



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:15 PM GMT

PDB ID : 2X7D
Title : CRYSTAL STRUCTURE OF HUMAN KINESIN EG5 IN COMPLEX WITH
(S)-DIMETHYLENASTRON
Authors : Kaan, H.Y.K.; Ulaganathan, V.; Rath, O.; Laggner, C.; Prokopcova, H.;
Dallinger, D.; Kappe, C.O.; Kozielski, F.
Deposited on : 2010-02-26
Resolution : 2.30 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>

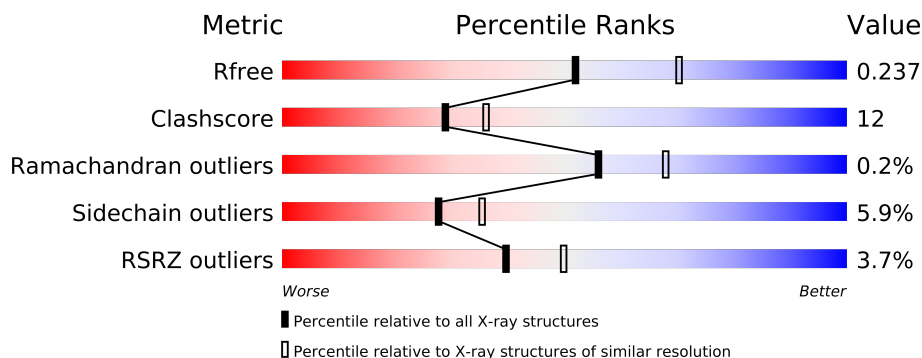
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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
3	MG	A	1368	-	X

2 Entry composition i

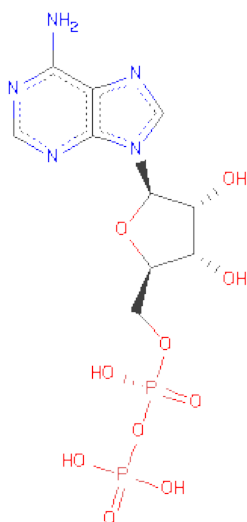
There are 5 unique types of molecules in this entry. The entry contains 5990 atoms, of which 0 are hydrogen and 0 are deuterium.

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	335	Total	C	N	O	S	0	10	0
			2670	1674	461	524	11			
1	B	334	Total	C	N	O	S	0	11	0
			2689	1689	465	524	11			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

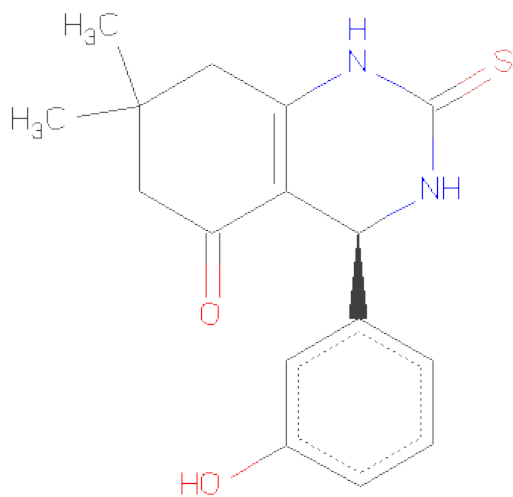


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

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

- Molecule 4 is (4S)-4-(3-HYDROXYPHENYL)-7,7-DIMETHYL-2-THIOXO-2,3,4,6,7,8-HEXAHYDROQUINAZOLIN-5(1H)-ONE (three-letter code: EGB) (formula: C₁₆H₁₈N₂O₂S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 21 16 2 2 1	0	0
4	B	1	Total C N O S 21 16 2 2 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	286	Total O 286 286	0	0
5	B	245	Total O 245 245	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.52Å 79.72Å 159.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.58 – 2.30 29.58 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.58-2.30) 99.9 (29.58-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.83 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.176 , 0.241 0.177 , 0.237	Depositor DCC
R_{free} test set	2003 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 25.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 39945 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5990	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.97 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.4053e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: EGB, 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	0.67	2/2740 (0.1%)	0.82	4/3709 (0.1%)
1	B	0.65	0/2761	0.98	3/3733 (0.1%)
All	All	0.66	2/5501 (0.0%)	0.90	7/7442 (0.1%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	270	GLU	CD-OE2	-6.85	1.18	1.25
1	A	270	GLU	CD-OE1	-5.48	1.19	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	58	ALA	CB-CA-C	29.94	155.01	110.10
1	B	59	ASP	N-CA-CB	-14.85	83.88	110.60
1	B	58	ALA	N-CA-C	-10.25	83.31	111.00
1	A	288	ILE	N-CA-CB	-7.44	93.69	110.80
1	A	59	ASP	N-CA-C	5.91	126.96	111.00
1	A	234	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	A	59	ASP	N-CA-CB	-5.25	101.14	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	59	ASP	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	2670	0	2686	59	0
1	B	2689	0	2730	76	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	21	0	18	1	0
4	B	21	0	18	1	0
5	A	286	0	0	13	0
5	B	245	0	0	12	0
All	All	5990	0	5476	135	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 12.

