



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:02 pm GMT

PDB ID : 3IDC
Title : Crystal structure of (102-265)RIIb:C holoenzyme of cAMP-dependent protein kinase
Authors : Brown, S.H.J.; Wu, J.; Kim, C.; Alberto, K.; Taylor, S.S.
Deposited on : 2009-07-20
Resolution : 2.70 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

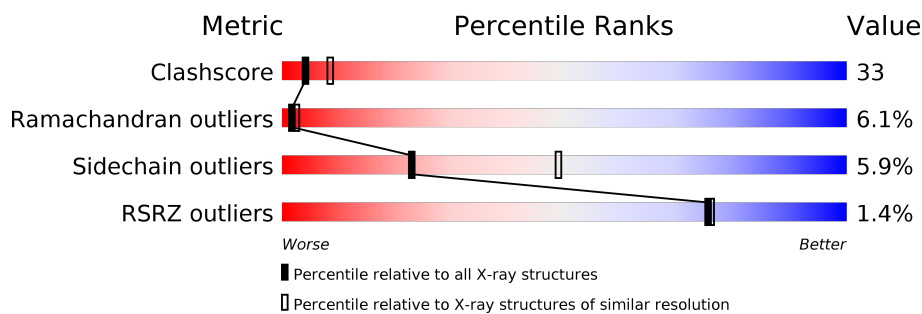
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.70 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))
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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	350	 49% 47% . .
2	B	164	 4% 48% 40% 9% . .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3948 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 cAMP-dependent protein kinase catalytic subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	P	S	0	0	0
			2736	1764	456	506	2	8			

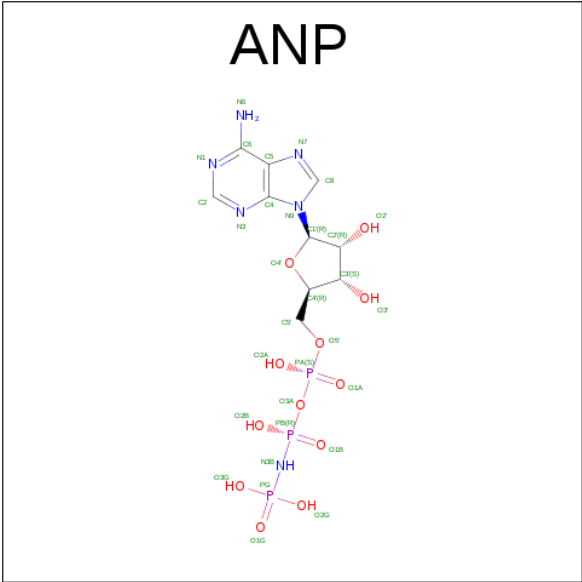
- Molecule 2 is a protein called cAMP-dependent protein kinase type II-beta regulatory subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	160	Total	C	N	O	S	0	0	1
			1136	706	208	215	7			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mn	0	0
			2	2		

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

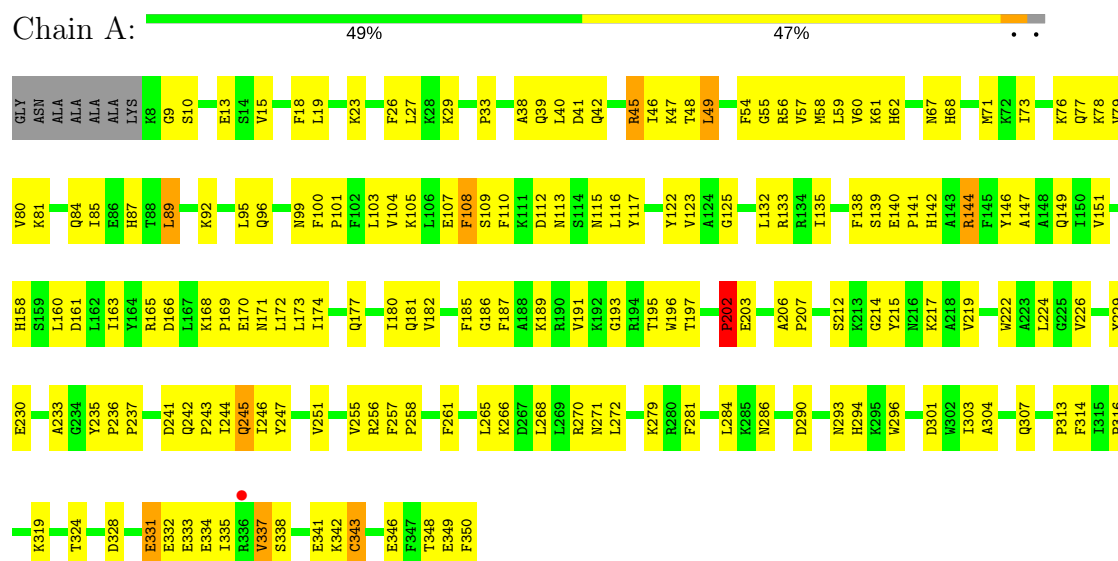
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	43	Total	0	0
			43 O 43 43		

