



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 03:57 pm GMT

PDB ID : 2X2R  
Title : CRYSTAL STRUCTURE OF HUMAN KINESIN EG5 IN COMPLEX WITH  
(R)-2-AMINO-3-((4-CHLOROPHENYL)DIPHENYLMETHYLTHIO)PROP  
ANOIC ACID  
Authors : Kaan, H.Y.K.; Weiss, J.; Menger, D.; Ulaganathan, V.; Laggner, C.;  
Popowycz, F.; Joseph, B.; Kozielski, F.  
Deposited on : 2010-01-15  
Resolution : 2.20 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

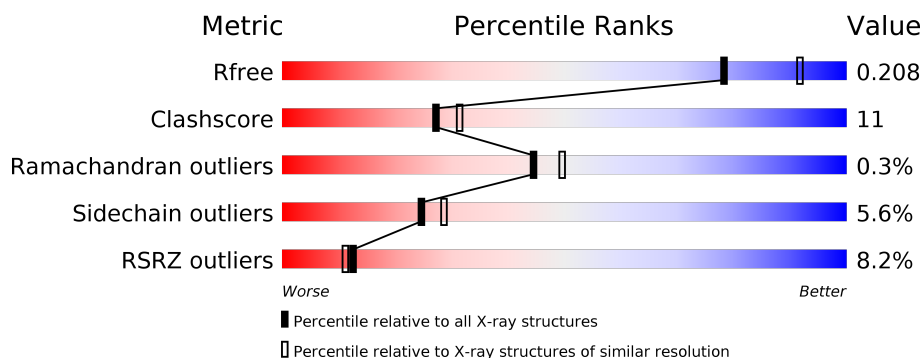
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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>7%</div> <div> <div></div> <div>70%</div> <div>18%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	368	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>13%</div> <div>•</div> <div>12%</div> </div> </div>
1	C	368	<div> <div>11%</div> <div> <div></div> <div>65%</div> <div>21%</div> <div>•</div> <div>11%</div> </div> </div>

## 2 Entry composition [i](#)

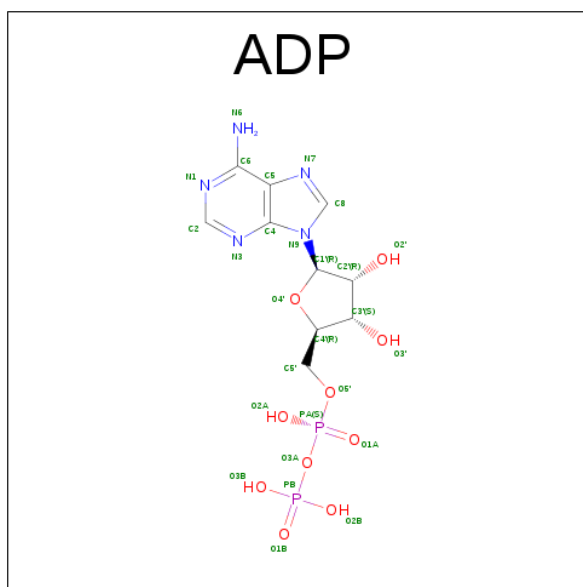
There are 5 unique types of molecules in this entry. The entry contains 8687 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

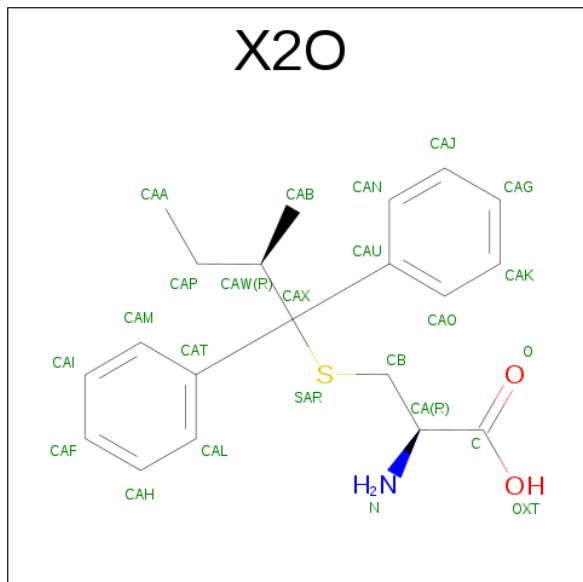
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	5	0
			2616	1641	452	512	11			
1	B	324	Total	C	N	O	S	0	10	0
			2588	1626	449	502	11			
1	C	329	Total	C	N	O	S	0	4	0
			2590	1624	447	509	10			

