



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:44 PM UTC

PDB ID : 6C95 / pdb_00006c95
Title : The Human NatA (Naa10/Naa15) amino-terminal acetyltransferase complex bound to HYPK
Authors : Gottlieb, L.; Marmorstein, R.
Deposited on : 2018-01-25
Resolution : 3.15 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

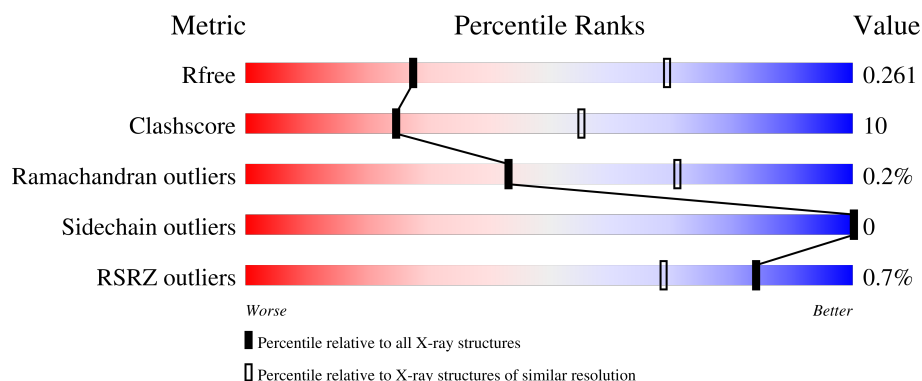
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	866	 69% 20% 11%
2	B	236	 51% 17% 32%
3	D	129	 64% 10% 26%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8454 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	773	Total	C	N	O	S	0	0	0
			6365	4076	1087	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
			1287	811	227	238	11			

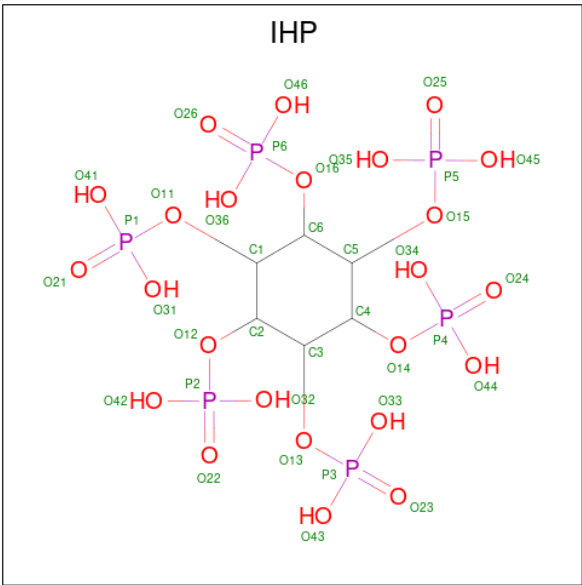
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is a protein called Huntingtin-interacting protein K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	95	Total	C	N	O	S	0	0	0
			732	442	131	155	4			

- Molecule 4 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆).



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

- Molecule 5 is water.

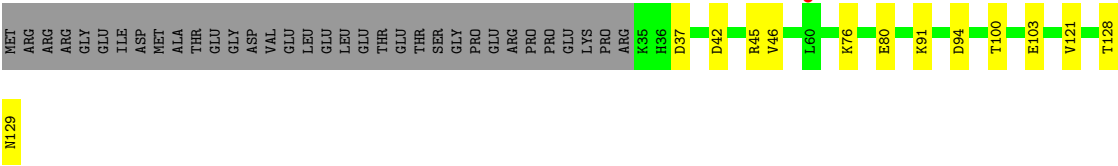
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	24	Total	O	0	0
			24	24		
5	B	6	Total	O	0	0
			6	6		
5	D	4	Total	O	0	0
			4	4		

