



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:10 PM GMT

PDB ID : 4A1Z
Title : Eg5-1
Authors : Talapatra, S.K.; Kozielski, F.
Deposited on : 2011-09-20
Resolution : 2.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

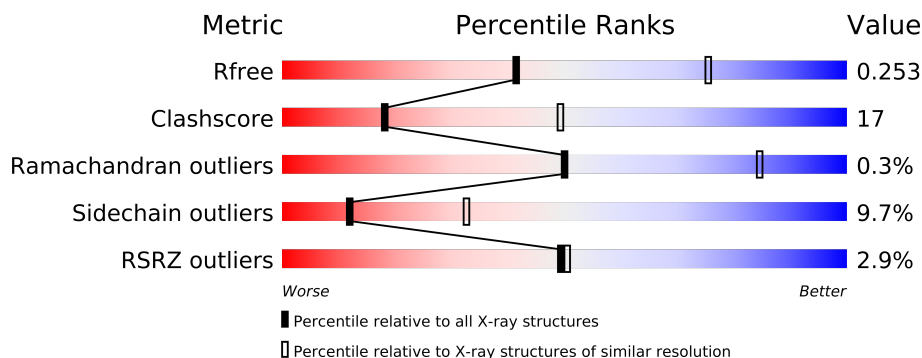
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	368	
1	B	368	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	A	1365	-	X
2	MG	B	1365	-	X
3	NO3	A	2000	X	-
3	NO3	A	2001	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5255 atoms, of which 0 are hydrogen and 0 are deuterium.

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 KINESIN-LIKE PROTEIN KIF11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	1	0
			2521	1587	434	490	10			
1	B	321	Total	C	N	O	S	0	0	0
			2500	1572	436	482	10			

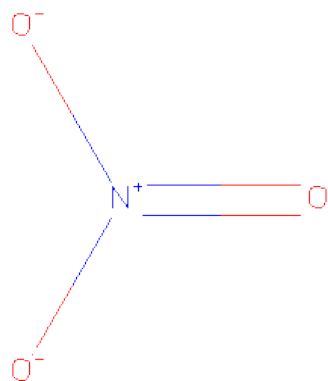
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	130	VAL	ASP	ENGINEERED MUTATION	UNP P52732
B	130	VAL	ASP	ENGINEERED MUTATION	UNP P52732

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

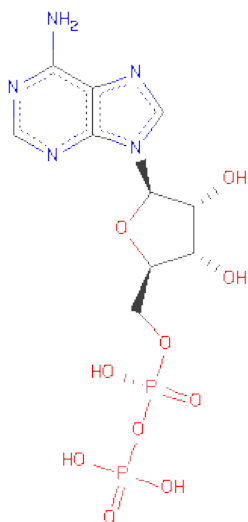
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	0
			4	1	3		
3	A	1	Total	N	O	0	0
			4	1	3		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is water.

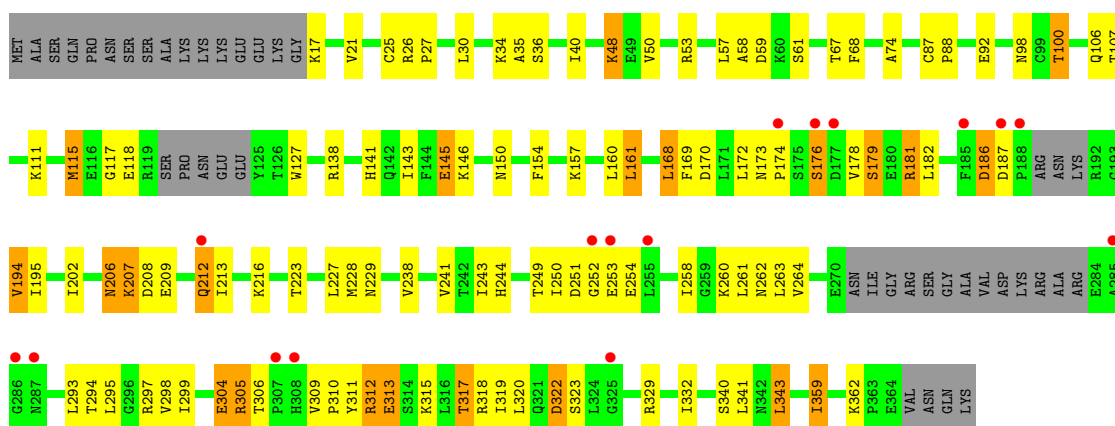
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	89	Total	O	0	0
			89	89		
5	B	81	Total	O	0	0
			81	81		

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 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.