All (135) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:61:SER:OG	1:B:63[A]:ARG:NH1	1.73	1.19
1:B:82[A]:TYR:CE1	1:B:87[A]:CYS:SG	2.48	1.06
1:A:162:GLU:HG3	1:A:171:LEU:HD23	1.41	0.98
1:B:82[A]:TYR:OH	1:B:142:GLN:HG3	1.65	0.97
1:A:116:GLU:OE2	1:A:221:ARG:NH2	1.99	0.95
1:A:92[A]:GLU:OE1	1:A:329[A]:ARG:HD2	1.68	0.94
1:A:355:ARG:NH2	5:A:2276:HOH:O	2.06	0.89
1:A:44:ASP:OD2	1:A:47[A]:ARG:NE	2.07	0.88
1:A:344[A]:GLU:OE2	5:A:2265:HOH:O	1.95	0.85
1:B:60:LYS:O	1:B:61:SER:HB3	1.74	0.84
1:B:271[A]:ASN:ND2	5:B:2190:HOH:O	2.10	0.84
1:B:82[A]:TYR:CZ	1:B:87[A]:CYS:SG	2.71	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:80:ASP:OD1	5:A:2062:HOH:O	2.00	0.79
1:A:344[A]:GLU:CD	5:A:2263:HOH:O	2.22	0.78
1:B:30:LEU:CD1	1:B:34:LYS:NZ	2.47	0.77
1:B:162:GLU:HG3	1:B:171:LEU:HD23	1.65	0.77
1:A:80:ASP:OD2	5:A:2063:HOH:O	2.03	0.77
1:B:61:SER:HB2	5:B:2031:HOH:O	1.84	0.76
1:B:260:LYS:HD3	5:B:2179:HOH:O	1.85	0.76
1:B:227[A]:LEU:HD22	1:B:228:MET:HG3	1.69	0.74
1:A:162:GLU:HG3	1:A:171:LEU:CD2	2.15	0.74
1:B:30:LEU:HD12	1:B:34:LYS:NZ	2.03	0.74
1:A:58:ALA:O	5:A:2040:HOH:O	2.05	0.74
1:A:187:ASP:OD1	1:A:189:ARG:HG3	1.90	0.72
1:A:344[A]:GLU:HG3	5:A:2263:HOH:O	1.89	0.71
1:B:175:SER:O	5:B:2119:HOH:O	2.09	0.71
1:A:251:ASP:OD1	5:A:2213:HOH:O	2.09	0.71
1:B:192:ARG:HG2	1:B:192:ARG:HH11	1.54	0.71
1:B:61:SER:HG	1:B:63[A]:ARG:HH12	1.32	0.70
1:B:92:GLU:HG3	1:B:97:TYR:CD2	2.28	0.68
1:A:43:CYS:HB3	1:A:71:VAL:HG12	1.76	0.68
1:B:30:LEU:HD12	1:B:34:LYS:HZ3	1.57	0.67
1:A:344[A]:GLU:OE1	5:A:2263:HOH:O	2.13	0.67
1:A:344[A]:GLU:CG	5:A:2263:HOH:O	2.43	0.67
1:A:91:ASP:OD1	1:A:146:LYS:HE2	1.94	0.67
1:B:166:GLU:O	1:B:315:LYS:HE2	1.94	0.67
1:B:57:LEU:O	1:B:58:ALA:CB	2.43	0.66
1:B:184:MET:HE3	1:B:318:ARG:NH1	2.10	0.66
1:B:193:GLY:HA2	5:B:2128:HOH:O	1.96	0.66
1:A:162:GLU:OE2	1:A:221:ARG:NH1	2.30	0.65
1:B:58:ALA:O	5:B:2032:HOH:O	2.14	0.65
1:B:184:MET:HE3	1:B:318:ARG:HD3	1.78	0.65
1:A:33:ARG:NH1	5:A:2009:HOH:O	2.29	0.65
1:A:184:MET:HE3	1:A:318:ARG:HD3	1.79	0.64