- 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		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is (2R)-2-AMINO-3-[(2R)-2-METHYL-1,1-DIPHENYL-BUTYL]SULFANYL-PROPANOIC ACID (three-letter code: X2O) (formula: C<sub>20</sub>H<sub>25</sub>NO<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			24	20	1	2	1		
3	B	1	Total	C	N	O	S	0	0
			24	20	1	2	1		
3	C	1	Total	C	N	O	S	0	0
			24	20	1	2	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	282	Total	O	0	0
			282	282		
5	B	283	Total	O	0	0
			283	283		

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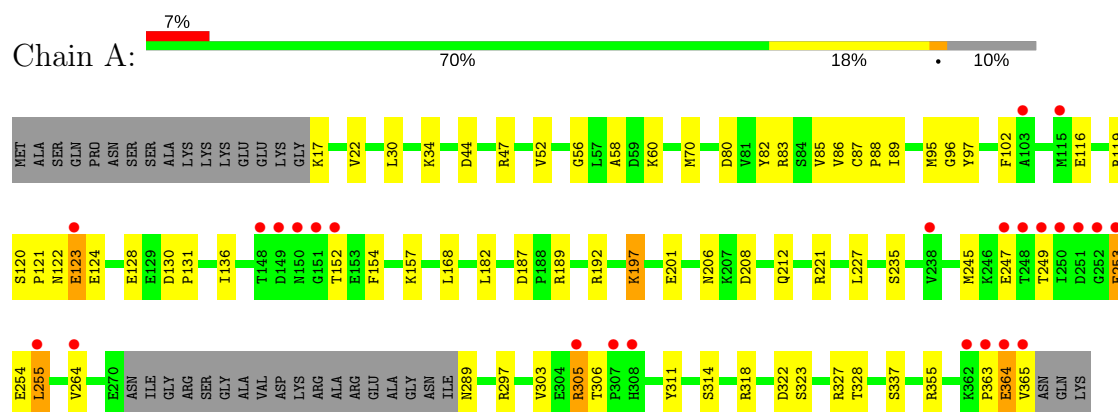
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	172	Total	O	0	0
			172	172		

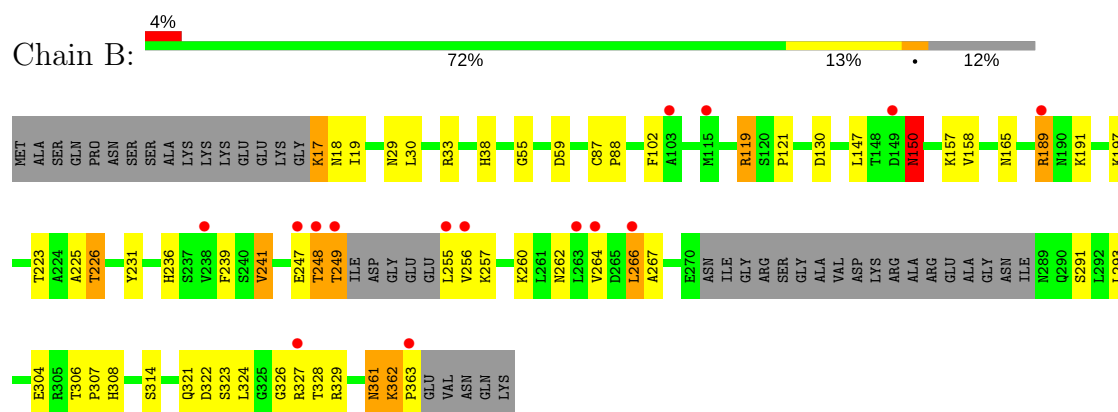
### 3 Residue-property plots [i](#)

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.

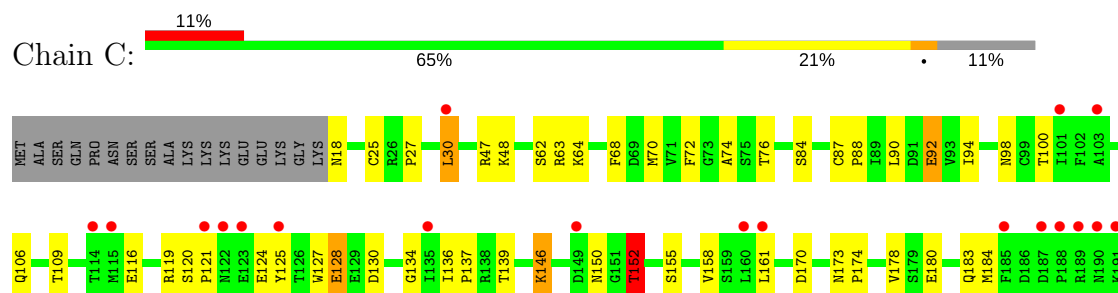
#### • Molecule 1: KINESIN-LIKE PROTEIN KIF11