- Molecule 1: N-alpha-acetyltransferase 15, NatA auxiliary subunit

D811	P653	ASP	C484	R315	L143	MET
L654	L654	THR	M485	M316	R144	PRO
G815	E655	ALA	C485	ALA	Q147	ALA
D816		ASN	W486	P324		VAL
C817	I658	MET	F487			S5
C818		SER	Q488	T328	I152	L6
E819	T662	ASP		L329		P7
A820	M666	LYS	A492	R330	I166	
	L667	GLU		S331	E10	N11
Y824		LEU	K496	L332	H159	
R825	R684	LYS	A497	Y333		
	K685	LYS	M498		M166	F14
	E686	LEU		K338		
L831	K687	ARG	F501	I342	I170	I17
		ASN	G502			
A834		LYS	E503		Y189	C20
A835	L692	GLN		Y349	S190	
R836	Q693	ARG	K506		E191	Q25
E837		ARG	K507	C356	L192	T26
F838	K696	ALA	C508	R357	L193	R27
M839		GLN				
P840	H705	LYS	I511	N360	E202	K31
P841		LYS	E512	P361		
GLY	L708	ALA	R513		L213	Q35
TYR		GLN		P390	C214	
GLU	M712	ILE	I516		T215	A50
GLU		GLU		A393	Y216	
ASP	F716	GLU	F523	I408	E217	Y66
MET		GLU	B594			E67
LYS	A719	LYS	F525		C338	L68
ILE	V720	LYS	H526	Y418	R239	V89
THR	C721	ASN	T527		L240	R70
VAL	E722	ALA	Y528	A421	E241	R71
ASN	S723	GLU		G422	D242	
GLY		LYS	I533	N423		R74
ASP	V730	GLU	T534		N254	
SER	R731	LYS	L535	A427	P255	V85
SER	T732	GLN			E256	
ALA	V733	GLN	L541	L437	N257	D93
GLU	L734	ARG				K94
ALA		ASN	V547	I444	Y260	K95
GLU	M738	GLN	L548		Y261	Y96
GLU		LYS	R549	C448		D97
LEU	F742	LYS			A267	E98
ALA		LYS	I560	M452		
ASN	E752	LYS			M273	D110
GLU		ASP	I564	N456		
ILE	D776	ASP		L457	W284	N113
	P777	ASP	H569			
	S778	ASP		E460	V292	L117
		GLU	L573	A461	P293	
	R782	ILE	THR		R294	L123
		ILE	ASP	M464	R295	Q124
	T788	GLY	GLU			I125
		GLY	ASN	R470	L301	
	R797	GLY	LYS	E471		R128
		P638	GLU	G472	F306	
E807		V650	GLU	T473		Q139
A808		F651	GLU		D311	L140
		T652	GLU	L470		

SER	R112	ACEO
LYS	K113	M1
ASP		N2
LEU		I3
SER	Y122	R4
GLU		N5
VAL	F128	A6
SER		R7
GLU	E142	
THR	D143	M12
THR		I13
GLU	F160	M14
SER	HIS	Q15
THR	LEU	H16
ASP	GLU	
ASP	LEU	L19
VAL	LEU	
LYS	LYS	
ASP	GLU	M28
SER	LYS	
SER	GLY	L36
GLU	ARG	S37
ALA	HIS	V38
SER	VAL	P39
ASP	VAL	Q40
SER	LEU	L41
ALA	GLY	
SER	ALA	I44
	IIE	A45
	GLU	E46
	ASN	D47
	LYS	E48
	VAL	
	GLU	Y55
	SER	V56
	LYS	L57
	GLY	A58
	ASN	K59
	SER	M60
	PRO	E61
	PRO	E62
	SER	D63
	SER	P64
	LYS	D65
	GLU	D66
	ALA	V67
	CYS	
	ARG	G70
	GLU	
	GLY	S80
	LYS	
	GLY	K89
	LEU	L90
	ALA	
	ALA	A94
	GLU	
	ASP	M98
	SER	
	GLY	K105
	GLY	
	ASP	L109

● Molecule 3: Huntingtin-interacting protein K



N129

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	182.32Å 182.32Å 86.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.04 – 3.15 49.04 – 3.15	Depositor EDS
% Data completeness (in resolution range)	95.3 (49.04-3.15) 95.2 (49.04-3.15)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.11.1-2575)	Depositor
R, R_{free}	0.221 , 0.255 0.226 , 0.261	Depositor DCC
R_{free} test set	1352 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	87.7	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8454	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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: ACE, 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	0.19	0/6501	0.38	1/8761 (0.0%)
2	B	0.26	1/1313 (0.1%)	0.40	0/1773
3	D	0.17	0/734	0.36	0/983
All	All	0.20	1/8548 (0.0%)	0.38	1/11517 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	0	ACE	C-N	6.13	1.45	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	488	GLN	CB-CA-C	5.02	119.38	110.85

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	6365	0	6404	135	0
2	B	1287	0	1244	33	0
3	D	732	0	718	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	36	0	6	1	0
5	A	24	0	0	1	0
5	B	6	0	0	0	0
5	D	4	0	0	0	0
All	All	8454	0	8372	165	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 10.