1:B:30:LEU:CD1	1:B:34:LYS:HZ3	2.11	0.64
1:B:56:GLY:O	1:B:60:LYS:O	2.14	0.64
1:B:227[A]:LEU:CD2	1:B:228:MET:HG3	2.29	0.63
1:A:184:MET:CE	1:A:318:ARG:NH1	2.62	0.62
1:B:212[B]:GLN:OE1	1:B:216:LYS:HE2	2.01	0.60
1:A:43:CYS:HB3	1:A:71:VAL:CG1	2.32	0.60
1:A:187:ASP:OD1	1:A:187:ASP:C	2.39	0.59
1:A:184:MET:HE2	1:A:318:ARG:NH1	2.19	0.57
1:B:184:MET:HE3	1:B:318:ARG:CZ	2.34	0.57
1:A:166:GLU:O	1:A:315:LYS:HE2	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:184:MET:CE	1:B:318:ARG:NH1	2.69	0.56
1:B:82[B]:TYR:OH	1:B:142:GLN:CG	2.55	0.55
1:B:54:THR:HG21	1:B:64:LYS:HG3	1.89	0.54
1:A:87[B]:CYS:HB3	1:A:88:PRO:HD3	1.90	0.54
1:B:299:ILE:HG23	1:B:359:ILE:HD11	1.90	0.53
1:B:18:ASN:OD1	1:B:360:LEU:CD2	2.57	0.53
1:B:363:PRO:O	5:B:2236:HOH:O	2.18	0.53
1:A:288:ILE:O	1:A:288:ILE:CG2	2.57	0.52
1:A:92[A]:GLU:OE1	1:A:329[A]:ARG:CD	2.51	0.52
1:B:146:LYS:HE2	5:B:2058:HOH:O	2.09	0.52
1:B:170:ASP:HB2	1:B:182:LEU:HD11	1.91	0.52
1:B:45:PRO:HD2	5:B:2021:HOH:O	2.11	0.51
1:A:289:ASN:HD22	1:A:292:LEU:H	1.58	0.51
1:B:171:LEU:HG	1:B:221:ARG:HG3	1.93	0.51
1:A:184:MET:HE3	1:A:318:ARG:CZ	2.40	0.51
1:B:173:ASN:HB2	1:B:200:GLU:HG3	1.92	0.51
1:B:30:LEU:CD1	1:B:34:LYS:HZ2	2.22	0.51
1:A:184:MET:HE3	1:A:318:ARG:CD	2.40	0.50
1:A:106:GLN:HG2	1:A:109:THR:CG2	2.42	0.50
1:B:57:LEU:O	1:B:58:ALA:HB2	2.12	0.50
1:B:184:MET:CE	1:B:318:ARG:HD3	2.41	0.50
1:A:288:ILE:O	1:A:288:ILE:HG23	2.12	0.49
1:A:87[A]:CYS:HB2	1:A:88:PRO:HD3	1.94	0.49
1:B:154:PHE:HA	1:B:244:HIS:O	2.12	0.49
1:B:192:ARG:HG2	1:B:192:ARG:NH1	2.25	0.49
1:A:289:ASN:ND2	1:A:292:LEU:H	2.10	0.49
1:B:82[B]:TYR:OH	1:B:142:GLN:HG3	2.13	0.49
1:B:291:SER:HA	1:B:314:SER:HB2	1.95	0.49
1:B:158:VAL:HA	1:B:240:SER:O	2.14	0.47
1:A:187:ASP:HB2	1:A:195:ILE:HG13	1.96	0.47
1:B:92:GLU:HG3	1:B:97:TYR:HD2	1.80	0.47
1:B:323:SER:HA	1:B:328:THR:HB	1.97	0.46
1:A:173:ASN:CB	1:A:200:GLU:HG3	2.46	0.46
1:B:30:LEU:HD11	1:B:34:LYS:NZ	2.29	0.46
1:B:53:ARG:HG3	5:B:2031:HOH:O	2.16	0.45
1:B:162:GLU:OE1	1:B:221:ARG:NE	2.43	0.45
