



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2020 – 01:07 PM EDT

PDB ID : 6C9M
Title : The Human NatA (Naa10/Naa15) amino-terminal acetyltransferase complex
Authors : Gottlieb, L.; Marmorstein, R.
Deposited on : 2018-01-26
Resolution : 2.80 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.14.6
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) : 2.14.6

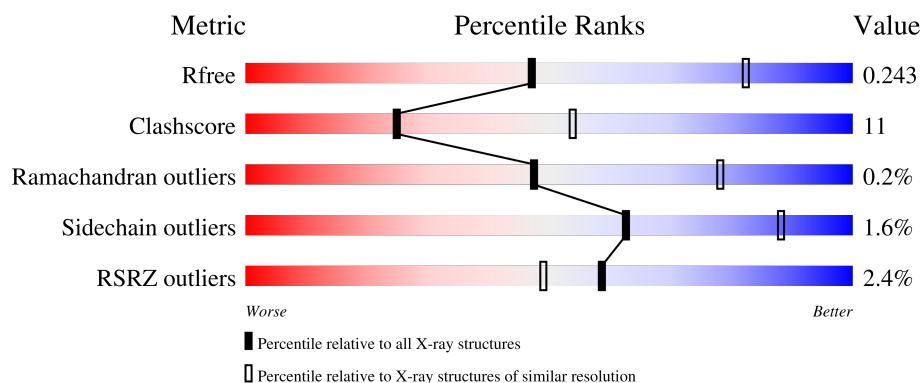
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on 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	866	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>24%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	866	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>20%</div> <div>•</div> <div>11%</div> </div> </div>
2	B	236	<div> <div></div> <div> <div>55%</div> <div>14%</div> <div>32%</div> </div> </div>
2	D	236	<div> <div></div> <div> <div>54%</div> <div>13%</div> <div>•</div> <div>32%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15331 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 N-alpha-acetyltransferase 15, NatA auxiliary subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	771	Total	C	N	O	S	0	0	0
			6279	4019	1075	1146	39			
1	C	773	Total	C	N	O	S	0	0	0
			6359	4071	1086	1162	40			

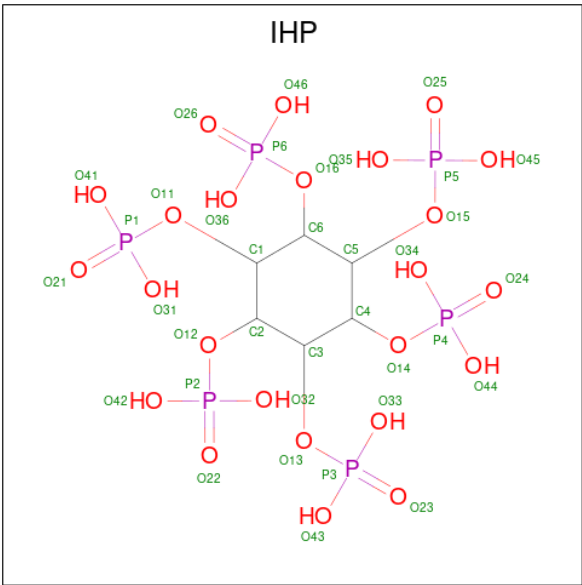
- Molecule 2 is a protein called N-alpha-acetyltransferase 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	161	Total	C	N	O	S	0	0	0
			1309	821	235	242	11			
2	D	161	Total	C	N	O	S	0	0	0
			1287	811	229	236	11			

There are 2 discrepancies between the modelled and reference sequences:

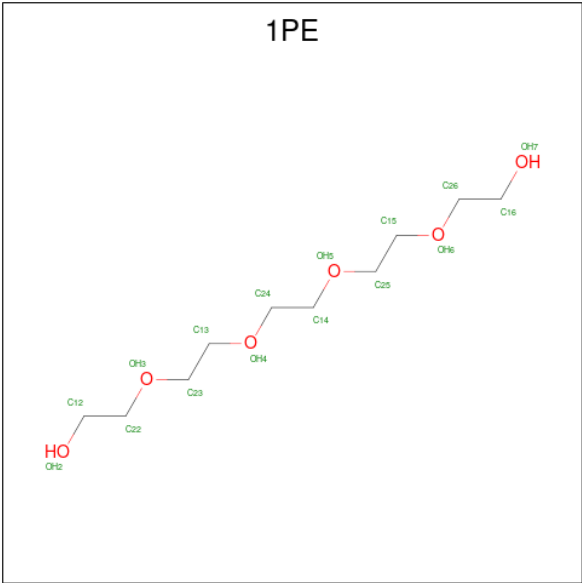
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ACE	-	acetylation	UNP P41227
D	0	ACE	-	acetylation	UNP P41227

- Molecule 3 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: C₆H₁₈O₂₄P₆).



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

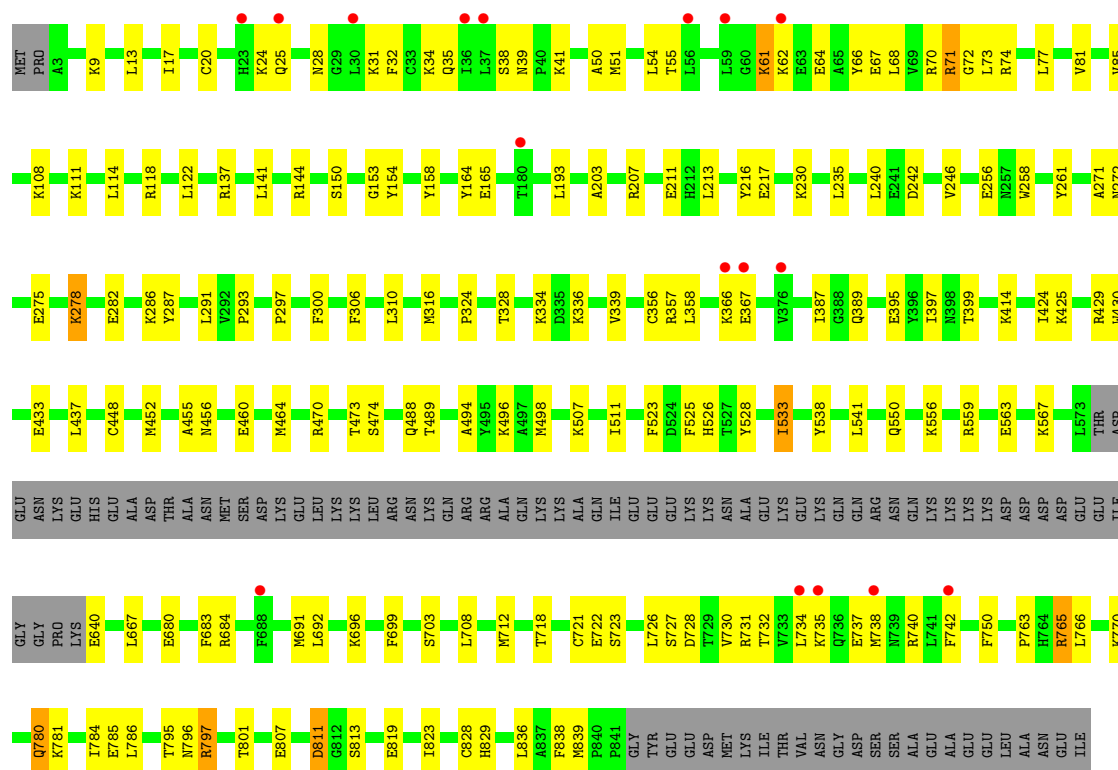
- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			16	10	6		