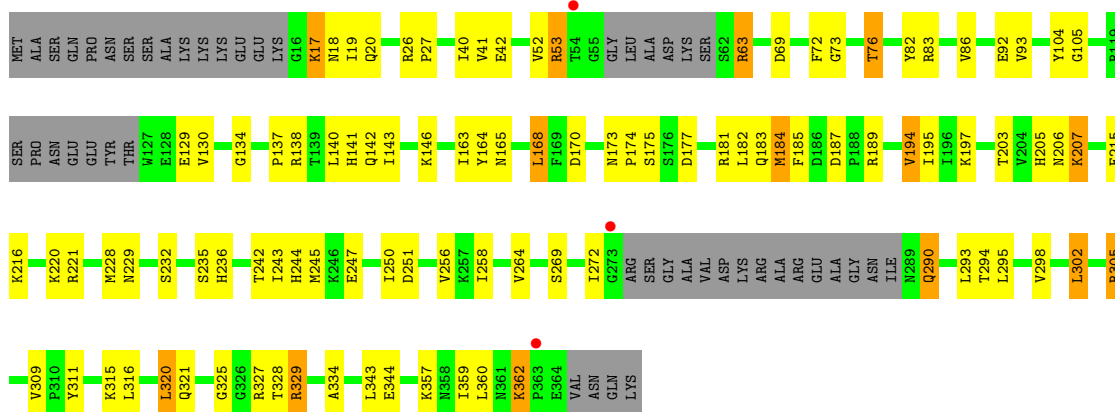
• Molecule 1: KINESIN-LIKE PROTEIN KIF11

Chain A:



• Molecule 1: KINESIN-LIKE PROTEIN KIF11

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.48Å 78.39Å 93.27Å 90.00° 93.47° 90.00°	Depositor
Resolution (Å)	29.23 – 2.80 29.23 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.0 (29.23-2.80) 100.0 (29.23-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.07 (at 2.80Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.173 , 0.257 0.174 , 0.253	Depositor DCC
R_{free} test set	940 reflections (5.12%)	DCC
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.631	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 23.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 18389 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5255	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, NO3

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	0.53	0/2559	0.74	0/3463
1	B	0.59	0/2535	0.72	0/3426
All	All	0.56	0/5094	0.73	0/6889

