



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:53 AM UTC

PDB ID : 6C9M / pdb_00006c9m
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 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

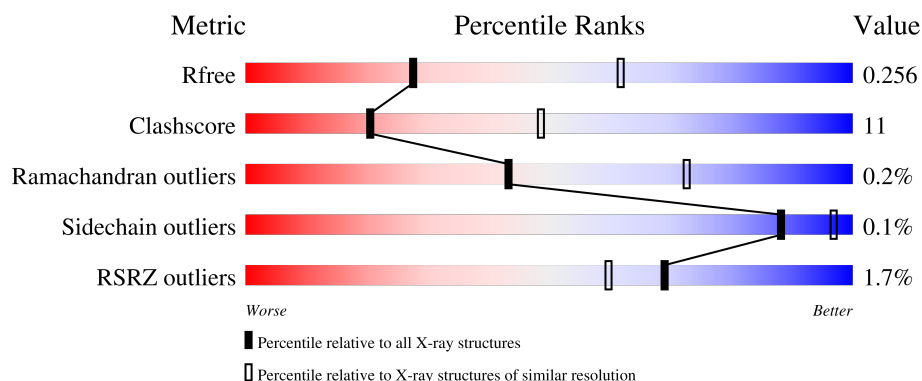
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 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	2% 65% 24% 11%
1	C	866	2% 68% 21% 11%
2	B	236	56% 12% 32%
2	D	236	2% 53% 14% 32%

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			

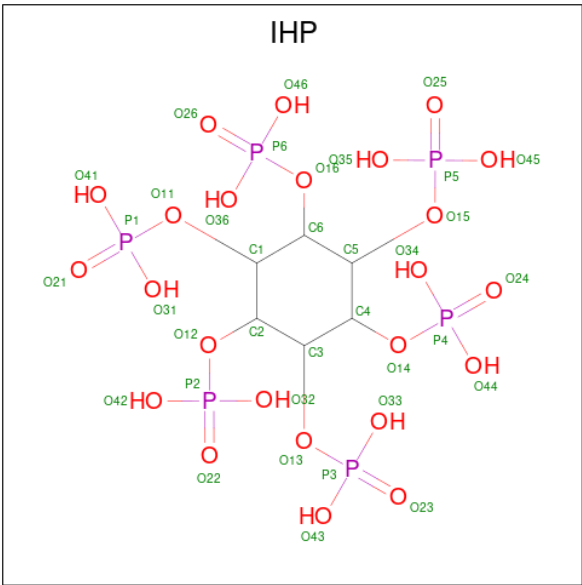
- Molecule 2 is a protein called N-alpha-acetyltransferase 10.

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:

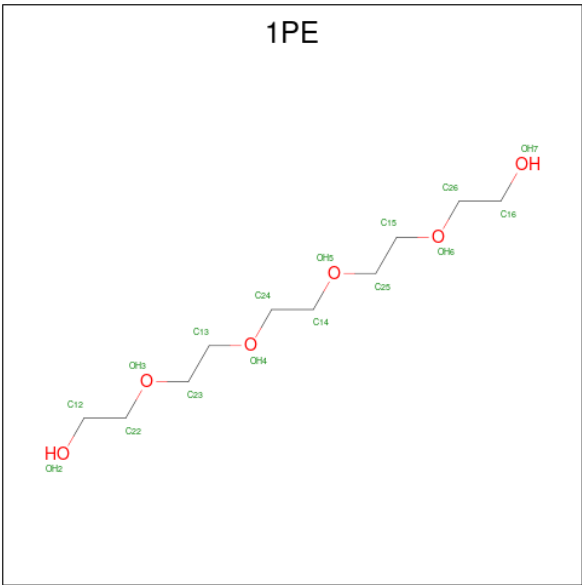
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ACE	-	acetylation	UNP P41227
D	0	ACE	-	acetylation	UNP P41227

- Molecule 3 is INOSITOL HEXAKISPHOSPHATE (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	C	1	Total	C	O	P	0	0
			36	6	24	6		

- Molecule 4 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



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

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.

- Chain A:

