W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 04:22 PM GMT

PDB ID	:	4A28
Title	:	Eg5-2
Authors	:	Talapatra, S.K.; Kozielski, F.
Deposited on	:	2011-09-22
Resolution	:	2.55 Å(reported)

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 2.55 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	Percentile Ranks	Value
Rfree		0.262
Clashscore		17
Ramachandran outliers		0.2%
Sidechain outliers		9.3%
RSRZ outliers		5.3%

Worse   Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
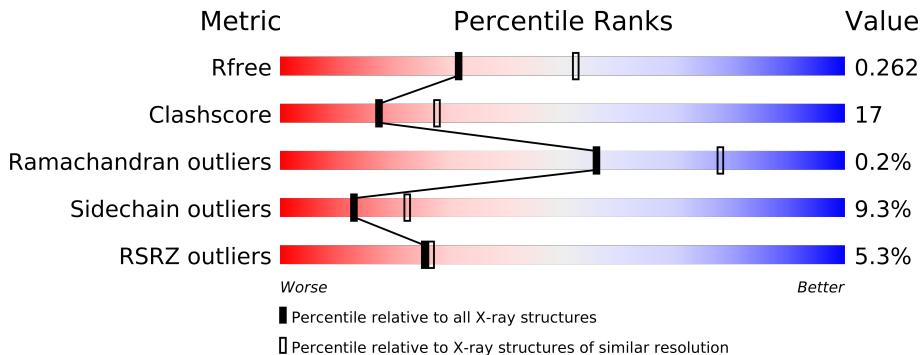
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	3413 (2.58-2.50)
Clashscore	79885	4284 (2.58-2.50)
Ramachandran outliers	78287	4193 (2.58-2.50)
Sidechain outliers	78261	4195 (2.58-2.50)
RSRZ outliers	66119	3414 (2.58-2.50)

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	
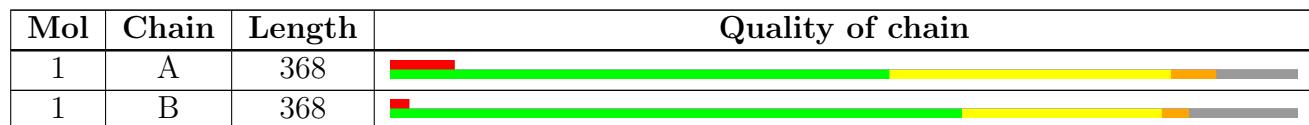
2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 5306 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	332	Total	C	N	O	S	0	0	0
			2534	1589	438	497	10			
1	B	322	Total	C	N	O	S	0	1	0
			2517	1579	436	492	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	133	ASP	ALA	ENGINEERED MUTATION	UNP P52732
B	133	ASP	ALA	ENGINEERED MUTATION	UNP P52732

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
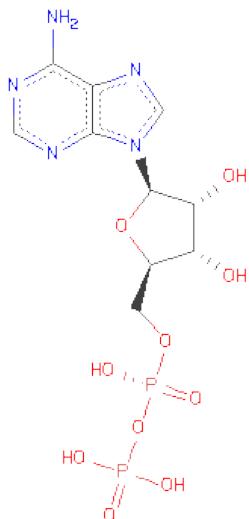
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	91	91	91	0	0
4	B	108	Total	O	0	0
			108	108		