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
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	325	GLY	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2521	0	2531	96	0
1	B	2500	0	2527	82	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	8	0	0	3	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
5	A	89	0	0	7	0
5	B	81	0	0	5	0
All	All	5255	0	5082	173	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (173) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:304:GLU:HB2	1:A:306:THR:HG23	1.34	1.05
1:B:53:ARG:HG3	1:B:53:ARG:HH11	1.27	0.99
1:A:206:ASN:HD21	1:A:208:ASP:HB2	1.31	0.94
1:B:362:LYS:HZ2	1:B:362:LYS:H	1.14	0.92
1:A:179:SER:HB2	1:A:181:ARG:NH2	1.87	0.90
1:A:312:ARG:HD3	1:A:312:ARG:H	1.38	0.89
1:A:170:ASP:HB2	1:A:182:LEU:HD11	1.53	0.89
1:A:143:ILE:HD13	1:A:243:ILE:HD11	1.55	0.88
1:A:249:THR:HB	1:A:252:GLY:HA3	1.57	0.87
1:B:73:GLY:O	1:B:76:THR:HG23	1.78	0.83
1:B:362:LYS:NZ	1:B:362:LYS:H	1.75	0.83
1:A:305:ARG:HH11	1:A:305:ARG:HG2	1.48	0.79
1:A:312:ARG:N	1:A:312:ARG:HD3	1.98	0.79
1:A:127:TRP:CZ2	1:A:145:GLU:HG3	2.19	0.77
1:B:168:LEU:O	1:B:181:ARG:HB2	1.84	0.76
1:A:304:GLU:HB2	1:A:306:THR:CG2	2.15	0.74
1:B:105:GLY:C	1:B:269:SER:HB2	2.08	0.74
1:B:53:ARG:CG	1:B:53:ARG:HH11	1.99	0.74
1:B:40:ILE:HD12	1:B:41:VAL:HG23	1.70	0.73
1:A:57:LEU:HB2	1:B:164:TYR:HE2	1.54	0.71
1:A:100:THR:HG23	1:A:262:ASN:HB2	1.70	0.71
1:A:223:THR:HG23	1:A:227:LEU:HD23	1.72	0.71
1:B:344:GLU:CD	1:B:344:GLU:H	1.94	0.70
1:B:17:LYS:HG3	1:B:18:ASN:H	1.56	0.70
1:A:127:TRP:CH2	1:A:145:GLU:HG3	2.28	0.69
1:A:305:ARG:CG	1:A:305:ARG:HH11	2.04	0.69
1:B:184:MET:HE2	1:B:194:VAL:HG21	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:305:ARG:NH1	1:A:305:ARG:HG2	2.05	0.67
1:B:170:ASP:HB2	1:B:182:LEU:HD11	1.76	0.66
1:A:146:LYS:O	1:A:150:ASN:HB2	1.96	0.65
1:A:206:ASN:HD21	1:A:208:ASP:CB	2.07	0.65
1:A:143:ILE:CD1	1:A:243:ILE:HD11	2.27	0.65
1:A:179:SER:HB2	1:A:181:ARG:HH21	1.60	0.64
1:B:321:GLN:HG2	1:B:321:GLN:O	1.98	0.64
1:B:311:TYR:CG	1:B:321:GLN:HG3	2.33	0.63
1:A:264:VAL:HG21	1:A:320:LEU:HD11	1.79	0.63
1:A:362:LYS:HG2	5:A:2020:HOH:O	1.98	0.63
1:A:58:ALA:HB2	1:B:228:MET:CE	2.29	0.63
1:B:272:ILE:HG23	1:B:293:LEU:HD21	1.81	0.63
1:B:362:LYS:N	1:B:362:LYS:NZ	2.49	0.60
1:A:172:LEU:HB2	5:A:2064:HOH:O	2.02	0.59
1:A:187:ASP:HB2	1:A:195:ILE:HG13	1.84	0.59
1:B:290:GLN:HA	1:B:293:LEU:HD23	1.84	0.59
1:B:311:TYR:CD1	1:B:321:GLN:HG3	2.38	0.59
1:A:161:LEU:HD12	1:A:161:LEU:O	2.01	0.59
1:A:87:CYS:HB2	1:A:88:PRO:HD3	1.84	0.58
1:B:143:ILE:CD1	1:B:243:ILE:HD11	2.33	0.58
1:B:243:ILE:HG22	1:B:245:MET:HG3	1.86	0.57
1:A:58:ALA:HB2	1:B:228:MET:HE3	1.87	0.57
1:A:340:SER:OG	3:A:2000:NO3:O1	2.15	0.57
1:A:117:GLY:O	1:A:118:GLU:HG3	2.05	0.57
1:A:298:VAL:HG21	1:A:317:THR:HG21	1.86	0.56