L806	H709	ALA	T527	L394	V292	R128	H1
E807	E710	GLU	Y528	E396	P293	D129	P2
A808	C711	LYS	C529	L395	P297	L130	A3
L809	H712	GLU		L397			V4
Y810	I713	LYS	I533	R398		Y133	S5
D811	R714	GLN		T399	F300	R134	L6
G812	T718	GLN	E545	L407	K305	R137	E10
S813	S723	ARG	R549	I408	F306	R144	R16
L814	K724	ASN	O550	E409			
E819	D725	LYS		L410	L310		
A820	L726	LYS	A557	F411	D311	R148	R19
	S727	LYS	I560	L412			C20
R825	D728	ASP	A561	K414	R315	Y158	Q25
	T729	ASP	I562	R415	F318	H159	
C828	V730	ASP		I417		L160	L30
H829	L741	ASP	S572	M423	P324	Y164	
L836	PHE	GLU	THR	I424	V325	E188	K41
F838	GLY	GLU	ASP		F326		F42
R839	ALA	GLY	ASP	K450	S331	L194	H45
M840	T745	GLY	ASN	Y451		Y195	
P841	H746	PRO	LYS	M452	K334	Q196	K52
	T747	LYS	GLU	L453		N197	S53
GLY	T753	E640	HIS	K454	E337	Q198	L54
TYR	F754	E641	GLU	A461	K338	V199	T55
GLU		L642	ALA		V339		L56
GLU			ASP		A340	A203	
ASP	R757	K646	THR	M464	I341		L68
MET	N758	ALA	THR	C465	I342	R207	V69
LYS	S759	ASN	ASN	S466	E343		R70
ILE	D760	V650	MET	E344		E211	
THR	S761	THR	SER	T469	L345	H212	D76
VAL	L762	E656	ASP	B470	V346	L213	
ASN	P763		LYS	E471	V347		S79
GLY	H764	K665	GLU	G472	G348	E217	H80
ASP	R765	N666	LEU	A475	Y349	R218	
SER		L667	LYS			I220	V85
SER	A768	V668	LEU	C484	R357		Y86
ALA	A769	K669	LYS		L358	K230	
GLU	K770	N670	ARG	F487	F359		Q90
ALA	H771	K671	ASN	Q488		L234	
GLU	V772	T674	LYS		L374		Y96
GLU	Y773		GLN	C491	W375	R239	N105
LEU	Y774	I681	ARG	A492	V376		K108
ALA	P777	V682	ALA	Q493		E256	
ASN		F683	GLN	K507	L380	Y261	K111
ILE	Q780	R684	LYS		H383	L277	L114
	I784	K685	LYS	E510			
		E686	GLN	Y511	K386	E281	L120
	T788	M691	GLN	E512	I387		S121
T789		V695	ILE	H513	G388	K286	L122
L790			GLU		Q389	Y287	P123
D791		V695	GLU	T519	P390		Q124
		H705	LYS		S391		I125
L794			GLY	F525	K392	G290	
T795		L708	ASN	H526	I393	Y291	

- Chain C:
-
- | Label | Color |
|-------|--------|
| MET | Grey |
| PRO | Grey |
| A3 | Green |
| V4 | Green |
| K9 | Yellow |
| L13 | Yellow |
| I17 | Yellow |
| C20 | Yellow |
| K24 | Yellow |
| Q25 | Yellow |
| N28 | Yellow |
| K31 | Yellow |
| P32 | Yellow |
| C33 | Green |
| K34 | Yellow |
| Q35 | Yellow |
| S38 | Yellow |
| N39 | Yellow |
| P40 | Green |
| K41 | Yellow |
| A50 | Yellow |
| M51 | Yellow |
| L54 | Yellow |
| T55 | Yellow |
| L59 | Green |
| G60 | Yellow |
| K61 | Yellow |
| K62 | Yellow |
| E63 | Green |
| E64 | Yellow |
| A65 | Yellow |
| V66 | Yellow |
| E67 | Green |
| L68 | Green |
| V69 | Yellow |
| R70 | Yellow |
| R71 | Yellow |
| G72 | Yellow |
| L73 | Yellow |
| R74 | Yellow |
| L77 | Yellow |
| V81 | Yellow |
| V85 | Yellow |
| K108 | Yellow |

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 0.205 , 0.256	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 , 73.0	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, IHP, 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	0.41	1/6412 (0.0%)	0.58	0/8648
1	C	0.45	1/6494 (0.0%)	0.64	2/8753 (0.0%)
2	B	0.47	1/1335 (0.1%)	0.66	0/1800
2	D	0.49	1/1313 (0.1%)	0.66	0/1773
All	All	0.44	4/15554 (0.0%)	0.62	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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	292	VAL	CA-CB	9.58	1.59	1.54
1	C	292	VAL	CA-CB	-8.40	1.49	1.54
2	D	0	ACE	C-N	6.82	1.47	1.33
2	B	0	ACE	C-N	6.08	1.45	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	737	GLU	N-CA-C	-6.44	104.34	111.36
1	C	68	LEU	N-CA-C	-5.84	104.92	111.28