All (165) 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:A:696:LYS:HD3	3:D:128:THR:HG22	1.55	0.88
1:A:693:GLN:HA	3:D:128:THR:HG23	1.60	0.83
1:A:693:GLN:HA	3:D:128:THR:CG2	2.08	0.82
1:A:331:SER:HB2	2:B:48:GLU:OE1	1.80	0.81
1:A:422:GLY:HA3	1:A:835:ALA:HA	1.65	0.78
1:A:693:GLN:CA	3:D:128:THR:HG23	2.13	0.77
1:A:50:ALA:HB1	1:A:85:VAL:HG21	1.72	0.70
2:B:47:ASP:OD1	2:B:48:GLU:N	2.24	0.70
1:A:331:SER:CB	2:B:48:GLU:OE1	2.40	0.69
1:A:470:ARG:HG2	1:A:472:GLY:H	1.58	0.68
1:A:295:ARG:HE	1:A:328:THR:HB	1.59	0.67
1:A:193:LEU:HD13	1:A:216:TYR:HB3	1.76	0.67
1:A:541:LEU:HD22	2:B:36:LEU:HD11	1.76	0.67
1:A:470:ARG:HH11	1:A:473:THR:HG21	1.60	0.66
2:B:14:MET:HE1	2:B:57:LEU:HD13	1.80	0.64
1:A:696:LYS:HD3	3:D:128:THR:CG2	2.26	0.64
1:A:418:TYR:HB2	1:A:427:ALA:HB2	1.81	0.62
1:A:294:ARG:NH2	1:A:316:MET:SD	2.74	0.61
1:A:730:VAL:O	1:A:734:LEU:N	2.28	0.61
1:A:685:LYS:NZ	3:D:103:GLU:OE2	2.26	0.60
1:A:423:ASN:HA	1:A:836:LEU:HG	1.83	0.59
1:A:693:GLN:HA	3:D:128:THR:HG22	1.84	0.59
2:B:41:LEU:HB3	2:B:58:ALA:HB3	1.85	0.59
1:A:452:MET:HE3	1:A:461:ALA:HA	1.86	0.58
1:A:788:THR:HG22	1:A:788:THR:O	2.03	0.58
1:A:513:ARG:HA	1:A:516:ILE:HD12	1.85	0.57
1:A:817:CYS:HB3	1:A:820:ALA:HB3	1.86	0.57
1:A:152:ILE:O	1:A:156:ILE:HG13	2.04	0.57
1:A:295:ARG:NH2	1:A:328:THR:O	2.27	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:LEU:HG	3:D:128:THR:HG21	1.85	0.57
2:B:113:LYS:HD3	2:B:143:ASP:HB2	1.85	0.57
2:B:5:ASN:OD1	2:B:7:ARG:NH2	2.38	0.56
1:A:807:GLU:O	1:A:811:ASP:N	2.36	0.56
1:A:284:TRP:HD1	1:A:293:PRO:HB2	1.70	0.56
1:A:501:PHE:HD2	1:A:564:ILE:HG23	1.71	0.56
1:A:816:ASP:OD1	1:A:818:LYS:HG3	2.07	0.55
2:B:56:VAL:CG2	2:B:90:LEU:HB3	2.36	0.55
1:A:723:SER:O	1:A:731:ARG:NH1	2.39	0.55
1:A:408:ILE:HG21	1:A:444:ILE:HD13	1.88	0.55
1:A:508:CYS:HA	1:A:511:ILE:HD12	1.88	0.55
1:A:525:PHE:HA	1:A:528:TYR:HB3	1.89	0.55
1:A:549:ARG:HB2	1:A:667:LEU:HD12	1.89	0.54
1:A:311:ASP:OD1	1:A:349:TYR:OH	2.22	0.54
1:A:569:HIS:HD2	1:A:684:ARG:HD3	1.73	0.53
1:A:457:LEU:HB3	1:A:460:GLU:HB2	1.90	0.53
1:A:6:LEU:HB2	1:A:11:ASN:HB2	1.90	0.52
1:A:239:ARG:NH2	1:A:242:ASP:OD2	2.38	0.52
1:A:254:ASN:ND2	1:A:257:ASN:HB2	2.24	0.52
1:A:329:LEU:HD12	1:A:342:ILE:HD13	1.92	0.52
1:A:329:LEU:HB3	1:A:333:TYR:HE1	1.74	0.52
1:A:836:LEU:HA	1:A:839:MET:HG2	1.91	0.52
1:A:110:ASP:HB3	1:A:113:ASN:HB2	1.92	0.52
1:A:70:ARG:O	1:A:74:ARG:HG2	2.10	0.52
1:A:719:ALA:O	1:A:723:SER:HB2	2.09	0.52
2:B:56:VAL:HG21	2:B:90:LEU:HB3	1.91	0.52
2:B:67:VAL:HB	2:B:105:LYS:HG3	1.91	0.52
1:A:547:VAL:HG12	1:A:667:LEU:HD22	1.91	0.52
1:A:422:GLY:CA	1:A:835:ALA:HA	2.39	0.51