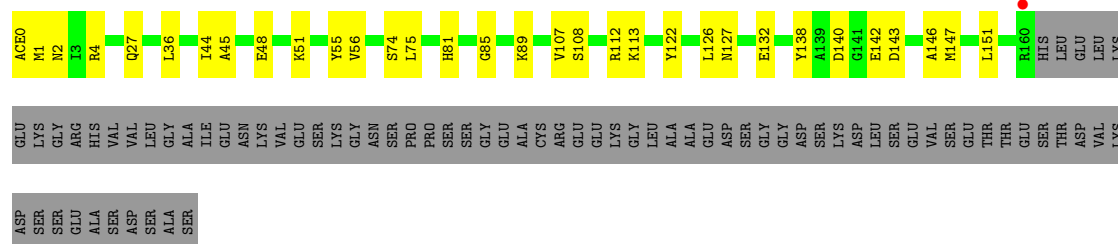
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total 4	O 4	0	0
5	B	1	Total 1	O 1	0	0
5	C	4	Total 4	O 4	0	0



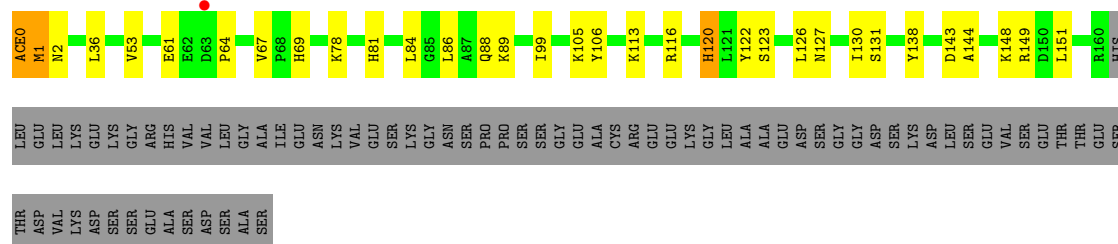
• Molecule 2: N-alpha-acetyltransferase 10

Chain B: 55% 14% 32%



• Molecule 2: N-alpha-acetyltransferase 10

Chain D: 54% 13% 32%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.11Å 171.83Å 178.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.95 – 2.80 48.95 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.95-2.80) 100.0 (48.95-2.80)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.11.1-2575)	Depositor
R, R_{free}	0.187 , 0.242 0.189 , 0.243	Depositor DCC
R_{free} test set	3640 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	82.4	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 69.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15331	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IHP, ACE, 1PE

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	0.46	0/6412	0.58	0/8648
1	C	0.49	0/6494	0.61	0/8753
2	B	0.52	0/1335	0.65	1/1800 (0.1%)
2	D	0.52	1/1313 (0.1%)	0.66	1/1773 (0.1%)
All	All	0.48	1/15554 (0.0%)	0.61	2/20974 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	0	ACE	C-N	5.63	1.47	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	MET	CG-SD-CE	6.34	110.34	100.20
2	B	1	MET	CG-SD-CE	5.50	109.00	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	1	MET	Mainchain

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	6279	0	6249	154	0
1	C	6359	0	6390	136	0
2	B	1309	0	1277	23	0
2	D	1287	0	1247	30	0
3	A	36	0	2	2	0
3	C	36	0	4	0	0
4	C	16	0	22	0	0
5	A	4	0	0	1	0
5	B	1	0	0	0	0
5	C	4	0	0	0	0
All	All	15331	0	15191	328	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 11.