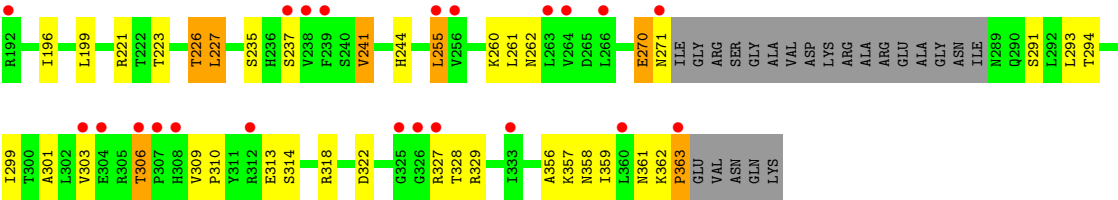


#### • Molecule 1: KINESIN-LIKE PROTEIN KIF11



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.35Å 96.35Å 124.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.41 – 2.20 29.41 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.41-2.20) 100.0 (29.41-2.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.33 (at 2.20Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.172 , 0.216 0.166 , 0.208	Depositor DCC
$R_{free}$ test set	3321 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.4	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l 0.027 for h,-h-k,-l 0.016 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8687	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: X2O, 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	0.47	1/2670 (0.0%)	0.57	0/3611
1	B	0.49	2/2655 (0.1%)	0.60	2/3589 (0.1%)
1	C	0.43	1/2641 (0.0%)	0.54	0/3573
All	All	0.46	4/7966 (0.1%)	0.57	2/10773 (0.0%)

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	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	150[A]	ASN	N-CA	7.42	1.61	1.46
1	B	150[B]	ASN	N-CA	7.42	1.61	1.46
1	A	311	TYR	CD1-CE1	-5.50	1.31	1.39
1	C	270	GLU	CD-OE1	-5.13	1.20	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	150[A]	ASN	N-CA-CB	5.98	121.37	110.60
1	B	150[B]	ASN	N-CA-CB	5.98	121.37	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	GLU	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2616	0	2651	54	0
1	B	2588	0	2643	57	0
1	C	2590	0	2614	68	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
3	A	24	0	24	2	0
3	B	24	0	24	1	0
3	C	24	0	24	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	282	0	0	9	0
5	B	283	0	0	5	0
5	C	172	0	0	6	0
All	All	8687	0	8016	181	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 11.