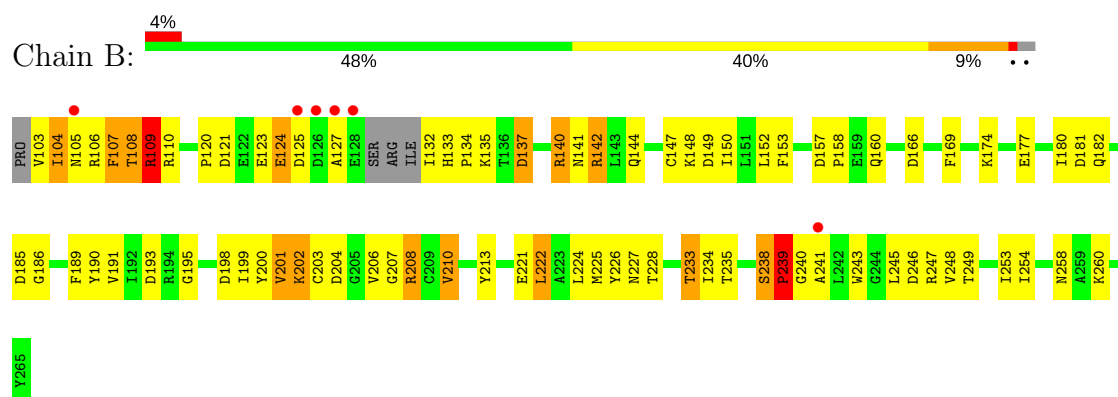
3 Residue-property plots

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: cAMP-dependent protein kinase catalytic subunit alpha



- Molecule 2: cAMP-dependent protein kinase type II-beta regulatory subunit



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	179.27Å 67.43Å 47.33Å 90.00° 99.51° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 31.50 – 2.05	Depositor EDS
% Data completeness (in resolution range)	95.2 (50.00-2.70) 67.8 (31.50-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.05Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.241 , 0.319 0.251 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.741	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.9	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	0.91	EDS
Total number of atoms	3948	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, MN, ANP, SEP

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	0.44	0/2783	0.64	0/3766
2	B	0.44	0/1156	0.67	0/1569
All	All	0.44	0/3939	0.65	0/5335

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

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	2736	0	2598	164	0
2	B	1136	0	965	87	0
3	A	2	0	0	1	0
4	A	31	0	13	1	0
5	A	43	0	0	6	0
All	All	3948	0	3576	244	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 33.