All (328) 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)
2:D:127:ASN:HB3	2:D:149:ARG:NH1	1.46	1.30
1:A:345:LEU:HG	1:A:349:TYR:HE2	1.20	1.03
1:C:734:LEU:O	1:C:738:MET:HG2	1.59	1.01
1:A:770:LYS:HD3	1:A:813:SER:HB2	1.44	1.00
2:D:127:ASN:CB	2:D:149:ARG:NH1	2.29	0.95
2:D:127:ASN:HB3	2:D:149:ARG:HH11	0.99	0.94
1:A:349:TYR:CD1	1:A:359:PHE:HD1	1.86	0.93
1:A:345:LEU:HG	1:A:349:TYR:CE2	2.04	0.91
1:C:734:LEU:HD12	1:C:735:LYS:N	1.93	0.84
2:D:113:LYS:HD2	2:D:143:ASP:HB2	1.60	0.82
2:B:113:LYS:HD2	2:B:143:ASP:HB2	1.63	0.80
1:C:25:GLN:NE2	1:C:28:ASN:HB3	1.99	0.78
1:C:25:GLN:HE22	1:C:28:ASN:HB3	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ASN:HD22	1:A:212:HIS:HD2	1.30	0.77
1:A:754:PHE:HE1	1:A:758:ASN:HD22	1.33	0.76
1:A:114:LEU:HD11	1:A:144:ARG:NH1	2.02	0.75
1:C:357:ARG:HB2	1:C:367:GLU:HB3	1.67	0.75
1:A:331:SER:HB3	2:B:48:GLU:OE2	1.87	0.75
1:A:197:ASN:HD22	1:A:212:HIS:CD2	2.05	0.74
1:A:345:LEU:O	1:A:349:TYR:CD2	2.40	0.74
1:C:692:LEU:HG	1:C:696:LYS:HE3	1.70	0.74
1:A:469:THR:HG21	1:A:475:ALA:HA	1.69	0.73
1:C:738:MET:HA	1:C:742:PHE:HD1	1.54	0.73
1:A:394:LEU:HD13	1:A:417:ILE:HG21	1.69	0.73
1:A:349:TYR:HD1	1:A:359:PHE:HD1	1.34	0.73
1:C:488:GLN:HB2	1:C:511:ILE:HD11	1.72	0.72
1:A:10:GLU:N	1:A:10:GLU:OE1	2.22	0.71
1:A:311:ASP:O	1:A:315:ARG:HG3	1.91	0.71
1:C:738:MET:HA	1:C:742:PHE:CD1	2.26	0.71
1:A:346:VAL:HA	1:A:349:TYR:HD2	1.55	0.70
1:C:696:LYS:HE2	1:C:737:GLU:OE1	1.92	0.70
1:A:761:SER:HA	1:A:795:THR:HG22	1.73	0.70
1:C:50:ALA:HB1	1:C:85:VAL:HG11	1.74	0.69
1:A:789:THR:O	1:A:790:LEU:HD12	1.93	0.69
1:A:395:GLU:O	1:A:399:THR:HG23	1.94	0.68
1:A:671:LYS:O	1:A:674:THR:HG22	1.93	0.67
3:A:901:IHP:O42	2:B:51:LYS:NZ	2.28	0.67
1:C:193:LEU:HD13	1:C:216:TYR:HB3	1.77	0.67
1:C:425:LYS:HE3	1:C:429:ARG:HH22	1.60	0.65
1:C:699:PHE:CE1	1:C:703:SER:HB2	2.32	0.65
1:A:349:TYR:CD1	1:A:359:PHE:CD1	2.77	0.65
1:C:640:GLU:N	1:C:640:GLU:OE2	2.30	0.65
1:C:25:GLN:OE1	1:C:28:ASN:HB3	1.95	0.65
1:C:395:GLU:O	1:C:399:THR:HG23	1.97	0.64
1:A:4:VAL:HG22	1:A:6:LEU:HD13	1.79	0.64
2:D:67:VAL:HG21	2:D:105:LYS:HG3	1.78	0.63
1:A:1:MET:O	1:A:4:VAL:HG12	1.98	0.63
1:C:25:GLN:CD	1:C:28:ASN:HB3	2.19	0.63
1:C:291:LEU:HD23	2:D:0:ACE:H2	1.81	0.63
1:C:489:THR:HB	1:C:556:LYS:HG2	1.80	0.62
1:A:148:ARG:NE	5:A:1001:HOH:O	2.31	0.62
1:C:742:PHE:HA	1:C:750:PHE:CE1	2.35	0.61
1:C:722:GLU:O	1:C:723:SER:C	2.35	0.61
1:A:331:SER:CB	2:B:48:GLU:OE2	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:ALA:N	1:C:275:GLU:OE2	2.32	0.61
1:C:217:GLU:OE2	1:C:230:LYS:NZ	2.24	0.60
1:C:718:THR:O	1:C:721:CYS:O	2.20	0.60
1:A:343:GLU:O	1:A:347:VAL:HG23	2.01	0.60
1:A:819:GLU:HG2	1:A:820:ALA:H	1.66	0.60
2:B:85:GLY:O	2:B:89:LYS:HG3	2.02	0.59
1:A:164:TYR:HB3	1:A:203:ALA:HB2	1.84	0.59
1:C:819:GLU:O	1:C:823:ILE:HG13	2.01	0.59
1:A:424:ILE:HD11	1:A:454:LYS:HB2	1.85	0.59
1:A:52:LYS:HG2	1:A:68:LEU:HD13	1.84	0.58
1:C:141:LEU:HA	1:C:150:SER:HB3	1.84	0.58
1:C:780:GLN:O	1:C:784:ILE:HG12	2.03	0.58
1:C:81:VAL:O	1:C:85:VAL:HG12	2.03	0.58
2:D:122:TYR:HD1	2:D:126:LEU:HD12	1.69	0.58
1:C:735:LYS:HA	1:C:738:MET:CG	2.34	0.58
1:A:529:CYS:SG	2:B:36:LEU:HD23	2.44	0.57
1:A:806:LEU:HD21	1:A:810:TYR:CE1	2.39	0.57
1:A:512:GLU:OE1	1:A:549:ARG:NH1	2.37	0.57
1:C:836:LEU:HA	1:C:839:MET:HG3	1.86	0.57
1:C:32:PHE:HA	1:C:35:GLN:HG3	1.85	0.57
1:C:66:TYR:O	1:C:70:ARG:HB2	2.05	0.57
1:C:807:GLU:O	1:C:811:ASP:HB2	2.06	0.56
2:D:130:ILE:H	2:D:130:ILE:HD12	1.70	0.56
1:A:789:THR:C	1:A:790:LEU:HD12	2.25	0.56
2:B:122:TYR:HD1	2:B:126:LEU:HD12	1.70	0.56
1:A:825:ARG:NH1	1:A:839:MET:O	2.37	0.56
1:C:727:SER:OG	1:C:730:VAL:HG12	2.05	0.56
1:A:770:LYS:NZ	1:A:774:TYR:HB2	2.21	0.56
1:C:286:LYS:HG2	1:C:287:TYR:CZ	2.39	0.56
1:A:297:PRO:HA	1:A:300:PHE:CE2	2.41	0.56
1:C:460:GLU:N	1:C:460:GLU:OE2	2.36	0.56
1:C:563:GLU:O	1:C:567:LYS:HG2	2.06	0.55
1:C:765:ARG:NH1	1:C:786:LEU:O	2.37	0.55
1:A:762:LEU:HD12	1:A:794:LEU:HD13	1.89	0.55
1:A:188:GLU:HB3	1:A:533:ILE:HD13	1.88	0.55
1:A:753:THR:O	1:A:757:ARG:HG3	2.06	0.55
1:A:407:LEU:HD23	1:A:410:LEU:HD11	1.88	0.55
1:A:806:LEU:HD21	1:A:810:TYR:HE1	1.71	0.55
1:C:61:LYS:N	1:C:64:GLU:OE1	2.40	0.55
1:A:828:CYS:HB3	1:A:838:PHE:CD2	2.41	0.55
1:C:496:LYS:HE3	1:C:563:GLU:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:ARG:HD2	1:C:153:GLY:HA3	1.87	0.54
2:D:84:LEU:HB2	2:D:86:LEU:HD13	1.89	0.54
1:A:768:ALA:O	1:A:772:VAL:HG13	2.07	0.54
1:C:13:LEU:O	1:C:17:ILE:HG13	2.08	0.54
2:D:127:ASN:HB3	2:D:149:ARG:HH12	1.60	0.54
1:A:685:LYS:O	1:A:686:GLU:HG3	2.08	0.54
1:A:760:ASP:N	1:A:760:ASP:OD1	2.39	0.54
1:A:784:ILE:O	1:A:788:THR:HG23	2.07	0.53
1:C:683:PHE:HA	1:C:691:MET:SD	2.48	0.53
1:C:51:MET:O	1:C:55:THR:HG22	2.08	0.53
1:A:286:LYS:HD2	1:A:286:LYS:O	2.07	0.53
1:A:196:GLN:OE1	1:A:212:HIS:HE1	1.91	0.53
1:A:6:LEU:HD11	1:A:45:HIS:NE2	2.23	0.53
2:D:99:ILE:HD11	2:D:151:LEU:HB3	1.89	0.53
2:D:67:VAL:CG2	2:D:105:LYS:HG3	2.38	0.53
2:B:108:SER:HA	2:B:147:MET:O	2.08	0.53