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	158	0
1	C	6359	0	6390	144	0
2	B	1309	0	1277	23	0
2	D	1287	0	1247	33	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	343	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 (343) 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:688:PHE:HA	1:C:691:MET:HE2	1.59	0.85
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:GLN:HE22	1:C:28:ASN:HB3	1.49	0.77
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:OE1	1:A:10:GLU:N	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:25:GLN:CD	1:C:28:ASN:HB3	2.19	0.66
1:A:770:LYS:HG3	1:A:771:MET:HE2	1.78	0.66
1:C:722:GLU:O	1:C:723:SER:C	2.35	0.65
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
1:C:713:ILE:HB	1:C:771:MET:HE2	1.80	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:331:SER:CB	2:B:48:GLU:OE2	2.48	0.61
1:A:789:THR:C	1:A:790:LEU:HD12	2.25	0.61
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:C:431:MET:HE2	1:C:447:LYS:HB3	1.84	0.60
1:A:819:GLU:HG2	1:A:820:ALA:H	1.66	0.60
1:C:691:MET:HE3	1:C:715:LEU:HD13	1.83	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:A:452:MET:HE3	1:A:461:ALA:HA	1.85	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
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:C:449:ALA:HA	1:C:452:MET:HE3	1.88	0.56
1:A:297:PRO:HA	1:A:300:PHE:CE2	2.41	0.56
1:C:460:GLU:OE2	1:C:460:GLU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:OE2	2:D:61:GLU:HA	2.10	0.51
1:A:234:LEU:HD22	1:A:239:ARG:HB2	1.91	0.51
1:A:331:SER:HB3	2:B:48:GLU:CD	2.35	0.51
2:D:130:ILE:HG13	2:D:147:MET:HE3	1.90	0.51
1:A:357:ARG:H	1:A:357:ARG:HD2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:452:MET:HE1	1:A:464:MET:CB	2.41	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:760:ASP:OD1	1:A:760:ASP:N	2.39	0.50
1:A:134:ARG:HD3	1:A:158:TYR:CZ	2.46	0.50
1:C:448:CYS:SG	1:C:464:MET:HE3	2.51	0.50
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: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: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
2:D:88:GLN:H	2:D:88:GLN:CD	2.20	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:452:MET:HE1	1:C:464:MET:HB2	1.95	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:C:734:LEU:HD12	1:C:734:LEU:C	2.38	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:68:LEU:O	1:C:72:GLY:N	2.32	0.48
1:C:559:ARG:O	1:C:563:GLU:HG2	2.13	0.48
1:A:324:PRO:HG3	2:B:81:HIS:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:PHE:CE1	1:A:758:ASN:ND2	2.81	0.48
1:C:297:PRO:HA	1:C:300:PHE:CE2	2.48	0.48
1:C:431:MET:HE2	1:C:447:LYS:CB	2.43	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:A:681:ILE:O	1:A:685:LYS:HB2	2.14	0.48
1:C:9:LYS:O	1:C:13:LEU:HD13	2.14	0.48
1:C:71:ARG:HA	1:C:74:ARG:HB2	1.95	0.48
1:C:452:MET:HE1	1:C:464:MET:CB	2.44	0.48
1:A:791:ASP:OD1	1:A:791:ASP:N	2.47	0.47
1:A:70:ARG:NH1	1:A:86:TYR:OH	2.43	0.47
1:A:780:GLN:O	1:A:784:ILE:HD13	2.14	0.47
1:A:86:TYR:O	1:A:90:GLN:HG3	2.14	0.47
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
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:73:LEU:O	1:C:77:LEU:HD23	2.14	0.47
1:C:523:PHE:HA	1:C:526:HIS:CD2	2.50	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: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:25:GLN:CD	1:C:25:GLN:O	2.59	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:76:ASP:OD2	1:A:79:SER:HB2	2.15	0.46
1:A:217:GLU:OE2	1:A:230:LYS:NZ	2.49	0.46
2:B:112:ARG:HB3	2:B:142:GLU:CD	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:28:ASN:OD1	1:C:28:ASN:C	2.59	0.45
1:C:473:THR:HG23	1:C:474:SER:O	2.17	0.45
1:C:494:ALA:O	1:C:498:MET:HG3	2.17	0.45
1:C:533:ILE:HG22	1:C:533:ILE:O	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:318:PHE:CE2	1:A:376:VAL:HG12	2.52	0.45
1:A:346:VAL:HA	1:A:349:TYR:CD2	2.44	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
1:C:448:CYS:SG	1:C:452:MET:HE2	2.57	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:31:LYS:O	1:C:35:GLN:HG3	2.17	0.45
1:C:306:PHE:CE2	1:C:310:LEU:HD22	2.52	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
1:A:374:LEU:HD21	1:A:407:LEU:CD2	2.47	0.44
1:C:24:LYS:HA	1:C:24:LYS:HD3	1.84	0.44
2:B:4:ARG:CZ	2:B:44:ILE:HD11	2.48	0.44
1:C:74:ARG:HH21	1:C:74:ARG:HG3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:LEU:HD23	1:A:160:LEU:HB3	2.00	0.44
1:A:813:SER:O	1:A:814:LEU:HD23	2.17	0.44
2:B:127:ASN:O	2:B:127:ASN:ND2	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:737:GLU:O	1:C:738:MET:C	2.59	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:404:THR:C	1:C:406:THR:H	2.27	0.43
1:A:4:VAL:HG23	1:A:45:HIS:CE1	2.54	0.43
1:A:470:ARG:HG2	1:A:472:GLY:H	1.82	0.43
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:C:680:GLU:CD	1:C:714:ARG:HH12	2.27	0.43
1:A:256:GLU:OE1	1:A:290:GLY:HA2	2.19	0.42
1:C:74:ARG:HB2	1:C:74:ARG:CZ	2.48	0.42
1:C:425:LYS:HE3	1:C:429:ARG:NH2	2.30	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:HD3	1:C:144:ARG:HA	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:72:ILE:HG13	2:D:91:MET:HE1	2.01	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:HD13	1:A:387:ILE:HA	1.81	0.41
2:B:112:ARG:HH12	2:B:140:ASP:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:TYR:CD1	1:A:123:LEU:HD22	2.54	0.41
1:A:111:LYS:HB3	1:A:111:LYS:HE2	1.87	0.41
1:C:258:TRP:CE2	2:D:2:ASN:HB2	2.55	0.41
2:D:127:ASN:CG	2:D:149:ARG:NH1	2.77	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:9:LYS:HD3	1:C:9:LYS:HA	1.67	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:A:305:LYS:HD3	1:A:305:LYS:HA	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:54:LEU:HD22	1:A:85:VAL:HG13	2.01	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
1:A:326:PHE:HZ	1:A:386:LYS:HD2	1.86	0.41
1:C:235:LEU:HD23	1:C:240:LEU:HD22	2.03	0.41
1:A:291:LEU:HD12	2:B:0:ACE:CH3	2.51	0.41
1:A:646:LYS:HA	1:A:649:LYS:HD2	2.02	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:25:GLN:OE1	1:C:165:GLU:HG3	2.20	0.41
1:A:387:ILE:HG22	1:A:389:GLN:HG3	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:C:272:ASN:CG	1:C:275:GLU:HG3	2.46	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:HD12	1:C:397:ILE:HA	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:A:839:MET:HE2	1:A:839:MET:HB3	1.94	0.40
1:A:423:ASN:CG	1:A:836:LEU:HD11	2.46	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	48	77
1	C	769/866 (89%)	746 (97%)	21 (3%)	2 (0%)	36	66
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%)	43	72

