



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 08:29 pm BST

PDB ID : 2BFY
Title : Complex of Aurora-B with INCENP and Hesperadin.
Authors : Sessa, F.; Mapelli, M.; Ciferri, C.; Tarricone, C.; Areces, L.B.; Schneider, T.R.;
Stukenberg, P.T.; Musacchio, A.
Deposited on : 2004-12-15
Resolution : 1.80 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	:	2.11
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)	:	2.11

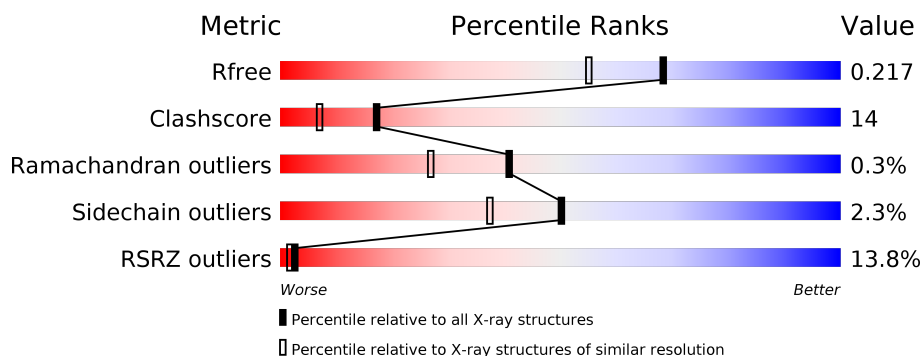
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	284	<div> <div>10%</div> <div>79%</div> <div>16%</div> <div>• •</div> </div>
1	B	284	<div> <div>8%</div> <div>80%</div> <div>17%</div> <div>• •</div> </div>
2	C	43	<div> <div>35%</div> <div>63%</div> <div>26%</div> <div>• 9%</div> </div>
2	D	43	<div> <div>44%</div> <div>47%</div> <div>30%</div> <div>• 21%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5636 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 AURORA KINASE B-A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	P	S	0	0	1
			2265	1452	409	390	1	13			
1	B	280	Total	C	N	O	P	S	0	0	1
			2323	1489	418	401	1	14			

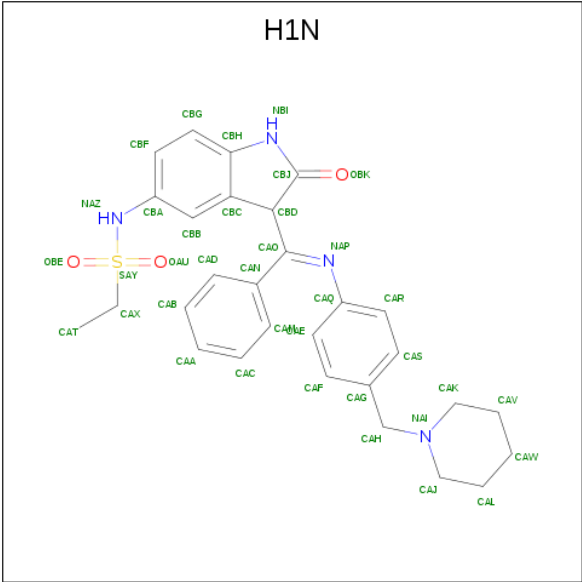
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	VAL	GLY	engineered mutation	UNP Q7ZYT9
B	96	VAL	GLY	engineered mutation	UNP Q7ZYT9

- Molecule 2 is a protein called INNER CENTROMERE PROTEIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	39	Total	C	N	O	S	0	0	1
			312	201	52	58	1			
2	D	34	Total	C	N	O	S	0	0	1
			279	179	46	53	1			

- Molecule 3 is N-[2-OXO-3-((E)-PHENYL{[4-(PIPERIDIN-1-YLMETHYL)PHENYL]IMINO}METHYL)-2,6-DIHYDRO-1H-INDOL-5-YL]ETHANESULFONAMIDE (three-letter code: H1N) (formula: C₂₉H₃₂N₄O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			37	29	4	3	1		
3	B	1	Total	C	N	O	S	0	0
			37	29	4	3	1		

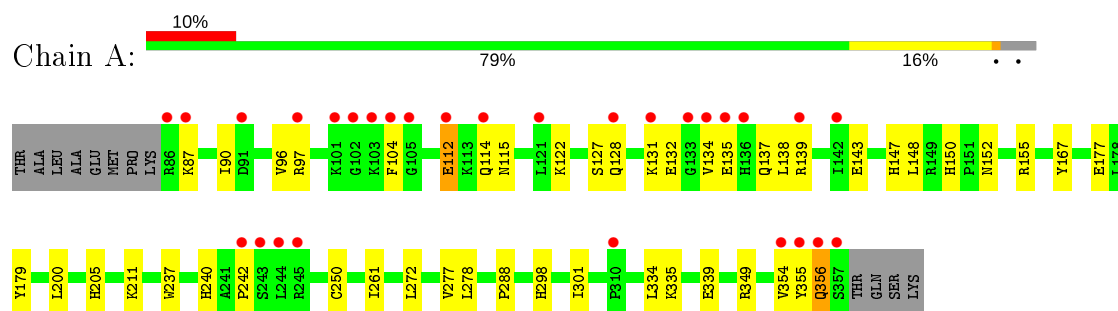
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	166	Total	O	0	0
			166	166		
4	B	194	Total	O	0	0
			194	194		
4	C	15	Total	O	0	0
			15	15		
4	D	8	Total	O	0	0
			8	8		

