



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 12:02 am GMT

PDB ID : 2X7E  
Title : CRYSTAL STRUCTURE OF HUMAN KINESIN EG5 IN COMPLEX WITH (R)-FLUORASTROL  
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 : 2.40 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](mailto: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.

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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

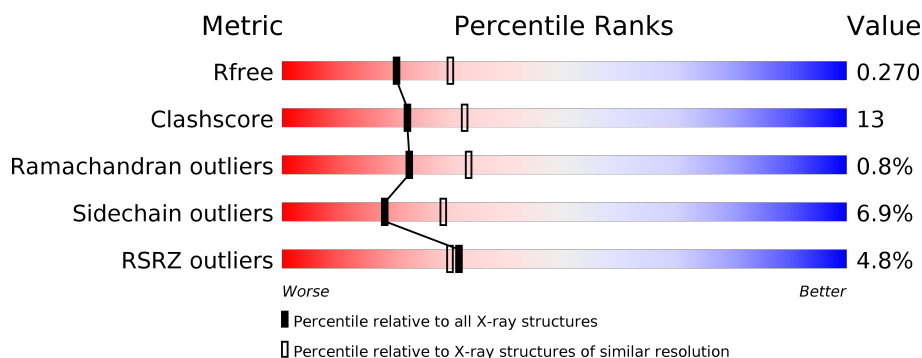
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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  $\geq 3$ , 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	368	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>19%</div> <div>• 10%</div> </div> </div>
1	B	368	<div> <div>6%</div> <div> <div></div> <div>71%</div> <div>16%</div> <div>• • 9%</div> </div> </div>

## 2 Entry composition [i](#)

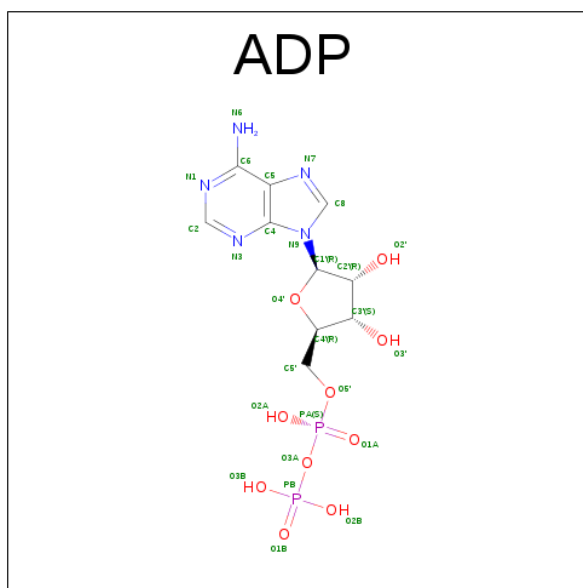
There are 5 unique types of molecules in this entry. The entry contains 5754 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 KINESIN-LIKE PROTEIN KIF11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	7	0
			2656	1666	461	518	11			
1	B	335	Total	C	N	O	S	0	4	0
			2654	1663	458	523	10			

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

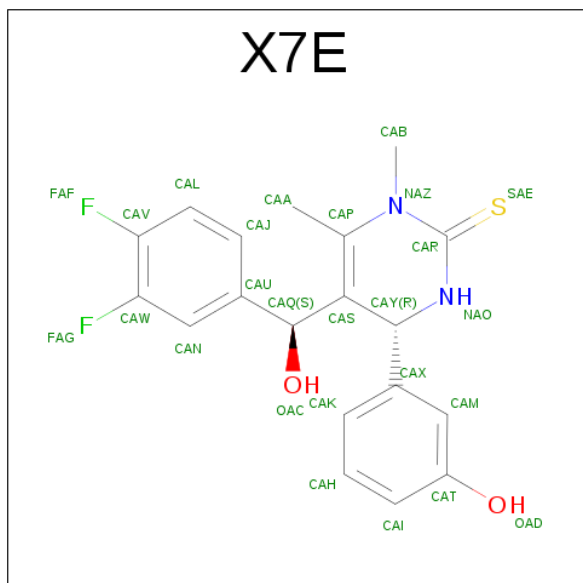


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

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

- Molecule 4 is (4R)-5-[(S)-(3,4-DIFLUOROPHENYL)(HYDROXY)METHYL]-4-(3-HYDROXYPHENYL)-1,6-DIMETHYL-3,4-DIHYDROPYRIMIDINE-2(1H)-THIONE (three-letter code: X7E) (formula: C<sub>19</sub>H<sub>18</sub>F<sub>2</sub>N<sub>2</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 26	C 19	F 2	N 2	O 2	S 1	0	0
4	B	1	Total 26	C 19	F 2	N 2	O 2	S 1	0	0