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 [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	665/769 (86%)	664 (100%)	1 (0%)	87	96
1	C	686/769 (89%)	686 (100%)	0	100	100
2	B	139/202 (69%)	139 (100%)	0	100	100
2	D	134/202 (66%)	134 (100%)	0	100	100
All	All	1624/1942 (84%)	1623 (100%)	1 (0%)	88	97

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

Mol	Chain	Res	Type
1	A	291	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	212	HIS
1	A	362	ASN
1	A	480	ASN
1	A	488	GLN
1	A	670	ASN
1	A	717	ASN
1	A	758	ASN
1	A	827	ASN
2	B	16	HIS
2	B	27	GLN
2	B	153	GLN
1	C	25	GLN
1	C	35	GLN
1	C	90	GLN
1	C	115	GLN
1	C	147	GLN
1	C	178	GLN
1	C	197	ASN
1	C	219	GLN
1	C	382	GLN
1	C	488	GLN
1	C	739	ASN
1	C	758	ASN
1	C	827	ASN
2	D	69	HIS
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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	901	-	36,36,36	1.57	9 (25%)	60,60,60	3.92	21 (35%)
3	IHP	C	902	-	36,36,36	1.84	10 (27%)	60,60,60	3.57	26 (43%)
4	1PE	C	901	-	15,15,15	0.53	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	A	901	-	-	9/30/54/54	0/1/1/1
3	IHP	C	902	-	-	13/30/54/54	0/1/1/1
4	1PE	C	901	-	-	4/13/13/13	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	902	IHP	P3-O13	4.61	1.67	1.59
3	A	901	IHP	P2-O12	3.76	1.66	1.59
3	C	902	IHP	P2-O12	3.62	1.65	1.59
3	C	902	IHP	C3-C2	3.61	1.59	1.52
3	C	902	IHP	P6-O16	3.33	1.65	1.59
3	A	901	IHP	P3-O13	3.31	1.65	1.59
3	A	901	IHP	P4-O14	3.29	1.65	1.59
3	C	902	IHP	O15-C5	-3.16	1.33	1.44
3	C	902	IHP	P4-O14	3.10	1.65	1.59
3	C	902	IHP	C6-C5	-2.69	1.46	1.52
3	A	901	IHP	C3-C2	2.66	1.57	1.52
3	C	902	IHP	C2-C1	2.65	1.57	1.52
3	C	902	IHP	C4-C3	2.54	1.57	1.52
3	A	901	IHP	P1-O11	2.48	1.63	1.59
3	A	901	IHP	C2-C1	2.39	1.57	1.52
3	A	901	IHP	C6-C5	-2.35	1.47	1.52
3	C	902	IHP	P1-O11	2.32	1.63	1.59
3	A	901	IHP	C4-C3	2.29	1.57	1.52
3	A	901	IHP	O15-C5	-2.26	1.36	1.44