2:B:59:LYS:NZ	3:D:42:ASP:OD2	2.42	0.51
1:A:31:LYS:O	1:A:35:GLN:HG3	2.11	0.51
1:A:492:ALA:HB2	1:A:507:LYS:HB2	1.93	0.51
1:A:752:GLU:OE2	1:A:782:ARG:NH1	2.43	0.51
1:A:662:THR:O	1:A:666:ASN:ND2	2.38	0.51
1:A:708:LEU:O	1:A:712:MET:HG3	2.10	0.51
1:A:733:VAL:HG22	3:D:121:VAL:HG13	1.92	0.51
1:A:479:LEU:HD13	1:A:487:PHE:CG	2.46	0.50
2:B:14:MET:HE3	2:B:55:TYR:CD2	2.46	0.50
2:B:6:ALA:HB2	2:B:44:ILE:HG23	1.93	0.50
1:A:788:THR:HG23	1:A:824:TYR:HD1	1.77	0.50
2:B:38:TRP:HB3	2:B:41:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:LEU:C	1:A:306:PHE:HB2	2.37	0.49
1:A:523:PHE:HA	1:A:526:HIS:CD2	2.47	0.49
1:A:20:CYS:O	1:A:25:GLN:N	2.45	0.49
1:A:533:ILE:O	1:A:535:LEU:N	2.45	0.49
1:A:166:MET:O	1:A:170:ILE:HG13	2.12	0.49
1:A:448:CYS:O	1:A:452:MET:HG3	2.13	0.49
1:A:696:LYS:NZ	3:D:129:ASN:OD1	2.36	0.49
1:A:738:MET:HG3	1:A:742:PHE:CD1	2.48	0.48
1:A:117:LEU:HB2	1:A:140:LEU:HD21	1.94	0.48
1:A:496:LYS:HD2	1:A:560:ILE:HG23	1.94	0.48
1:A:652:THR:O	1:A:652:THR:OG1	2.27	0.48
2:B:12:MET:HG2	2:B:28:MET:HE3	1.95	0.48
1:A:569:HIS:CD2	1:A:684:ARG:HD3	2.48	0.48
1:A:693:GLN:HB2	3:D:128:THR:HA	1.95	0.48
1:A:360:ASN:OD1	1:A:361:PRO:HD2	2.14	0.47
1:A:68:LEU:HD23	1:A:71:ARG:NH1	2.29	0.47
1:A:191:GLU:OE2	2:B:40:GLN:NE2	2.47	0.47
1:A:470:ARG:HH11	1:A:473:THR:CG2	2.27	0.47
2:B:4:ARG:HE	2:B:46:GLU:CD	2.22	0.47
1:A:14:PHE:HA	1:A:17:ILE:HG13	1.95	0.47
1:A:390:PRO:HA	1:A:393:ALA:HB3	1.96	0.47
1:A:159:HIS:NE2	1:A:202:GLU:OE1	2.39	0.47
1:A:479:LEU:HD12	1:A:487:PHE:CE2	2.50	0.47
1:A:356:CYS:O	1:A:357:ARG:HG2	2.15	0.47
1:A:484:CYS:HA	2:B:19:LEU:HD13	1.95	0.47
1:A:716:PHE:HB2	1:A:742:PHE:CE2	2.50	0.47
1:A:189:TYR:CE2	1:A:193:LEU:HD11	2.50	0.47
2:B:112:ARG:NH1	2:B:142:GLU:OE1	2.41	0.47
1:A:255:PRO:O	1:A:261:TYR:HE2	1.99	0.46
2:B:122:TYR:HB3	2:B:128:PHE:HB2	1.96	0.46
1:A:125:ILE:O	1:A:128:ARG:HD3	2.16	0.46
1:A:338:LYS:O	1:A:342:ILE:HG13	2.15	0.45
1:A:408:ILE:HG12	1:A:437:LEU:HD12	1.98	0.45
1:A:479:LEU:CD1	1:A:487:PHE:CD2	2.99	0.45
3:D:76:LYS:O	3:D:80:GLU:HG3	2.17	0.45
1:A:421:ALA:HB1	1:A:834:TYR:HB2	1.99	0.45
1:A:734:LEU:O	1:A:738:MET:HB2	2.16	0.45
1:A:788:THR:HG23	1:A:824:TYR:CD1	2.51	0.45
2:B:94:ALA:O	2:B:98:MET:HG3	2.17	0.45
3:D:91:LYS:HB3	3:D:94:ASP:OD2	2.17	0.45
2:B:109:LEU:HD12	2:B:109:LEU:C	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:MET:HA	2:B:28:MET:HE1	1.98	0.44
1:A:257:ASN:HB3	1:A:260:TYR:CD2	2.53	0.44
1:A:94:LYS:HA	1:A:96:TYR:CE1	2.53	0.44
2:B:41:LEU:HD21	2:B:60:MET:HG2	1.98	0.44
2:B:70:GLY:HA3	2:B:98:MET:SD	2.57	0.44
1:A:650:VAL:HG22	1:A:652:THR:H	1.83	0.44
1:A:705:HIS:HB3	1:A:708:LEU:HB3	1.99	0.44