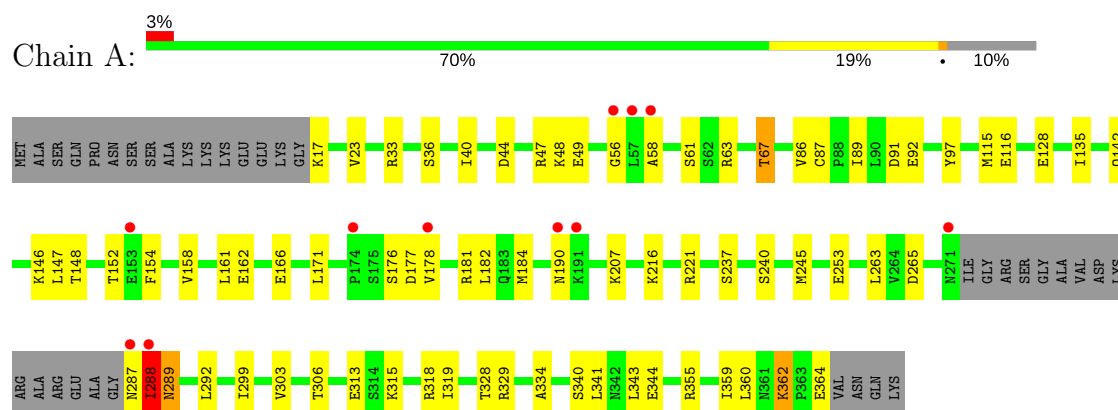
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	171	Total O 171 171	0	0
5	B	165	Total O 165 165	0	0

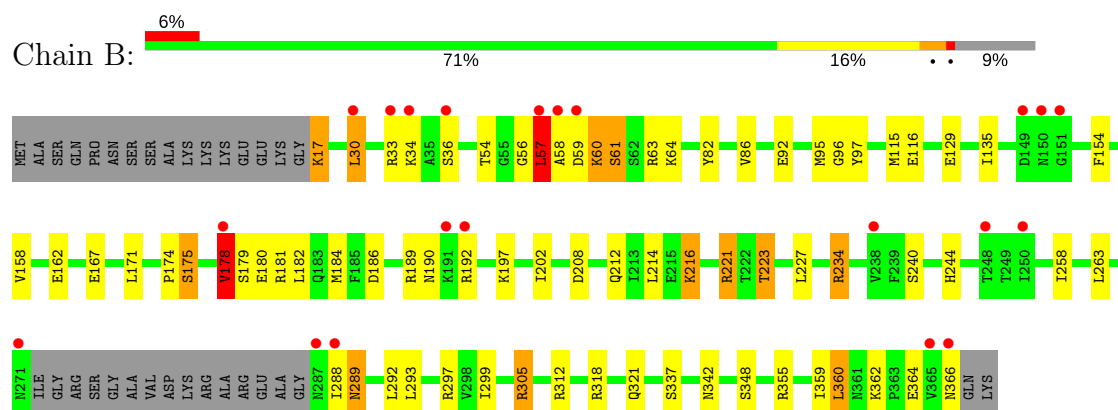
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: KINESIN-LIKE PROTEIN KIF11