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:
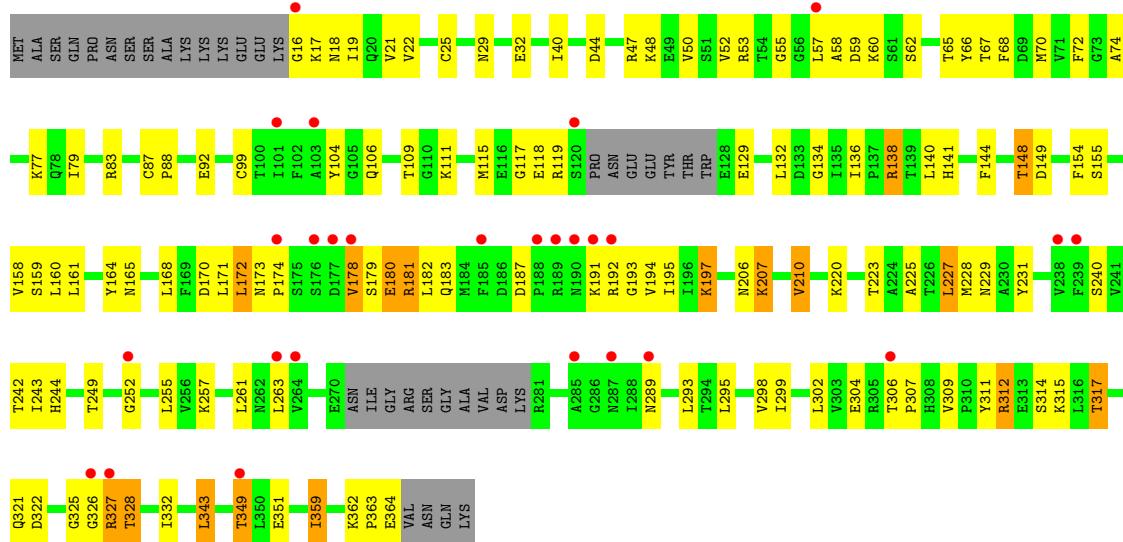
• Molecule 1: KINESIN-LIKE PROTEIN KIF11

Chain B:
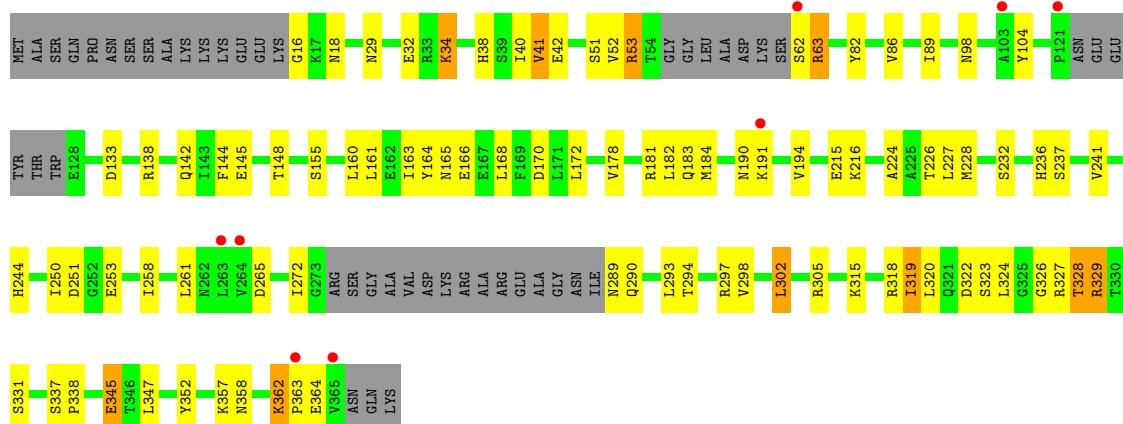
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	52.90Å 78.39Å 92.69Å 90.00° 93.16° 90.00°	Depositor
Resolution (Å)	29.50 – 2.55 29.91 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.50-2.55) 98.7 (29.91-2.55)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.60 (at 2.54Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.180 , 0.264 0.176 , 0.262	Depositor DCC
R_{free} test set	1238 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	38.3	Xtriage
Anisotropy	0.643	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Outliers	0 of 24512 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5306	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities 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

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	0.54	0/2567	0.69	0/3473
1	B	0.53	0/2554	0.70	0/3451
All	All	0.53	0/5121	0.69	0/6924