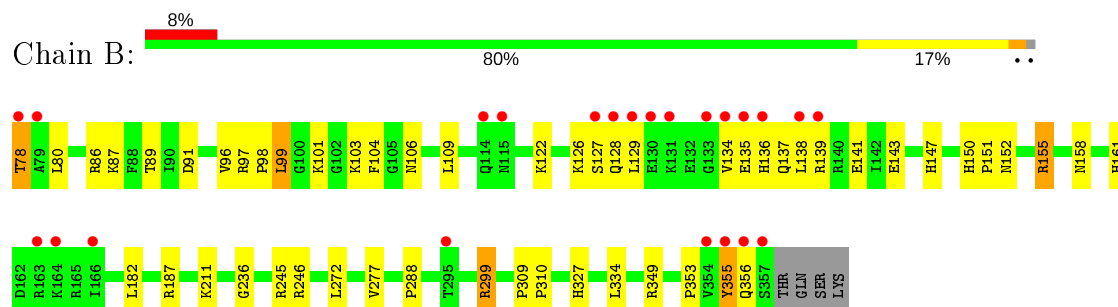
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

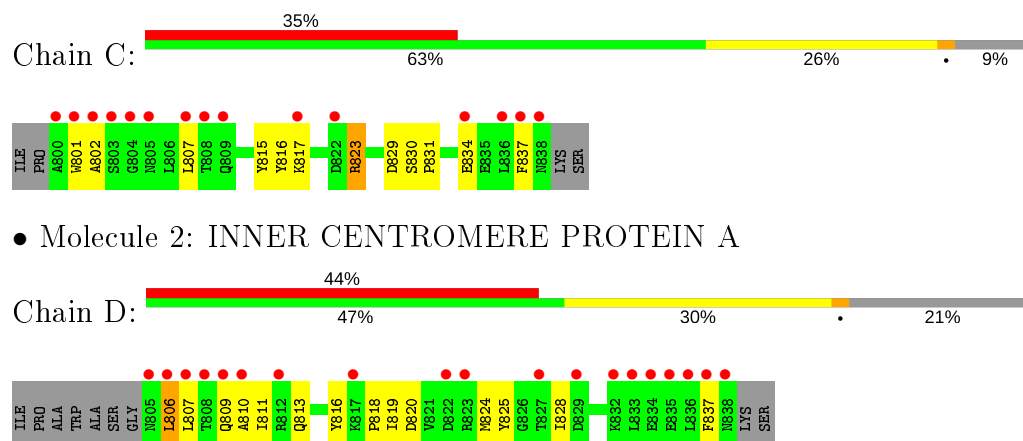
• Molecule 1: AURORA KINASE B-A



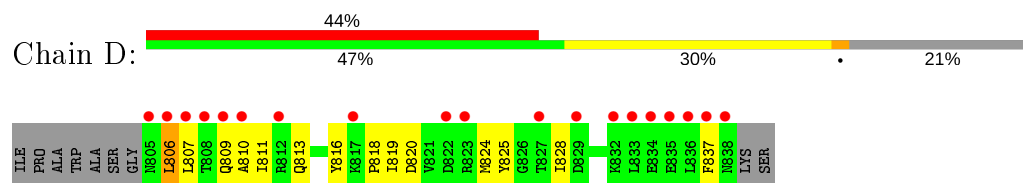
• Molecule 1: AURORA KINASE B-A



• Molecule 2: INNER CENTROMERE PROTEIN A



• Molecule 2: INNER CENTROMERE PROTEIN A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	45.95Å 67.04Å 116.46Å 90.00° 96.51° 90.00°	Depositor
Resolution (Å)	19.34 – 1.80 19.34 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.2 (19.34-1.80) 93.7 (19.34-1.70)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.203 , 0.226 0.192 , 0.217	Depositor DCC
R_{free} test set	3689 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5636	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% 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: TPO, H1N

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	0.56	0/2315	0.75	0/3116
1	B	0.56	0/2374	0.76	0/3196
2	C	0.48	0/319	0.65	0/433
2	D	0.47	0/284	0.63	0/384
All	All	0.55	0/5292	0.74	0/7129

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2265	0	2273	45	0
1	B	2323	0	2336	68	0
2	C	312	0	302	25	0
2	D	279	0	277	18	0
3	A	37	0	31	12	0
3	B	37	0	31	10	0
4	A	166	0	0	4	0
4	B	194	0	0	9	0
4	C	15	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	8	0	0	0	0
All	All	5636	0	5250	146	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 14.