1:A:139:GLN:O	1:A:143:LEU:HG	2.18	0.44
1:A:66:TYR:OH	1:A:93:ASP:OD2	2.22	0.44
1:A:256:GLU:HG3	2:B:89:LYS:HD3	2.00	0.44
1:A:7:PRO:O	1:A:11:ASN:N	2.45	0.43
1:A:797:ARG:HH22	1:A:831:LEU:HD22	1.84	0.43
1:A:496:LYS:HB2	1:A:564:ILE:HD11	2.00	0.43
1:A:528:TYR:CG	3:D:46:VAL:HG13	2.53	0.43
1:A:693:GLN:N	3:D:128:THR:HG23	2.33	0.43
3:D:37:ASP:OD1	3:D:37:ASP:N	2.51	0.43
1:A:788:THR:O	1:A:788:THR:CG2	2.67	0.43
1:A:27:ARG:HA	1:A:27:ARG:HD2	1.78	0.42
1:A:456:ASN:HB3	1:A:498:MET:SD	2.60	0.42
1:A:96:TYR:CD1	1:A:123:LEU:HD11	2.54	0.42
1:A:256:GLU:O	1:A:292:VAL:HG21	2.20	0.42
1:A:273:MET:HE3	1:A:273:MET:HB2	1.95	0.42
1:A:7:PRO:HD2	1:A:10:GLU:HB2	2.01	0.42
1:A:240:LEU:HB3	1:A:267:ALA:O	2.19	0.42
1:A:311:ASP:OD2	1:A:315:ARG:NH1	2.52	0.42
1:A:213:LEU:O	1:A:217:GLU:HB3	2.19	0.42
1:A:486:TRP:HB3	2:B:16:HIS:CE1	2.54	0.42
2:B:113:LYS:HG2	2:B:143:ASP:O	2.20	0.42
3:D:42:ASP:HA	3:D:45:ARG:HH11	1.83	0.42
1:A:479:LEU:HD12	1:A:487:PHE:CD2	2.54	0.42
1:A:98:GLU:OE1	1:A:98:GLU:N	2.52	0.42
1:A:295:ARG:NE	1:A:328:THR:HB	2.32	0.42
1:A:776:ASP:OD1	1:A:778:SER:OG	2.36	0.42
1:A:687:LYS:NZ	3:D:100:THR:O	2.45	0.41
1:A:808:ALA:HB1	1:A:814:LEU:HD13	2.02	0.41
1:A:479:LEU:HB3	1:A:484:CYS:HB3	2.03	0.41
1:A:484:CYS:SG	1:A:486:TRP:NE1	2.93	0.41
1:A:324:PRO:HB3	2:B:80:SER:O	2.20	0.41
1:A:654:LEU:O	1:A:658:ILE:HG13	2.20	0.41
1:A:255:PRO:O	1:A:261:TYR:CE2	2.74	0.41
1:A:503:GLU:O	1:A:506:LYS:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:MET:O	1:A:742:PHE:HB2	2.20	0.41
1:A:144:ARG:HB3	1:A:147:GLN:HG3	2.03	0.41
1:A:261:TYR:OH	1:A:293:PRO:HG3	2.21	0.41
2:B:2:ASN:HB3	2:B:46:GLU:HG2	2.03	0.41
2:B:60:MET:HE3	2:B:60:MET:HB3	1.94	0.41
1:A:655:GLU:OE2	1:A:685:LYS:NZ	2.52	0.40
1:A:721:CYS:O	1:A:722:GLU:HG3	2.21	0.40
4:A:901:IHP:O42	5:A:1001:HOH:O	2.22	0.40
1:A:448:CYS:SG	1:A:464:MET:HE3	2.61	0.40
1:A:444:ILE:H	1:A:444:ILE:HG13	1.70	0.40
1:A:452:MET:O	1:A:457:LEU:HB2	2.21	0.40
1:A:825:ARG:NH2	1:A:838:PHE:O	2.54	0.40
2:B:113:LYS:CD	2:B:143:ASP:HB2	2.51	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	769/866 (89%)	747 (97%)	20 (3%)	2 (0%)	36	64
2	B	159/236 (67%)	157 (99%)	2 (1%)	0	100	100
3	D	93/129 (72%)	89 (96%)	4 (4%)	0	100	100
All	All	1021/1231 (83%)	993 (97%)	26 (2%)	2 (0%)	43	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	533	ILE
1	A	534	THR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	688/769 (90%)	688 (100%)	0	100	100
2	B	134/202 (66%)	134 (100%)	0	100	100
3	D	77/111 (69%)	77 (100%)	0	100	100
All	All	899/1082 (83%)	899 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	ASN
2	B	15	GLN
2	B	101	ASN
2	B	110	HIS