All (181) 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:B:327:ARG:O	1:B:363:PRO:CB	1.88	1.21
1:B:327:ARG:O	1:B:363:PRO:HB3	1.05	1.18
1:B:362:LYS:H	1:B:363:PRO:HD3	1.07	1.15
1:C:362:LYS:CB	1:C:363:PRO:HD3	1.80	1.10
1:B:327:ARG:HG3	1:B:363:PRO:HA	1.42	1.00
1:B:361:ASN:O	1:B:362:LYS:HD2	1.65	0.94
1:B:362:LYS:N	1:B:363:PRO:HD3	1.84	0.89
1:C:362:LYS:HB3	1:C:363:PRO:HD3	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:GLU:O	1:C:271:ASN:HB2	1.70	0.88
1:C:362:LYS:HB2	1:C:363:PRO:HD3	1.55	0.88
1:C:363:PRO:HG2	1:C:363:PRO:O	1.74	0.86
1:B:306:THR:HB	1:B:307:PRO:HD2	1.59	0.84
1:B:362:LYS:H	1:B:363:PRO:CD	1.90	0.82
1:B:239:PHE:HE1	1:B:241:VAL:HG22	1.44	0.81
1:B:361:ASN:O	1:B:362:LYS:CG	2.30	0.80
1:C:92:GLU:HG3	1:C:329:ARG:HH11	1.47	0.80
1:B:361:ASN:O	1:B:362:LYS:CD	2.30	0.79
1:B:327:ARG:C	1:B:363:PRO:HB3	2.03	0.78
1:B:361:ASN:O	1:B:362:LYS:CB	2.31	0.78
1:B:327:ARG:HG3	1:B:363:PRO:CA	2.13	0.78
1:C:362:LYS:CB	1:C:363:PRO:CD	2.63	0.77
1:B:323:SER:HA	1:B:328:THR:HB	1.67	0.76
1:C:363:PRO:CG	1:C:363:PRO:O	2.30	0.74
1:A:364:GLU:O	1:A:365:VAL:HG22	1.87	0.73
1:A:157:LYS:HE3	1:A:201:GLU:OE1	1.89	0.72
1:C:47:ARG:HH22	1:C:363:PRO:CD	2.02	0.72
1:C:226:THR:HG22	1:C:227:LEU:HD13	1.71	0.72
1:B:260:LYS:HE2	1:B:262:ASN:HD21	1.54	0.72
1:A:247:GLU:HG2	1:A:255:LEU:HG	1.72	0.71
1:C:235:SER:O	5:C:2127:HOH:O	2.09	0.70
1:C:293:LEU:HD12	1:C:294:THR:N	2.07	0.69
1:B:329:ARG:HG2	1:B:363:PRO:HG3	1.74	0.69
1:A:96:GLY:O	1:A:365:VAL:HB	1.95	0.67
1:A:87[B]:CYS:HB3	1:A:88:PRO:HD3	1.76	0.67
1:A:235:SER:O	5:A:2209:HOH:O	2.14	0.66
1:C:146:LYS:O	1:C:150:ASN:HB2	1.96	0.65
1:A:327:ARG:O	1:A:363:PRO:HA	1.96	0.64
1:B:361:ASN:ND2	5:B:2272:HOH:O	2.30	0.62
1:A:364:GLU:O	1:A:365:VAL:CG2	2.47	0.62
1:B:87[A]:CYS:HB2	1:B:88:PRO:HD3	1.82	0.61
1:B:239:PHE:CE1	1:B:241:VAL:HG22	2.32	0.61
1:B:361:ASN:O	1:B:362:LYS:HB2	2.00	0.60
1:C:362:LYS:HB2	1:C:363:PRO:CD	2.30	0.59
1:C:18:ASN:HD22	1:C:357:LYS:HE3	1.67	0.58
1:C:47:ARG:NH2	1:C:363:PRO:HD2	2.18	0.58
1:B:29:ASN:O	1:B:33:ARG:HG3	2.03	0.58
1:A:82:TYR:CD2	1:A:86:VAL:HB	2.38	0.58
1:C:184:MET:HE3	1:C:318:ARG:NH1	2.18	0.58
1:C:139:THR:HG21	1:C:261:LEU:HD23	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:ARG:HH21	1:B:130:ASP:HB2	1.70	0.56
1:C:119:ARG:HH21	1:C:130:ASP:HB2	1.70	0.56
1:A:17:LYS:HE3	5:A:2001:HOH:O	2.04	0.56
1:B:236:HIS:CD2	1:B:267:ALA:H	2.24	0.56
1:C:70:MET:HE1	1:C:84:SER:HB2	1.88	0.56
1:C:47:ARG:HH22	1:C:363:PRO:HD2	1.69	0.55
1:C:152:THR:HG23	1:C:152:THR:O	2.04	0.55
1:C:184:MET:HE1	1:C:318:ARG:HD3	1.87	0.55
1:A:289:ASN:N	5:A:2228:HOH:O	2.39	0.55
1:B:322:ASP:O	1:B:326:GLY:HA3	2.07	0.54
1:A:221:ARG:HD2	5:A:2210:HOH:O	2.08	0.54
1:C:152:THR:CG2	1:C:152:THR:O	2.57	0.53
1:C:184:MET:HE3	1:C:318:ARG:CZ	2.39	0.53