All (146) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:LYS:NZ	2:C:831:PRO:HA	1.59	1.15
1:B:299:ARG:HH11	1:B:299:ARG:HG2	1.20	1.04
1:B:155:ARG:HH11	1:B:155:ARG:HB3	1.21	1.02
1:B:87:LYS:HZ3	2:C:831:PRO:HA	1.25	0.94
1:B:155:ARG:NH1	1:B:155:ARG:HB3	1.82	0.93
1:B:97:ARG:HD2	2:C:802:ALA:HB3	1.54	0.87
1:A:150:HIS:HD2	1:A:152:ASN:H	1.19	0.86
1:A:211:LYS:HD3	1:A:242:PRO:HA	1.59	0.85
1:B:89:THR:HG22	1:B:91:ASP:H	1.39	0.85
3:B:1357:H1N:HAX2	3:B:1357:H1N:HBF	1.58	0.85
1:B:96:VAL:HG12	2:C:802:ALA:HB2	1.59	0.84
1:B:87:LYS:HZ2	2:C:831:PRO:HA	1.40	0.84
1:A:112:GLU:HG2	2:D:825:TYR:OH	1.79	0.83
1:B:87:LYS:NZ	2:C:831:PRO:CA	2.42	0.81
1:B:78:THR:HG23	1:B:80:LEU:H	1.43	0.81
1:A:139:ARG:HG2	2:D:837:PHE:CE1	2.14	0.81
1:B:150:HIS:HD2	1:B:152:ASN:H	1.27	0.81
1:B:299:ARG:HG2	1:B:299:ARG:NH1	1.91	0.78
1:A:150:HIS:CD2	1:A:152:ASN:H	2.01	0.78
3:B:1357:H1N:HAR	3:B:1357:H1N:CAN	2.17	0.75
3:A:1357:H1N:HBF	3:A:1357:H1N:HAX2	1.67	0.74
3:A:1357:H1N:CAN	3:A:1357:H1N:HAR	2.17	0.73
1:B:87:LYS:HZ3	2:C:831:PRO:CA	2.02	0.71
1:B:150:HIS:CD2	1:B:152:ASN:H	2.08	0.71
2:D:806:LEU:HD12	2:D:809:GLN:HB2	1.75	0.69
1:A:135:GLU:HG3	2:D:837:PHE:CD2	2.28	0.69
1:B:96:VAL:CG1	2:C:802:ALA:HB2	2.23	0.68
1:A:122:LYS:HD3	4:A:2006:HOH:O	1.93	0.67
1:B:136:HIS:CD2	1:B:139:ARG:HH21	2.13	0.66
1:B:87:LYS:HZ2	2:C:831:PRO:CA	2.05	0.66
2:C:802:ALA:CB	2:C:807:LEU:HD11	2.25	0.66
1:A:152:ASN:HD21	1:A:349:ARG:HH21	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:GLU:O	1:A:139:ARG:HG3	1.97	0.64
1:B:152:ASN:HD21	1:B:349:ARG:HH21	1.44	0.64
1:B:155:ARG:HH11	1:B:155:ARG:CB	2.04	0.63
3:A:1357:H1N:CBF	3:A:1357:H1N:HAX2	2.27	0.63
3:B:1357:H1N:HAX2	3:B:1357:H1N:CBF	2.27	0.63
3:A:1357:H1N:HAR	3:A:1357:H1N:CAD	2.29	0.62
1:A:335:LYS:O	1:A:339:GLU:HG3	1.99	0.62
1:B:137:GLN:O	1:B:141:GLU:HG3	2.01	0.61
1:A:127:SER:O	1:A:131:LYS:HG3	2.01	0.60
1:B:135:GLU:HG3	2:C:837:PHE:CD2	2.36	0.60
2:C:802:ALA:HB1	2:C:807:LEU:HD11	1.83	0.60
1:A:143:GLU:O	1:A:147:HIS:HD2	1.85	0.59
3:A:1357:H1N:HBB	3:A:1357:H1N:CAN	2.32	0.58
1:A:138:LEU:HD23	2:D:837:PHE:CZ	2.39	0.58
1:A:237:TRP:CD2	1:A:250:CYS:HB2	2.38	0.58
1:B:86:ARG:HG2	1:B:87:LYS:N	2.17	0.58
3:A:1357:H1N:CAM	3:A:1357:H1N:HBB	2.34	0.57
1:B:187:ARG:NH1	4:B:2072:HOH:O	2.36	0.57
1:B:299:ARG:HH11	1:B:299:ARG:CG	2.06	0.57
3:B:1357:H1N:CAD	3:B:1357:H1N:HAR	2.33	0.57
1:A:122:LYS:HE2	3:A:1357:H1N:OAU	2.05	0.56
1:B:99:LEU:CD1	1:B:109:LEU:HB2	2.35	0.56
3:B:1357:H1N:CAX	3:B:1357:H1N:HBF	2.34	0.56
1:B:99:LEU:HD13	1:B:109:LEU:HB2	1.88	0.55
2:D:819:ILE:HG22	2:D:820:ASP:N	2.21	0.55
1:B:138:LEU:HA	1:B:141:GLU:OE2	2.06	0.54
1:A:112:GLU:HG3	1:A:112:GLU:O	2.06	0.54
1:B:103:LYS:HE2	4:B:2109:HOH:O	2.07	0.54
1:B:143:GLU:O	1:B:147:HIS:HD2	1.90	0.54
1:B:152:ASN:ND2	1:B:349:ARG:HH21	2.07	0.53
1:B:355:TYR:N	4:B:2194:HOH:O	2.41	0.53
1:A:139:ARG:HH11	1:A:139:ARG:HB3	1.74	0.53
1:B:182:LEU:HB3	4:B:2069:HOH:O	2.08	0.52
1:A:155:ARG:HD3	4:A:2019:HOH:O	2.09	0.52
1:B:122:LYS:NZ	3:B:1357:H1N:OAU	2.35	0.52
1:A:104:PHE:CZ	1:A:134:VAL:HG11	2.45	0.51
3:A:1357:H1N:HAJ2	3:A:1357:H1N:CAF	2.40	0.51
1:B:187:ARG:NE	4:B:2073:HOH:O	2.43	0.51
1:B:127:SER:C	1:B:129:LEU:H	2.14	0.51
2:D:828:ILE:N	2:D:828:ILE:HD12	2.25	0.51
1:A:211:LYS:CD	1:A:242:PRO:HA	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:GLN:NE2	2:C:816:TYR:O	2.41	0.50
1:A:90:ILE:HG21	1:A:167:TYR:CZ	2.47	0.50
1:A:137:GLN:HG2	4:A:2013:HOH:O	2.12	0.50