1:C:67:GLU:OE2	1:C:70:ARG:HB3	2.08	0.53
1:A:668:VAL:O	1:A:674:THR:HG21	2.09	0.53
1:C:692:LEU:CG	1:C:696:LYS:HE3	2.38	0.53
1:A:754:PHE:HE1	1:A:758:ASN:ND2	2.06	0.52
1:C:54:LEU:HD22	1:C:85:VAL:HG23	1.91	0.52
1:C:324:PRO:HG3	2:D:81:HIS:HA	1.90	0.52
1:A:356:CYS:O	1:A:358:LEU:N	2.38	0.52
2:D:53:VAL:HA	2:D:78:LYS:HG3	1.92	0.52
1:A:345:LEU:CG	1:A:349:TYR:CE2	2.87	0.52
1:C:25:GLN:HE22	1:C:28:ASN:CB	2.19	0.52
1:C:781:LYS:NZ	1:C:785:GLU:OE2	2.42	0.52
1:A:310:LEU:HD21	1:A:342:ILE:HG12	1.92	0.52
1:C:525:PHE:HA	1:C:528:TYR:HB3	1.91	0.52
1:A:114:LEU:HD11	1:A:144:ARG:HH11	1.73	0.51
2:D:61:GLU:HA	2:D:61:GLU:OE2	2.10	0.51
1:A:234:LEU:HD22	1:A:239:ARG:HB2	1.91	0.51
1:A:357:ARG:HD2	1:A:357:ARG:H	1.75	0.51
1:A:337:GLU:O	1:A:341:ILE:HD12	2.11	0.51
1:A:788:THR:O	1:A:790:LEU:HD13	2.10	0.51
1:A:218:LYS:HA	1:A:218:LYS:HE2	1.93	0.50
1:A:410:LEU:HD12	1:A:410:LEU:H	1.75	0.50
1:A:788:THR:O	1:A:790:LEU:CD1	2.59	0.50
1:C:207:ARG:NH2	1:C:211:GLU:OE2	2.44	0.50
1:A:519:THR:HA	1:A:545:GLU:OE1	2.11	0.50
1:A:134:ARG:HD3	1:A:158:TYR:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ALA:HB2	1:A:80:HIS:CE1	2.47	0.50
1:C:550:GLN:HG3	1:C:667:LEU:HB3	1.93	0.50
1:C:356:CYS:HB2	1:C:358:LEU:HD23	1.93	0.50
1:A:207:ARG:O	1:A:211:GLU:HG3	2.12	0.49
1:C:452:MET:HE1	1:C:464:MET:HE3	1.93	0.49
1:C:763:PRO:HG3	1:C:801:THR:HG21	1.94	0.49
1:A:389:GLN:OE1	1:A:392:ILE:HG13	2.13	0.49
1:C:526:HIS:ND1	1:C:538:TYR:OH	2.37	0.49
1:A:513:ARG:CZ	1:A:642:LEU:HD11	2.42	0.49
1:A:789:THR:HG22	1:A:791:ASP:OD1	2.12	0.49
1:C:766:LEU:HG	1:C:770:LYS:HE3	1.93	0.49
1:A:261:TYR:OH	1:A:293:PRO:HG3	2.11	0.49
1:A:714:ARG:O	1:A:718:THR:HG23	2.12	0.49
2:D:64:PRO:HG3	2:D:69:HIS:HE1	1.77	0.49
1:A:487:PHE:O	1:A:491:CYS:HB2	2.13	0.49
1:A:513:ARG:NE	1:A:642:LEU:HD11	2.27	0.49
1:C:291:LEU:HD12	1:C:316:MET:CE	2.43	0.49
1:A:665:LYS:O	1:A:669:LYS:HE3	2.12	0.49
1:A:829:HIS:HB2	1:A:838:PHE:O	2.12	0.48
1:A:525:PHE:HA	1:A:528:TYR:HB3	1.96	0.48
1:C:433:GLU:O	1:C:437:LEU:HD13	2.13	0.48
1:C:680:GLU:O	1:C:684:ARG:NH1	2.45	0.48
1:A:120:LEU:O	1:A:124:GLN:HG3	2.14	0.48
1:A:194:LEU:HD21	1:A:220:ILE:HG21	1.95	0.48
1:A:286:LYS:HG3	1:A:287:TYR:CZ	2.47	0.48
1:A:339:VAL:HG11	1:A:387:ILE:HD11	1.96	0.48
1:C:559:ARG:O	1:C:563:GLU:HG2	2.13	0.48
1:C:68:LEU:O	1:C:72:GLY:N	2.32	0.48
1:A:754:PHE:CE1	1:A:758:ASN:ND2	2.81	0.48
1:A:324:PRO:HG3	2:B:81:HIS:HA	1.96	0.48
1:C:297:PRO:HA	1:C:300:PHE:CE2	2.48	0.48
1:C:735:LYS:HA	1:C:738:MET:HG2	1.94	0.48
1:A:691:MET:O	1:A:695:VAL:HG23	2.14	0.48
1:C:114:LEU:O	1:C:118:ARG:HG2	2.14	0.48
1:C:691:MET:HB2	1:C:691:MET:HE2	1.73	0.48
1:A:681:ILE:O	1:A:685:LYS:HB2	2.14	0.48
1:C:71:ARG:HA	1:C:74:ARG:HB2	1.95	0.48
1:C:9:LYS:O	1:C:13:LEU:HD13	2.14	0.48
1:A:791:ASP:N	1:A:791:ASP:OD1	2.47	0.47
1:A:780:GLN:O	1:A:784:ILE:HD13	2.14	0.47
1:A:70:ARG:NH1	1:A:86:TYR:OH	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:TYR:O	1:A:137:ARG:HG2	2.14	0.47
1:A:762:LEU:O	1:A:765:ARG:N	2.47	0.47
1:A:86:TYR:O	1:A:90:GLN:HG3	2.14	0.47
2:B:56:VAL:HG23	2:B:75:LEU:HD12	1.96	0.47
1:C:261:TYR:OH	1:C:293:PRO:HG3	2.14	0.47
1:C:726:LEU:HD23	1:C:734:LEU:CD2	2.45	0.47
1:A:125:ILE:O	1:A:128:ARG:HD3	2.15	0.47
2:B:107:VAL:HG22	2:B:151:LEU:HD11	1.96	0.47
1:C:324:PRO:HG2	2:D:84:LEU:HD11	1.95	0.47
1:C:54:LEU:HB2	1:C:85:VAL:HG23	1.95	0.47
2:D:106:TYR:CZ	2:D:148:LYS:HE3	2.49	0.47
1:A:562:ILE:HG23	1:A:681:ILE:HD11	1.96	0.47
1:C:523:PHE:HA	1:C:526:HIS:CD2	2.50	0.47
1:C:73:LEU:O	1:C:77:LEU:HD23	2.14	0.47
1:A:277:LEU:HD13	1:A:281:GLU:HG3	1.97	0.47
1:A:550:GLN:HG3	1:A:667:LEU:HB3	1.97	0.47
1:C:242:ASP:O	1:C:246:VAL:HG23	2.15	0.47
1:A:331:SER:HB3	2:B:48:GLU:CD	2.35	0.47
1:C:738:MET:CA	1:C:742:PHE:HD1	2.25	0.46
1:A:710:GLU:O	1:A:714:ARG:HD3	2.14	0.46
1:C:336:LYS:HD3	1:C:339:VAL:CG2	2.45	0.46
1:C:71:ARG:HA	1:C:74:ARG:CB	2.46	0.46
1:C:34:LYS:O	1:C:38:SER:HB3	2.16	0.46
1:C:728:ASP:O	1:C:732:THR:HG23	2.16	0.46
1:C:39:ASN:ND2	1:C:41:LYS:HB2	2.30	0.46
1:A:217:GLU:OE2	1:A:230:LYS:NZ	2.49	0.46
1:A:76:ASP:OD2	1:A:79:SER:HB2	2.15	0.46
1:C:708:LEU:O	1:C:712:MET:HG3	2.15	0.46
2:D:127:ASN:CB	2:D:149:ARG:HH12	2.21	0.46
1:C:387:ILE:HG22	1:C:389:GLN:HG3	1.98	0.46
1:A:345:LEU:O	1:A:349:TYR:HD2	1.95	0.45
1:C:737:GLU:O	1:C:740:ARG:N	2.49	0.45
1:A:409:GLU:HA	1:A:412:LEU:HD12	1.98	0.45
2:B:2:ASN:O	2:B:45:ALA:HA	2.16	0.45
1:C:62:LYS:HB3	1:C:66:TYR:CD1	2.51	0.45
1:A:343:GLU:O	1:A:347:VAL:CG2	2.64	0.45
1:A:453:LEU:HD23	1:A:453:LEU:HA	1.86	0.45
1:A:380:LEU:HA	1:A:383:HIS:HB3	1.97	0.45
1:A:646:LYS:O	1:A:649:LYS:HG2	2.16	0.45
1:C:291:LEU:HD12	1:C:316:MET:HE1	1.99	0.45
1:C:473:THR:HG23	1:C:474:SER:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:494:ALA:O	1:C:498:MET:HG3	2.17	0.45
1:C:533:ILE:O	1:C:533:ILE:HG22	2.17	0.45
2:D:116:ARG:O	2:D:120:HIS:HB2	2.17	0.45
1:A:122:LEU:HD12	1:A:527:THR:HG23	1.99	0.45
1:C:20:CYS:CB	1:C:25:GLN:HE21	2.29	0.45
1:A:346:VAL:HA	1:A:349:TYR:CD2	2.44	0.45