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2534	0	2529	111	0
1	B	2517	0	2545	77	0
2	A	27	0	12	2	0
2	B	27	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	91	0	0	5	0
4	B	108	0	0	2	0
All	All	5306	0	5098	178	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 (178) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:178:VAL:HG12	1:A:179:SER:H	1.13	1.09
1:B:362:LYS:HZ2	1:B:362:LYS:H	1.11	0.98
1:A:144:PHE:O	1:A:148:THR:HG23	1.69	0.93
1:A:179:SER:HB2	1:A:181:ARG:HH21	1.31	0.92
1:A:304:GLU:HB3	1:A:306:THR:HG23	1.53	0.90
1:A:140:LEU:HG	1:A:210:VAL:HG13	1.58	0.85
1:A:327:ARG:HA	1:A:327:ARG:HE	1.41	0.83
1:A:178:VAL:HG12	1:A:179:SER:N	1.94	0.83
1:A:178:VAL:CG1	1:A:179:SER:H	1.91	0.82
1:A:57:LEU:HD13	1:B:164:TYR:CD2	2.15	0.81
1:B:53:ARG:N	1:B:63:ARG:HH11	1.83	0.77
1:B:289:ASN:CG	1:B:290:GLN:H	1.88	0.74
1:A:178:VAL:HB	1:A:180:GLU:HG2	1.69	0.74
1:A:249:THR:HB	1:A:252:GLY:HA3	1.70	0.73
1:A:53:ARG:NH1	1:A:60:LYS:HE3	2.05	0.72
1:A:225:ALA:O	1:A:229:ASN:HA	1.89	0.72
1:B:362:LYS:HB3	1:B:363:PRO:HD2	1.71	0.72
1:A:67:THR:HG22	1:A:359:ILE:HD11	1.71	0.72
1:A:327:ARG:NE	1:A:327:ARG:HA	2.00	0.71
1:A:311:TYR:OH	1:A:325:GLY:HA3	1.90	0.71
1:B:170:ASP:HB2	1:B:182:LEU:HD11	1.75	0.69
1:B:323:SER:O	4:B:2029:HOH:O	2.12	0.68
1:A:104:TYR:HE1	1:A:349:THR:OG1	1.76	0.67
1:A:228:MET:O	1:A:229:ASN:OD1	2.12	0.67
1:B:362:LYS:NZ	1:B:362:LYS:H	1.91	0.67
1:A:16:GLY:C	1:A:17:LYS:HD2	2.16	0.66
1:B:53:ARG:HG2	1:B:53:ARG:HH11	1.60	0.66
1:A:183:GLN:H	1:A:197:LYS:HE3	1.59	0.66
1:A:315:LYS:NZ	4:A:2069:HOH:O	2.29	0.65
1:A:171:LEU:O	1:A:220:LYS:HE3	1.96	0.65
1:A:179:SER:HB2	1:A:181:ARG:NH2	2.09	0.64
1:A:104:TYR:CE1	1:A:349:THR:OG1	2.49	0.64
1:A:118:GLU:O	1:A:132:LEU:HB2	1.98	0.64
1:B:16:GLY:HA3	1:B:357:LYS:HE3	1.80	0.64
1:B:29:ASN:HB2	4:B:2011:HOH:O	1.98	0.64
1:B:289:ASN:OD1	1:B:290:GLN:N	2.30	0.63
1:A:170:ASP:O	1:A:220:LYS:NZ	2.32	0.63
1:A:58:ALA:HB2	1:B:228:MET:CE	2.29	0.62
1:A:170:ASP:HB2	1:A:182:LEU:HD11	1.80	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:298:VAL:O	1:B:302:LEU:HD22	1.99	0.62
1:B:144:PHE:O	1:B:148:THR:HG23	1.99	0.62
1:A:140:LEU:HG	1:A:210:VAL:CG1	2.29	0.62
1:A:57:LEU:HB2	1:B:164:TYR:HE2	1.64	0.62
1:B:244:HIS:CD2	1:B:258:ILE:HG12	2.35	0.62
1:A:326:GLY:O	1:A:328:THR:HG22	1.99	0.61
1:B:82:TYR:CE2	1:B:86:VAL:HG11	2.36	0.61
1:A:104:TYR:HE1	1:A:349:THR:HG1	1.48	0.61
1:A:187:ASP:HB3	1:A:195:ILE:HG13	1.83	0.59
1:A:44:ASP:OD2	1:A:47:ARG:HB2	2.02	0.59
1:B:319:ILE:HG22	1:B:320:LEU:HG	1.83	0.59
1:A:289:ASN:O	1:A:293:LEU:HB2	2.03	0.59
1:B:226:THR:HG22	1:B:227:LEU:HD23	1.83	0.59
1:A:364:GLU:CG	1:A:364:GLU:O	2.51	0.59
1:B:41:VAL:CG2	1:B:338:PRO:HA	2.33	0.59
1:B:98:ASN:HB3	1:B:323:SER:OG	2.03	0.58
1:A:192:ARG:NH2	1:A:326:GLY:H	2.01	0.58