1:A:172:LEU:HD13	1:A:202:ILE:HG12	1.87	0.56
1:B:357:LYS:HE2	1:B:359:ILE:HD11	1.87	0.56
1:A:179:SER:HB2	1:A:181:ARG:HH22	1.71	0.56
1:A:30:LEU:HG	1:A:34:LYS:HE3	1.88	0.56
1:A:21:VAL:HG22	1:A:332:ILE:HD12	1.88	0.56
1:B:247:GLU:HG2	5:B:2065:HOH:O	2.05	0.55
1:B:17:LYS:CG	1:B:18:ASN:H	2.19	0.55
1:B:244:HIS:ND1	1:B:258:ILE:HG12	2.21	0.55
1:A:207:LYS:HG3	1:A:208:ASP:N	2.21	0.55
1:B:143:ILE:HD13	1:B:243:ILE:HD11	1.88	0.54
1:A:61:SER:HA	5:A:2023:HOH:O	2.07	0.54
1:B:19:ILE:HD11	1:B:302:LEU:HB3	1.90	0.54
1:B:18:ASN:HD21	1:B:327:ARG:HA	1.73	0.54
1:A:194:VAL:HG21	1:A:318:ARG:HD2	1.89	0.54
1:A:173:ASN:OD1	1:A:174:PRO:HD2	2.08	0.53
1:A:252:GLY:O	1:A:253:GLU:HB3	2.09	0.53
1:B:142:GLN:O	1:B:146:LYS:HG3	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:40:ILE:CD1	1:B:41:VAL:HG23	2.39	0.52
1:B:264:VAL:HG21	1:B:320:LEU:HD21	1.90	0.52
1:B:184:MET:HA	1:B:195:ILE:O	2.09	0.52
1:B:129:GLU:OE2	1:B:141:HIS:HD2	1.92	0.52
1:A:100:THR:HG23	1:A:262:ASN:CB	2.40	0.52
1:A:98[B]:ASN:HD21	1:A:260:LYS:NZ	2.08	0.52
1:A:57:LEU:HB2	1:B:164:TYR:CE2	2.41	0.51
1:B:244:HIS:HD2	5:B:2039:HOH:O	1.94	0.51
1:B:129:GLU:OE2	1:B:141:HIS:CD2	2.63	0.51
1:B:165:ASN:N	5:B:2046:HOH:O	2.26	0.51
1:A:127:TRP:HZ2	1:A:145:GLU:HG3	1.69	0.51
1:B:134:GLY:O	1:B:137:PRO:HD2	2.11	0.50
1:B:42:GLU:OE1	1:B:63:ARG:NH1	2.44	0.50
1:B:72:PHE:HB3	1:B:76:THR:HG21	1.93	0.50
1:B:18:ASN:HB3	1:B:328:THR:O	2.11	0.50
1:B:244:HIS:CE1	1:B:258:ILE:HG12	2.47	0.50
1:A:322:ASP:HB2	5:A:2080:HOH:O	2.10	0.50
1:A:169:PHE:CE1	1:A:228:MET:HE1	2.47	0.50
1:A:209:GLU:O	1:A:213:ILE:HG13	2.12	0.50
1:A:154:PHE:HA	1:A:244:HIS:O	2.12	0.49
1:A:50:VAL:CG1	1:A:68:PHE:HE2	2.26	0.49
1:A:329:ARG:HB3	5:A:2003:HOH:O	2.11	0.49
1:B:92:GLU:OE2	1:B:329:ARG:HG2	2.12	0.49
1:B:205:HIS:O	1:B:206:ASN:HB3	2.12	0.49
1:B:329:ARG:HB3	1:B:329:ARG:HH11	1.77	0.49
1:B:17:LYS:HG3	1:B:18:ASN:N	2.25	0.49
1:B:53:ARG:NH1	1:B:53:ARG:HG3	2.09	0.49
1:B:207:LYS:NZ	1:B:207:LYS:HB2	2.28	0.49
1:A:241:VAL:HG13	1:A:261:LEU:HB3	1.94	0.48
1:A:297:ARG:NH2	1:A:313:GLU:OE2	2.46	0.48
1:B:134:GLY:O	1:B:138:ARG:HG3	2.13	0.48
1:B:20:GLN:HA	1:B:69:ASP:OD2	2.14	0.48
1:B:250:ILE:O	1:B:251:ASP:HB2	2.14	0.48
1:A:48:LYS:HE3	1:A:68:PHE:O	2.13	0.48
1:B:105:GLY:C	1:B:269:SER:CB	2.81	0.48
1:B:294:THR:O	1:B:295:LEU:C	2.51	0.48
1:A:161:LEU:HD12	1:A:161:LEU:C	2.35	0.47
1:A:212:GLN:HG2	1:A:213:ILE:N	2.25	0.47
1:B:320:LEU:HD12	1:B:320:LEU:HA	1.65	0.47
1:A:53:ARG:HD2	5:A:2021:HOH:O	2.14	0.47
1:A:168:LEU:HD11	1:A:319:ILE:HD11	1.97	0.47
1:B:104:TYR:O	1:B:334:ALA:HA	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:67:THR:HG22	1:A:359:ILE:HD11	1.97	0.47
1:A:35:ALA:O	1:A:36:SER:HB2	2.15	0.47
1:A:160:LEU:HB3	1:A:172:LEU:HG	1.95	0.46
1:B:185:PHE:HE2	1:B:197:LYS:HE3	1.80	0.46
