



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:46 AM GMT

PDB ID : 2BFY
Title : complex of Aurora-B with INCENP and Hesperidin.
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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

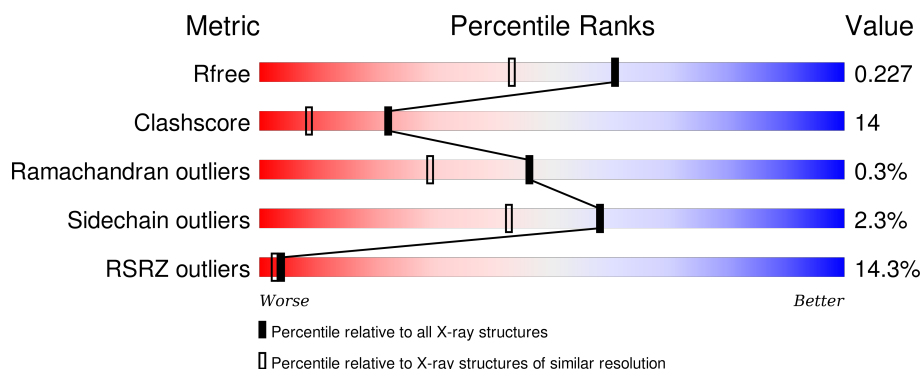
1 Overall quality at a glance

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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (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. 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>11%</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>49%</div> <div>47%</div> <div>30%</div> <div>• 21%</div> </div>

2 Entry composition

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			

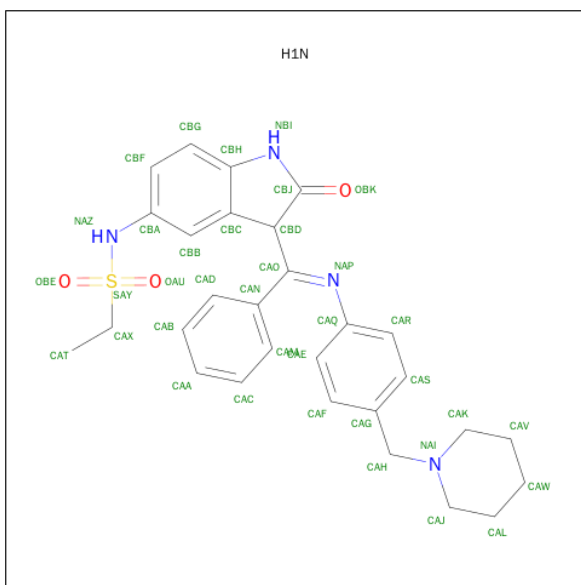
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	VAL	GLY	ENGINEERED	UNP Q7ZYT9
B	96	VAL	GLY	ENGINEERED	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 37	C 29	N 4	O 3	S 1	0	0
3	B	1	Total 37	C 29	N 4	O 3	S 1	0	0

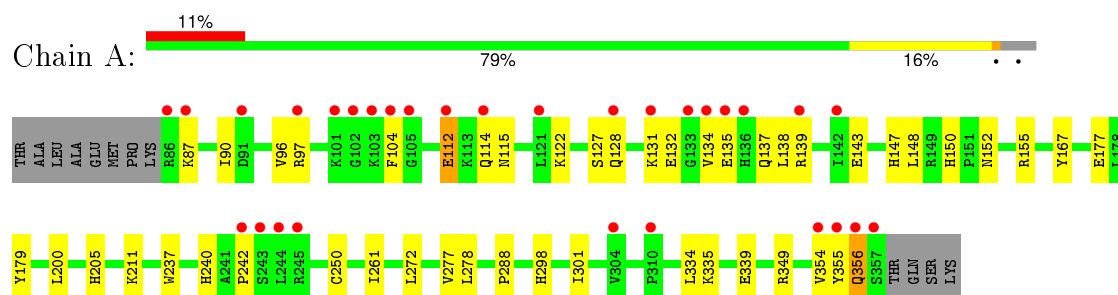
- Molecule 4 is water.