1:B:18:ASN:HB2	1:B:328:THR:O	2.04	0.58
1:B:178:VAL:CG2	1:B:224:ALA:HA	2.34	0.57
1:A:244:HIS:CD2	4:A:2060:HOH:O	2.58	0.56
1:A:223:THR:HG23	1:A:227:LEU:HD22	1.88	0.56
1:A:312:ARG:HD3	1:A:312:ARG:H	1.71	0.56
1:B:52:VAL:HG11	1:B:347:LEU:HD21	1.88	0.55
1:A:183:GLN:H	1:A:197:LYS:CE	2.18	0.55
1:A:243:ILE:HD12	1:A:243:ILE:N	2.22	0.55
1:B:53:ARG:NH1	1:B:53:ARG:HG2	2.21	0.54
1:A:364:GLU:HG3	1:A:364:GLU:O	2.08	0.54
1:A:57:LEU:HD13	1:B:164:TYR:CE2	2.44	0.53
1:A:66:TYR:OH	1:A:351:GLU:OE2	2.13	0.53
1:B:184:MET:CE	1:B:319:ILE:HD11	2.39	0.53
1:A:161:LEU:HD12	1:A:161:LEU:C	2.29	0.53
1:A:58:ALA:HB2	1:B:228:MET:HE3	1.91	0.52
1:B:253:GLU:HA	1:B:253:GLU:OE1	2.09	0.52
1:A:57:LEU:HD13	1:B:164:TYR:HD2	1.70	0.52
1:B:16:GLY:CA	1:B:357:LYS:HE3	2.39	0.52
1:A:164:TYR:O	1:A:165:ASN:HB2	2.10	0.51
1:A:16:GLY:O	1:A:17:LYS:HD2	2.11	0.51
1:B:184:MET:SD	1:B:319:ILE:HD11	2.50	0.51
1:A:225:ALA:HB1	1:B:38:HIS:CE1	2.45	0.50
1:A:50:VAL:HG12	1:A:68:PHE:HE2	1.76	0.50
1:A:178:VAL:HB	1:A:180:GLU:CG	2.40	0.50
1:A:159:SER:OG	1:A:240:SER:HB2	2.12	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:295:LEU:O	1:A:299:ILE:HG12	2.11	0.50
1:A:119:ARG:NH1	1:A:119:ARG:HB3	2.26	0.50
1:A:183:GLN:N	1:A:197:LYS:HE3	2.26	0.49
1:A:304:GLU:C	1:A:306:THR:H	2.15	0.49
1:B:29:ASN:N	1:B:32:GLU:OE1	2.31	0.49
1:A:70:MET:HG2	1:A:72:PHE:CZ	2.48	0.49
1:B:178:VAL:HG23	1:B:224:ALA:HA	1.93	0.49
1:A:141:HIS:HD2	1:A:207:LYS:NZ	2.10	0.48
1:A:19:ILE:HD11	1:A:327:ARG:HH22	1.77	0.48
1:B:34:LYS:HD3	1:B:34:LYS:O	2.13	0.48
1:A:311:TYR:OH	1:A:325:GLY:CA	2.59	0.48
1:A:62:SER:HA	4:A:2023:HOH:O	2.13	0.48
1:B:18:ASN:HD21	1:B:327:ARG:HA	1.78	0.48
1:A:18:ASN:HB3	1:A:328:THR:O	2.14	0.48
1:A:40:ILE:HD12	1:A:343:LEU:HD23	1.94	0.48
1:B:289:ASN:CG	1:B:290:GLN:N	2.58	0.48
1:B:133:ASP:O	1:B:138:ARG:NE	2.46	0.48
1:B:237:SER:HB3	1:B:265:ASP:HB3	1.96	0.47
1:A:50:VAL:CG1	1:A:68:PHE:HE2	2.27	0.47
1:A:77:LYS:HG2	4:A:2031:HOH:O	2.14	0.47
1:A:55:GLY:HA3	1:A:59:ASP:O	2.14	0.47
1:A:192:ARG:NH2	1:A:321:GLN:O	2.48	0.47
1:B:184:MET:SD	1:B:319:ILE:CD1	3.02	0.47
1:A:173:ASN:HA	1:A:174:PRO:HD3	1.72	0.47
1:B:324:LEU:C	1:B:326:GLY:H	2.18	0.47
1:A:304:GLU:HB3	1:A:306:THR:CG2	2.36	0.47
1:B:155:SER:OG	1:B:244:HIS:HB2	2.15	0.47
1:A:40:ILE:O	1:A:52:VAL:HA	2.15	0.47
1:B:161:LEU:HD12	1:B:161:LEU:C	2.34	0.47
1:A:57:LEU:HB2	1:B:164:TYR:CE2	2.48	0.47
1:A:309:VAL:HB	1:A:311:TYR:CE2	2.50	0.46
1:B:318:ARG:HA	1:B:318:ARG:HD2	1.64	0.46
1:B:358:ASN:C	1:B:358:ASN:OD1	2.54	0.46
1:A:160:LEU:HB3	1:A:172:LEU:HD13	1.98	0.46
1:A:25:CYS:O	1:A:74:ALA:HA	2.16	0.45
1:A:257:LYS:HE3	1:A:257:LYS:HB2	1.68	0.45
1:A:312:ARG:CD	1:A:312:ARG:H	2.30	0.45
1:B:250:ILE:O	1:B:251:ASP:HB2	2.17	0.45
2:A:1365:ADP:N6	4:A:2003:HOH:O	2.13	0.45
1:A:231:TYR:HE1	1:B:38:HIS:ND1	2.15	0.45