1:B:305:ARG:HB2	1:B:305:ARG:HE	1.48	0.46
1:A:40:ILE:CD1	1:A:343:LEU:HB2	2.44	0.46
1:B:187:ASP:OD1	1:B:189:ARG:NH1	2.49	0.46
1:A:141:HIS:ND1	1:A:207:LYS:HE3	2.31	0.46
1:A:295:LEU:HD11	1:A:299:ILE:HD11	1.97	0.46
1:B:164:TYR:O	1:B:165:ASN:HB3	2.16	0.46
1:B:174:PRO:HD2	1:B:175:SER:H	1.81	0.46
1:B:53:ARG:NH1	1:B:53:ARG:CG	2.66	0.45
1:B:26:ARG:HD2	1:B:27:PRO:O	2.16	0.45
1:B:105:GLY:CA	1:B:269:SER:HB2	2.46	0.45
1:A:238:VAL:HG22	1:A:264:VAL:HG22	1.98	0.45
1:A:106:GLN:HG2	1:A:107:THR:O	2.16	0.45
1:A:98[B]:ASN:ND2	1:A:322:ASP:HB3	2.31	0.45
1:A:26:ARG:HB2	1:A:27:PRO:HD2	1.99	0.45
1:A:138:ARG:O	1:A:141:HIS:HB3	2.17	0.44
1:A:176:SER:OG	1:A:176:SER:O	2.32	0.44
1:B:221:ARG:HD3	5:B:2043:HOH:O	2.16	0.44
1:A:40:ILE:HD13	1:A:340:SER:HA	1.99	0.44
1:A:143:ILE:HD13	1:A:243:ILE:CD1	2.37	0.44
1:A:298:VAL:HG21	1:A:317:THR:CG2	2.46	0.44
1:A:297:ARG:HH22	1:A:313:GLU:CD	2.21	0.44
1:A:309:VAL:HG22	1:A:311:TYR:CE2	2.53	0.44
1:B:215:GLU:O	1:B:216:LYS:C	2.56	0.44
1:B:138:ARG:HD2	5:B:2015:HOH:O	2.18	0.44
1:A:187:ASP:HB2	1:A:195:ILE:CD1	2.48	0.44
1:B:82:TYR:CE1	1:B:86:VAL:HG11	2.53	0.43
1:A:115:MET:HE3	1:A:263:LEU:HD22	2.00	0.43
1:A:157:LYS:HG2	5:A:2059:HOH:O	2.19	0.43
1:A:25:CYS:O	1:A:74:ALA:HA	2.17	0.43
1:B:163:ILE:HG12	1:B:168:LEU:HD12	2.00	0.43
1:A:98[B]:ASN:OD1	1:A:260:LYS:HG2	2.18	0.43
1:B:163:ILE:O	1:B:235:SER:HB2	2.19	0.43
1:B:360:LEU:HA	1:B:360:LEU:HD12	1.88	0.43
1:A:309:VAL:HG22	1:A:311:TYR:CD2	2.54	0.43
1:A:309:VAL:HA	1:A:310:PRO:HD3	1.75	0.42
1:B:362:LYS:N	1:B:362:LYS:HZ2	1.97	0.42
1:A:206:ASN:ND2	1:A:208:ASP:HB2	2.15	0.42
1:A:88:PRO:HB3	1:A:329:ARG:NH2	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:18:ASN:ND2	1:B:327:ARG:HA	2.35	0.41
1:A:173:ASN:ND2	1:A:176:SER:HB3	2.35	0.41
1:A:244:HIS:CD2	1:A:258:ILE:HG12	2.55	0.41
1:A:59:ASP:O	1:B:229:ASN:ND2	2.53	0.41
1:A:340:SER:CB	3:A:2000:NO3:O1	2.67	0.41
1:A:111:LYS:HE2	1:A:111:LYS:HB2	1.67	0.41
1:A:294:THR:O	1:A:295:LEU:C	2.57	0.41
1:B:221:ARG:HD2	1:B:232:SER:HB3	2.02	0.41
1:A:341:LEU:HA	3:A:2000:NO3:O2	2.20	0.41
1:B:173:ASN:OD1	1:B:174:PRO:HD2	2.20	0.41
1:A:100:THR:OG1	1:A:323:SER:HB2	2.21	0.41
1:B:302:LEU:HA	1:B:302:LEU:HD12	1.99	0.41
1:B:236:HIS:CD2	1:B:316:LEU:HD22	2.56	0.41
1:B:174:PRO:CD	1:B:175:SER:H	2.35	0.40
1:B:298:VAL:HG22	1:B:309:VAL:HG12	2.03	0.40
1:B:140:LEU:HA	1:B:140:LEU:HD13	1.87	0.40
1:A:172:LEU:HA	1:A:172:LEU:HD23	1.78	0.40
1:A:186:ASP:OD2	1:A:318:ARG:NH1	2.49	0.40
1:A:98[B]:ASN:HD21	1:A:260:LYS:HZ3	1.69	0.40
1:A:250:ILE:O	1:A:251:ASP:HB2	2.21	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	320/368 (87%)	308 (96%)	10 (3%)	2 (1%)	33	72
1	B	313/368 (85%)	305 (97%)	8 (3%)	0	100	100
All	All	633/736 (86%)	613 (97%)	18 (3%)	2 (0%)	50	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	VAL
1	A	179	SER