1:A:318:PHE:CE2	1:A:376:VAL:HG12	2.52	0.45
1:A:507:LYS:HD3	1:A:510:GLU:OE1	2.17	0.45
1:C:414:LYS:HE2	1:C:430:TRP:CE2	2.51	0.45
1:A:511:ILE:HD13	1:A:557:ALA:HB2	1.99	0.45
2:B:132:GLU:HG3	2:B:146:ALA:HB3	1.99	0.45
1:C:291:LEU:HD23	2:D:0:ACE:CH3	2.47	0.45
2:D:61:GLU:HG3	2:D:64:PRO:HD3	1.99	0.45
2:B:132:GLU:OE2	1:C:108:LYS:HD2	2.17	0.45
2:D:138:TYR:CE1	2:D:144:ALA:HB2	2.52	0.45
1:A:388:GLY:O	1:A:390:PRO:HD3	2.17	0.45
1:A:397:ILE:HG12	1:A:414:LYS:HB2	1.98	0.45
1:A:761:SER:O	1:A:765:ARG:HB2	2.17	0.45
1:C:306:PHE:CE2	1:C:310:LEU:HD22	2.52	0.45
1:C:31:LYS:O	1:C:35:GLN:HG3	2.17	0.45
1:A:30:LEU:HD21	1:A:56:LEU:CD1	2.47	0.44
1:C:507:LYS:O	1:C:511:ILE:HG12	2.16	0.44
2:D:88:GLN:CD	2:D:88:GLN:H	2.20	0.44
1:A:374:LEU:HD21	1:A:407:LEU:CD2	2.47	0.44
1:C:24:LYS:HD3	1:C:24:LYS:HA	1.84	0.44
2:B:4:ARG:CZ	2:B:44:ILE:HD11	2.48	0.44
1:C:74:ARG:HG3	1:C:74:ARG:HH21	1.83	0.44
1:A:130:LEU:HD23	1:A:160:LEU:HB3	2.00	0.44
1:C:734:LEU:HD12	1:C:734:LEU:C	2.38	0.44
1:A:813:SER:O	1:A:814:LEU:HD23	2.17	0.44
2:B:127:ASN:ND2	2:B:127:ASN:O	2.49	0.44
1:C:256:GLU:HG3	2:D:89:LYS:HD3	1.98	0.44
1:A:213:LEU:O	1:A:217:GLU:HB2	2.18	0.43
1:C:324:PRO:O	1:C:328:THR:HG23	2.18	0.43
2:D:127:ASN:OD1	2:D:149:ARG:NH1	2.51	0.43
1:C:71:ARG:O	1:C:74:ARG:HB3	2.17	0.43
1:C:154:TYR:CZ	1:C:158:TYR:HE2	2.37	0.43
1:C:448:CYS:O	1:C:452:MET:HE2	2.18	0.43
1:A:4:VAL:HG23	1:A:45:HIS:CE1	2.54	0.43
1:A:452:MET:HB2	1:A:452:MET:HE3	1.77	0.43
1:A:470:ARG:HG2	1:A:472:GLY:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:CYS:O	1:A:488:GLN:HG3	2.18	0.43
1:A:683:PHE:HA	1:A:691:MET:SD	2.59	0.43
1:C:811:ASP:HB3	1:C:813:SER:H	1.83	0.43
1:A:349:TYR:CE1	1:A:359:PHE:CD1	3.07	0.43
1:A:650:VAL:HG11	1:A:656:GLU:HG3	1.99	0.43
1:A:708:LEU:O	1:A:712:MET:HG3	2.19	0.43
1:A:705:HIS:HB3	1:A:708:LEU:HB3	2.00	0.43
1:A:256:GLU:OE1	1:A:290:GLY:HA2	2.19	0.42
1:C:425:LYS:HE3	1:C:429:ARG:NH2	2.30	0.42
1:C:74:ARG:CZ	1:C:74:ARG:HB2	2.48	0.42
2:B:56:VAL:CG2	2:B:75:LEU:HD12	2.49	0.42
1:C:541:LEU:HD22	2:D:36:LEU:HD11	2.02	0.42
1:C:456:ASN:HB3	1:C:498:MET:SD	2.59	0.42
1:A:159:HIS:CD2	1:A:199:VAL:HG12	2.54	0.42
1:A:424:ILE:CD1	1:A:454:LYS:HB2	2.48	0.42
2:B:112:ARG:HG2	2:B:138:TYR:CE2	2.55	0.42
1:C:144:ARG:HA	1:C:144:ARG:HD3	1.72	0.42
1:A:811:ASP:HB3	1:A:813:SER:H	1.84	0.42
1:C:488:GLN:HB3	1:C:507:LYS:HD2	2.02	0.42
2:D:138:TYR:HE1	2:D:144:ALA:HB2	1.85	0.42
1:A:493:GLN:HG3	1:A:560:ILE:HD11	2.02	0.42
1:A:41:LYS:HD2	1:A:42:PHE:CZ	2.55	0.42
1:A:4:VAL:HG23	1:A:45:HIS:HE1	1.84	0.42
1:C:137:ARG:HD3	1:C:137:ARG:HA	1.83	0.42
1:A:387:ILE:HA	1:A:387:ILE:HD13	1.81	0.41
2:B:112:ARG:HH12	2:B:140:ASP:HB2	1.85	0.41
1:A:111:LYS:HB3	1:A:111:LYS:HE2	1.87	0.41
1:A:96:TYR:CD1	1:A:123:LEU:HD22	2.54	0.41
1:C:258:TRP:CE2	2:D:2:ASN:HB2	2.55	0.41
1:A:16:ARG:HH21	1:A:19:ARG:NH2	2.17	0.41
1:A:450:LYS:NZ	3:A:901:IHP:H3	2.35	0.41
1:C:25:GLN:O	1:C:25:GLN:CD	2.59	0.41
1:C:20:CYS:HB3	1:C:25:GLN:HE21	1.84	0.41
1:C:424:ILE:HG23	1:C:455:ALA:HB2	2.02	0.41
1:C:9:LYS:HA	1:C:9:LYS:HD3	1.67	0.41
1:A:305:LYS:HA	1:A:305:LYS:HD3	1.83	0.41
1:C:118:ARG:O	1:C:122:LEU:HG	2.19	0.41
1:C:795:THR:O	1:C:796:ASN:HB2	2.19	0.41
1:C:797:ARG:HD2	1:C:797:ARG:O	2.20	0.41
1:A:306:PHE:CZ	1:A:338:LYS:HG2	2.55	0.41
1:A:825:ARG:HG3	1:A:838:PHE:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:HD22	1:A:85:VAL:HG13	2.01	0.41
1:A:326:PHE:HZ	1:A:386:LYS:HD2	1.86	0.41
2:B:112:ARG:HB3	2:B:142:GLU:CD	2.41	0.41
1:C:235:LEU:HD23	1:C:240:LEU:HD22	2.03	0.41
1:A:646:LYS:HA	1:A:649:LYS:HD2	2.02	0.41
1:A:291:LEU:HD12	2:B:0:ACE:CH3	2.51	0.41
1:C:278:LYS:O	1:C:282:GLU:HG3	2.21	0.41
1:C:334:LYS:HE2	1:C:334:LYS:HB2	1.71	0.41
1:C:712:MET:HB3	1:C:742:PHE:CE2	2.55	0.41
2:D:131:SER:HB2	2:D:148:LYS:HD2	2.03	0.41
1:A:754:PHE:HE1	1:A:764:HIS:HD2	1.68	0.41
1:C:164:TYR:HB3	1:C:203:ALA:HB2	2.03	0.41
1:A:25:GLN:OE1	1:C:165:GLU:HG3	2.20	0.41
1:C:448:CYS:SG	1:C:464:MET:HE3	2.61	0.41
1:A:387:ILE:HG22	1:A:389:GLN:HG3	2.03	0.41
1:C:272:ASN:OD1	1:C:275:GLU:HG3	2.20	0.41
1:A:334:LYS:HA	1:A:334:LYS:HD3	1.76	0.41
1:C:397:ILE:HA	1:C:397:ILE:HD12	1.88	0.41
1:C:829:HIS:HB2	1:C:838:PHE:O	2.21	0.41
1:A:20:CYS:HB3	1:A:25:GLN:O	2.21	0.40
1:C:213:LEU:O	1:C:217:GLU:HB2	2.22	0.40
1:A:105:ASN:O	1:A:108:LYS:HB2	2.22	0.40
1:A:466:SER:HA	1:A:469:THR:HB	2.03	0.40
1:C:28:ASN:OD1	1:C:28:ASN:C	2.59	0.40
1:C:828:CYS:HB3	1:C:838:PHE:CD2	2.56	0.40
1:A:808:ALA:HA	1:A:811:ASP:HB2	2.02	0.40
2:B:55:TYR:HE2	2:B:74:SER:HB3	1.86	0.40
1:C:731:ARG:HA	1:C:734:LEU:CD2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	765/866 (88%)	736 (96%)	28 (4%)	1 (0%)	51	81
1	C	769/866 (89%)	746 (97%)	21 (3%)	2 (0%)	41	72
2	B	159/236 (67%)	155 (98%)	4 (2%)	0	100	100
2	D	159/236 (67%)	158 (99%)	1 (1%)	0	100	100
All	All	1852/2204 (84%)	1795 (97%)	54 (3%)	3 (0%)	47	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	811	ASP
1	A	686	GLU
1	C	533	ILE