1:A:178:VAL:HG22	1:A:220:LYS:HE2	1.98	0.45
1:A:104:TYR:O	1:A:334:ALA:HA	2.17	0.44
1:B:173:ASN:HA	1:B:174:PRO:HD3	1.74	0.44
1:A:106:GLN:HG2	1:A:109:THR:HG21	1.99	0.44
1:B:173:ASN:CB	1:B:200:GLU:HG3	2.47	0.44
1:B:184:MET:HE3	1:B:318:ARG:CD	2.46	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:321:GLN:NE2	5:B:2209:HOH:O	2.50	0.44
1:A:178:VAL:HG21	1:A:223:THR:HB	2.00	0.44
1:A:253[A]:GLU:HG3	1:A:254:GLU:N	2.32	0.43
1:A:306:THR:O	5:A:2240:HOH:O	2.22	0.43
1:B:258:ILE:O	1:B:366:ASN:ND2	2.49	0.43
1:B:116:GLU:HB3	4:B:1369:EGB:NAM	2.34	0.43
1:A:116:GLU:HB3	4:A:1369:EGB:HAM	1.84	0.43
1:B:82[A]:TYR:OH	1:B:87[A]:CYS:SG	2.76	0.43
1:B:82[A]:TYR:HE1	1:B:87[A]:CYS:SG	2.30	0.42
1:A:161:LEU:HD21	1:A:319:ILE:HD13	2.01	0.42
1:B:61:SER:HG	1:B:63[A]:ARG:NH1	1.99	0.42
1:A:26:ARG:HB2	1:A:27:PRO:HD2	2.01	0.42
1:B:337:SER:CB	1:B:342:ASN:HD22	2.31	0.42
1:A:184:MET:CE	1:A:318:ARG:CZ	2.97	0.42
1:A:56:GLY:HA3	1:A:61[A]:SER:HA	2.01	0.42
1:B:53:ARG:HH21	1:B:63[A]:ARG:NH2	2.17	0.42
1:B:18:ASN:OD1	1:B:360:LEU:HD23	2.19	0.42
1:A:154:PHE:HA	1:A:244:HIS:O	2.19	0.42
1:A:253[B]:GLU:OE1	1:A:253[B]:GLU:HA	2.19	0.42
1:B:57:LEU:O	1:B:58:ALA:HB3	2.20	0.42
1:B:212[B]:GLN:HB3	1:B:212[B]:GLN:HE21	1.72	0.42
1:B:172:LEU:HD23	1:B:172:LEU:HA	1.92	0.42
1:A:173:ASN:HA	1:A:200:GLU:HG3	2.01	0.42
1:B:57:LEU:HD12	1:B:57:LEU:H	1.84	0.41
1:A:184:MET:HE3	1:A:318:ARG:NE	2.35	0.41
1:B:240:SER:OG	1:B:262:ASN:ND2	2.52	0.41
1:B:162:GLU:CG	1:B:171:LEU:HD23	2.44	0.41
1:A:173:ASN:HB2	1:A:200:GLU:HG3	2.03	0.41
1:B:269:SER:HA	1:B:292:LEU:HD21	2.03	0.41
1:B:291:SER:HA	1:B:314:SER:CB	2.52	0.40
1:A:304:GLU:O	1:A:305:ARG:HB2	2.21	0.40
1:A:47[A]:ARG:CZ	5:A:2031:HOH:O	2.70	0.40
1:A:52:VAL:O	1:A:63:ARG:HA	2.22	0.40
1:B:194:VAL:N	5:B:2128:HOH:O	2.49	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	341/368 (93%)	333 (98%)	8 (2%)	0	100	100
1	B	340/368 (92%)	329 (97%)	10 (3%)	1 (0%)	50	60
All	All	681/736 (92%)	662 (97%)	18 (3%)	1 (0%)	56	72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	58	ALA