All (244) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LYS:HE2	1:A:171:ASN:ND2	1.70	1.06
2:B:222:LEU:HD12	2:B:228:THR:HG21	1.44	0.98
1:A:303:ILE:HD12	1:A:304:ALA:N	1.80	0.96
1:A:241:ASP:HA	2:B:106:ARG:NH2	1.81	0.95
2:B:185:ASP:HB3	2:B:227:ASN:HD21	1.33	0.90
1:A:10:SER:H	1:A:293:ASN:HD21	1.18	0.89
1:A:125:GLY:HA3	1:A:174:ILE:O	1.73	0.88
1:A:42:GLN:HB3	1:A:62:HIS:CE1	2.10	0.86
2:B:152:LEU:HD11	2:B:225:MET:HG2	1.59	0.84
1:A:73:ILE:HD13	1:A:335:ILE:HD13	1.64	0.80
1:A:189:LYS:HE2	1:A:195:THR:OG1	1.82	0.79
2:B:133:HIS:HB3	2:B:134:PRO:HD2	1.63	0.78
1:A:244:ILE:HD11	2:B:222:LEU:HD23	1.65	0.77
1:A:149:GLN:HE22	1:A:180:ILE:H	1.29	0.77
2:B:152:LEU:HD11	2:B:225:MET:CG	2.14	0.77
2:B:203:CYS:H	2:B:208:ARG:NH2	1.83	0.77
1:A:266:LYS:O	1:A:270:ARG:HG3	1.85	0.76
2:B:107:PHE:CD1	2:B:108:THR:N	2.54	0.75
1:A:18:PHE:HD1	1:A:19:LEU:HD12	1.54	0.73
1:A:303:ILE:O	1:A:307:GLN:HG3	1.90	0.72
2:B:132:ILE:HA	2:B:166:ASP:HB3	1.72	0.72
1:A:168:LYS:HE2	1:A:171:ASN:HD21	1.54	0.71
2:B:203:CYS:N	2:B:208:ARG:NH2	2.37	0.71
2:B:201:VAL:O	2:B:208:ARG:NH2	2.24	0.71
1:A:241:ASP:HA	2:B:106:ARG:HH21	1.53	0.71
1:A:13:GLU:HG2	1:A:15:VAL:HG13	1.73	0.71
1:A:115:ASN:HB2	1:A:117:TYR:CZ	2.27	0.70
3:A:401:MN:MN	4:A:450:ANP:O2G	1.50	0.69
2:B:225:MET:HE2	2:B:226:TYR:HE1	1.58	0.69
1:A:45:ARG:HH12	1:A:335:ILE:HG13	1.57	0.69
1:A:303:ILE:HD12	1:A:304:ALA:H	1.57	0.69
1:A:135:ILE:O	1:A:135:ILE:HG22	1.92	0.69
1:A:42:GLN:HB3	1:A:62:HIS:HE1	1.57	0.69
2:B:193:ASP:HB3	2:B:241:ALA:O	1.92	0.68
2:B:222:LEU:CD1	2:B:228:THR:HG21	2.22	0.68
1:A:110:PHE:CE1	1:A:117:TYR:CD2	2.81	0.67
1:A:265:LEU:HD13	1:A:296:TRP:CE2	2.30	0.67
2:B:142:ARG:HH11	2:B:142:ARG:HG2	1.59	0.67
2:B:208:ARG:NE	2:B:208:ARG:H	1.92	0.67
2:B:227:ASN:HB2	2:B:247:ARG:HH22	1.59	0.67
1:A:9:GLY:HA3	1:A:293:ASN:ND2	2.10	0.66
2:B:195:GLY:HA3	2:B:240:GLY:HA3	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ILE:HG23	1:A:117:TYR:CE1	2.32	0.65
1:A:99:ASN:ND2	1:A:105:LYS:NZ	2.45	0.65
1:A:87:HIS:HB3	1:A:186:GLY:O	1.98	0.64
1:A:60:VAL:O	1:A:68:HIS:HA	1.97	0.64
2:B:140:ARG:NH2	2:B:141:ASN:HA	2.13	0.64
2:B:147:CYS:C	2:B:149:ASP:H	2.00	0.64
1:A:73:ILE:HG23	1:A:117:TYR:HE1	1.64	0.63
1:A:26:PHE:CG	1:A:160:LEU:HD13	2.34	0.63
2:B:182:GLN:NE2	2:B:202:LYS:O	2.33	0.62
1:A:42:GLN:O	1:A:62:HIS:HA	1.99	0.62
1:A:147:ALA:O	1:A:151:VAL:HG23	2.00	0.62
1:A:203:GLU:HG3	1:A:246:ILE:HD13	1.82	0.61
1:A:132:LEU:HD13	1:A:138:PHE:CE1	2.35	0.61
1:A:55:GLY:HA3	1:A:73:ILE:O	1.99	0.61
1:A:163:ILE:HD12	1:A:191:VAL:HG21	1.81	0.61
1:A:9:GLY:HA3	1:A:293:ASN:HD22	1.63	0.61
1:A:29:LYS:HB3	1:A:29:LYS:NZ	2.15	0.60
2:B:202:LYS:HA	2:B:207:GLY:HA2	1.84	0.60