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

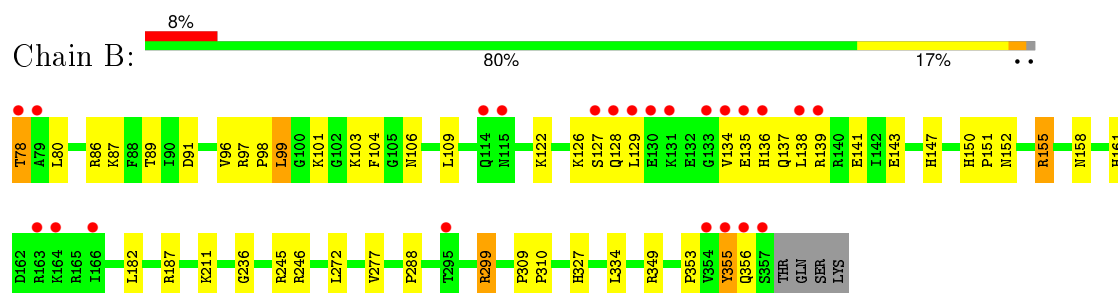
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

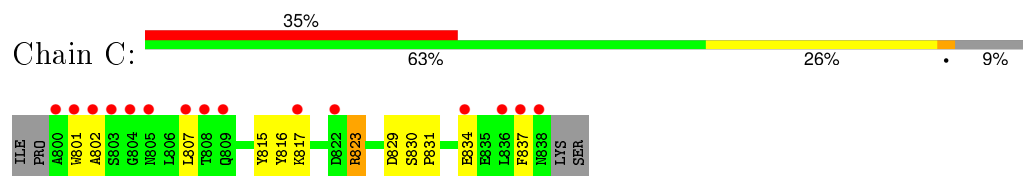
• Molecule 1: AURORA KINASE B-A



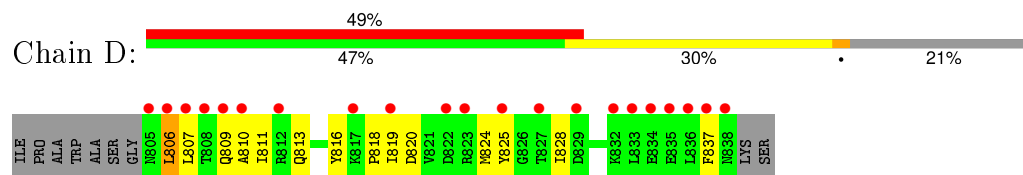
• Molecule 1: AURORA KINASE B-A



• 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 0.203 , 0.227	Depositor DCC
R_{free} test set	3270 reflections (5.38%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 72454 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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:87:LYS:HZ2	2:C:831:PRO:CA	2.05	0.66
1:B:136:HIS:CD2	1:B:139:ARG:HH21	2.13	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:HB3	1:A:139:ARG:HH11	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
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:A:104:PHE:CZ	1:A:134:VAL:HG11	2.45	0.51
1:B:127:SER:C	1:B:129:LEU:H	2.14	0.51
2:D:828:ILE:HD12	2:D:828:ILE:N	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:B:187:ARG:CZ	4:B:2073:HOH:O	2.58	0.50
1:A:128:GLN:HG3	1:A:132:GLU:OE2	2.11	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:135:GLU:CD	2:D:837:PHE:HB3	2.32	0.48
1:A:355:TYR:O	1:A:356:GLN:HG3	2.13	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:NH1	1:A:139:ARG:CB	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:HA	2:D:806:LEU:HD12	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:O	1:B:129:LEU:HD23	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
2:D:806:LEU:CD1	2:D:809:GLN:CD	2.85	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
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:CAN	3:B:1357:H1N:HBB	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:CBF	3:A:1357:H1N:CAX	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:B:126:LYS:NZ	1:B:161:HIS:HD2	2.17	0.42
1:A:200:LEU:HD22	1:A:278:LEU:HD23	2.02	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:B:96:VAL:HG11	2:C:807:LEU:CD2	2.50	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:355:TYR:N	1:B:355:TYR:CD1	2.87	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:104:PHE:CE1	1:B:134:VAL:HG21	2.54	0.41
1:B:99:LEU:HD11	1:B:109:LEU:HB2	2.03	0.41
1:B:103:LYS:HE3	1:B:104:PHE:CE2	2.55	0.41
1:B:101:LYS:HD2	1:B:106:ASN:HD22	1.85	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 [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	269/284 (95%)	259 (96%)	9 (3%)	1 (0%)	39	23
1	B	277/284 (98%)	264 (95%)	12 (4%)	1 (0%)	39	23
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%)	46	29