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	IHP	O11-C1-C6	-12.54	82.08	108.76
3	C	902	IHP	C6-C5-C4	12.01	136.79	110.43
3	C	902	IHP	O11-C1-C6	-11.09	85.16	108.76
3	A	901	IHP	O16-C6-C1	10.72	131.56	108.76
3	A	901	IHP	C6-C5-C4	10.35	133.14	110.43
3	A	901	IHP	O14-C4-C3	10.24	130.54	108.76
3	C	902	IHP	O16-C6-C1	9.63	129.24	108.76
3	A	901	IHP	O11-C1-C2	-8.38	90.94	108.76
3	C	902	IHP	O14-C4-C3	8.37	126.57	108.76
3	A	901	IHP	O15-C5-C4	6.91	123.45	108.76
3	A	901	IHP	P4-O14-C4	6.70	141.34	123.43
3	C	902	IHP	P4-O14-C4	6.15	139.85	123.43
3	C	902	IHP	O15-C5-C6	-6.10	95.79	108.76
3	A	901	IHP	O12-C2-C1	6.04	121.61	108.76
3	A	901	IHP	C3-C2-C1	5.89	123.36	110.43
3	A	901	IHP	O13-C3-C4	5.76	121.01	108.76
3	C	902	IHP	O12-C2-C3	5.58	120.64	108.76
3	A	901	IHP	O14-C4-C5	5.55	120.58	108.76
3	C	902	IHP	O13-C3-C2	5.03	119.46	108.76
3	A	901	IHP	P2-O12-C2	4.86	136.42	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	902	IHP	C3-C2-C1	4.80	120.96	110.43
3	C	902	IHP	O14-C4-C5	4.71	118.78	108.76
3	A	901	IHP	P6-O16-C6	4.19	134.61	123.43
3	C	902	IHP	P2-O12-C2	4.14	134.50	123.43
3	C	902	IHP	C6-C1-C2	4.13	119.49	110.43
3	A	901	IHP	O15-C5-C6	-3.87	100.53	108.76
3	C	902	IHP	O11-C1-C2	-3.76	100.77	108.76
3	A	901	IHP	P1-O11-C1	3.74	133.42	123.43
3	A	901	IHP	C4-C3-C2	3.22	117.49	110.43
3	C	902	IHP	O33-P3-O13	3.17	118.19	105.85
3	A	901	IHP	O33-P3-O13	3.03	117.67	105.85
3	C	902	IHP	O42-P2-O12	2.95	117.35	105.85
3	C	902	IHP	O15-C5-C4	2.83	114.78	108.76
3	C	902	IHP	O13-C3-C4	2.70	114.50	108.76
3	A	901	IHP	O13-P3-O23	-2.63	99.97	109.33
3	C	902	IHP	P6-O16-C6	2.57	130.31	123.43
3	C	902	IHP	O16-P6-O26	-2.56	100.20	109.33
3	A	901	IHP	C5-C6-C1	2.40	115.68	110.43
3	C	902	IHP	P5-O15-C5	2.37	129.75	123.43
3	C	902	IHP	O12-C2-C1	-2.25	103.98	108.76
3	C	902	IHP	O46-P6-O16	2.19	114.40	105.85
3	A	901	IHP	O12-C2-C3	-2.18	104.12	108.76
3	C	902	IHP	P1-O11-C1	2.15	129.19	123.43
3	A	901	IHP	O35-P5-O15	2.10	114.04	105.85
3	C	902	IHP	O44-P4-O14	2.08	113.95	105.85
3	C	902	IHP	O36-P6-O16	2.04	113.81	105.85
3	C	902	IHP	O16-C6-C5	2.04	113.10	108.76

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	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