2:B:208:ARG:H	2:B:208:ARG:HE	1.49	0.60
1:A:173:LEU:HB2	1:A:181:GLN:HB2	1.83	0.60
1:A:47:LYS:HG2	1:A:332:GLU:OE1	2.02	0.60
2:B:190:TYR:HA	2:B:243:TRP:O	2.01	0.60
1:A:169:PRO:HA	1:A:172:LEU:HD12	1.84	0.59
1:A:255:VAL:HG22	1:A:256:ARG:N	2.17	0.59
2:B:157:ASP:HB2	2:B:160:GLN:HG3	1.83	0.59
2:B:200:TYR:C	2:B:202:LYS:H	2.06	0.59
1:A:45:ARG:NH1	1:A:335:ILE:HG13	2.16	0.58
1:A:92:LYS:NZ	1:A:350:PHE:C	2.57	0.58
1:A:212:SER:HA	5:A:508:HOH:O	2.02	0.58
1:A:76:LYS:O	1:A:80:VAL:HG23	2.03	0.58
2:B:181:ASP:HA	2:B:233:THR:HG23	1.83	0.58
1:A:244:ILE:CD1	2:B:222:LEU:HD23	2.33	0.58
1:A:92:LYS:HZ2	1:A:350:PHE:C	2.06	0.58
2:B:107:PHE:CG	2:B:108:THR:N	2.72	0.57
1:A:133:ARG:HE	2:B:107:PHE:HD1	1.50	0.57
1:A:158:HIS:HB3	1:A:217:LYS:HE3	1.87	0.57
2:B:107:PHE:O	2:B:108:THR:HB	2.03	0.57
1:A:123:VAL:HB	1:A:173:LEU:HD13	1.87	0.56
1:A:331:GLU:O	1:A:333:GLU:HG3	2.04	0.56
1:A:57:VAL:HA	1:A:71:MET:O	2.06	0.56
1:A:168:LYS:HE2	1:A:171:ASN:HD22	1.61	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:SER:HB2	1:A:141:PRO:HD2	1.87	0.56
1:A:247:TYR:O	1:A:251:VAL:HG23	2.05	0.56
2:B:140:ARG:HH11	2:B:140:ARG:HB3	1.70	0.55
1:A:39:GLN:HB2	1:A:42:GLN:HG2	1.88	0.55
1:A:112:ASP:OD2	1:A:337:VAL:HG12	2.06	0.55
1:A:61:LYS:HA	1:A:67:ASN:O	2.06	0.55
1:A:116:LEU:HD13	1:A:350:PHE:CE1	2.43	0.54
1:A:40:LEU:C	1:A:42:GLN:H	2.11	0.54
1:A:99:ASN:ND2	1:A:105:LYS:HZ3	2.06	0.54
1:A:242:GLN:HB2	1:A:245:GLN:HB2	1.88	0.54
1:A:49:LEU:HD21	1:A:122:TYR:CE2	2.43	0.54
1:A:89:LEU:CD2	1:A:349:GLU:HB2	2.38	0.53
2:B:103:VAL:HG23	2:B:104:ILE:N	2.24	0.53
1:A:38:ALA:HB3	1:A:110:PHE:CD2	2.43	0.53
2:B:180:ILE:O	2:B:233:THR:HA	2.08	0.53
1:A:48:THR:CB	1:A:56:ARG:HH21	2.21	0.53
2:B:227:ASN:CB	2:B:247:ARG:HH22	2.21	0.53
1:A:142:HIS:HA	1:A:313:PRO:HG3	1.91	0.52
1:A:10:SER:N	1:A:293:ASN:HD21	1.96	0.52
2:B:140:ARG:HH22	2:B:141:ASN:HA	1.73	0.52
1:A:203:GLU:OE2	2:B:110:ARG:HD2	2.10	0.52
1:A:215:TYR:CD1	1:A:219:VAL:HG11	2.45	0.51
1:A:85:ILE:HD11	1:A:346:GLU:O	2.10	0.51
2:B:147:CYS:C	2:B:149:ASP:N	2.64	0.51
1:A:113:ASN:OD1	1:A:341:GLU:HB2	2.10	0.51
2:B:246:ASP:HB3	2:B:249:THR:OG1	2.11	0.51
1:A:115:ASN:HB2	1:A:117:TYR:OH	2.11	0.51
1:A:42:GLN:NE2	1:A:42:GLN:HA	2.26	0.51
1:A:99:ASN:HD22	1:A:105:LYS:HZ3	1.59	0.51
1:A:286:ASN:HB2	1:A:290:ASP:OD2	2.10	0.50
1:A:243:PRO:O	1:A:246:ILE:HB	2.10	0.50
1:A:45:ARG:HB3	1:A:58:MET:CE	2.41	0.50
2:B:189:PHE:HB2	2:B:224:LEU:HG	1.93	0.50
1:A:207:PRO:HD3	1:A:222:TRP:CZ2	2.45	0.50
1:A:42:GLN:O	1:A:62:HIS:ND1	2.30	0.50
1:A:196:TRP:O	1:A:197:TPO:C	2.58	0.50
1:A:45:ARG:HB3	1:A:58:MET:HE1	1.93	0.50
2:B:199:ILE:HD11	2:B:213:TYR:CE1	2.47	0.50
2:B:185:ASP:HB3	2:B:227:ASN:ND2	2.15	0.50