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	665/769 (86%)	651 (98%)	14 (2%)	53	84
1	C	686/769 (89%)	677 (99%)	9 (1%)	69	91
2	B	139/202 (69%)	138 (99%)	1 (1%)	84	95
2	D	134/202 (66%)	132 (98%)	2 (2%)	65	89
All	All	1624/1942 (84%)	1598 (98%)	26 (2%)	62	88

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	169	LYS
1	A	183	ASP
1	A	278	LYS
1	A	286	LYS
1	A	289	ARG
1	A	291	LEU
1	A	357	ARG

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Mol	Chain	Res	Type
1	A	366	LYS
1	A	491	CYS
1	A	670	ASN
1	A	800	GLN
1	A	811	ASP
1	A	822	GLU
2	B	27	GLN
1	C	61	LYS
1	C	71	ARG
1	C	111	LYS
1	C	278	LYS
1	C	366	LYS
1	C	470	ARG
1	C	765	ARG
1	C	780	GLN
1	C	797	ARG
2	D	120	HIS
2	D	123	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	212	HIS
2	B	27	GLN
1	C	25	GLN
1	C	35	GLN
1	C	147	GLN
1	C	456	ASN
1	C	758	ASN
2	D	124	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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	C	902	-	36,36,36	1.78	10 (27%)	54,60,60	3.32	16 (29%)
3	IHP	A	901	-	36,36,36	1.52	9 (25%)	54,60,60	3.60	15 (27%)
4	1PE	C	901	-	15,15,15	0.52	0	14,14,14	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IHP	C	902	-	-	13/30/54/54	0/1/1/1
3	IHP	A	901	-	-	12/30/54/54	0/1/1/1
4	1PE	C	901	-	-	5/13/13/13	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	902	IHP	P3-O13	4.39	1.67	1.59
3	A	901	IHP	P2-O12	3.60	1.66	1.59
3	C	902	IHP	C3-C2	3.59	1.59	1.52
3	C	902	IHP	P2-O12	3.47	1.65	1.59
3	C	902	IHP	P6-O16	3.20	1.65	1.59
3	A	901	IHP	P3-O13	3.18	1.65	1.59
3	A	901	IHP	P4-O14	3.17	1.65	1.59
3	C	902	IHP	P4-O14	2.99	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	902	IHP	O15-C5	-2.97	1.33	1.44
3	C	902	IHP	C6-C5	-2.65	1.46	1.52
3	A	901	IHP	C3-C2	2.65	1.57	1.52
3	C	902	IHP	C2-C1	2.63	1.57	1.52
3	C	902	IHP	C4-C3	2.52	1.57	1.52
3	A	901	IHP	P1-O11	2.42	1.63	1.59
3	A	901	IHP	C2-C1	2.38	1.57	1.52
3	A	901	IHP	C6-C5	-2.31	1.47	1.52
3	A	901	IHP	C4-C3	2.27	1.57	1.52
3	C	902	IHP	P1-O11	2.27	1.63	1.59
3	A	901	IHP	O15-C5	-2.13	1.36	1.44

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	902	IHP	C6-C5-C4	12.05	136.79	110.41
3	A	901	IHP	O11-C1-C6	-11.29	82.08	108.69
3	A	901	IHP	C6-C5-C4	10.38	133.14	110.41
3	C	902	IHP	O11-C1-C6	-9.98	85.16	108.69
3	A	901	IHP	O16-C6-C1	9.70	131.56	108.69
3	A	901	IHP	O14-C4-C3	9.27	130.54	108.69
3	C	902	IHP	O16-C6-C1	8.72	129.24	108.69
3	C	902	IHP	O14-C4-C3	7.59	126.57	108.69
3	A	901	IHP	O11-C1-C2	-7.53	90.94	108.69
3	A	901	IHP	O15-C5-C4	6.26	123.45	108.69
3	A	901	IHP	C3-C2-C1	5.91	123.36	110.41
3	A	901	IHP	O12-C2-C1	5.48	121.61	108.69
3	C	902	IHP	O15-C5-C6	-5.47	95.79	108.69
3	A	901	IHP	O13-C3-C4	5.23	121.01	108.69
3	C	902	IHP	O12-C2-C3	5.07	120.64	108.69
3	A	901	IHP	O14-C4-C5	5.04	120.58	108.69
3	C	902	IHP	C3-C2-C1	4.82	120.96	110.41
3	C	902	IHP	O13-C3-C2	4.57	119.46	108.69
3	C	902	IHP	O14-C4-C5	4.28	118.78	108.69
3	C	902	IHP	C6-C1-C2	4.14	119.49	110.41
3	A	901	IHP	O15-C5-C6	-3.46	100.53	108.69
3	C	902	IHP	O11-C1-C2	-3.36	100.77	108.69
3	A	901	IHP	C4-C3-C2	3.23	117.49	110.41
3	C	902	IHP	O33-P3-O13	2.72	118.19	105.99
3	A	901	IHP	O33-P3-O13	2.61	117.67	105.99
3	C	902	IHP	O15-C5-C4	2.58	114.78	108.69
3	C	902	IHP	O42-P2-O12	2.54	117.35	105.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	902	IHP	O13-C3-C4	2.47	114.50	108.69
3	A	901	IHP	O13-P3-O23	-2.44	99.97	109.39
3	A	901	IHP	C5-C6-C1	2.41	115.68	110.41
3	C	902	IHP	O16-P6-O26	-2.38	100.20	109.39

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	902	IHP	C2-C1-O11-P1
3	C	902	IHP	C6-C1-O11-P1
3	C	902	IHP	C3-C2-O12-P2
3	C	902	IHP	C1-C6-O16-P6
3	C	902	IHP	C5-C6-O16-P6
3	C	902	IHP	C2-O12-P2-O22
3	C	902	IHP	C3-O13-P3-O33
3	C	902	IHP	C6-O16-P6-O26
3	A	901	IHP	C1-C2-O12-P2
3	A	901	IHP	C4-C3-O13-P3
3	A	901	IHP	C3-C4-O14-P4
3	A	901	IHP	C4-C5-O15-P5
3	A	901	IHP	C6-C5-O15-P5
3	A	901	IHP	C1-C6-O16-P6
3	A	901	IHP	C3-O13-P3-O23
3	C	902	IHP	C1-C2-O12-P2
3	A	901	IHP	C6-O16-P6-O26
4	C	901	1PE	C24-C14-OH5-C25
4	C	901	1PE	C16-C26-OH6-C15
3	C	902	IHP	C4-C3-O13-P3
3	C	902	IHP	C3-C4-O14-P4
3	A	901	IHP	C2-O12-P2-O42
3	C	902	IHP	C4-C5-O15-P5
4	C	901	1PE	C23-C13-OH4-C24
4	C	901	1PE	OH7-C16-C26-OH6
3	C	902	IHP	C3-O13-P3-O23
3	A	901	IHP	C4-O14-P4-O24
3	A	901	IHP	C1-O11-P1-O31
3	A	901	IHP	C2-O12-P2-O32
4	C	901	1PE	OH5-C14-C24-OH4

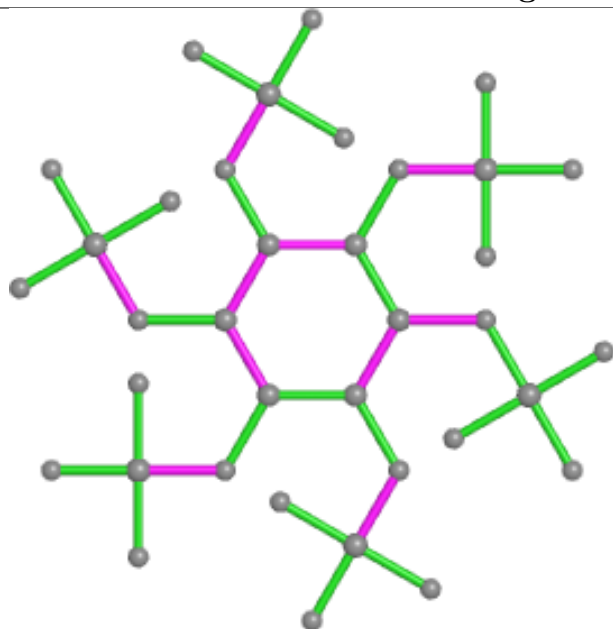
There are no ring outliers.