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](#)

1 ligand is 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	$\# Z > 2$
4	IHP	A	901	-	36,36,36	2.01	12 (33%)	60,60,60	3.76	19 (31%)

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
4	IHP	A	901	-	-	12/30/54/54	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	IHP	P2-O12	4.50	1.67	1.59
4	A	901	IHP	P3-O13	4.03	1.66	1.59
4	A	901	IHP	C3-C2	4.03	1.60	1.52
4	A	901	IHP	P4-O14	3.91	1.66	1.59
4	A	901	IHP	P6-O16	3.07	1.64	1.59
4	A	901	IHP	C2-C1	3.02	1.58	1.52
4	A	901	IHP	C6-C5	-2.96	1.46	1.52
4	A	901	IHP	P5-O15	2.96	1.64	1.59
4	A	901	IHP	C4-C3	2.94	1.58	1.52
4	A	901	IHP	O15-C5	-2.69	1.34	1.44
4	A	901	IHP	C5-C4	-2.58	1.47	1.52
4	A	901	IHP	P1-O11	2.08	1.63	1.59

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	IHP	O15-C5-C6	-15.02	76.82	108.76
4	A	901	IHP	O15-C5-C4	-11.76	83.75	108.76
4	A	901	IHP	C6-C5-C4	10.38	133.20	110.43
4	A	901	IHP	O11-C1-C6	-8.97	89.68	108.76
4	A	901	IHP	O16-C6-C1	7.57	124.87	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	IHP	O14-C4-C3	6.63	122.86	108.76
4	A	901	IHP	P4-O14-C4	5.31	137.60	123.43
4	A	901	IHP	C3-C2-C1	4.43	120.15	110.43
4	A	901	IHP	O14-C4-C5	4.11	117.51	108.76
4	A	901	IHP	P2-O12-C2	4.01	134.13	123.43
4	A	901	IHP	O12-C2-C3	3.98	117.23	108.76
4	A	901	IHP	P6-O16-C6	3.68	133.26	123.43
4	A	901	IHP	C6-C1-C2	3.48	118.07	110.43
4	A	901	IHP	C4-C3-C2	3.26	117.57	110.43
4	A	901	IHP	O16-C6-C5	3.04	115.23	108.76
4	A	901	IHP	O13-C3-C2	2.46	114.00	108.76
4	A	901	IHP	O32-P2-O12	2.38	115.12	105.85
4	A	901	IHP	O13-C3-C4	2.08	113.19	108.76
4	A	901	IHP	O46-P6-O16	2.08	113.96	105.85