1:A:128:GLN:HG3	1:A:132:GLU:OE2	2.11	0.50
1:B:187:ARG:CZ	4:B:2073:HOH:O	2.58	0.50
1:B:272:LEU:HD21	1:B:334:LEU:HG	1.93	0.50
1:B:137:GLN:HG2	1:B:141:GLU:OE2	2.12	0.49
1:B:96:VAL:HG11	2:C:807:LEU:HD21	1.95	0.49
2:D:809:GLN:O	2:D:813:GLN:HG3	2.13	0.49
1:A:355:TYR:O	1:A:356:GLN:HG3	2.13	0.48
1:A:135:GLU:CD	2:D:837:PHE:HB3	2.32	0.48
1:B:141:GLU:HG2	1:B:236:GLY:HA2	1.93	0.48
1:A:277:VAL:HG13	1:A:288:PRO:HD2	1.96	0.48
1:A:152:ASN:ND2	1:A:349:ARG:HH21	2.10	0.48
1:A:355:TYR:HD1	2:D:818:PRO:O	1.96	0.48
1:B:353:PRO:HD3	2:C:815:TYR:CZ	2.49	0.48
1:B:89:THR:HG22	1:B:91:ASP:N	2.19	0.47
1:B:135:GLU:HG3	2:C:837:PHE:CG	2.49	0.47
3:A:1357:H1N:CBB	3:A:1357:H1N:CAN	2.92	0.47
1:A:138:LEU:HD23	2:D:837:PHE:CE2	2.49	0.47
2:C:823:ARG:HG2	4:C:2009:HOH:O	2.14	0.47
1:A:139:ARG:CB	1:A:139:ARG:NH1	2.78	0.47
1:A:96:VAL:O	1:A:97:ARG:HG3	2.15	0.46
3:A:1357:H1N:CAR	3:A:1357:H1N:CAN	2.84	0.46
2:D:806:LEU:HD12	2:D:806:LEU:HA	1.49	0.46
2:D:816:TYR:C	2:D:818:PRO:HD3	2.36	0.46
1:A:211:LYS:HD2	4:A:2087:HOH:O	2.15	0.46
1:B:129:LEU:HD23	1:B:129:LEU:O	2.16	0.46
1:B:245:ARG:O	1:B:246:ARG:HD2	2.16	0.46
1:B:211:LYS:NZ	4:B:2095:HOH:O	2.48	0.46
1:B:96:VAL:CG1	2:C:807:LEU:HD21	2.46	0.46
1:A:135:GLU:HG3	2:D:837:PHE:CG	2.51	0.45
1:B:138:LEU:HD13	1:B:138:LEU:O	2.17	0.45
1:B:98:PRO:HD3	2:C:801:TRP:CD2	2.52	0.45
1:A:90:ILE:CG2	1:A:167:TYR:CZ	3.00	0.45
1:B:158:ASN:OD1	2:C:830:SER:HB3	2.17	0.45
2:D:806:LEU:CD1	2:D:809:GLN:CD	2.85	0.45
3:B:1357:H1N:CAX	3:B:1357:H1N:CBF	2.92	0.45
1:B:327:HIS:HB3	4:B:2179:HOH:O	2.16	0.45
3:B:1357:H1N:CAD	3:B:1357:H1N:CAR	2.95	0.45
3:B:1357:H1N:HBB	3:B:1357:H1N:CAN	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:HIS:C	1:A:242:PRO:HD3	2.38	0.44
3:B:1357:H1N:HBB	3:B:1357:H1N:CAM	2.47	0.43
1:A:205:HIS:CE1	1:A:335:LYS:HE3	2.54	0.43
1:B:98:PRO:HD3	2:C:801:TRP:CE2	2.54	0.43
2:D:806:LEU:O	2:D:810:ALA:HB2	2.19	0.43
3:A:1357:H1N:CAX	3:A:1357:H1N:CBF	2.96	0.43
1:B:138:LEU:HD12	2:C:837:PHE:HZ	1.83	0.43
2:C:834:GLU:HG3	4:C:2015:HOH:O	2.17	0.43
1:A:261:ILE:HD12	1:A:301:ILE:HG21	2.00	0.43
2:C:817:LYS:NZ	4:C:2008:HOH:O	2.50	0.43
1:A:177:GLU:OE2	3:A:1357:H1N:HAB	2.19	0.42
1:A:200:LEU:HD22	1:A:278:LEU:HD23	2.02	0.42
1:B:126:LYS:NZ	1:B:161:HIS:HD2	2.17	0.42
1:A:272:LEU:HD21	1:A:334:LEU:HG	2.01	0.42
2:D:807:LEU:O	2:D:811:ILE:HG13	2.19	0.42
1:A:150:HIS:HD2	1:A:152:ASN:N	2.01	0.42
1:B:87:LYS:HE3	4:B:2006:HOH:O	2.19	0.41
1:A:115:ASN:OD1	2:D:824:MET:HG3	2.20	0.41
1:B:150:HIS:CG	1:B:151:PRO:HD2	2.55	0.41
1:B:277:VAL:HG13	1:B:288:PRO:HD2	2.02	0.41
1:A:355:TYR:O	1:A:356:GLN:CB	2.69	0.41
1:A:112:GLU:OE2	1:A:114:GLN:HB3	2.21	0.41
1:B:103:LYS:O	1:B:104:PHE:HB2	2.21	0.41
1:B:96:VAL:HG11	2:C:807:LEU:CD2	2.50	0.41
1:A:354:VAL:HG12	1:A:355:TYR:N	2.34	0.41
1:B:309:PRO:HA	1:B:310:PRO:HD3	1.94	0.41
1:B:355:TYR:N	1:B:355:TYR:CD1	2.87	0.41
1:B:104:PHE:CE1	1:B:134:VAL:HG21	2.54	0.41
1:B:101:LYS:HD2	1:B:106:ASN:HD22	1.85	0.41
1:B:103:LYS:HE3	1:B:104:PHE:CE2	2.55	0.41
1:B:99:LEU:HD11	1:B:109:LEU:HB2	2.03	0.41
1:B:143:GLU:O	1:B:147:HIS:CD2	2.73	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	269/284 (95%)	259 (96%)	9 (3%)	1 (0%)	34	21
1	B	277/284 (98%)	264 (95%)	12 (4%)	1 (0%)	34	21
2	C	37/43 (86%)	35 (95%)	2 (5%)	0	100	100
2	D	32/43 (74%)	29 (91%)	3 (9%)	0	100	100
All	All	615/654 (94%)	587 (95%)	26 (4%)	2 (0%)	41	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	356	GLN
1	B	128	GLN