1 monomer is involved in 2 short contacts:

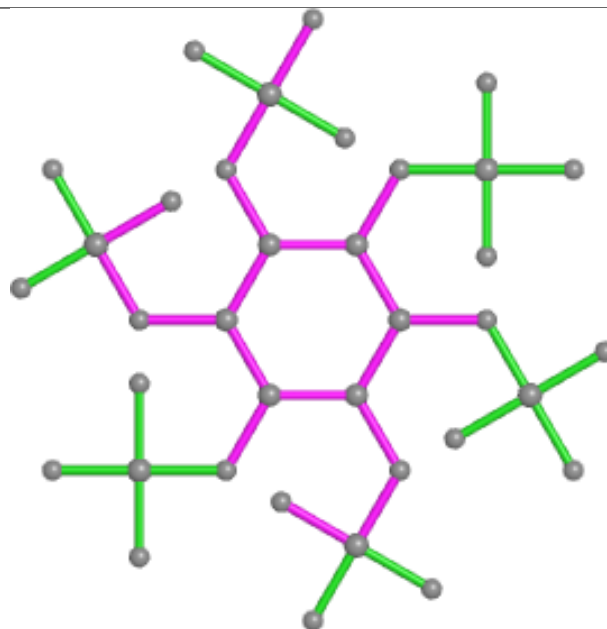
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	IHP	2	0