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%)	63	49
1	B	251/256 (98%)	246 (98%)	5 (2%)	63	49
2	C	32/38 (84%)	30 (94%)	2 (6%)	22	8
2	D	31/38 (82%)	30 (97%)	1 (3%)	46	29
All	All	559/588 (95%)	546 (98%)	13 (2%)	58	42

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	1.72	3 (37%)	7,14,16	4.66	4 (57%)
1	TPO	B	248	1	8,10,11	1.47	1 (12%)	7,14,16	4.82	4 (57%)

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	-	0/8/11/13	0/0/0/0
1	TPO	B	248	1	-	0/8/11/13	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	248	TPO	P-OG1	-3.20	1.50	1.60
1	B	248	TPO	P-OG1	-3.06	1.50	1.60
1	A	248	TPO	P-O3P	-2.25	1.46	1.54
1	A	248	TPO	CB-CA	-2.15	1.50	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	248	TPO	O3P-P-O1P	-7.79	85.50	110.58
1	A	248	TPO	O3P-P-O1P	-7.78	85.53	110.58
1	A	248	TPO	O3P-P-O2P	-4.51	90.20	107.38
1	B	248	TPO	O3P-P-O2P	-4.04	91.99	107.38
1	B	248	TPO	O2P-P-O1P	2.86	119.79	110.58
1	A	248	TPO	O2P-P-O1P	4.08	123.71	110.58
1	A	248	TPO	OG1-P-O1P	7.07	124.77	107.11
1	B	248	TPO	OG1-P-O1P	8.63	128.67	107.11

There are no chirality outliers.

There are no torsion outliers.

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	A	1357	-	38,41,41	2.01	6 (15%)	47,58,58	1.23	3 (6%)
3	H1N	B	1357	-	38,41,41	2.01	8 (21%)	47,58,58	1.15	2 (4%)

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	A	1357	-	-	0/24/44/44	0/5/5/5
3	H1N	B	1357	-	-	0/24/44/44	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1357	H1N	CBA-NAZ	-5.78	1.33	1.43
3	B	1357	H1N	CBA-NAZ	-5.71	1.33	1.43
3	B	1357	H1N	CAN-CAO	-5.48	1.39	1.48
3	A	1357	H1N	CAQ-NAP	-5.17	1.33	1.42
3	A	1357	H1N	CAN-CAO	-5.15	1.40	1.48
3	B	1357	H1N	CAQ-NAP	-4.97	1.34	1.42
3	B	1357	H1N	CBC-CBD	-2.12	1.39	1.45
3	B	1357	H1N	CBJ-NBI	-2.09	1.33	1.37
3	B	1357	H1N	CAO-NAP	3.04	1.33	1.28
3	A	1357	H1N	CAO-NAP	3.11	1.33	1.28
3	B	1357	H1N	OAU-SAY	4.29	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1357	H1N	OBE-SAY	4.34	1.50	1.43
3	B	1357	H1N	OBE-SAY	4.34	1.50	1.43
3	A	1357	H1N	OAU-SAY	4.37	1.50	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1357	H1N	OAU-SAY-OBE	-4.87	110.92	119.34
3	A	1357	H1N	OAU-SAY-OBE	-4.72	111.20	119.34
3	A	1357	H1N	CBF-CBA-NAZ	2.12	124.55	120.02
3	B	1357	H1N	CAQ-NAP-CAO	3.98	129.03	122.03
3	A	1357	H1N	CAQ-NAP-CAO	4.15	129.31	122.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 22 short contacts:

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

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	271/284 (95%)	0.62	30 (11%) 7 5	13, 26, 54, 67	0
1	B	279/284 (98%)	0.32	23 (8%) 14 11	12, 23, 53, 67	0
2	C	39/43 (90%)	1.91	15 (38%) 0 0	25, 41, 58, 63	0
2	D	34/43 (79%)	2.89	21 (61%) 0 0	29, 51, 70, 72	0
All	All	623/654 (95%)	0.69	89 (14%) 4 2	12, 26, 58, 72	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	357	SER	15.9
1	A	244	LEU	9.3
2	C	802	ALA	8.8
2	D	837	PHE	8.7
1	A	136	HIS	8.6
2	D	806	LEU	8.4
2	D	807	LEU	7.8
1	A	86	ARG	7.5
1	B	136	HIS	7.5
1	A	356	GLN	7.4
1	A	104	PHE	6.6
2	D	805	ASN	6.2
2	D	834	GLU	6.0
2	D	838	ASN	5.7
1	B	133	GLY	5.6
2	C	803	SER	5.3
1	B	355	TYR	5.1
2	D	808	THR	4.9
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	4.3
1	A	97	ARG	4.2
2	C	800	ALA	4.2
2	D	809	GLN	4.1
2	C	834	GLU	4.1
1	A	114	GLN	4.1
1	B	128	GLN	4.1
2	C	837	PHE	4.0
1	B	129	LEU	3.9
1	B	78	THR	3.9
1	B	135	GLU	3.7
2	D	829	ASP	3.7
1	B	131	LYS	3.6
1	B	130	GLU	3.5
1	B	356	GLN	3.5
2	C	817	LYS	3.5
2	D	833	LEU	3.5
2	C	805	ASN	3.4
2	D	832	LYS	3.4
2	D	835	GLU	3.3
1	A	121	LEU	3.3
1	A	133	GLY	3.3
1	A	354	VAL	3.2
2	D	822	ASP	3.2
1	A	139	ARG	3.1
1	A	245	ARG	3.1
1	B	295	THR	3.0
2	D	817	LYS	2.9
1	A	105	GLY	2.9
1	A	103	LYS	2.8
2	C	804	GLY	2.8
1	A	131	LYS	2.8
1	A	102	GLY	2.8
1	A	128	GLN	2.7
2	C	809	GLN	2.7
1	B	357	SER	2.7
1	A	101	LYS	2.6
2	D	836	LEU	2.6
2	C	836	LEU	2.6
1	A	135	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	91	ASP	2.6
2	C	822	ASP	2.6
1	A	134	VAL	2.5
1	B	164	LYS	2.5
2	D	823	ARG	2.5
2	C	838	ASN	2.4
2	D	827	THR	2.4
1	B	354	VAL	2.4
1	B	79	ALA	2.4
1	A	310	PRO	2.3
1	A	142	ILE	2.3
1	B	166	ILE	2.3
2	D	812	ARG	2.3
1	B	127	SER	2.3
1	B	139	ARG	2.2
1	B	138	LEU	2.2
1	B	134	VAL	2.2
1	A	242	PRO	2.2
1	A	112	GLU	2.2
1	B	114	GLN	2.1
2	C	807	LEU	2.1
1	B	115	ASN	2.1
2	D	825	TYR	2.1
1	A	87	LYS	2.1
1	A	304	VAL	2.0
2	D	819	ILE	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
1	TPO	A	248	11/12	0.97	0.09	-	28,30,33,35	0
1	TPO	B	248	11/12	0.95	0.09	-	25,26,31,37	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	H1N	B	1357	37/37	0.87	0.13	0.12	21,29,47,48	0
3	H1N	A	1357	37/37	0.89	0.13	-0.18	21,32,47,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.