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	IHP	C2-C1-O11-P1
4	A	901	IHP	C6-C1-O11-P1
4	A	901	IHP	C1-C2-O12-P2
4	A	901	IHP	C3-C2-O12-P2
4	A	901	IHP	C5-C4-O14-P4
4	A	901	IHP	C1-C6-O16-P6
4	A	901	IHP	C4-C3-O13-P3
4	A	901	IHP	C3-O13-P3-O33
4	A	901	IHP	C3-O13-P3-O23
4	A	901	IHP	C3-C4-O14-P4
4	A	901	IHP	C1-O11-P1-O21
4	A	901	IHP	C6-O16-P6-O26

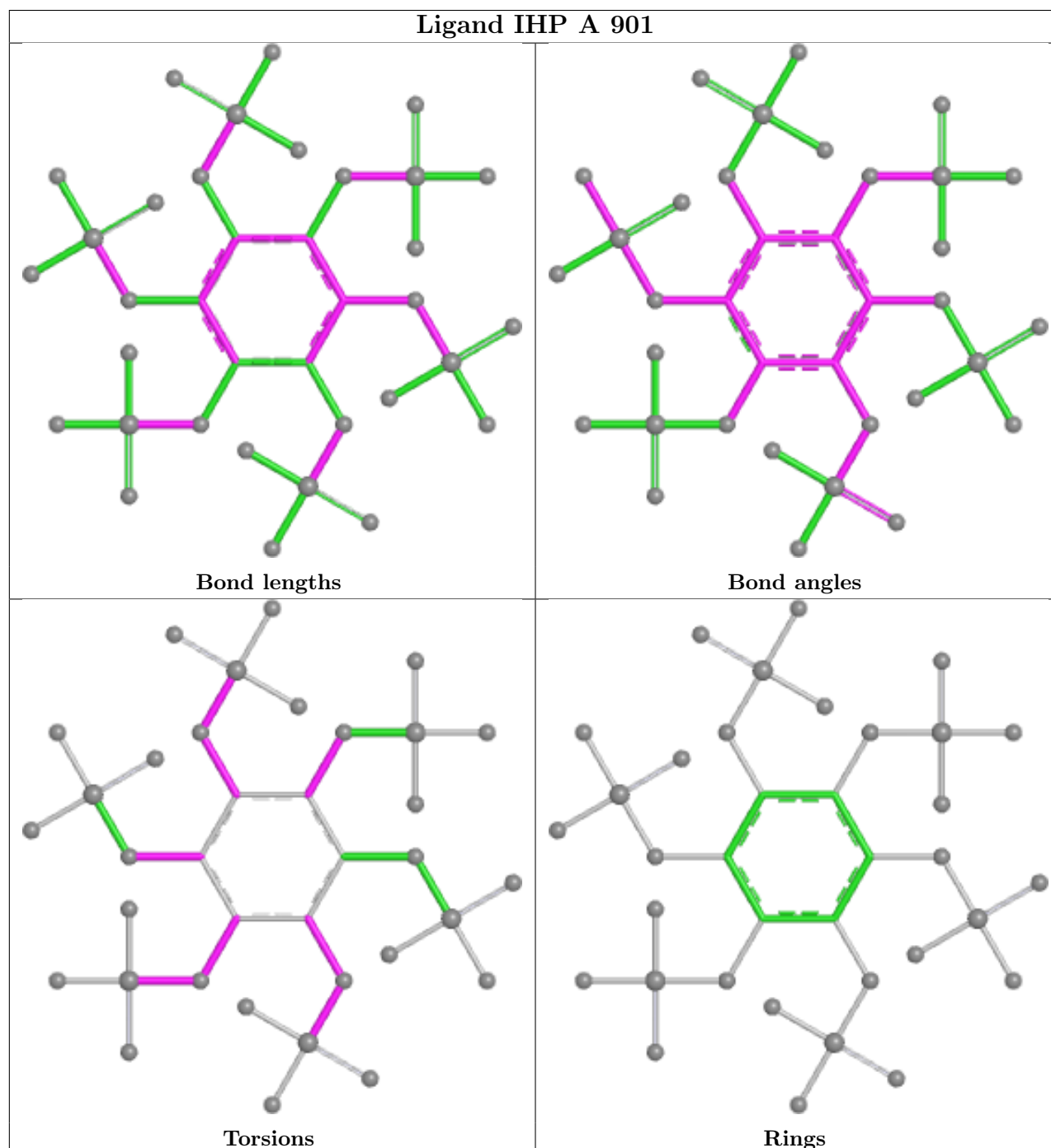
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	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.