1:A:268:LEU:HB2	1:A:294:HIS:CE1	2.46	0.49
1:A:133:ARG:NE	2:B:107:PHE:CD1	2.75	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:GLN:NE2	1:A:180:ILE:H	2.06	0.49
1:A:10:SER:H	1:A:293:ASN:ND2	1.98	0.49
2:B:135:LYS:C	2:B:137:ASP:H	2.16	0.49
1:A:241:ASP:HA	2:B:106:ARG:CZ	2.41	0.49
2:B:123:GLU:O	2:B:124:GLU:CB	2.61	0.49
2:B:137:ASP:O	2:B:140:ARG:CB	2.61	0.49
2:B:203:CYS:O	2:B:208:ARG:NH2	2.46	0.49
1:A:314:PHE:HE1	1:A:316:PRO:HG3	1.77	0.48
2:B:140:ARG:HB3	2:B:140:ARG:NH1	2.28	0.48
2:B:246:ASP:OD1	2:B:248:VAL:HB	2.13	0.48
1:A:202:PRO:HG3	1:A:247:TYR:OH	2.14	0.48
1:A:258:PRO:HD2	1:A:261:PHE:CD1	2.49	0.48
1:A:104:VAL:HG12	1:A:182:VAL:O	2.14	0.48
1:A:163:ILE:CD1	1:A:191:VAL:HG21	2.43	0.48
2:B:191:VAL:HB	2:B:243:TRP:HB2	1.95	0.48
1:A:48:THR:HG21	1:A:56:ARG:NH2	2.29	0.48
1:A:89:LEU:HD23	5:A:542:HOH:O	2.14	0.48
2:B:254:ILE:O	2:B:258:ASN:ND2	2.47	0.48
1:A:217:LYS:HD2	5:A:510:HOH:O	2.14	0.47
2:B:133:HIS:HB3	2:B:134:PRO:CD	2.39	0.47
2:B:246:ASP:OD2	2:B:247:ARG:N	2.47	0.47
1:A:170:GLU:N	1:A:170:GLU:OE2	2.43	0.47
1:A:40:LEU:O	1:A:42:GLN:N	2.47	0.47
1:A:337:VAL:HG23	1:A:338:SEP:N	2.29	0.47
2:B:150:ILE:HG23	2:B:221:GLU:CD	2.35	0.47
2:B:132:ILE:HG13	2:B:132:ILE:O	2.15	0.47
1:A:335:ILE:O	1:A:335:ILE:HG13	2.15	0.47
1:A:54:PHE:HA	1:A:78:LYS:HD3	1.96	0.47
1:A:177:GLN:OE1	1:A:177:GLN:N	2.48	0.46
2:B:108:THR:O	2:B:109:ARG:C	2.53	0.46
2:B:109:ARG:HH11	2:B:109:ARG:HG2	1.79	0.46
1:A:135:ILE:O	1:A:135:ILE:CG2	2.62	0.46
1:A:146:TYR:CB	1:A:180:ILE:HD11	2.46	0.46
2:B:157:ASP:HB3	2:B:158:PRO:HD2	1.97	0.46
2:B:109:ARG:HG2	2:B:109:ARG:NH1	2.31	0.46
1:A:144:ARG:NH1	1:A:296:TRP:O	2.48	0.46
1:A:207:PRO:HD3	1:A:222:TRP:CE2	2.50	0.46
2:B:137:ASP:O	2:B:140:ARG:HB3	2.14	0.46
2:B:140:ARG:HH21	2:B:144:GLN:CB	2.28	0.46
2:B:147:CYS:O	2:B:149:ASP:N	2.48	0.46
1:A:29:LYS:HB3	1:A:29:LYS:HZ2	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:ARG:HG2	2:B:142:ARG:NH1	2.28	0.46
2:B:177:GLU:O	2:B:235:THR:HA	2.16	0.46
1:A:160:LEU:O	1:A:161:ASP:HB2	2.16	0.46
1:A:132:LEU:HD21	1:A:230:GLU:HG2	1.97	0.46
2:B:203:CYS:O	2:B:204:ASP:CB	2.64	0.46
1:A:100:PHE:HB3	1:A:103:LEU:HG	1.98	0.45
2:B:221:GLU:HA	2:B:224:LEU:HD12	1.97	0.45
1:A:242:GLN:H	1:A:245:GLN:HE21	1.64	0.45
1:A:87:HIS:CE1	1:A:197:TPO:HG21	2.51	0.45
1:A:265:LEU:HD13	1:A:296:TRP:CZ2	2.52	0.45
2:B:208:ARG:HE	2:B:208:ARG:N	2.13	0.45
1:A:314:PHE:CD1	1:A:314:PHE:C	2.90	0.45
2:B:245:LEU:HD23	2:B:246:ASP:N	2.31	0.45
1:A:140:GLU:N	1:A:141:PRO:CD	2.80	0.45
1:A:38:ALA:HB3	1:A:110:PHE:HD2	1.81	0.45
1:A:92:LYS:HZ3	1:A:350:PHE:HA	1.82	0.45
2:B:234:ILE:HG22	2:B:234:ILE:O	2.16	0.45