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	245/256 (96%)	240 (98%)	5 (2%)	55	44
1	B	251/256 (98%)	246 (98%)	5 (2%)	55	44
2	C	32/38 (84%)	30 (94%)	2 (6%)	18	6
2	D	31/38 (82%)	30 (97%)	1 (3%)	39	25
All	All	559/588 (95%)	546 (98%)	13 (2%)	50	37

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	LYS
1	A	112	GLU
1	A	148	LEU
1	A	179	TYR

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Mol	Chain	Res	Type
1	A	298	HIS
1	B	78	THR
1	B	99	LEU
1	B	155	ARG
1	B	299	ARG
1	B	355	TYR
2	C	823	ARG
2	C	829	ASP
2	D	806	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	HIS
1	A	150	HIS
1	A	152	ASN
1	B	106	ASN
1	B	136	HIS
1	B	137	GLN
1	B	147	HIS
1	B	150	HIS
1	B	152	ASN
1	B	161	HIS
2	C	813	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	TPO	A	248	1	8,10,11	2.04	2 (25%)	10,14,16	3.77	6 (60%)
1	TPO	B	248	1	8,10,11	1.86	1 (12%)	10,14,16	3.78	6 (60%)

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
1	TPO	A	248	1	-	1/9/11/13	-
1	TPO	B	248	1	-	1/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	248	TPO	P-OG1	-4.76	1.50	1.59
1	B	248	TPO	P-OG1	-4.54	1.50	1.59
1	A	248	TPO	P-O3P	-2.13	1.46	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	248	TPO	O3P-P-O1P	-6.43	85.50	110.68
1	A	248	TPO	O3P-P-O1P	-6.42	85.53	110.68
1	B	248	TPO	O3P-P-OG1	-6.30	77.76	105.99
1	A	248	TPO	O3P-P-OG1	-5.47	81.47	105.99
1	B	248	TPO	OG1-P-O1P	4.99	128.67	109.39
1	A	248	TPO	O3P-P-O2P	-4.56	90.20	107.64
1	A	248	TPO	P-OG1-CB	-4.25	110.38	123.21
1	B	248	TPO	O3P-P-O2P	-4.09	91.99	107.64
1	A	248	TPO	OG1-P-O1P	3.98	124.77	109.39
1	A	248	TPO	O2P-P-O1P	3.33	123.71	110.68
1	B	248	TPO	P-OG1-CB	-3.24	113.43	123.21
1	B	248	TPO	O2P-P-O1P	2.33	119.79	110.68

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	248	TPO	CB-OG1-P-O1P
1	B	248	TPO	CB-OG1-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	H1N	B	1357	-	39,41,41	2.29	9 (23%)	45,58,58	1.29	3 (6%)
3	H1N	A	1357	-	39,41,41	2.27	7 (17%)	45,58,58	1.41	4 (8%)

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	H1N	B	1357	-	-	11/24/57/57	0/5/5/5
3	H1N	A	1357	-	-	8/24/57/57	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1357	H1N	CAX-SAY	5.89	1.83	1.76
3	A	1357	H1N	CBA-NAZ	-5.85	1.33	1.43
3	B	1357	H1N	CBA-NAZ	-5.78	1.33	1.43
3	A	1357	H1N	CAX-SAY	5.67	1.83	1.76
3	B	1357	H1N	CAN-CAO	-5.44	1.39	1.48
3	A	1357	H1N	CAN-CAO	-5.11	1.40	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1357	H1N	CAQ-NAP	-5.09	1.33	1.42
3	B	1357	H1N	CAQ-NAP	-4.90	1.34	1.42
3	A	1357	H1N	OAU-SAY	4.89	1.50	1.43
3	B	1357	H1N	OBE-SAY	4.85	1.50	1.43
3	A	1357	H1N	OBE-SAY	4.85	1.50	1.43
3	B	1357	H1N	OAU-SAY	4.80	1.50	1.43
3	A	1357	H1N	CAO-NAP	3.61	1.33	1.28
3	B	1357	H1N	CAO-NAP	3.53	1.33	1.28
3	B	1357	H1N	CBJ-NBI	-2.36	1.33	1.37
3	B	1357	H1N	CBC-CBD	-2.01	1.39	1.44

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1357	H1N	OAU-SAY-OBE	-5.82	110.92	119.35
3	A	1357	H1N	OAU-SAY-OBE	-5.63	111.20	119.35
3	A	1357	H1N	CAQ-NAP-CAO	3.71	129.31	121.83
3	B	1357	H1N	CAQ-NAP-CAO	3.57	129.03	121.83
3	A	1357	H1N	CAT-CAX-SAY	-3.44	108.08	112.93
3	B	1357	H1N	CAT-CAX-SAY	-2.71	109.12	112.93
3	A	1357	H1N	CBF-CBA-NAZ	2.06	124.55	120.09

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1357	H1N	NAP-CAO-CBD-CBJ
3	B	1357	H1N	CBA-NAZ-SAY-OAU
3	B	1357	H1N	CBA-NAZ-SAY-CAX
3	A	1357	H1N	CBA-NAZ-SAY-OAU
3	A	1357	H1N	CBA-NAZ-SAY-CAX
3	A	1357	H1N	CAR-CAQ-NAP-CAO
3	B	1357	H1N	CAR-CAQ-NAP-CAO
3	B	1357	H1N	CAE-CAQ-NAP-CAO
3	A	1357	H1N	CAE-CAQ-NAP-CAO
3	B	1357	H1N	CAN-CAO-NAP-CAQ
3	A	1357	H1N	NAP-CAO-CBD-CBJ
3	B	1357	H1N	CAN-CAO-CBD-CBC
3	B	1357	H1N	CAN-CAO-CBD-CBJ
3	B	1357	H1N	CBA-NAZ-SAY-OBE
3	A	1357	H1N	CAN-CAO-CBD-CBC
3	A	1357	H1N	CAN-CAO-CBD-CBJ

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Mol	Chain	Res	Type	Atoms
3	B	1357	H1N	CAM-CAN-CAO-NAP
3	B	1357	H1N	CAD-CAN-CAO-NAP
3	A	1357	H1N	CAM-CAN-CAO-NAP