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	773/866 (89%)	-0.10	3 (0%) 88 78	47, 90, 133, 175	0
2	B	160/236 (67%)	-0.12	3 (1%) 66 45	50, 84, 138, 185	0
3	D	95/129 (73%)	0.04	1 (1%) 78 60	74, 112, 152, 168	0
All	All	1028/1231 (83%)	-0.09	7 (0%) 84 69	47, 91, 137, 185	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	238	CYS	3.0
1	A	214	CYS	2.8
1	A	329	LEU	2.5
2	B	65	ASP	2.2
3	D	60	LEU	2.2
2	B	62	GLU	2.1
2	B	63	ASP	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

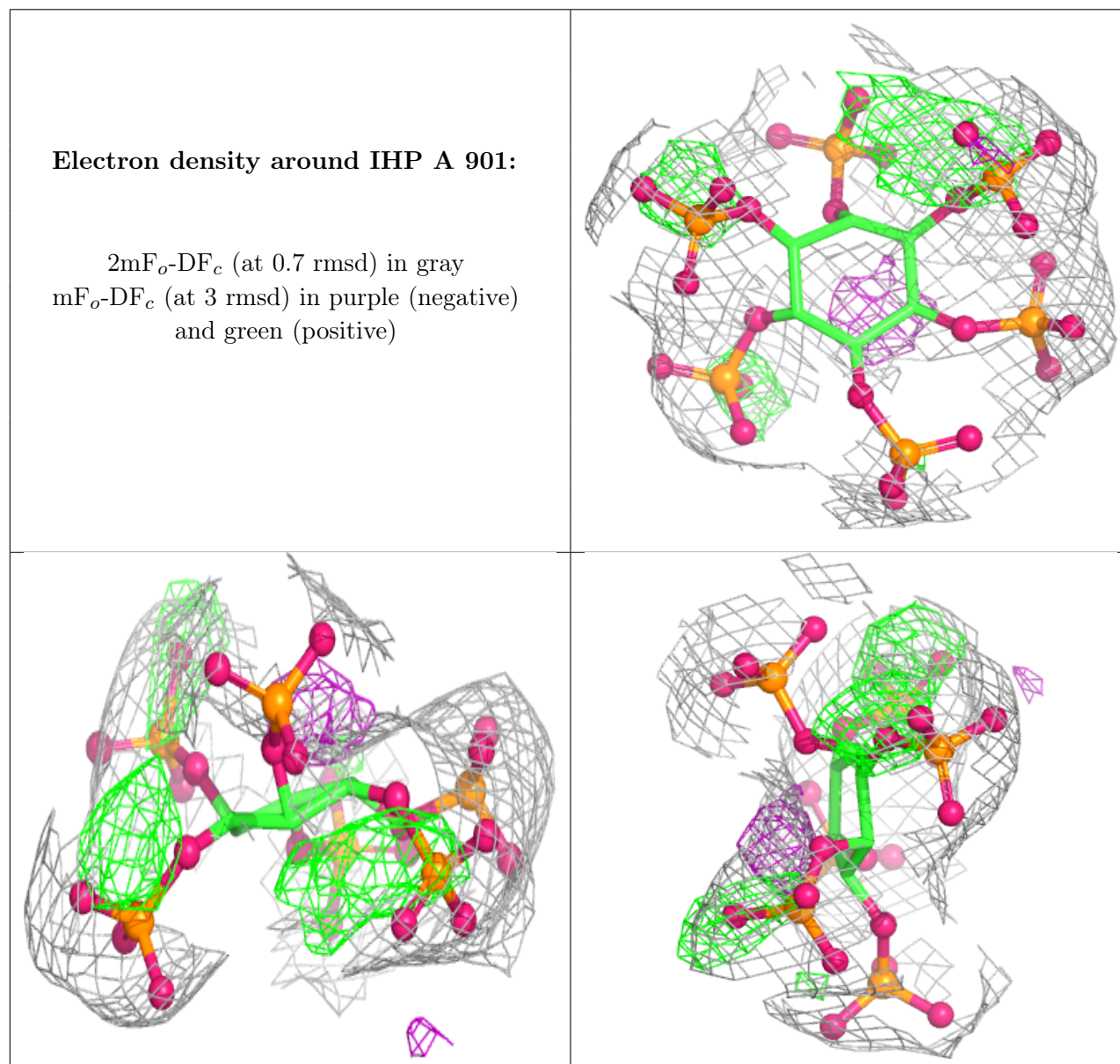
6.4 Ligands [i](#)

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

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	IHP	A	901	36/36	0.80	0.14	118,178,187,189	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.