#### • Molecule 1: KINESIN-LIKE PROTEIN KIF11



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.60Å 79.85Å 160.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 29.71 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.4 (30.00-2.40) 95.4 (29.71-2.40)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.90 (at 2.42Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.196 , 0.273 0.196 , 0.270	Depositor DCC
$R_{free}$ test set	1709 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.6	Xtrriage
Anisotropy	0.179	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5754	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.19 % 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 1.0280e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, X7E, 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	0.62	0/2717	0.82	0/3672
1	B	0.64	0/2705	0.94	6/3658 (0.2%)
All	All	0.63	0/5422	0.88	6/7330 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	178	VAL	N-CA-C	9.15	135.70	111.00
1	B	179	SER	N-CA-C	-8.26	88.70	111.00
1	B	234	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	B	297	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	221	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	B	58	ALA	N-CA-C	5.16	124.92	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2656	0	2691	72	0
1	B	2654	0	2676	67	0
2	A	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	27	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	26	0	17	3	0
4	B	26	0	18	4	0
5	A	171	0	0	9	0
5	B	165	0	0	18	0
All	All	5754	0	5426	143	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 13.

All (143) 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:154:PHE:HB3	1:A:245[B]:MET:CE	1.53	1.37
1:A:154:PHE:CB	1:A:245[B]:MET:HE3	1.59	1.30
1:B:54:THR:HG21	1:B:64:LYS:HG3	1.26	1.06
1:A:154:PHE:HB3	1:A:245[B]:MET:HE3	1.04	1.01
1:A:288:ILE:HG21	5:A:2132:HOH:O	1.61	1.00
1:B:178:VAL:O	1:B:178:VAL:HG13	1.58	0.99
1:A:288:ILE:CG2	5:A:2132:HOH:O	2.11	0.98
1:A:288:ILE:O	1:A:288:ILE:HD13	1.70	0.92
1:B:178:VAL:O	1:B:178:VAL:CG1	2.17	0.91
1:A:287:ASN:O	1:A:288:ILE:HG22	1.71	0.91
1:B:223:THR:HG22	5:B:2091:HOH:O	1.70	0.90
1:B:92[B]:GLU:OE2	1:B:95:MET:HE3	1.71	0.90
1:B:92[B]:GLU:OE2	1:B:95:MET:CE	2.23	0.85
1:A:154:PHE:HB2	1:A:245[B]:MET:HE3	1.59	0.84
1:B:216:LYS:HE3	5:B:2080:HOH:O	1.77	0.83
1:A:128:GLU:HG2	5:A:2059:HOH:O	1.79	0.83
1:B:54:THR:CG2	1:B:64:LYS:HG3	2.10	0.81
1:B:189:ARG:HD2	5:B:2072:HOH:O	1.81	0.81
1:A:162:GLU:HG3	1:A:171:LEU:HD23	1.62	0.80
1:A:40:ILE:HD13	1:A:340:SER:HA	1.65	0.78
1:B:61:SER:OG	1:B:63:ARG:NH1	2.13	0.78
1:A:89:ILE:HG12	1:A:329[B]:ARG:HH11	1.46	0.78
1:A:89:ILE:CG1	1:A:329[B]:ARG:HH11	1.95	0.77