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

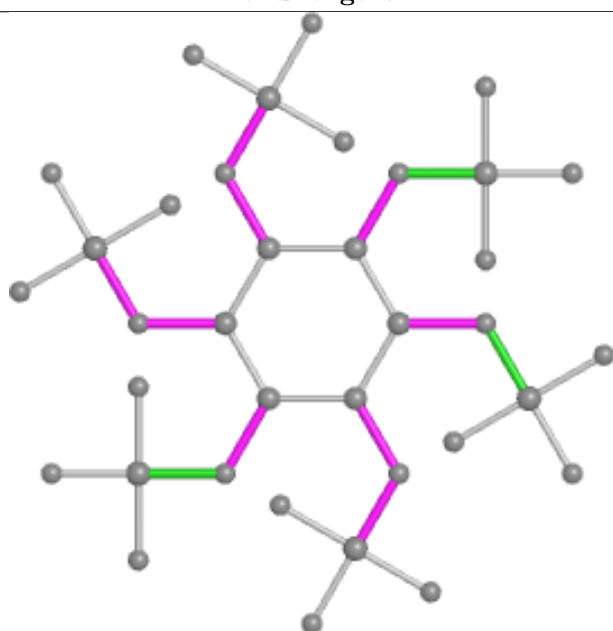
Ligand IHP C 902



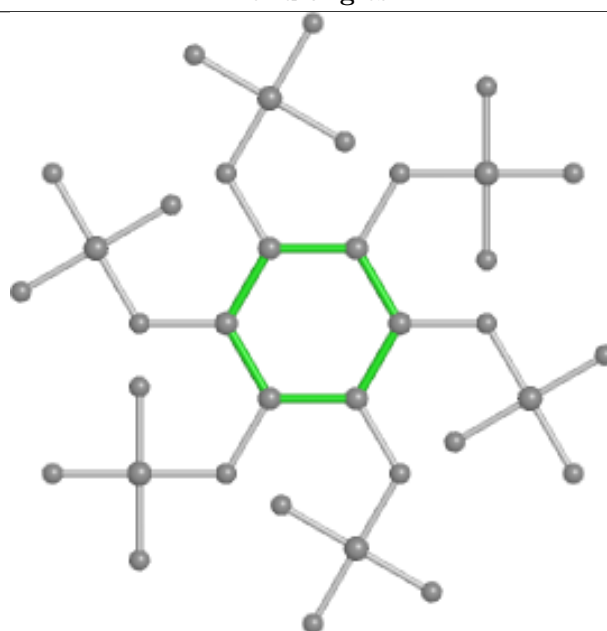
Bond lengths



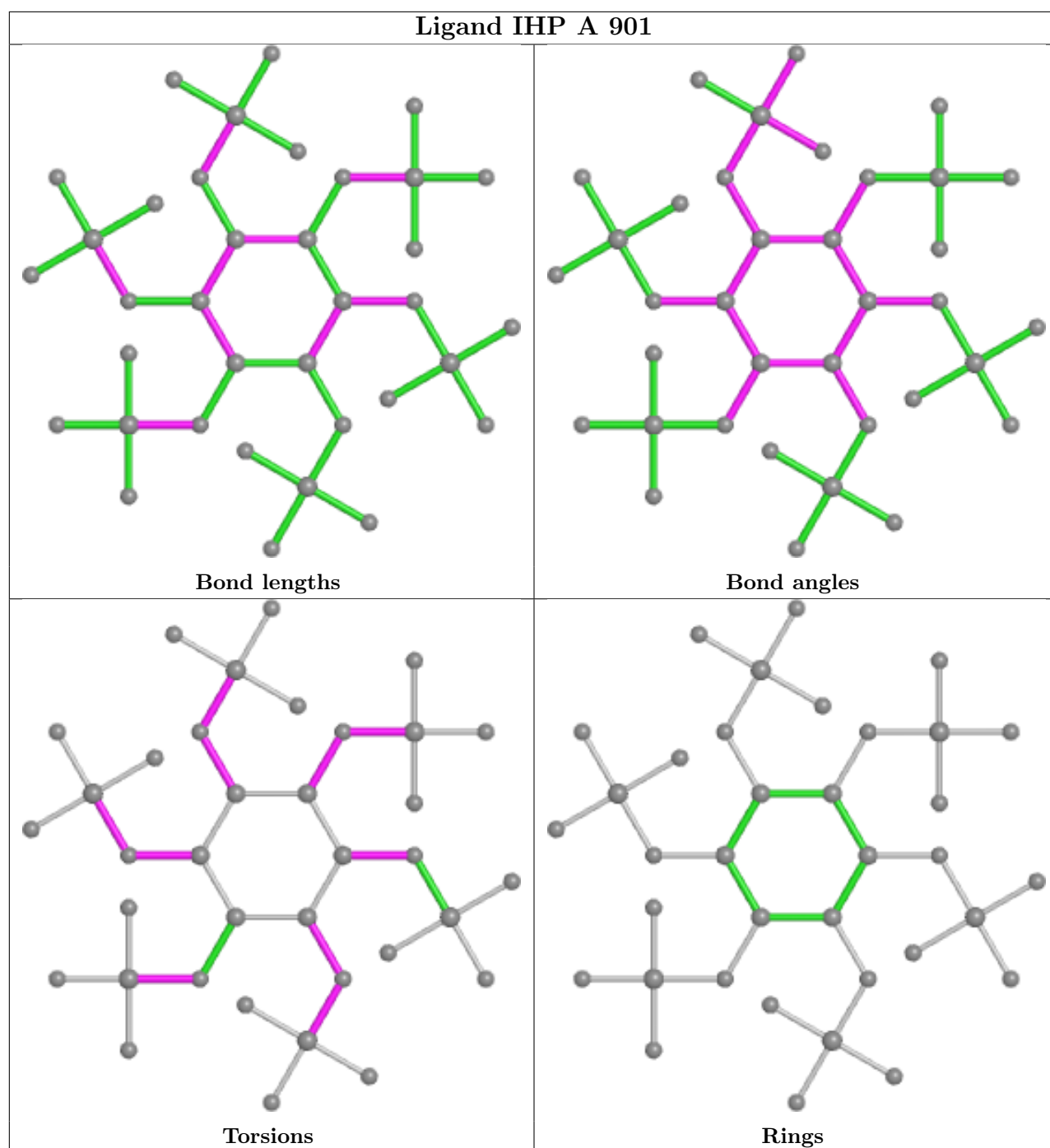
Bond angles



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	771/866 (89%)	0.25	25 (3%) 47 37	51, 95, 155, 210	0
1	C	773/866 (89%)	0.20	17 (2%) 62 52	52, 79, 138, 181	0
2	B	160/236 (67%)	0.17	1 (0%) 89 86	52, 73, 111, 151	0
2	D	160/236 (67%)	0.22	1 (0%) 89 86	57, 79, 143, 182	0
All	All	1864/2204 (84%)	0.22	44 (2%) 59 49	51, 85, 145, 210	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	734	LEU	4.8
1	A	182	PRO	4.6
1	C	180	THR	3.9
1	A	783	ALA	3.3
1	C	735	LYS	3.3
1	C	36	ILE	3.2
1	C	30	LEU	3.0
1	C	742	PHE	2.9
1	A	721	CYS	2.8
1	C	59	LEU	2.8
1	A	376	VAL	2.8
1	A	785	GLU	2.7
1	C	376	VAL	2.7
1	A	649	LYS	2.7
1	A	688	PHE	2.7
1	C	366	LYS	2.7
1	C	738	MET	2.6
1	C	688	PHE	2.6
1	A	719	ALA	2.6
1	A	817	CYS	2.5
1	A	825	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	56	LEU	2.5
1	A	568	LEU	2.4
2	B	160	ARG	2.4
1	A	831	LEU	2.4
1	A	789	THR	2.4
1	A	641	GLU	2.4
1	C	37	LEU	2.3
1	A	650	VAL	2.3
1	A	689	LEU	2.3
1	C	367	GLU	2.3
1	A	735	LYS	2.3
2	D	63	ASP	2.2
1	A	787	ALA	2.2
1	A	814	LEU	2.2
1	A	359	PHE	2.1
1	A	728	ASP	2.1
1	A	304	GLU	2.1
1	C	23	HIS	2.1
1	A	564	ILE	2.1
1	C	62	LYS	2.1
1	A	394	LEU	2.0
1	A	458	ILE	2.0
1	C	25	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

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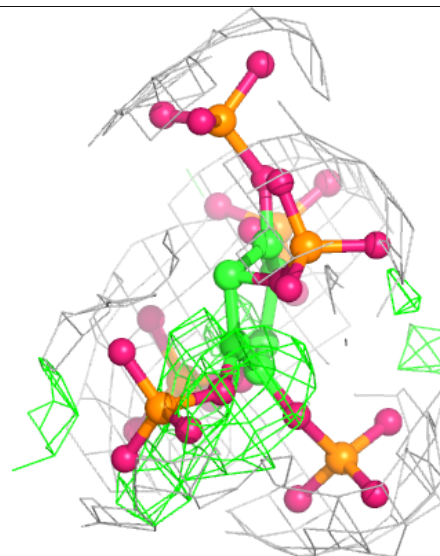
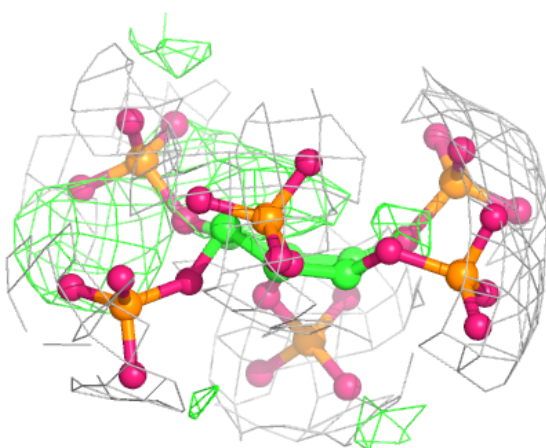
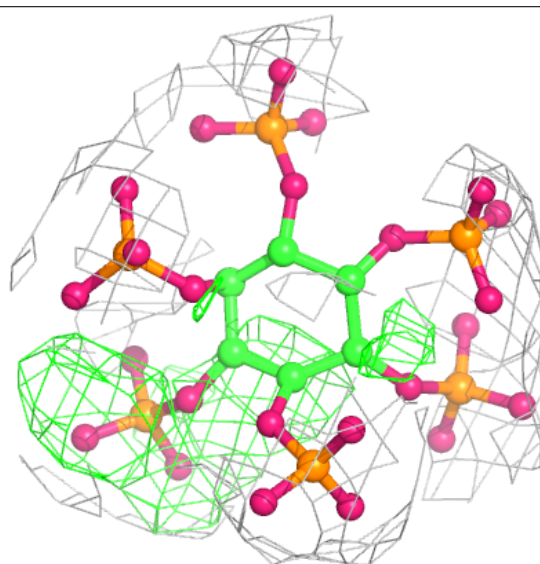
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	1PE	C	901	16/16	0.85	0.15	98,112,122,122	0
3	IHP	A	901	36/36	0.86	0.32	121,152,164,167	0
3	IHP	C	902	36/36	0.87	0.29	87,156,167,168	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.

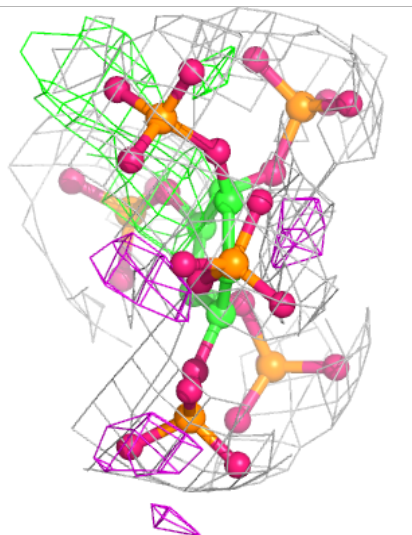
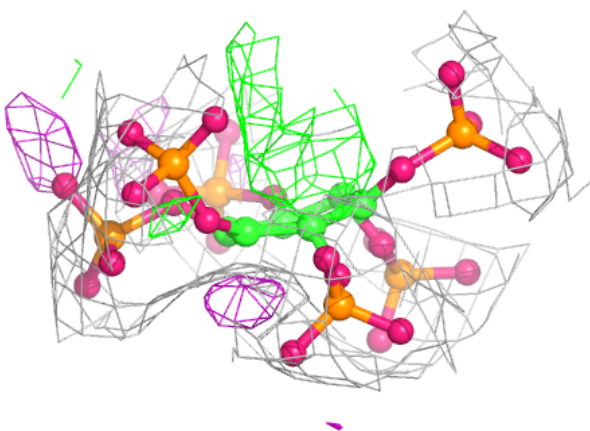
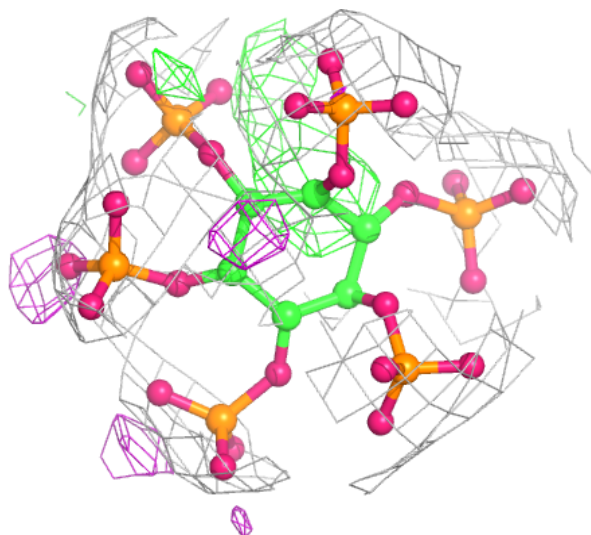
Electron density around IHP A 901:

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 C 902:

$2mF_o-DF_c$ (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.