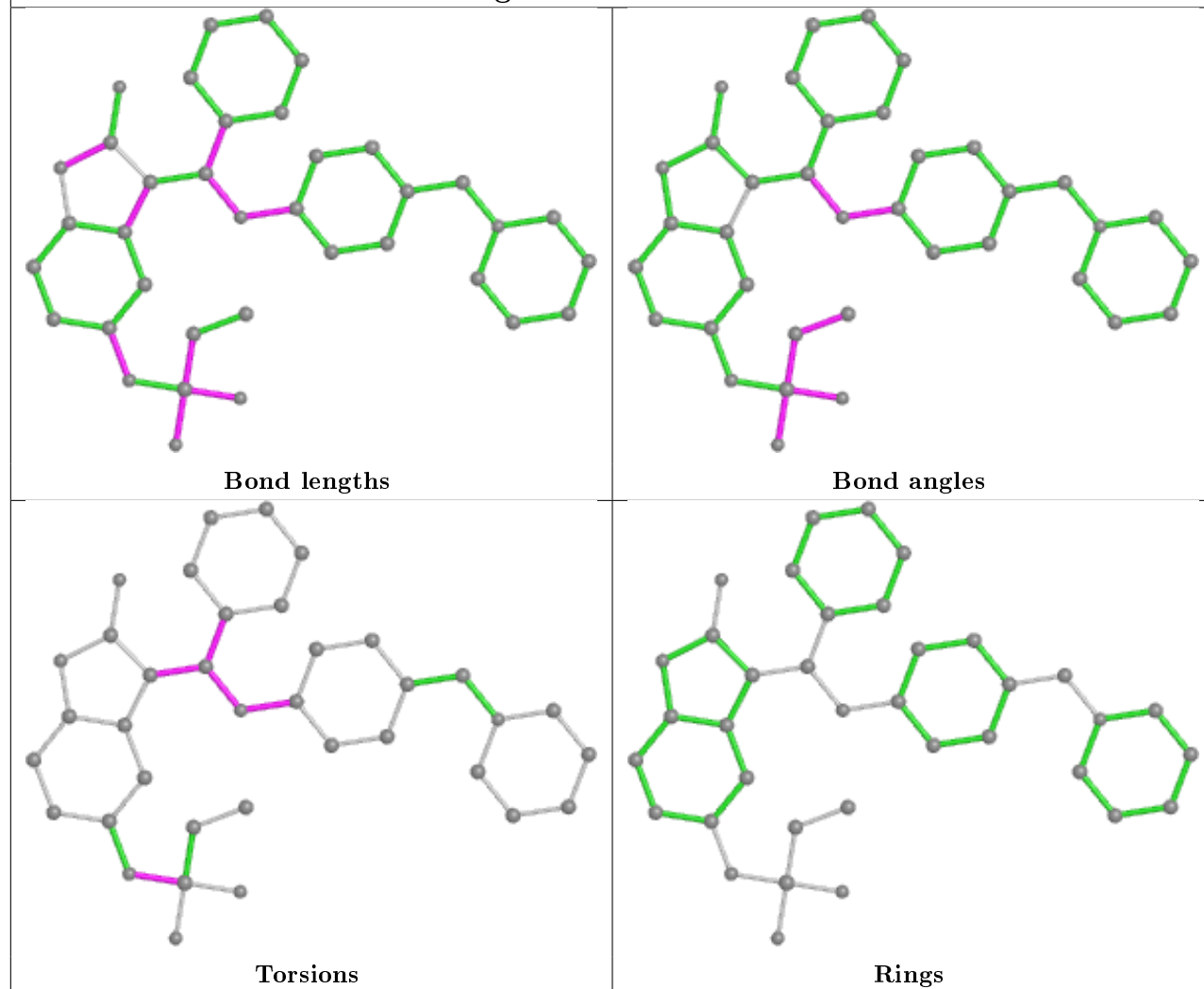
There are no ring outliers.

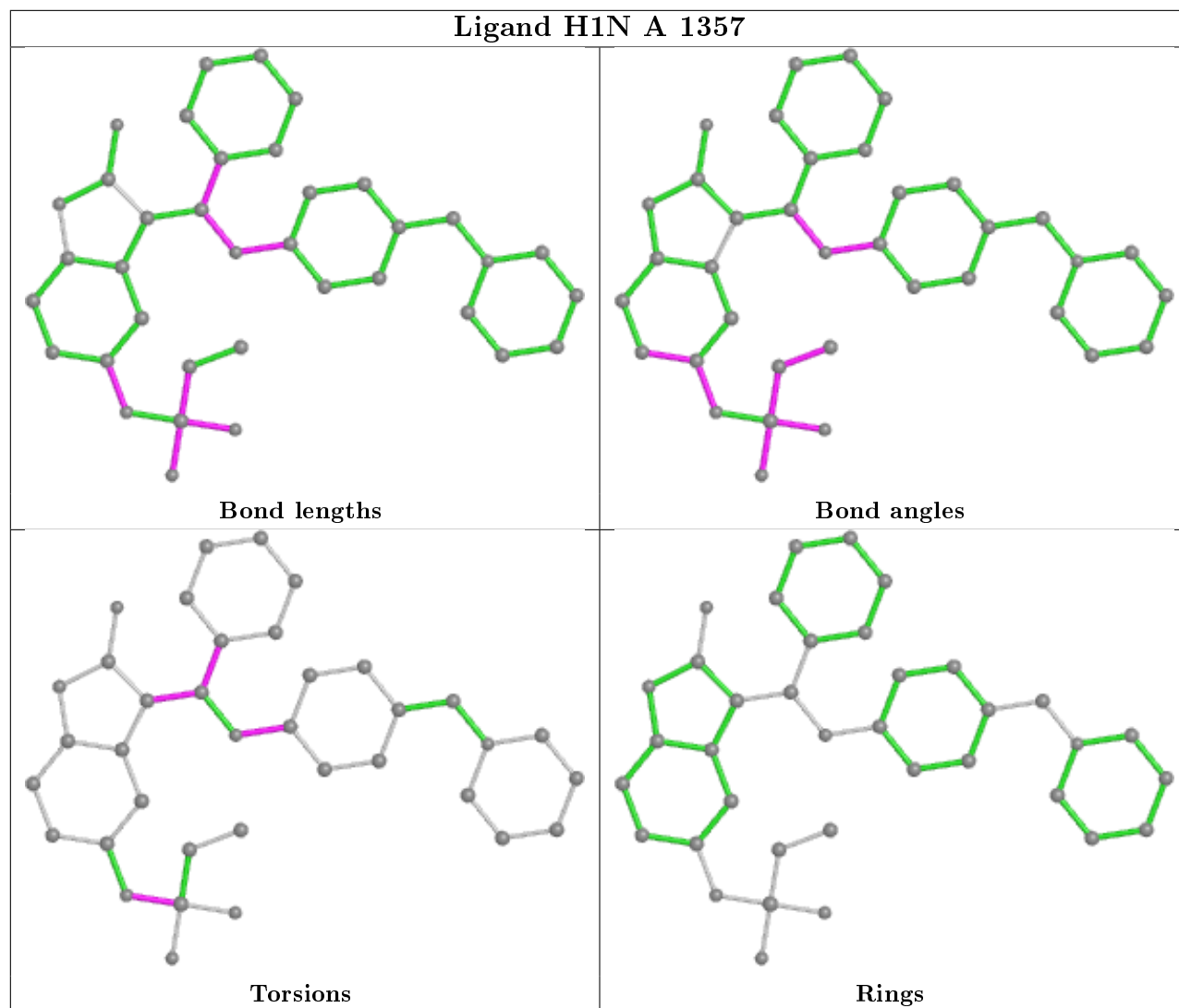
2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1357	H1N	10	0
3	A	1357	H1N	12	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 H1N B 1357