1:A:287:ASN:O	1:A:288:ILE:CG2	2.34	0.74
1:A:288:ILE:CD1	1:A:288:ILE:O	2.36	0.74
1:B:258:ILE:O	1:B:366:ASN:ND2	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:PHE:CB	1:A:245[B]:MET:CE	2.33	0.73
1:B:60:LYS:O	1:B:61:SER:HB3	1.90	0.72
1:B:186:ASP:CG	1:B:312:ARG:HH22	1.94	0.70
1:A:89:ILE:CG1	1:A:329[B]:ARG:NH1	2.56	0.69
1:A:184:MET:HE3	1:A:318:ARG:CZ	2.23	0.68
1:A:287:ASN:O	1:A:288:ILE:CB	2.41	0.67
1:A:115:MET:CE	1:A:263:LEU:HB3	2.24	0.67
1:B:175:SER:O	5:B:2065:HOH:O	2.12	0.67
1:A:89:ILE:HG13	1:A:329[B]:ARG:NH1	2.08	0.67
1:B:115:MET:CE	1:B:263:LEU:HB3	2.25	0.67
1:A:289:ASN:HD22	1:A:292:LEU:H	1.41	0.66
1:A:154:PHE:HB3	1:A:245[B]:MET:HE2	1.67	0.66
1:B:95:MET:SD	5:B:2027:HOH:O	2.54	0.66
1:B:56:GLY:O	1:B:57:LEU:HB2	1.98	0.64
1:B:92[A]:GLU:HG3	1:B:97:TYR:CD2	2.32	0.64
1:B:186:ASP:OD1	1:B:312:ARG:NH2	2.29	0.63
1:A:313:GLU:HG2	1:B:288:ILE:HG21	1.80	0.63
4:A:1365:X7E:HAQ	4:A:1365:X7E:HAK	1.81	0.63
1:B:92[B]:GLU:CD	1:B:95:MET:HE3	2.19	0.62
1:A:184:MET:CE	1:A:318:ARG:NH1	2.63	0.62
1:A:49:GLU:HG2	1:A:67:THR:HG22	1.82	0.61
1:B:289:ASN:HD22	1:B:292:LEU:H	1.47	0.61
1:A:152:THR:CG2	1:A:245[B]:MET:HE1	2.29	0.61
4:A:1365:X7E:CAQ	4:A:1365:X7E:HAK	2.30	0.61
1:B:154:PHE:HA	1:B:244:HIS:O	2.00	0.61
1:A:166:GLU:O	1:A:315:LYS:HE2	2.01	0.60
1:A:152:THR:HG22	1:A:245[B]:MET:HE1	1.83	0.60
1:B:60:LYS:O	1:B:61:SER:CB	2.49	0.60
1:B:174:PRO:HB3	1:B:216:LYS:HE2	1.83	0.60
1:B:115:MET:HE1	1:B:263:LEU:HB3	1.84	0.59
1:B:288:ILE:CG2	1:B:293:LEU:HD11	2.33	0.58
1:A:287:ASN:O	1:A:288:ILE:HB	2.04	0.58
1:B:184:MET:CE	1:B:318:ARG:HD3	2.35	0.56
1:B:162:GLU:HG3	1:B:171:LEU:HD23	1.88	0.55
1:A:288:ILE:O	1:A:288:ILE:HG23	2.05	0.55
1:B:216:LYS:HB2	5:B:2083:HOH:O	2.07	0.55
1:B:33:ARG:HG3	5:B:2009:HOH:O	2.07	0.54
1:A:147:LEU:HD13	1:A:245[B]:MET:CE	2.37	0.54
1:A:289:ASN:ND2	1:A:292:LEU:H	2.05	0.54
1:A:116:GLU:CD	1:A:221:ARG:HH22	2.10	0.54
1:B:197:LYS:HD3	5:B:2071:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92[B]:GLU:OE2	1:B:95:MET:HE1	2.05	0.53
1:B:184:MET:HE3	1:B:318:ARG:CZ	2.39	0.53
1:A:162:GLU:HG3	1:A:171:LEU:CD2	2.36	0.53
1:A:40:ILE:CD1	1:A:340:SER:HA	2.38	0.53
1:B:116:GLU:OE2	1:B:221:ARG:NH1	2.37	0.53
1:B:95:MET:HE2	5:B:2013:HOH:O	2.09	0.53
1:A:17:LYS:N	5:A:2002:HOH:O	2.42	0.52
1:A:23:VAL:HG22	1:A:334:ALA:HB3	1.92	0.52
1:A:184:MET:HE2	1:A:318:ARG:NH1	2.25	0.51
1:B:288:ILE:HA	5:B:2121:HOH:O	2.11	0.51
1:B:17:LYS:N	1:B:360:LEU:CD1	2.74	0.51
4:B:1365:X7E:HAQ	4:B:1365:X7E:HAK	1.93	0.51
1:B:30:LEU:HD22	1:B:34:LYS:NZ	2.26	0.51
1:A:184:MET:HE3	1:A:318:ARG:NH1	2.25	0.50
1:B:63:ARG:HD2	5:B:2017:HOH:O	2.11	0.49
1:B:116:GLU:HB3	4:B:1365:X7E:HAY	1.94	0.49
1:B:30:LEU:HD22	1:B:34:LYS:HZ3	1.77	0.49
1:A:362:LYS:HD3	5:A:2166:HOH:O	2.12	0.49
1:B:192:ARG:HG2	5:B:2073:HOH:O	2.10	0.49