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

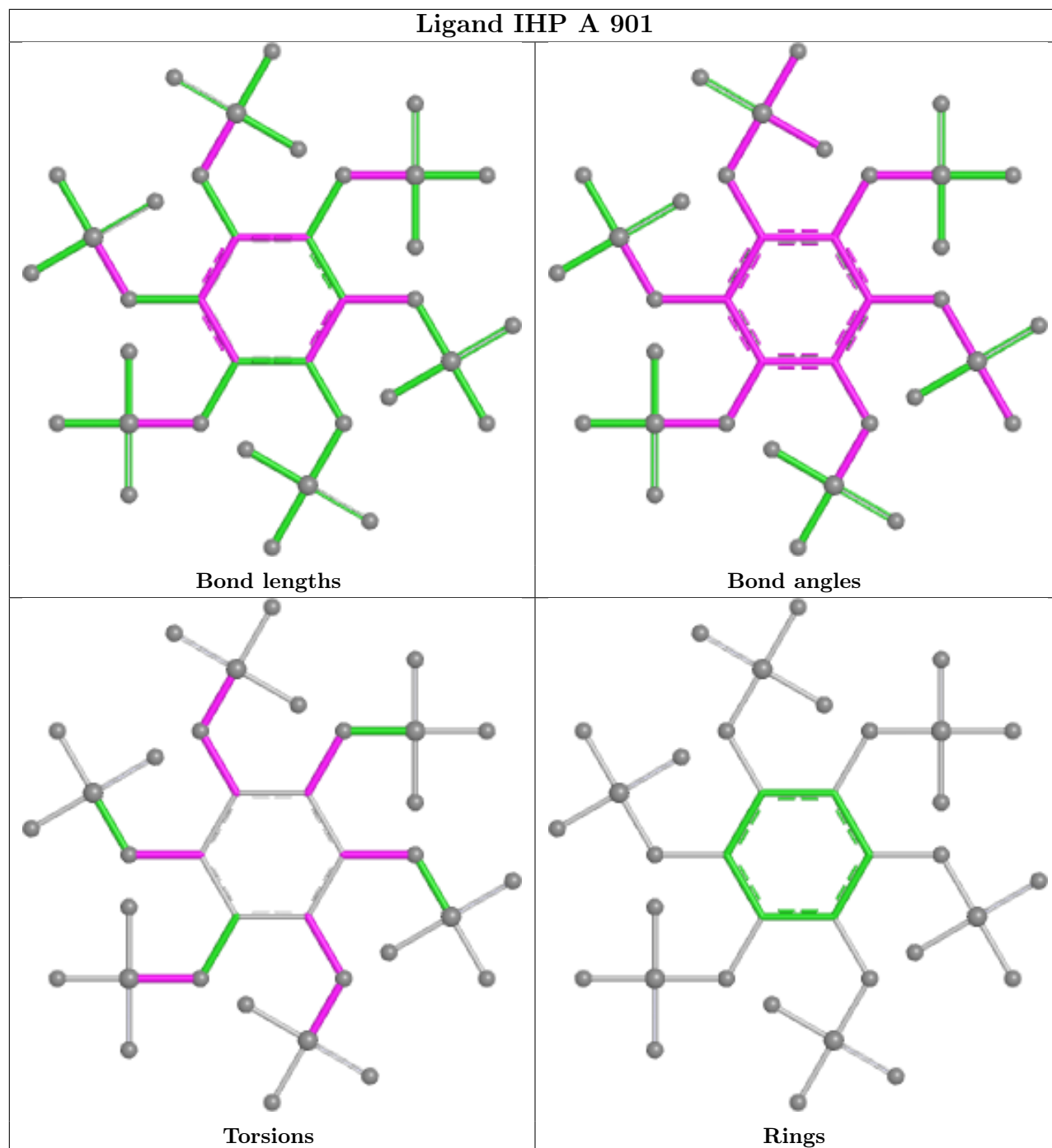
There are no ring outliers.

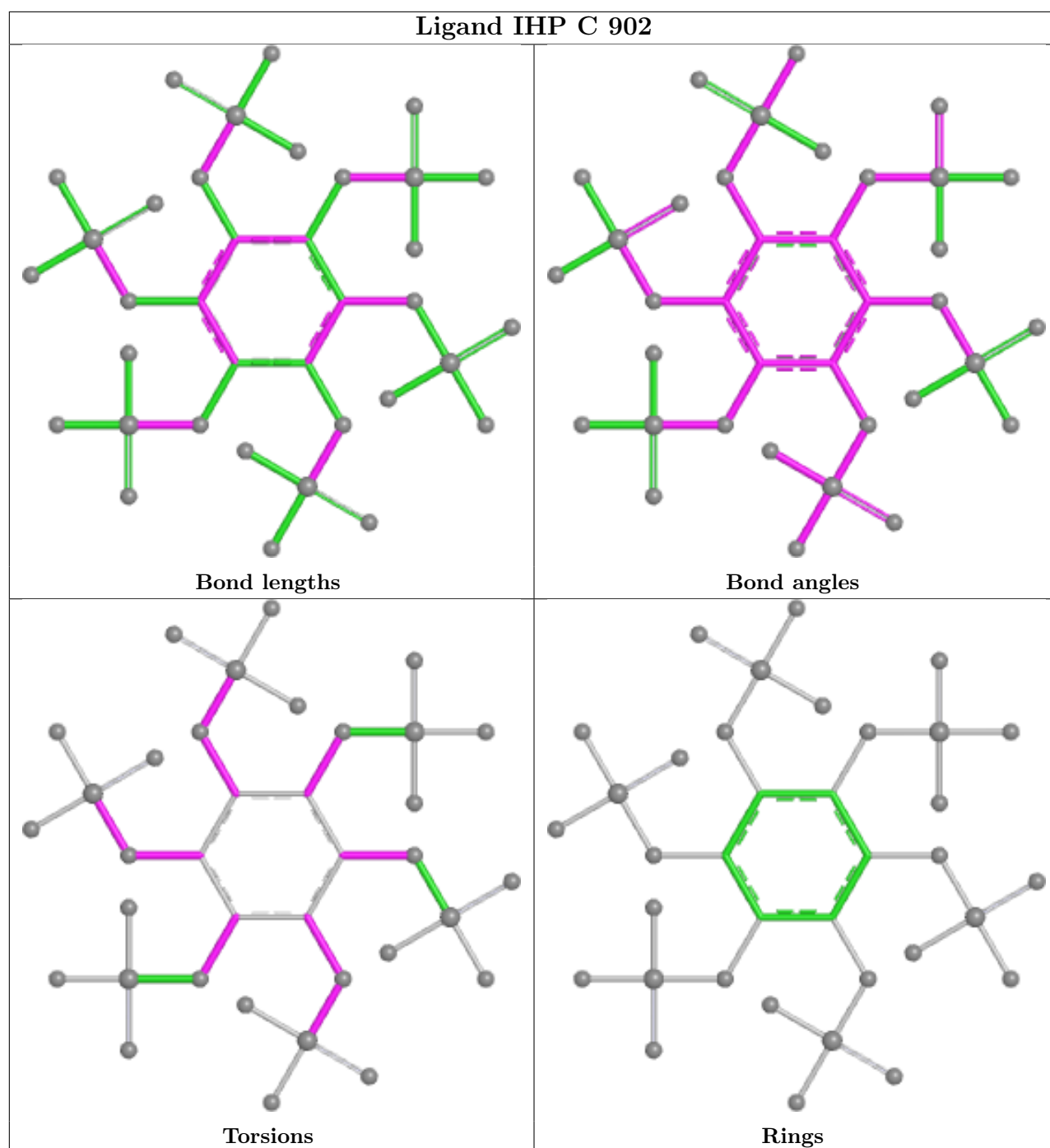
1 monomer is involved in 2 short contacts:

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 A 901





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%)	-0.15	13 (1%) 69 60	51, 95, 155, 210	0
1	C	773/866 (89%)	-0.36	13 (1%) 69 60	52, 79, 138, 181	0
2	B	160/236 (67%)	-0.49	1 (0%) 85 80	52, 73, 111, 151	0
2	D	160/236 (67%)	-0.33	4 (2%) 58 48	57, 79, 143, 182	0
All	All	1864/2204 (84%)	-0.28	31 (1%) 69 60	51, 85, 145, 210	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3	ALA	6.1
1	C	376	VAL	5.0
1	A	723	SER	4.7
1	A	741	LEU	3.9
1	C	734	LEU	3.3
1	C	322	CYS	3.3
1	A	730	VAL	3.2
1	A	725	ASP	3.1
1	A	728	ASP	3.0
2	D	66	ASP	2.9
1	A	727	SER	2.9
2	D	65	ASP	2.8
1	A	777	PRO	2.8
1	C	4	VAL	2.8
1	A	724	LYS	2.7
1	C	841	PRO	2.6
1	A	376	VAL	2.5
2	B	65	ASP	2.5
1	A	745	THR	2.5
1	C	735	LYS	2.5
1	C	68	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	291	LEU	2.4
1	A	572	PRO	2.4
1	C	742	PHE	2.3
1	C	59	LEU	2.2
1	A	1	MET	2.1
1	C	67	GLU	2.1
1	C	738	MET	2.0
2	D	88	GLN	2.0
1	A	747	PRO	2.0
2	D	160	ARG	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](#)

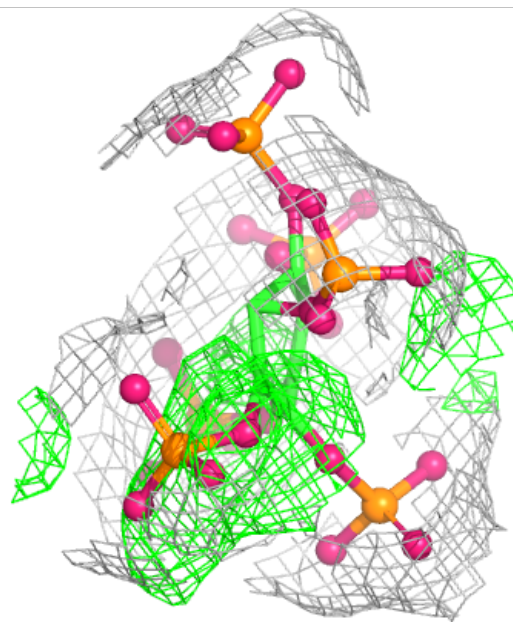
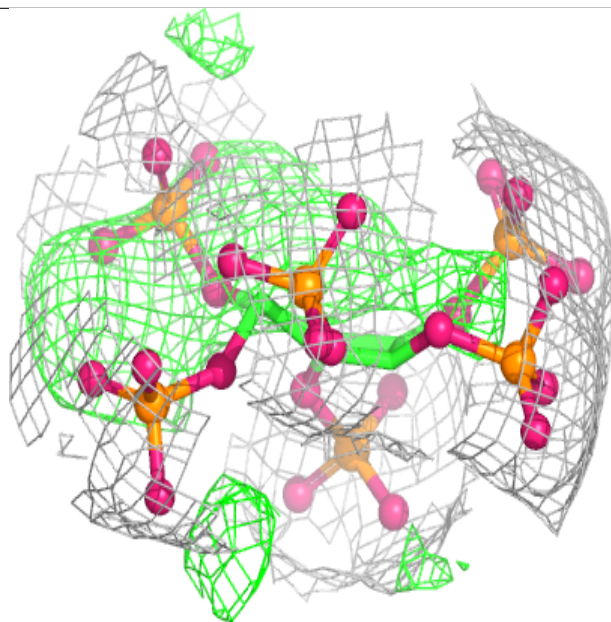
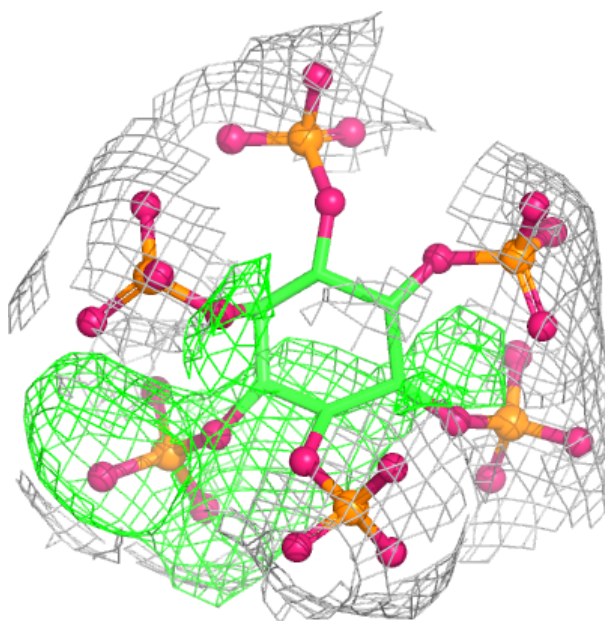
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	1PE	C	901	16/16	0.81	0.16	98,112,122,122	0
3	IHP	A	901	36/36	0.82	0.11	121,152,164,167	0
3	IHP	C	902	36/36	0.83	0.12	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.