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	303/322 (94%)	282 (93%)	21 (7%)	22	27
1	B	307/322 (95%)	292 (95%)	15 (5%)	35	45
All	All	610/644 (95%)	574 (94%)	36 (6%)	28	35

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	57	LEU
1	A	148	THR
1	A	165	ASN
1	A	167	GLU
1	A	176	SER
1	A	177	ASP
1	A	178	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	181	ARG
1	A	183	GLN
1	A	189	ARG
1	A	220	LYS
1	A	253[A]	GLU
1	A	253[B]	GLU
1	A	287	ASN
1	A	288	ILE
1	A	289	ASN
1	A	306	THR
1	A	321	GLN
1	A	341	LEU
1	A	360	LEU
1	B	30	LEU
1	B	34	LYS
1	B	36	SER
1	B	57	LEU
1	B	77	LYS
1	B	145	GLU
1	B	177	ASP
1	B	178	VAL
1	B	190	ASN
1	B	192	ARG
1	B	216	LYS
1	B	289	ASN
1	B	305	ARG
1	B	360	LEU
1	B	365	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	262	ASN
1	A	289	ASN
1	B	262	ASN
1	B	289	ASN
1	B	290	GLN
1	B	308	HIS
1	B	321	GLN
1	B	342	ASN

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 8 ligands modelled in this entry, 4 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$
4	EGB	A	1369	-	23,23,23	3.95	6 (26%)	35,35,35	3.52	11 (31%)
2	ADP	A	601	3	29,29,29	1.23	4 (13%)	45,45,45	1.95	9 (20%)
4	EGB	B	1369	-	23,23,23	3.81	7 (30%)	35,35,35	3.49	11 (31%)
2	ADP	B	602	3	29,29,29	1.09	2 (6%)	45,45,45	1.85	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
4	EGB	A	1369	-	-	0/4/34/34	0/1/3/3
2	ADP	A	601	3	-	0/16/32/32	0/1/3/3
4	EGB	B	1369	-	-	0/4/34/34	0/1/3/3
2	ADP	B	602	3	-	0/16/32/32	0/1/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1369	EGB	CAO-NAM	14.66	1.46	1.33
4	A	1369	EGB	CAO-NAM	14.19	1.45	1.33
4	A	1369	EGB	CAO-NAL	7.27	1.45	1.36
4	B	1369	EGB	CAO-NAL	7.26	1.45	1.36
4	A	1369	EGB	CAK-CAP	5.77	1.57	1.50
4	A	1369	EGB	CAO-SAE	5.27	1.80	1.68
4	B	1369	EGB	CAO-SAE	4.97	1.79	1.68
4	B	1369	EGB	CAN-CAQ	-3.82	1.38	1.45
2	A	601	ADP	C4-N9	-3.80	1.32	1.37
4	A	1369	EGB	CAN-CAQ	-3.43	1.39	1.45
2	B	602	ADP	C4-N9	-3.16	1.33	1.37
2	B	602	ADP	C5-C4	3.02	1.47	1.40
4	B	1369	EGB	CAT-NAM	2.67	1.49	1.47
4	A	1369	EGB	CAT-CAQ	2.67	1.54	1.51
2	A	601	ADP	C5-C4	2.56	1.46	1.40
4	B	1369	EGB	CAP-CAQ	2.33	1.39	1.36
2	A	601	ADP	O4'-C1'	2.31	1.44	1.41
4	B	1369	EGB	CAK-CAP	2.28	1.53	1.50
2	A	601	ADP	C8-N9	-2.04	1.33	1.36