1:B:158:VAL:HA	1:B:240:SER:O	2.13	0.49
1:A:91:ASP:OD1	1:A:146:LYS:HE2	2.13	0.49
1:B:82:TYR:CD2	1:B:86:VAL:HB	2.48	0.49
4:B:1365:X7E:CAQ	4:B:1365:X7E:HAK	2.42	0.49
1:B:17:LYS:N	1:B:360:LEU:HD13	2.27	0.49
1:B:321:GLN:NE2	5:B:2136:HOH:O	2.46	0.49
1:B:366:ASN:HB2	5:B:2112:HOH:O	2.13	0.48
1:A:184:MET:HE3	1:A:318:ARG:NE	2.29	0.48
1:A:152:THR:HG22	1:A:245[B]:MET:CE	2.44	0.48
1:B:192:ARG:O	1:B:192:ARG:HG3	2.14	0.48
1:B:167:GLU:OE1	1:B:181:ARG:CZ	2.62	0.47
1:B:86:VAL:HG21	1:B:135:ILE:HG12	1.97	0.47
1:A:184:MET:HE3	1:A:318:ARG:HD3	1.97	0.47
1:A:299:ILE:HG23	1:A:359:ILE:HD11	1.97	0.47
1:A:115:MET:HE1	1:A:263:LEU:HB3	1.95	0.47
1:A:97:TYR:CE1	1:A:364:GLU:HB3	2.50	0.46
1:A:92[B]:GLU:OE2	1:A:97:TYR:CD2	2.68	0.46
1:A:245[B]:MET:HA	1:A:245[B]:MET:HE2	1.98	0.46
1:A:344:GLU:HG3	5:A:2155:HOH:O	2.15	0.46
1:B:305:ARG:NH1	5:B:2125:HOH:O	2.49	0.45
1:B:244:HIS:HE1	5:B:2106:HOH:O	2.00	0.45
1:A:47:ARG:HB3	1:A:49:GLU:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:VAL:HG21	1:A:135:ILE:HG12	1.97	0.45
1:B:182:LEU:HA	5:B:2070:HOH:O	2.16	0.45
1:A:299:ILE:O	1:A:303:VAL:HG13	2.17	0.44
1:A:237:SER:OG	1:A:265:ASP:HB3	2.17	0.44
1:A:116:GLU:CD	1:A:221:ARG:NH2	2.71	0.44
1:B:184:MET:HE3	1:B:318:ARG:HD3	1.99	0.44
1:B:234:ARG:NH1	5:B:2101:HOH:O	2.49	0.43
1:B:289:ASN:ND2	1:B:292:LEU:H	2.14	0.43
1:B:214:LEU:HD22	4:B:1365:X7E:HAN	1.99	0.43
1:B:299:ILE:HG23	1:B:359:ILE:HD11	2.00	0.43
1:B:184:MET:HE3	1:B:318:ARG:NE	2.34	0.43
1:A:92[B]:GLU:HG3	1:A:97:TYR:HB2	2.01	0.42
1:A:184:MET:HE3	1:A:318:ARG:CD	2.49	0.42
1:B:96:GLY:O	1:B:366:ASN:ND2	2.53	0.42
1:A:56:GLY:HA3	1:A:61:SER:HA	2.00	0.41
1:A:44:ASP:O	1:A:48:LYS:N	2.52	0.41
1:A:161:LEU:HD21	1:A:319:ILE:HD13	2.02	0.41
1:B:30:LEU:CD2	1:B:34:LYS:NZ	2.83	0.41
1:A:154:PHE:CG	1:A:245[B]:MET:HE3	2.45	0.41
1:A:33:ARG:O	1:A:36:SER:N	2.39	0.41
1:A:355[B]:ARG:HH11	1:A:355[B]:ARG:HG2	1.85	0.41
1:B:184:MET:CE	1:B:318:ARG:NH1	2.83	0.41
1:B:184:MET:HE1	1:B:318:ARG:HD3	2.02	0.41
4:A:1365:X7E:HAJ	5:A:2171:HOH:O	2.20	0.41
1:A:216:LYS:HE3	5:A:2096:HOH:O	2.21	0.41
1:A:152:THR:CG2	1:A:245[B]:MET:CE	2.97	0.40
1:A:40:ILE:HD12	1:A:343:LEU:HD13	2.02	0.40
1:A:92[A]:GLU:HA	1:A:92[A]:GLU:OE2	2.21	0.40
1:A:158:VAL:HA	1:A:240:SER:O	2.22	0.40
1:A:360:LEU:HB3	5:A:2002:HOH:O	2.19	0.40
1:B:184:MET:HE2	1:B:318:ARG:NH1	2.37	0.40
1:B:292:LEU:HD12	1:B:292:LEU:HA	1.84	0.40
1:B:337:SER:OG	1:B:342:ASN:ND2	2.47	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	336/368 (91%)	324 (96%)	10 (3%)	2 (1%)	28	41
1	B	335/368 (91%)	325 (97%)	7 (2%)	3 (1%)	20	29
All	All	671/736 (91%)	649 (97%)	17 (2%)	5 (1%)	22	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	288	ILE
1	B	57	LEU
1	B	178	VAL
1	B	61	SER
1	A	58	ALA