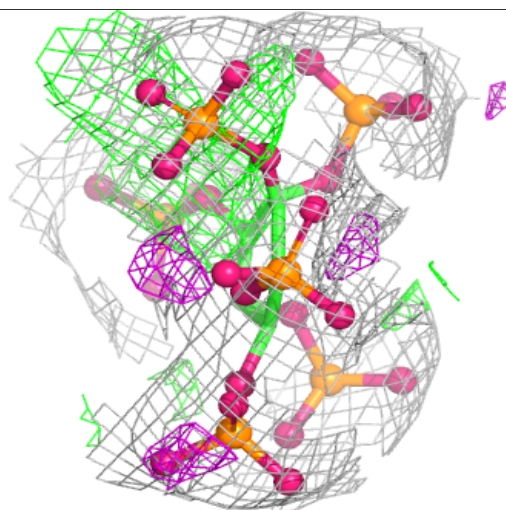
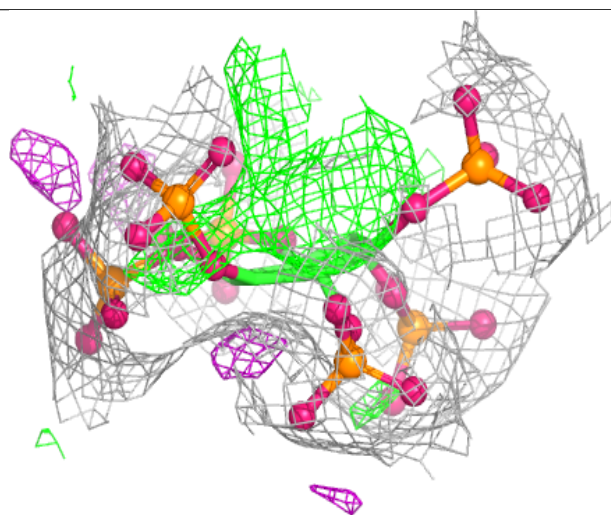
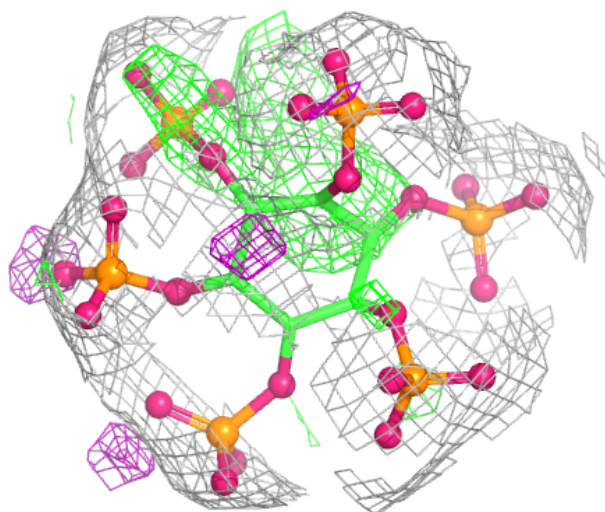
Electron density around IHP A 901:

$2mF_o-DF_c$ (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.