2:B:238:SER:CB	2:B:239:PRO:C	2.84	0.45
1:A:139:SER:CB	1:A:141:PRO:HD2	2.47	0.45
1:A:268:LEU:O	1:A:268:LEU:HD12	2.18	0.44
1:A:99:ASN:ND2	1:A:105:LYS:HZ1	2.14	0.44
1:A:173:LEU:O	1:A:180:ILE:HA	2.17	0.44
1:A:116:LEU:HD22	1:A:350:PHE:CD2	2.52	0.44
1:A:235:TYR:HB2	1:A:236:PRO:HD2	1.99	0.44
1:A:107:GLU:HB2	1:A:108:PHE:CE1	2.53	0.44
2:B:260:LYS:NZ	2:B:260:LYS:HB2	2.32	0.44
2:B:140:ARG:NH1	2:B:141:ASN:N	2.66	0.44
2:B:135:LYS:C	2:B:137:ASP:N	2.70	0.44
1:A:255:VAL:CG2	1:A:256:ARG:N	2.81	0.43
2:B:203:CYS:N	2:B:208:ARG:HH22	2.15	0.43
1:A:84:GLN:HE22	1:A:187:PHE:HE2	1.66	0.43
1:A:151:VAL:HG22	1:A:224:LEU:HD21	2.00	0.43
1:A:23:LYS:O	1:A:27:LEU:HG	2.19	0.43
2:B:227:ASN:HA	2:B:247:ARG:NH2	2.33	0.43
1:A:76:LYS:HE3	1:A:342:LYS:O	2.18	0.43
2:B:203:CYS:N	2:B:208:ARG:HH21	2.13	0.43
1:A:146:TYR:HB3	1:A:180:ILE:HD11	2.01	0.43
1:A:301:ASP:OD2	1:A:303:ILE:HG13	2.18	0.43
1:A:79:VAL:CG1	1:A:85:ILE:HA	2.49	0.43
1:A:229:TYR:CE2	1:A:237:PRO:HA	2.53	0.43
1:A:68:HIS:HD2	5:A:503:HOH:O	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ALA:HA	1:A:222:TRP:NE1	2.34	0.42
2:B:133:HIS:CD2	2:B:169:PHE:HA	2.54	0.42
1:A:168:LYS:CE	1:A:171:ASN:ND2	2.61	0.42
1:A:279:LYS:HA	1:A:284:LEU:HD21	2.01	0.42
2:B:202:LYS:HA	2:B:207:GLY:CA	2.46	0.42
1:A:110:PHE:CE1	1:A:117:TYR:HD2	2.32	0.42
1:A:146:TYR:O	1:A:149:GLN:HB2	2.19	0.42
1:A:226:VAL:HG13	1:A:237:PRO:HD2	2.02	0.42
1:A:242:GLN:HG3	1:A:245:GLN:NE2	2.34	0.42
2:B:249:THR:O	2:B:253:ILE:HG13	2.19	0.42
1:A:95:LEU:HD13	1:A:185:PHE:CD2	2.55	0.42
1:A:229:TYR:HE1	1:A:257:PHE:HD1	1.66	0.42
2:B:153:PHE:N	2:B:153:PHE:CD1	2.87	0.42
1:A:268:LEU:HD11	1:A:272:LEU:HD11	2.02	0.42
1:A:92:LYS:HE3	1:A:109:SER:OG	2.19	0.42
1:A:141:PRO:HG3	5:A:528:HOH:O	2.18	0.42
2:B:222:LEU:HD13	2:B:222:LEU:O	2.20	0.42
1:A:13:GLU:HB2	1:A:303:ILE:HG23	2.02	0.42
1:A:166:ASP:OD2	1:A:171:ASN:ND2	2.53	0.41
1:A:271:ASN:HB3	1:A:281:PHE:CD1	2.55	0.41
1:A:80:VAL:HG21	1:A:343:CYS:SG	2.60	0.41
2:B:106:ARG:HG2	2:B:106:ARG:HH11	1.84	0.41
1:A:265:LEU:HA	1:A:265:LEU:HD12	1.82	0.41
1:A:303:ILE:CD1	1:A:304:ALA:N	2.68	0.41
1:A:71:MET:HE3	1:A:73:ILE:HG12	2.03	0.41
2:B:200:TYR:O	2:B:202:LYS:N	2.53	0.41
1:A:139:SER:O	1:A:140:GLU:C	2.58	0.41
1:A:165:ARG:HH12	1:A:197:TPO:P	2.44	0.41
1:A:77:GLN:O	1:A:81:LYS:N	2.39	0.41
1:A:95:LEU:HD13	1:A:185:PHE:CG	2.56	0.41
1:A:233:ALA:HB2	1:A:261:PHE:CZ	2.56	0.41
1:A:132:LEU:HB2	1:A:138:PHE:CZ	2.57	0.40
1:A:226:VAL:O	1:A:229:TYR:HB3	2.21	0.40
2:B:203:CYS:H	2:B:208:ARG:HH21	1.64	0.40
1:A:58:MET:HE1	5:A:502:HOH:O	2.21	0.40
1:A:100:PHE:HA	1:A:101:PRO:HD3	1.89	0.40
1:A:132:LEU:HA	1:A:138:PHE:CZ	2.57	0.40
1:A:87:HIS:CD2	1:A:87:HIS:H	2.40	0.40