3:C:1367:X2O:HAB2	3:C:1367:X2O:CAL	2.40	0.52
1:C:98:ASN:ND2	1:C:260:LYS:HB3	2.24	0.52
1:B:87[B]:CYS:HB3	1:B:88:PRO:HD3	1.90	0.52
1:C:70:MET:CE	1:C:84:SER:HB2	2.40	0.52
1:A:60:LYS:HE3	5:A:2057:HOH:O	2.09	0.52
1:B:329:ARG:HG2	1:B:363:PRO:CG	2.40	0.52
1:C:301:ALA:HA	1:C:306:THR:HG23	1.90	0.52
1:A:102:PHE:HB3	1:A:264:VAL:HB	1.92	0.52
1:A:56:GLY:O	1:A:60:LYS:HE2	2.10	0.51
1:B:102:PHE:HB3	1:B:264:VAL:HB	1.91	0.51
1:A:58:ALA:O	1:B:197:LYS:HD2	2.11	0.50
1:C:223:THR:O	1:C:226:THR:HB	2.11	0.50
1:A:121:PRO:O	1:A:122:ASN:HB2	2.11	0.50
1:A:44:ASP:OD2	1:A:47:ARG:HD2	2.12	0.49
1:C:158:VAL:HG12	1:C:241:VAL:HG13	1.94	0.49
1:A:30:LEU:HD23	1:A:34:LYS:HE2	1.93	0.49
1:C:270:GLU:O	1:C:271:ASN:CB	2.49	0.49
1:C:87:CYS:HB2	1:C:88:PRO:HD3	1.94	0.49
1:B:29:ASN:HB3	5:B:2276:HOH:O	2.13	0.49
1:A:189:ARG:HD2	5:A:2161:HOH:O	2.14	0.48
1:B:362:LYS:N	1:B:363:PRO:CD	2.58	0.48
1:A:82:TYR:CE2	1:A:86:VAL:HG11	2.49	0.48
1:B:321:GLN:O	1:B:324:LEU:O	2.32	0.48
1:A:197:LYS:HA	1:A:197:LYS:HD3	1.51	0.48
1:B:157:LYS:HE2	1:B:157:LYS:HB2	1.49	0.48
1:A:116:GLU:HG2	1:A:136:ILE:HD12	1.96	0.47
1:C:27:PRO:HG3	1:C:74:ALA:O	2.14	0.47
1:B:121:PRO:HD2	5:B:2119:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:HIS:HE1	5:B:2235:HOH:O	1.97	0.47
1:A:255:LEU:N	1:A:255:LEU:HD23	2.29	0.47
1:A:116:GLU:OE1	1:A:221:ARG:NH2	2.47	0.47
1:C:68:PHE:HA	1:C:359:ILE:HD12	1.97	0.47
1:C:329:ARG:HA	5:C:2002:HOH:O	2.15	0.47
1:B:248:THR:HA	1:B:249:THR:C	2.35	0.47
1:B:307:PRO:HG2	1:B:308:HIS:H	1.79	0.47
3:C:1367:X2O:HAL	3:C:1367:X2O:HAB2	1.97	0.47
1:B:323:SER:HA	1:B:328:THR:CB	2.43	0.47
1:C:309:VAL:HA	1:C:310:PRO:HD3	1.52	0.46
1:A:365:VAL:HG23	5:A:2099:HOH:O	2.14	0.46
1:A:95:MET:CE	1:A:95:MET:HA	2.46	0.46
1:B:223:THR:O	1:B:226:THR:HB	2.15	0.46
1:A:303:VAL:O	1:A:305:ARG:NH1	2.49	0.46
1:C:90:LEU:O	1:C:94:ILE:HG12	2.16	0.46
1:A:152:THR:HG22	1:A:154:PHE:HB3	1.97	0.46
1:A:121:PRO:C	1:A:122:ASN:O	2.50	0.46
1:A:323:SER:HA	1:A:328:THR:HB	1.98	0.46
1:A:80:ASP:OD1	1:A:83:ARG:NH2	2.49	0.46
1:B:327:ARG:CG	1:B:363:PRO:HA	2.31	0.45
1:A:152:THR:HG21	1:A:245:MET:HG2	1.99	0.45
1:C:72:PHE:CD1	1:C:76:THR:HG21	2.52	0.45
1:B:33:ARG:NE	5:B:2019:HOH:O	2.45	0.45
1:A:30:LEU:CD2	1:A:34:LYS:HE2	2.47	0.45
1:C:255:LEU:HD12	1:C:255:LEU:O	2.17	0.45
1:A:120:SER:HA	1:A:121:PRO:HD3	1.80	0.45
1:C:221:ARG:HD2	5:C:2128:HOH:O	2.16	0.45
1:A:87[A]:CYS:HB2	1:A:88:PRO:HD3	1.96	0.45
1:A:82:TYR:CE2	1:A:86:VAL:CG1	3.00	0.45
1:A:364:GLU:C	1:A:365:VAL:CG2	2.84	0.44
1:C:303:VAL:HG21	1:C:356:ALA:O	2.17	0.44
1:C:48:LYS:HE3	1:C:48:LYS:HB2	1.76	0.44
1:C:155:SER:HB3	1:C:244:HIS:HB2	1.98	0.44
1:C:116:GLU:OE1	1:C:221:ARG:NH2	2.49	0.44
1:B:291:SER:HA	1:B:314:SER:HB2	2.00	0.44
1:B:158:VAL:HG12	1:B:241:VAL:HG13	2.00	0.43