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	279/322 (87%)	251 (90%)	28 (10%)	11	30
1	B	279/322 (87%)	253 (91%)	26 (9%)	13	35
All	All	558/644 (87%)	504 (90%)	54 (10%)	12	32

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	48	LYS
1	A	92	GLU
1	A	100	THR
1	A	115	MET
1	A	145	GLU
1	A	161	LEU
1	A	168	LEU
1	A	176	SER
1	A	181	ARG
1	A	186	ASP
1	A	194	VAL
1	A	206	ASN
1	A	207	LYS
1	A	212	GLN
1	A	216	LYS
1	A	229	ASN
1	A	254	GLU
1	A	293	LEU
1	A	304	GLU
1	A	305	ARG
1	A	312	ARG
1	A	313	GLU
1	A	315	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	317	THR
1	A	322	ASP
1	A	343	LEU
1	A	359	ILE
1	B	17	LYS
1	B	52	VAL
1	B	53	ARG
1	B	63	ARG
1	B	76	THR
1	B	83	ARG
1	B	93	VAL
1	B	130	VAL
1	B	168	LEU
1	B	177	ASP
1	B	183	GLN
1	B	184	MET
1	B	194	VAL
1	B	203	THR
1	B	207	LYS
1	B	220	LYS
1	B	242	THR
1	B	256	VAL
1	B	290	GLN
1	B	302	LEU
1	B	305	ARG
1	B	315	LYS
1	B	320	LEU
1	B	329	ARG
1	B	343	LEU
1	B	362	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	ASN
1	B	18	ASN
1	B	141	HIS
1	B	183	GLN
1	B	212	GLN
1	B	244	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z > 2$
3	NO3	A	2000	-	3,3,3	3.12	3 (100%)	3,3,3	0.33	0
3	NO3	A	2001	-	3,3,3	3.40	3 (100%)	3,3,3	0.37	0
4	ADP	A	2601	2	29,29,29	1.24	2 (6%)	45,45,45	1.71	7 (15%)
4	ADP	B	2600	2	29,29,29	1.17	3 (10%)	45,45,45	1.98	9 (20%)