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	339/350 (97%)	299 (88%)	29 (9%)	11 (3%)	5	11
2	B	156/164 (95%)	115 (74%)	22 (14%)	19 (12%)	0	0
All	All	495/514 (96%)	414 (84%)	51 (10%)	30 (6%)	2	2

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	PRO
1	A	337	VAL
2	B	104	ILE
2	B	105	ASN
2	B	108	THR
2	B	120	PRO
2	B	124	GLU
2	B	125	ASP
2	B	137	ASP
2	B	238	SER
1	A	33	PRO
1	A	41	ASP
1	A	331	GLU
1	A	334	GLU
2	B	127	ALA
2	B	186	GLY
2	B	201	VAL
2	B	202	LYS
1	A	319	LYS
1	A	328	ASP
2	B	148	LYS
2	B	109	ARG
2	B	239	PRO
2	B	121	ASP
2	B	174	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	210	VAL
1	A	46	ILE
1	A	214	GLY
2	B	206	VAL
1	A	193	GLY

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	277/303 (91%)	265 (96%)	12 (4%)	33	64
2	B	95/141 (67%)	85 (90%)	10 (10%)	8	18
All	All	372/444 (84%)	350 (94%)	22 (6%)	23	49

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ARG
1	A	49	LEU
1	A	59	LEU
1	A	89	LEU
1	A	96	GLN
1	A	108	PHE
1	A	144	ARG
1	A	202	PRO
1	A	245	GLN
1	A	324	THR
1	A	343	CYS
1	A	348	THR
2	B	107	PHE
2	B	109	ARG
2	B	140	ARG
2	B	142	ARG
2	B	198	ASP
2	B	208	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	210	VAL
2	B	222	LEU
2	B	233	THR
2	B	239	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	42	GLN
1	A	68	HIS
1	A	87	HIS
1	A	90	ASN
1	A	96	GLN
1	A	99	ASN
1	A	131	HIS
1	A	149	GLN
1	A	176	GLN
1	A	245	GLN
1	A	283	ASN
1	A	289	ASN
1	A	293	ASN
2	B	160	GLN
2	B	227	ASN