1:B:38:HIS:HD2	1:C:180:GLU:OE2	2.00	0.43
1:C:30:LEU:HA	1:C:30:LEU:HD22	1.84	0.43
1:A:365:VAL:CG2	5:A:2099:HOH:O	2.65	0.43
1:B:247:GLU:HB2	1:B:255:LEU:HD23	1.99	0.43
1:C:310:PRO:HB3	1:C:313:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:TYR:HE2	1:A:86:VAL:HG11	1.82	0.43
1:B:249:THR:O	1:B:255:LEU:HB2	2.19	0.43
1:C:161:LEU:HD12	1:C:161:LEU:C	2.39	0.43
1:A:85:VAL:O	1:A:89:ILE:HG12	2.18	0.43
1:A:119:ARG:HG2	3:A:1367:X2O:HAP1	2.01	0.43
1:C:361:ASN:HA	5:C:2036:HOH:O	2.18	0.43
3:A:1367:X2O:HAB2	3:A:1367:X2O:CAL	2.48	0.43
1:C:178:VAL:HG22	1:C:178:VAL:O	2.19	0.43
1:A:206:ASN:OD1	1:A:208:ASP:HB2	2.19	0.42
3:B:1367:X2O:HAB2	3:B:1367:X2O:CAL	2.49	0.42
1:B:361:ASN:HB3	1:B:363:PRO:HD3	2.00	0.42
1:C:62:SER:O	1:C:63:ARG:HD3	2.19	0.42
1:A:355:ARG:NH1	5:A:2264:HOH:O	2.47	0.42
1:A:130:ASP:HA	1:A:131:PRO:HD3	1.95	0.42
1:A:314:SER:O	1:A:318:ARG:HG3	2.19	0.42
1:A:22:VAL:CG1	1:A:70:MET:HB2	2.49	0.42
1:C:25:CYS:O	1:C:74:ALA:HA	2.20	0.42
1:B:55:GLY:HA3	1:B:59:ASP:O	2.20	0.42
1:C:136:ILE:HB	1:C:137:PRO:HD3	2.01	0.42
1:C:299:ILE:O	1:C:303:VAL:HG23	2.20	0.42
1:A:249:THR:HG22	1:A:253:GLU:H	1.85	0.42
1:C:106:GLN:HG2	1:C:109:THR:CG2	2.50	0.42
1:C:183:GLN:HG2	5:C:2045:HOH:O	2.20	0.42
1:C:127:TRP:CE2	1:C:128[B]:GLU:HG3	2.54	0.42
1:C:100:THR:HG23	1:C:262:ASN:HB2	2.01	0.42
1:B:17:LYS:HA	1:B:17:LYS:HD3	1.72	0.42
1:B:256:VAL:O	1:B:256:VAL:HG13	2.20	0.41
1:B:306:THR:HB	1:B:307:PRO:CD	2.41	0.41
1:C:291:SER:HA	1:C:314:SER:HB2	2.01	0.41
1:B:225:ALA:HA	1:B:231:TYR:HB3	2.02	0.41
1:B:264:VAL:HG12	1:B:266:LEU:HD13	2.02	0.41
1:C:92:GLU:OE2	1:C:329:ARG:HG3	2.19	0.41
1:C:170:ASP:CG	1:C:173:ASN:HB2	2.41	0.41
1:A:192:ARG:HD2	1:A:322:ASP:OD1	2.20	0.41
1:A:97:TYR:HA	1:A:365:VAL:CG2	2.50	0.41
1:B:361:ASN:O	1:B:362:LYS:HG3	2.19	0.41
1:C:120:SER:HA	1:C:121:PRO:HD2	1.88	0.41
1:C:18:ASN:N	5:C:2001:HOH:O	2.53	0.41
1:B:17:LYS:HD2	1:B:18:ASN:H	1.86	0.41
1:C:291:SER:HA	1:C:314:SER:CB	2.50	0.41
1:A:157:LYS:HE3	1:A:201:GLU:CD	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LEU:HB2	1:A:182:LEU:HB2	2.02	0.41
1:C:134:GLY:O	1:C:137:PRO:HD2	2.21	0.41
1:A:187:ASP:OD1	1:A:189:ARG:HG2	2.20	0.41
1:B:147:LEU:HA	1:B:150[A]:ASN:HB2	2.03	0.41
1:B:189:ARG:H	1:B:189:ARG:HG3	1.64	0.41
1:C:173:ASN:HA	1:C:174:PRO:HD3	1.94	0.41
1:C:196:ILE:HG22	1:C:199:LEU:HB2	2.03	0.40
1:A:121:PRO:O	1:A:122:ASN:CB	2.64	0.40
1:C:64:LYS:HD2	1:C:64:LYS:HA	1.86	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	332/368 (90%)	326 (98%)	6 (2%)	0	100	100
1	B	327/368 (89%)	320 (98%)	5 (2%)	2 (1%)	28	29
1	C	329/368 (89%)	321 (98%)	7 (2%)	1 (0%)	44	49
All	All	988/1104 (90%)	967 (98%)	18 (2%)	3 (0%)	44	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	361	ASN
1	B	362	LYS
1	C	152	THR