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	NO3	A	2000	-	-	0/0/0/0	0/0/0/0
3	NO3	A	2001	-	-	0/0/0/0	0/0/0/0
4	ADP	A	2601	2	-	0/16/32/32	0/1/3/3
4	ADP	B	2600	2	-	0/16/32/32	0/1/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001	NO3	O1-N	4.06	1.41	1.24
3	A	2000	NO3	O1-N	3.65	1.39	1.24
4	A	2601	ADP	C5-C4	3.46	1.48	1.40
4	A	2601	ADP	C4-N9	-3.35	1.32	1.37
3	A	2001	NO3	O3-N	3.15	1.42	1.25
4	B	2600	ADP	C5-C4	2.95	1.47	1.40
3	A	2000	NO3	O2-N	2.92	1.40	1.25
3	A	2001	NO3	O2-N	2.87	1.40	1.25
3	A	2000	NO3	O3-N	2.71	1.39	1.25
4	B	2600	ADP	C4-N9	-2.54	1.34	1.37
4	B	2600	ADP	C2'-C1'	-2.45	1.50	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2600	ADP	N3-C2-N1	-6.50	123.27	128.71
4	B	2600	ADP	N3-C4-N9	6.23	136.69	125.43
4	A	2601	ADP	N3-C4-N9	5.53	135.43	125.43
4	B	2600	ADP	O4'-C1'-N9	-3.76	104.95	108.44
4	A	2601	ADP	C4-C5-N7	-3.49	106.53	109.52
4	B	2600	ADP	C8-N9-C4	3.44	109.52	106.90
4	A	2601	ADP	PA-O3A-PB	-3.28	122.06	131.68
4	A	2601	ADP	N3-C2-N1	-3.27	125.97	128.71
4	B	2600	ADP	C5-C4-N3	-3.23	118.66	125.70
4	A	2601	ADP	C5-C4-N3	-3.23	118.67	125.70
4	A	2601	ADP	C8-N9-C4	3.14	109.30	106.90
4	B	2600	ADP	PA-O3A-PB	-2.99	122.92	131.68
4	A	2601	ADP	O3'-C3'-C4'	-2.62	103.35	111.08
4	B	2600	ADP	N6-C6-N1	2.39	124.05	119.36
4	B	2600	ADP	C2-N3-C4	2.33	120.65	114.01
4	B	2600	ADP	C8-N9-C1'	-2.13	122.18	126.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	327/368 (88%)	-0.17	16 (4%) 28 29	7, 24, 56, 81	0
1	B	321/368 (87%)	-0.35	3 (0%) 81 81	10, 21, 46, 63	0
All	All	648/736 (88%)	-0.26	19 (2%) 49 50	7, 22, 54, 81	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	252	GLY	3.6
1	A	177	ASP	3.2
1	B	54	THR	3.2
1	B	273	GLY	3.0
1	A	287	ASN	2.6
1	A	253	GLU	2.5
1	A	307	PRO	2.4
1	A	188	PRO	2.4
1	A	187	ASP	2.3
1	B	363	PRO	2.3
1	A	308	HIS	2.3
1	A	185	PHE	2.2
1	A	174	PRO	2.2
1	A	255	LEU	2.2
1	A	286	GLY	2.1
1	A	176	SER	2.1
1	A	325	GLY	2.1
1	A	285	ALA	2.1
1	A	212	GLN	2.1

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

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

6.3 Carbohydrates

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. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MG	A	1365	1/1	0.24	2.97	30,30,30,30	0
2	MG	B	1365	1/1	0.32	2.47	30,30,30,30	0
3	NO3	A	2001	4/4	0.22	0.47	36,38,43,45	0
3	NO3	A	2000	4/4	0.12	0.28	15,17,19,22	0
4	ADP	A	2601	27/27	0.12	-0.63	7,9,16,22	0
4	ADP	B	2600	27/27	0.13	-0.69	10,13,17,18	0

6.5 Other polymers

There are no such residues in this entry.