### 5.3.2 Protein sidechains [i](#)

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	302/322 (94%)	284 (94%)	18 (6%)	22	35
1	B	301/322 (94%)	276 (92%)	25 (8%)	13	20
All	All	603/644 (94%)	560 (93%)	43 (7%)	18	27

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ARG

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Mol	Chain	Res	Type
1	A	67	THR
1	A	87	CYS
1	A	142	GLN
1	A	148	THR
1	A	176	SER
1	A	177	ASP
1	A	178	VAL
1	A	181	ARG
1	A	182	LEU
1	A	190	ASN
1	A	207	LYS
1	A	253	GLU
1	A	288	ILE
1	A	289	ASN
1	A	306	THR
1	A	341	LEU
1	A	362	LYS
1	B	17	LYS
1	B	30	LEU
1	B	36	SER
1	B	57	LEU
1	B	59[A]	ASP
1	B	59[B]	ASP
1	B	60	LYS
1	B	129	GLU
1	B	175	SER
1	B	180[A]	GLU
1	B	180[B]	GLU
1	B	190	ASN
1	B	202	ILE
1	B	208	ASP
1	B	212	GLN
1	B	216	LYS
1	B	223	THR
1	B	227	LEU
1	B	289	ASN
1	B	305	ARG
1	B	348	SER
1	B	355	ARG
1	B	360	LEU
1	B	362	LYS
1	B	364	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	262	ASN
1	A	289	ASN
1	A	321	GLN
1	B	165	ASN
1	B	244	HIS
1	B	271	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 [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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
4	X7E	A	1365	-	25,28,28	1.95	4 (16%)	31,41,41	2.87	10 (32%)
2	ADP	A	600	3	25,29,29	1.19	3 (12%)	24,45,45	1.69	3 (12%)
4	X7E	B	1365	-	25,28,28	1.79	4 (16%)	31,41,41	2.65	8 (25%)
2	ADP	B	603	3	25,29,29	0.96	1 (4%)	24,45,45	2.09	4 (16%)