### 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	298/322 (92%)	283 (95%)	15 (5%)	28	34
1	B	297/322 (92%)	279 (94%)	18 (6%)	22	25
1	C	294/322 (91%)	274 (93%)	20 (7%)	18	20
All	All	889/966 (92%)	836 (94%)	53 (6%)	25	25

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	123	GLU
1	A	124	GLU
1	A	128	GLU
1	A	197	LYS
1	A	212	GLN
1	A	227	LEU
1	A	253	GLU
1	A	254	GLU
1	A	255	LEU
1	A	297	ARG
1	A	305	ARG
1	A	306	THR
1	A	337	SER
1	A	364	GLU
1	B	17	LYS
1	B	19[A]	ILE
1	B	19[B]	ILE
1	B	30	LEU
1	B	119	ARG
1	B	150[A]	ASN
1	B	150[B]	ASN
1	B	165	ASN
1	B	189	ARG
1	B	191	LYS
1	B	226	THR

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Mol	Chain	Res	Type
1	B	241	VAL
1	B	248	THR
1	B	249	THR
1	B	257	LYS
1	B	266	LEU
1	B	293	LEU
1	B	304	GLU
1	C	30	LEU
1	C	92	GLU
1	C	124	GLU
1	C	125	TYR
1	C	128[A]	GLU
1	C	128[B]	GLU
1	C	146	LYS
1	C	152	THR
1	C	226	THR
1	C	227	LEU
1	C	237[A]	SER
1	C	237[B]	SER
1	C	241	VAL
1	C	255	LEU
1	C	306	THR
1	C	322	ASP
1	C	327	ARG
1	C	328	THR
1	C	358	ASN
1	C	363	PRO

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

Mol	Chain	Res	Type
1	A	38	HIS
1	A	141	HIS
1	A	262	ASN
1	A	321	GLN
1	B	38	HIS
1	B	236	HIS
1	B	262	ASN
1	B	321	GLN
1	B	361	ASN
1	C	18	ASN
1	C	38	HIS

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Mol	Chain	Res	Type
1	C	98	ASN
1	C	150	ASN
1	C	262	ASN
1	C	321	GLN
1	C	358	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	1366	4	25,29,29	0.98	1 (4%)	24,45,45	1.67	2 (8%)
3	X2O	A	1367	-	17,25,25	0.50	0	16,34,34	0.73	0
2	ADP	B	1366	4	25,29,29	1.08	2 (8%)	24,45,45	1.68	3 (12%)
3	X2O	B	1367	-	17,25,25	0.58	0	16,34,34	0.58	0
2	ADP	C	1366	4	25,29,29	0.91	1 (4%)	24,45,45	1.85	3 (12%)
3	X2O	C	1367	-	17,25,25	0.52	0	16,34,34	0.49	0