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	248:TPO	C	249:MET	N	1.63
1	A	248:TPO	C	249:MET	N	1.62

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	271/284 (95%)	0.58	29 (10%) 6 4	13, 26, 54, 67	0
1	B	279/284 (98%)	0.29	23 (8%) 11 9	12, 23, 53, 67	0
2	C	39/43 (90%)	1.85	15 (38%) 0 0	25, 41, 58, 63	0
2	D	34/43 (79%)	2.82	19 (55%) 0 0	29, 51, 70, 72	0
All	All	623/654 (95%)	0.65	86 (13%) 2 2	12, 26, 58, 72	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	357	SER	14.8
1	A	244	LEU	9.0
2	D	837	PHE	8.5
2	C	802	ALA	8.5
1	A	136	HIS	8.5
2	D	806	LEU	8.3
2	D	807	LEU	7.8
1	A	86	ARG	7.5
1	B	136	HIS	7.4
1	A	356	GLN	7.3
1	A	104	PHE	6.3
2	D	805	ASN	6.1
2	D	834	GLU	6.0
1	B	133	GLY	5.6
2	D	838	ASN	5.3
2	C	803	SER	5.1
1	B	355	TYR	5.0
2	D	808	THR	4.8
1	B	163	ARG	4.8
1	A	355	TYR	4.6
1	A	243	SER	4.5

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Mol	Chain	Res	Type	RSRZ
2	D	810	ALA	4.5
2	C	801	TRP	4.4
2	C	808	THR	4.2
1	A	97	ARG	4.2
2	D	809	GLN	4.1
1	A	114	GLN	4.1
2	C	834	GLU	4.1
2	C	800	ALA	4.1
1	B	128	GLN	4.0
2	C	837	PHE	3.9
1	B	78	THR	3.8
1	B	129	LEU	3.8
1	B	135	GLU	3.6
2	D	829	ASP	3.5
1	B	131	LYS	3.5
2	C	817	LYS	3.5
1	B	130	GLU	3.5
1	B	356	GLN	3.5
2	D	833	LEU	3.4
2	C	805	ASN	3.3
2	D	832	LYS	3.3
2	D	835	GLU	3.3
1	A	121	LEU	3.2
1	A	133	GLY	3.2
2	D	822	ASP	3.1
1	A	354	VAL	3.1
1	A	139	ARG	3.1
1	A	245	ARG	3.1
1	B	295	THR	2.9
1	A	103	LYS	2.9
2	D	817	LYS	2.9
1	A	105	GLY	2.8
1	A	102	GLY	2.8
2	C	804	GLY	2.7
1	B	357	SER	2.7
1	A	131	LYS	2.7
1	A	128	GLN	2.7
1	A	101	LYS	2.6
2	C	809	GLN	2.6
1	A	135	GLU	2.6
1	A	91	ASP	2.5
2	D	836	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	822	ASP	2.5
1	B	164	LYS	2.5
1	A	134	VAL	2.5
2	C	836	LEU	2.5
2	D	827	THR	2.4
2	D	823	ARG	2.4
2	C	838	ASN	2.4
1	B	354	VAL	2.3
1	B	79	ALA	2.3
2	D	812	ARG	2.3
1	A	310	PRO	2.2
1	A	142	ILE	2.2
1	B	166	ILE	2.2
1	B	139	ARG	2.2
1	A	242	PRO	2.1
1	B	127	SER	2.1
1	A	112	GLU	2.1
1	B	134	VAL	2.1
1	B	138	LEU	2.1
1	B	114	GLN	2.1
1	B	115	ASN	2.1
2	C	807	LEU	2.0
1	A	87	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	TPO	B	248	11/12	0.95	0.09	25,26,31,37	0
1	TPO	A	248	11/12	0.97	0.09	28,30,33,35	0