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1369	EGB	CAO-NAL-CAP	-11.04	115.49	123.61
4	B	1369	EGB	SAE-CAO-NAL	-10.17	108.40	121.99
4	A	1369	EGB	SAE-CAO-NAM	-9.86	110.49	122.76
4	A	1369	EGB	SAE-CAO-NAL	-9.44	109.38	121.99
4	B	1369	EGB	SAE-CAO-NAM	-9.00	111.56	122.76
4	A	1369	EGB	CAT-NAM-CAO	-8.62	111.61	125.33
4	A	1369	EGB	CAO-NAL-CAP	-8.25	117.54	123.61
2	A	601	ADP	N3-C2-N1	-7.41	122.51	128.71
4	B	1369	EGB	CAT-NAM-CAO	-7.29	113.72	125.33
2	B	602	ADP	N3-C2-N1	-6.45	123.31	128.71
2	A	601	ADP	N3-C4-N9	6.07	136.39	125.43
2	B	602	ADP	N3-C4-N9	4.93	134.33	125.43
4	A	1369	EGB	OAC-CAN-CAQ	-4.57	116.68	121.29
4	A	1369	EGB	CAJ-CAN-CAQ	4.36	124.50	118.22
2	A	601	ADP	C8-N9-C4	4.18	110.09	106.90
2	B	602	ADP	C8-N9-C4	3.89	109.87	106.90
4	A	1369	EGB	CAS-CAT-NAM	3.26	114.13	110.83
2	B	602	ADP	C4-C5-N7	-3.20	106.78	109.52
4	B	1369	EGB	CAQ-CAT-NAM	3.07	111.42	109.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1369	EGB	NAL-CAO-NAM	-3.07	114.21	116.27
2	A	601	ADP	C5-C4-N3	-3.05	119.05	125.70
4	B	1369	EGB	CAJ-CAN-CAQ	2.95	122.46	118.22
2	B	602	ADP	C2-N1-C6	2.86	123.94	118.77
4	A	1369	EGB	CAU-CAJ-CAN	-2.62	110.08	114.37
4	B	1369	EGB	CAU-CAJ-CAN	-2.45	110.36	114.37
2	A	601	ADP	C2-N3-C4	2.38	120.79	114.01
2	B	602	ADP	C5-C4-N3	-2.38	120.52	125.70
2	A	601	ADP	O3B-PB-O2B	2.29	116.53	107.61
4	B	1369	EGB	OAC-CAN-CAQ	-2.25	119.01	121.29
4	B	1369	EGB	CAS-CAT-CAQ	-2.24	109.88	112.85
4	A	1369	EGB	CAR-CAI-CAS	2.21	121.96	120.05
4	A	1369	EGB	CAT-CAQ-CAP	2.21	122.64	120.03
2	A	601	ADP	C4-C5-N7	-2.19	107.65	109.52
2	B	602	ADP	O3'-C3'-C4'	-2.17	104.67	111.08
2	B	602	ADP	O3'-C3'-C2'	-2.15	104.84	111.83
2	A	601	ADP	N6-C6-N1	2.13	123.55	119.36
4	B	1369	EGB	CAR-CAI-CAS	2.08	121.85	120.05
4	B	1369	EGB	CAT-CAQ-CAP	2.05	122.45	120.03
2	A	601	ADP	C2-N1-C6	2.03	122.44	118.77

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	335/368 (91%)	-0.24	10 (2%) 48 58	6, 18, 45, 60	0
1	B	334/368 (90%)	-0.13	15 (4%) 32 42	6, 17, 44, 67	0
All	All	669/736 (90%)	-0.19	25 (3%) 39 50	6, 17, 44, 67	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	58	ALA	11.8
1	A	57	LEU	8.3
1	B	57	LEU	7.0
1	B	149[A]	ASP	4.7
1	A	178	VAL	4.6
1	A	58	ALA	4.4
1	B	190	ASN	4.2
1	A	190	ASN	4.0
1	B	192	ARG	3.8
1	A	271	ASN	3.7
1	B	56	GLY	3.7
1	B	365	VAL	2.9
1	B	34	LYS	2.8
1	A	287	ASN	2.7
1	B	191	LYS	2.7
1	B	178	VAL	2.4
1	A	56	GLY	2.4
1	B	264	VAL	2.4
1	A	34	LYS	2.3
1	B	36	SER	2.3
1	B	305	ARG	2.1
1	B	188	PRO	2.1
1	A	191	LYS	2.1
1	A	189	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	271[A]	ASN	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
3	MG	A	1368	1/1	0.22	2.26	17,17,17,17	0
3	MG	B	1368	1/1	0.15	1.39	3,3,3,3	0
4	EGB	B	1369	21/21	0.11	0.22	6,8,11,14	0
4	EGB	A	1369	21/21	0.11	0.06	6,11,15,18	0
2	ADP	A	601	27/27	0.11	-0.00	6,17,21,26	0
3	MG	A	1367	1/1	0.12	-0.62	12,12,12,12	0
2	ADP	B	602	27/27	0.08	-0.81	7,12,17,18	0
3	MG	B	1367	1/1	0.06	-1.45	8,8,8,8	0

6.5 Other polymers ⓘ

There are no such residues in this entry.