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	1366	4	-	0/12/32/32	0/3/3/3
3	X2O	A	1367	-	-	0/24/30/30	0/2/2/2
2	ADP	B	1366	4	-	0/12/32/32	0/3/3/3
3	X2O	B	1367	-	-	0/24/30/30	0/2/2/2
2	ADP	C	1366	4	-	0/12/32/32	0/3/3/3
3	X2O	C	1367	-	-	0/24/30/30	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1366	ADP	C2-N3	2.13	1.35	1.32
2	C	1366	ADP	C5-C4	2.67	1.46	1.40
2	A	1366	ADP	C5-C4	2.78	1.46	1.40
2	B	1366	ADP	C5-C4	3.31	1.48	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1366	ADP	N3-C2-N1	-7.16	122.62	128.86
2	A	1366	ADP	N3-C2-N1	-6.17	123.48	128.86
2	B	1366	ADP	N3-C2-N1	-5.84	123.77	128.86
2	B	1366	ADP	C4-C5-N7	-2.73	106.78	109.41
2	A	1366	ADP	C4-C5-N7	-2.54	106.96	109.41
2	C	1366	ADP	C4-C5-N7	-2.37	107.12	109.41
2	B	1366	ADP	C2-N1-C6	2.18	122.58	118.77
2	C	1366	ADP	C2-N1-C6	2.50	123.14	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1367	X2O	2	0
3	B	1367	X2O	1	0
3	C	1367	X2O	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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	331/368 (89%)	-0.03	25 (7%)	15 13	17, 30, 70, 131	0
1	B	324/368 (88%)	-0.18	15 (4%)	33 32	17, 29, 67, 89	0
1	C	329/368 (89%)	0.33	41 (12%)	4 4	23, 41, 72, 97	0
All	All	984/1104 (89%)	0.04	81 (8%)	12 11	17, 33, 70, 131	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	250	ILE	8.8
1	A	249	THR	6.1
1	A	252	GLY	5.9
1	B	248	THR	5.8
1	A	248	THR	5.3
1	C	308	HIS	5.3
1	B	363	PRO	5.3
1	A	151	GLY	5.1
1	A	149	ASP	4.9
1	A	251	ASP	4.9
1	C	255	LEU	4.9
1	C	307	PRO	4.8
1	C	326	GLY	4.6
1	B	149	ASP	4.5
1	C	304	GLU	4.4
1	A	365	VAL	4.4
1	A	152	THR	4.4
1	C	271	ASN	4.4
1	A	363	PRO	4.3
1	C	189	ARG	4.1
1	A	253	GLU	4.1
1	C	188	PRO	4.0
1	C	264	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	238	VAL	3.8
1	B	255	LEU	3.8
1	A	247	GLU	3.8
1	B	247	GLU	3.7
1	C	327	ARG	3.7
1	C	363	PRO	3.7
1	C	239	PHE	3.5
1	C	190	ASN	3.5
1	C	123	GLU	3.4
1	C	306	THR	3.4
1	B	256	VAL	3.4
1	A	307	PRO	3.3
1	B	189	ARG	3.2
1	A	123	GLU	3.1
1	C	325	GLY	3.1
1	C	191	LYS	3.0
1	A	264	VAL	3.0
1	A	255	LEU	2.9
1	A	362	LYS	2.9
1	C	101	ILE	2.8
1	C	192	ARG	2.8
1	A	364	GLU	2.8
1	C	237[A]	SER	2.8
1	A	308	HIS	2.7
1	C	187	ASP	2.7
1	B	263	LEU	2.7
1	C	114	THR	2.7
1	C	312	ARG	2.6
1	C	149	ASP	2.6
1	C	125	TYR	2.6
1	C	160	LEU	2.6
1	B	264	VAL	2.6
1	C	263	LEU	2.5
1	C	115	MET	2.5
1	C	103	ALA	2.5
1	A	148	THR	2.5
1	C	333	ILE	2.5
1	A	150[A]	ASN	2.4
1	A	238	VAL	2.4
1	C	185	PHE	2.4
1	B	249	THR	2.3
1	C	121	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	360	LEU	2.3
1	A	305	ARG	2.2
1	C	135	ILE	2.2
1	C	256	VAL	2.2
1	B	103	ALA	2.2
1	C	30	LEU	2.2
1	C	161	LEU	2.2
1	B	238	VAL	2.1
1	C	266	LEU	2.1
1	B	266	LEU	2.1
1	A	103	ALA	2.1
1	B	115	MET	2.1
1	B	327	ARG	2.1
1	C	122	ASN	2.1
1	C	303	VAL	2.1
1	A	115	MET	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
3	X2O	B	1367	24/24	0.94	0.13	0.09	18,22,31,33	0
3	X2O	A	1367	24/24	0.95	0.11	-0.55	21,30,36,43	0
2	ADP	B	1366	27/27	0.99	0.11	-0.71	16,21,27,33	0
3	X2O	C	1367	24/24	0.94	0.12	-0.74	27,36,40,54	0
2	ADP	A	1366	27/27	0.98	0.09	-0.85	16,21,27,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ADP	C	1366	27/27	0.97	0.10	-1.04	23,32,37,39	0
4	MG	C	1368	1/1	0.97	0.20	-	37,37,37,37	0
4	MG	A	1368	1/1	0.98	0.15	-	23,23,23,23	0
4	MG	B	1368	1/1	0.99	0.21	-	22,22,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.