6.3 Carbohydrates [i](#)

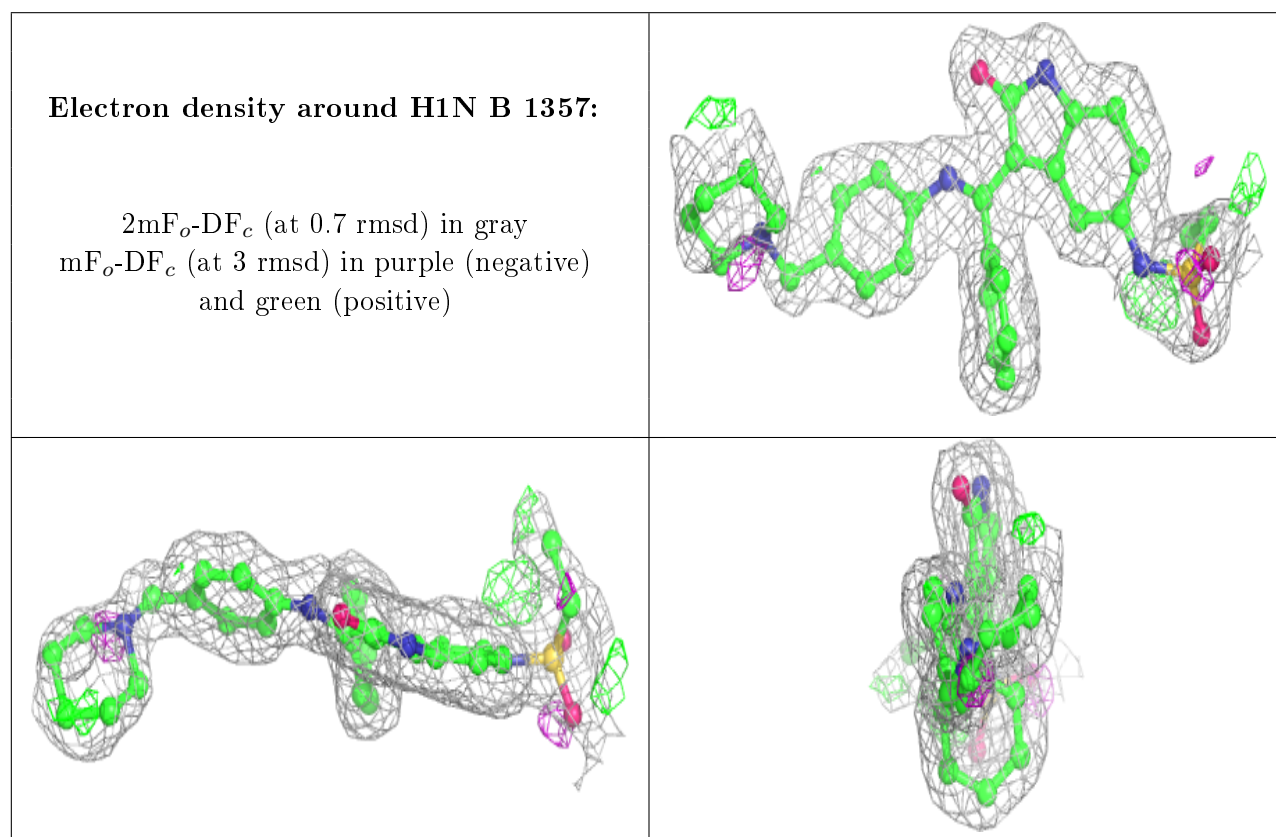
There are no carbohydrates in this entry.

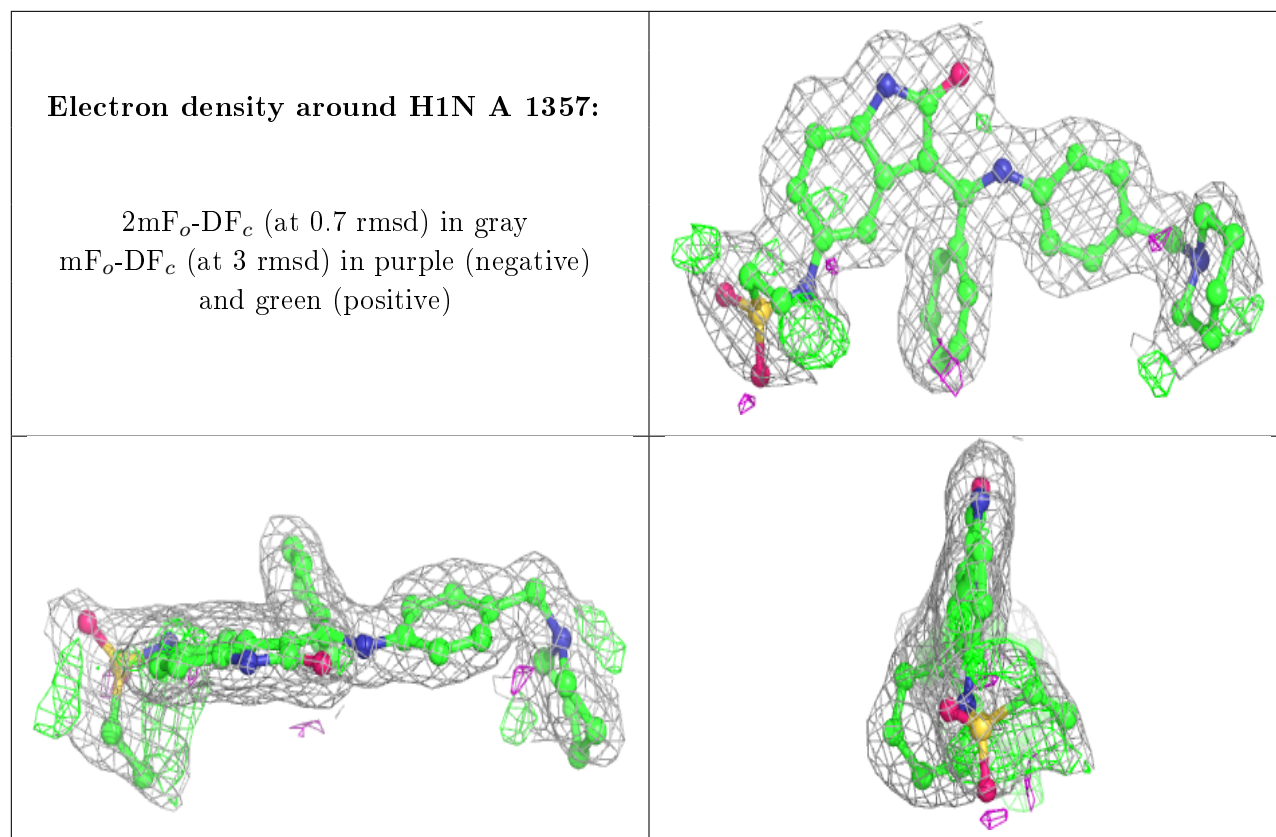
6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	H1N	B	1357	37/37	0.87	0.13	21,29,47,48	0
3	H1N	A	1357	37/37	0.89	0.13	21,32,47,49	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 [i](#)

There are no such residues in this entry.