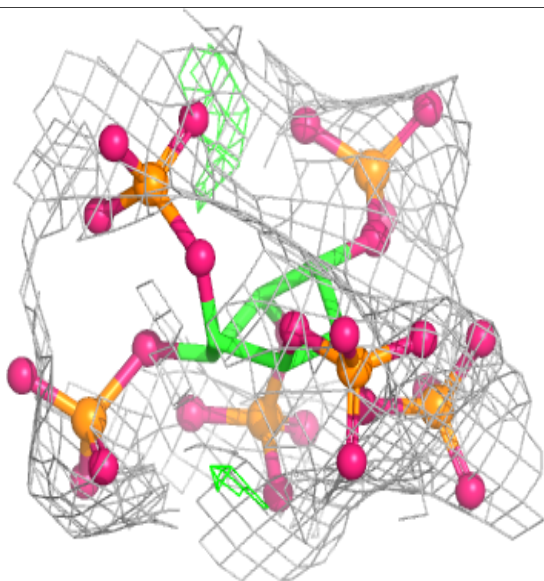
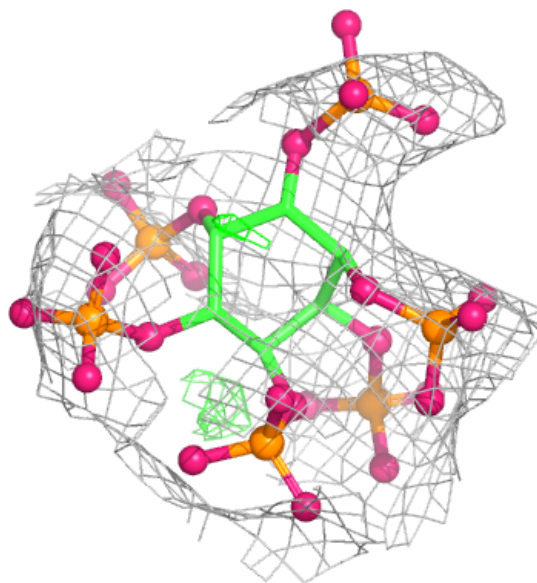
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	IHP	A	302	36/36	0.46	0.13	87,89,92,92	36
3	IHP	A	301	36/36	0.58	0.13	97,100,103,104	36

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.

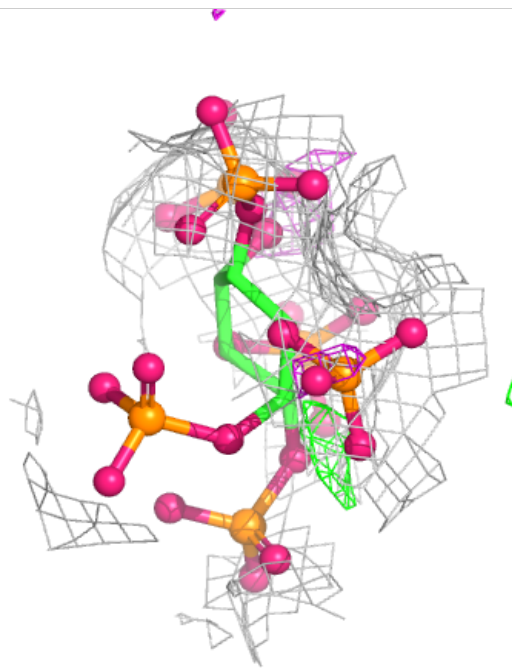
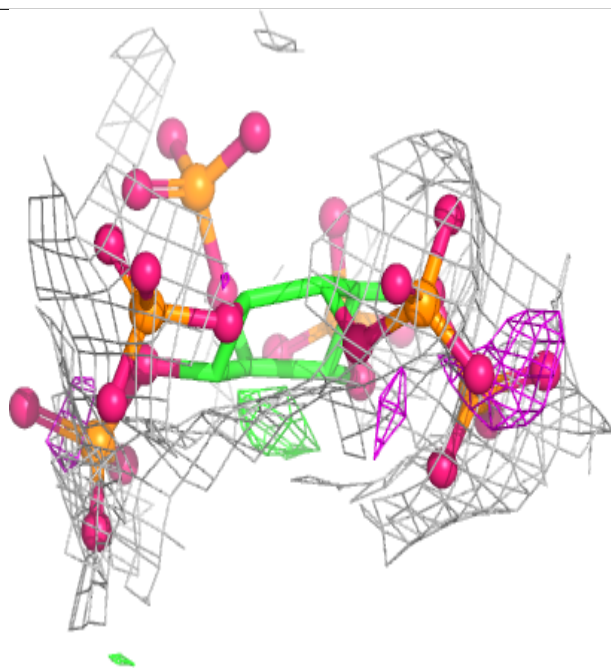
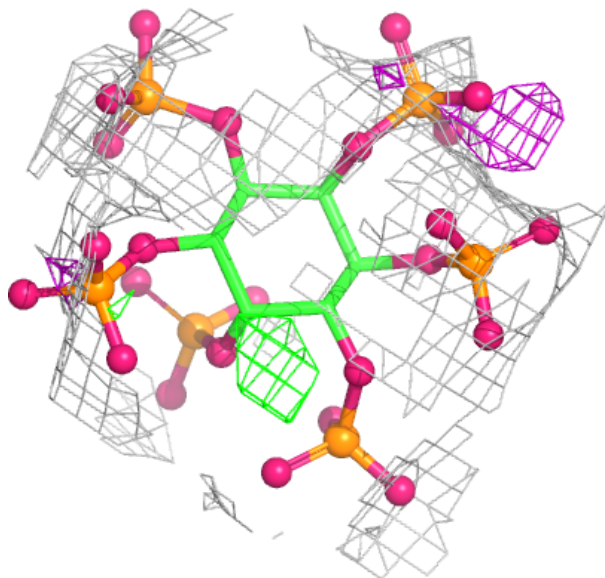
Electron density around IHP A 302:

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 IHP 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.