1:A:362:LYS:HA	1:A:363:PRO:HD3	1.78	0.45
1:B:226:THR:HG22	1:B:227:LEU:CD2	2.47	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:322:ASP:N	1:A:322:ASP:OD1	2.50	0.44
1:B:168:LEU:O	1:B:181:ARG:HB2	2.18	0.44
1:A:178:VAL:CG1	1:A:179:SER:N	2.64	0.44
1:A:191:LYS:C	1:A:193:GLY:H	2.20	0.43
1:B:18:ASN:ND2	1:B:327:ARG:HA	2.32	0.43
1:B:216:LYS:HE2	1:B:216:LYS:HB3	1.71	0.43
1:A:183:GLN:H	1:A:197:LYS:CD	2.32	0.43
1:B:183:GLN:HA	1:B:183:GLN:OE1	2.18	0.43
1:A:29:ASN:OD1	1:A:32:GLU:HG3	2.18	0.43
1:B:16:GLY:HA3	1:B:357:LYS:CE	2.47	0.43
1:A:314:SER:OG	1:A:317:THR:OG1	2.26	0.43
1:A:92:GLU:HG2	1:A:99:CYS:SG	2.59	0.43
1:A:79:ILE:O	1:A:83:ARG:HG3	2.18	0.43
1:B:178:VAL:HG22	1:B:228:MET:CG	2.49	0.43
1:B:190:ASN:ND2	1:B:322:ASP:OD1	2.50	0.43
1:A:53:ARG:HH12	1:A:60:LYS:HE3	1.81	0.42
1:A:21:VAL:HG22	1:A:332:ILE:HD12	2.00	0.42
1:A:57:LEU:HD22	1:B:165:ASN:HB3	2.00	0.42
1:A:154:PHE:HA	1:A:244:HIS:O	2.19	0.42
1:A:87:CYS:HB2	1:A:88:PRO:HD3	2.01	0.42
1:B:178:VAL:HG21	1:B:227:LEU:HB2	2.01	0.42
1:A:117:GLY:O	1:A:118:GLU:HB3	2.19	0.42
1:B:42:GLU:OE2	1:B:63:ARG:NH2	2.53	0.42
1:B:345:GLU:HA	1:B:345:GLU:OE1	2.19	0.42
1:B:294:THR:OG1	1:B:297:ARG:NH2	2.53	0.42
1:A:155:SER:OG	1:A:244:HIS:HB2	2.20	0.41
1:A:65:THR:HG22	1:A:66:TYR:N	2.35	0.41
1:B:104:TYR:CE2	1:B:352:TYR:CE2	3.08	0.41
1:A:231:TYR:CE1	1:B:38:HIS:ND1	2.87	0.41
1:B:160:LEU:HB3	1:B:172:LEU:HG	2.01	0.41
1:B:324:LEU:O	1:B:326:GLY:N	2.54	0.41
1:A:22:VAL:CG1	1:A:70:MET:HB3	2.50	0.41
1:A:223:THR:CG2	1:A:227:LEU:HD22	2.49	0.41
1:B:329:ARG:HD2	1:B:329:ARG:HA	1.83	0.41
1:B:164:TYR:O	1:B:165:ASN:HB3	2.20	0.41
1:A:134:GLY:O	1:A:138:ARG:HB2	2.20	0.41
1:B:362:LYS:N	1:B:362:LYS:HZ2	1.95	0.41
1:B:163:ILE:HB	1:B:236:HIS:HB2	2.02	0.41
1:A:106:GLN:HB3	1:A:109:THR:HG23	2.03	0.41
1:A:306:THR:HA	1:A:307:PRO:HD3	1.80	0.41
1:B:178:VAL:HG22	1:B:228:MET:HG3	2.02	0.41
1:A:47:ARG:O	1:A:48:LYS:HB2	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:326:GLY:O	1:B:327:ARG:C	2.58	0.41
1:A:22:VAL:HG12	1:A:70:MET:CB	2.51	0.41
1:A:136:ILE:HG12	1:A:263:LEU:CD1	2.51	0.41
1:A:170:ASP:OD1	1:A:172:LEU:N	2.43	0.40
1:A:298:VAL:HG21	1:A:317:THR:HG21	2.02	0.40
1:B:166:GLU:O	1:B:315:LYS:HE3	2.21	0.40
1:A:141:HIS:HD2	1:A:207:LYS:CE	2.34	0.40
1:B:319:ILE:HD12	1:B:319:ILE:HA	1.83	0.40
1:A:111:LYS:NZ	2:A:1365:ADP:O2B	2.50	0.40
1:B:89:ILE:HD11	1:B:331:SER:HB2	2.04	0.40
1:A:57:LEU:O	1:A:58:ALA:HB3	2.21	0.40
1:A:158:VAL:HA	1:A:240:SER:O	2.22	0.40
1:B:89:ILE:HG12	1:B:329:ARG:HB3	2.03	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	326/368 (89%)	312 (96%)	13 (4%)	1 (0%)	50	71
1	B	315/368 (86%)	306 (97%)	9 (3%)	0	100	100
All	All	641/736 (87%)	618 (96%)	22 (3%)	1 (0%)	56	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	VAL