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	197	1	9,10,11	1.67	2 (22%)	10,14,16	1.22	1 (10%)
1	SEP	A	338	1	9,9,10	0.72	0	9,12,14	1.12	1 (11%)

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	197	1	-	0/8/11/13	0/0/0/0
1	SEP	A	338	1	-	0/5/8/10	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	197	TPO	P-OG1	2.58	1.64	1.59
1	A	197	TPO	CA-C	3.72	1.55	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	TPO	O-C-CA	-2.26	119.89	125.15
1	A	338	SEP	OG-CB-CA	2.26	110.39	108.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	197	TPO	3	0
1	A	338	SEP	1	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ANP	A	450	3	29,33,33	1.53	4 (13%)	28,52,52	1.24	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ANP	A	450	3	-	0/13/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	450	ANP	PB-O2B	-2.70	1.49	1.56
4	A	450	ANP	PG-O2G	-2.20	1.50	1.56
4	A	450	ANP	PB-O1B	2.47	1.48	1.46
4	A	450	ANP	PG-O1G	6.25	1.53	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	450	ANP	PA-O3A-PB	-4.37	116.95	132.38
4	A	450	ANP	O1B-PB-N3B	-2.29	108.36	111.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	450	ANP	1	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	341/350 (97%)	-0.48	1 (0%) 93 94	21, 50, 76, 90	0
2	B	160/164 (97%)	-0.18	6 (3%) 41 39	20, 73, 92, 99	0
All	All	501/514 (97%)	-0.38	7 (1%) 75 76	20, 56, 87, 99	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	127	ALA	3.1
2	B	241	ALA	2.7
1	A	336	ARG	2.6
2	B	128	GLU	2.3
2	B	125	ASP	2.2
2	B	105	ASN	2.1
2	B	126	ASP	2.1

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	SEP	A	338	10/11	0.88	0.10	-	77,78,79,80	0
1	TPO	A	197	11/12	0.97	0.10	-	35,42,45,45	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
4	ANP	A	450	31/31	0.94	0.18	0.23	46,50,55,57	0
3	MN	A	402	1/1	0.98	0.13	-1.54	40,40,40,40	0
3	MN	A	401	1/1	0.97	0.16	-	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.