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	X7E	A	1365	-	-	0/10/32/32	0/3/3/3
2	ADP	A	600	3	-	0/12/32/32	0/3/3/3
4	X7E	B	1365	-	-	0/10/32/32	0/3/3/3
2	ADP	B	603	3	-	0/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1365	X7E	CAY-NAO	-2.58	1.44	1.47
4	B	1365	X7E	CAY-NAO	-2.23	1.44	1.47
2	A	600	ADP	C2-N3	2.08	1.35	1.32
4	B	1365	X7E	CAA-CAP	2.38	1.53	1.49
2	A	600	ADP	O4'-C1'	2.50	1.44	1.41
2	B	603	ADP	C5-C4	2.79	1.46	1.40
2	A	600	ADP	C5-C4	3.16	1.47	1.40
4	B	1365	X7E	CAX-CAY	4.15	1.59	1.52
4	A	1365	X7E	CAA-CAP	4.21	1.56	1.49
4	A	1365	X7E	CAX-CAY	4.83	1.60	1.52
4	A	1365	X7E	CAR-NAO	5.69	1.37	1.33
4	B	1365	X7E	CAR-NAO	6.27	1.37	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1365	X7E	SAE-CAR-NAZ	-9.09	114.89	123.57
4	A	1365	X7E	CAY-NAO-CAR	-7.64	113.74	125.26
4	B	1365	X7E	CAX-CAY-NAO	-7.20	102.73	110.80
2	B	603	ADP	N3-C2-N1	-7.16	122.62	128.86
4	B	1365	X7E	SAE-CAR-NAZ	-6.99	116.89	123.57
2	A	600	ADP	N3-C2-N1	-6.01	123.62	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1365	X7E	CAX-CAY-NAO	-5.70	104.41	110.80
4	B	1365	X7E	CAY-NAO-CAR	-5.20	117.42	125.26
2	B	603	ADP	O3'-C3'-C4'	-4.50	97.94	111.09
4	A	1365	X7E	CAK-CAX-CAM	-4.39	113.67	118.79
4	B	1365	X7E	CAK-CAX-CAM	-3.65	114.53	118.79
4	A	1365	X7E	CAH-CAI-CAT	-2.81	115.39	119.37
2	B	603	ADP	O2'-C2'-C1'	-2.39	104.13	111.61
4	A	1365	X7E	CAJ-CAL-CAV	-2.27	116.59	119.01
4	B	1365	X7E	SAE-CAR-NAO	-2.12	118.35	121.17
2	B	603	ADP	C2-N1-C6	2.06	122.38	118.77
4	A	1365	X7E	CAM-CAX-CAY	2.10	123.50	119.77
2	A	600	ADP	C2-N1-C6	2.16	122.56	118.77
4	A	1365	X7E	CAI-CAT-CAM	2.30	122.75	120.20
4	B	1365	X7E	FAF-CAV-CAL	2.98	125.14	118.49
4	B	1365	X7E	FAG-CAW-CAN	2.98	124.26	118.63
4	A	1365	X7E	CAH-CAK-CAX	3.00	124.33	120.64
2	A	600	ADP	N6-C6-N1	3.25	125.20	118.77
4	A	1365	X7E	CAT-CAM-CAX	3.29	122.91	120.06
4	B	1365	X7E	CAT-CAM-CAX	4.60	124.04	120.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1365	X7E	3	0
4	B	1365	X7E	4	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	333/368 (90%)	-0.09	11 (3%) 47 45	7, 21, 46, 58	0
1	B	335/368 (91%)	-0.05	21 (6%) 21 19	6, 19, 48, 60	0
All	All	668/736 (90%)	-0.07	32 (4%) 31 30	6, 20, 48, 60	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	58	ALA	10.3
1	A	57	LEU	8.3
1	B	57	LEU	4.5
1	B	178	VAL	4.2
1	B	34	LYS	3.7
1	B	36	SER	3.6
1	B	149	ASP	3.6
1	A	288	ILE	3.5
1	A	287	ASN	3.5
1	B	287	ASN	3.4
1	A	271	ASN	3.3
1	A	191	LYS	3.2
1	B	250	ILE	2.9
1	B	33	ARG	2.9
1	A	56	GLY	2.9
1	B	365	VAL	2.7
1	B	192	ARG	2.7
1	B	271	ASN	2.7
1	A	174	PRO	2.5
1	A	190	ASN	2.4
1	B	191	LYS	2.4
1	B	238	VAL	2.2
1	B	30	LEU	2.2
1	B	288	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	178	VAL	2.1
1	B	248	THR	2.1
1	B	366	ASN	2.1
1	B	151	GLY	2.1
1	A	58	ALA	2.1
1	B	150	ASN	2.1
1	A	153	GLU	2.1
1	B	59[A]	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	X7E	B	1365	26/26	0.96	0.13	-0.18	8,13,20,25	0
4	X7E	A	1365	26/26	0.96	0.13	-0.24	11,15,22,25	0
2	ADP	A	600	27/27	0.98	0.11	-1.05	8,23,29,30	0
2	ADP	B	603	27/27	0.99	0.09	-1.45	8,12,18,23	0
3	MG	B	604	1/1	0.98	0.07	-	12,12,12,12	0
3	MG	A	601	1/1	0.93	0.09	-	15,15,15,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.