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	277/323 (86%)	251 (91%)	26 (9%)	13	22
1	B	285/323 (88%)	259 (91%)	26 (9%)	14	23
All	All	562/646 (87%)	510 (91%)	52 (9%)	13	22

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	MET
1	A	129	GLU
1	A	138	ARG
1	A	148	THR
1	A	149	ASP
1	A	168	LEU
1	A	172	LEU
1	A	180	GLU
1	A	181	ARG
1	A	194	VAL
1	A	197	LYS
1	A	206	ASN
1	A	207	LYS
1	A	210	VAL
1	A	227	LEU
1	A	242	THR
1	A	255	LEU
1	A	261	LEU
1	A	302	LEU
1	A	312	ARG
1	A	317	THR
1	A	327	ARG
1	A	328	THR
1	A	343	LEU
1	A	349	THR
1	A	359	ILE
1	B	34	LYS
1	B	40	ILE
1	B	41	VAL
1	B	51	SER
1	B	53	ARG
1	B	62	SER
1	B	63	ARG
1	B	142	GLN

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Mol	Chain	Res	Type
1	B	145	GLU
1	B	191	LYS
1	B	194	VAL
1	B	215	GLU
1	B	232	SER
1	B	241	VAL
1	B	261	LEU
1	B	272	ILE
1	B	293	LEU
1	B	302	LEU
1	B	305	ARG
1	B	319	ILE
1	B	328	THR
1	B	329	ARG
1	B	337	SER
1	B	345	GLU
1	B	362	LYS
1	B	364	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#|Z| > 2$
2	ADP	A	1365	3	29,29,29	0.99	2 (6%)	45,45,45	1.83	8 (17%)
2	ADP	B	1366	3	29,29,29	1.22	2 (6%)	45,45,45	1.62	8 (17%)

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
2	ADP	A	1365	3	-	0/16/32/32	0/1/3/3
2	ADP	B	1366	3	-	0/16/32/32	0/1/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1366	ADP	C5-C4	3.52	1.48	1.40
2	A	1365	ADP	C4-N9	-2.94	1.33	1.37
2	B	1366	ADP	C4-N9	-2.67	1.33	1.37
2	A	1365	ADP	C5-C4	2.53	1.46	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1365	ADP	N3-C2-N1	-5.87	123.80	128.71
2	B	1366	ADP	N3-C4-N9	5.27	134.96	125.43
2	A	1365	ADP	N3-C4-N9	5.13	134.70	125.43
2	B	1366	ADP	N3-C2-N1	-4.76	124.73	128.71
2	A	1365	ADP	C8-N9-C4	4.53	110.36	106.90
2	A	1365	ADP	C4-C5-N7	-3.65	106.39	109.52
2	B	1366	ADP	O4'-C1'-N9	-3.14	105.52	108.44
2	B	1366	ADP	C4-C5-N7	-3.06	106.90	109.52
2	B	1366	ADP	C5-C4-N3	-3.03	119.11	125.70
2	A	1365	ADP	C5-C4-N3	-2.70	119.82	125.70
2	A	1365	ADP	O4'-C1'-N9	-2.68	105.95	108.44
2	B	1366	ADP	PA-O3A-PB	-2.36	124.76	131.68
2	A	1365	ADP	O3B-PB-O2B	2.35	116.77	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1366	ADP	C8-N9-C4	2.27	108.63	106.90
2	A	1365	ADP	C2-N3-C4	2.20	120.27	114.01
2	B	1366	ADP	C2-N3-C4	2.02	119.77	114.01

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(Å²)	Q<0.9
1	A	332/368 (90%)	0.20	27 (8%)	12	11	20, 44, 83, 112	0
1	B	322/368 (87%)	-0.01	8 (2%)	54	58	19, 38, 67, 102	0
All	All	654/736 (88%)	0.10	35 (5%)	25	26	19, 41, 79, 112	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	188	PRO	4.2
1	A	192	ARG	3.7
1	B	363	PRO	3.4
1	A	190	ASN	3.3
1	B	365	VAL	3.3
1	A	177	ASP	3.3
1	B	264	VAL	3.2
1	B	121	PRO	3.2
1	A	263	LEU	3.1
1	A	264	VAL	3.0
1	B	62	SER	2.8
1	A	289	ASN	2.8
1	A	252	GLY	2.8
1	A	16	GLY	2.6
1	A	101	ILE	2.6
1	A	185	PHE	2.5
1	B	191	LYS	2.5
1	A	191	LYS	2.5
1	A	57	LEU	2.4
1	A	174	PRO	2.4
1	A	120	SER	2.4
1	A	103	ALA	2.3
1	A	327	ARG	2.3
1	A	178	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	326	GLY	2.2
1	A	176	SER	2.2
1	A	238	VAL	2.2
1	A	239	PHE	2.2
1	A	349	THR	2.2
1	A	285	ALA	2.1
1	A	287	ASN	2.1
1	A	189	ARG	2.1
1	B	263	LEU	2.1
1	A	306	THR	2.1
1	B	103	ALA	2.0

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
3	MG	A	1366	1/1	0.22	0.48	24,24,24,24	0
3	MG	B	1367	1/1	0.23	-0.38	23,23,23,23	0
2	ADP	B	1366	27/27	0.13	-0.80	18,27,34,35	0
2	ADP	A	1365	27/27	0.12	-0.89	21,25,35,39	0

6.5 Other polymers ⓘ

There are no such residues in this entry.