



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2016 – 03:53 PM EST

PDB ID : 2XAM  
Title : Inositol 1,3,4,5,6-pentakisphosphate 2-kinase from *A. thaliana* in complex with ADP and IP6.  
Authors : Gonzalez, B.; Banos-Sanz, J.I.; Villate, M.; Brearley, C.A.; Sanz-Aparicio, J.  
Deposited on : 2010-03-31  
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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : rb-20028442

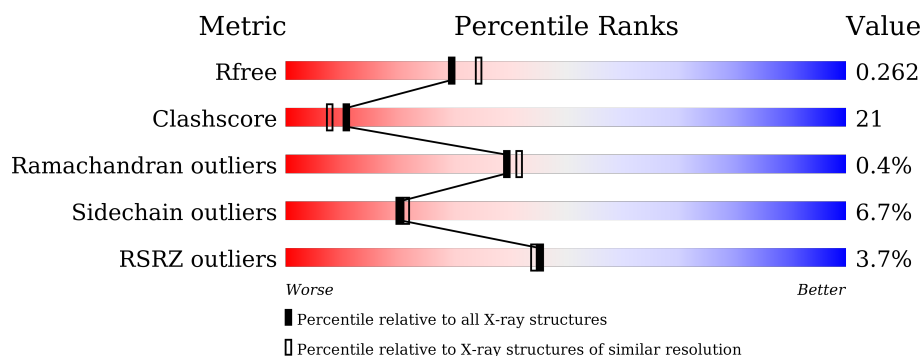
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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	451	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>23%</div> <div>• 8%</div> </div> </div>
1	B	451	<div> <div>4%</div> <div> <div></div> <div>61%</div> <div>28%</div> <div>5% 6%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7013 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.

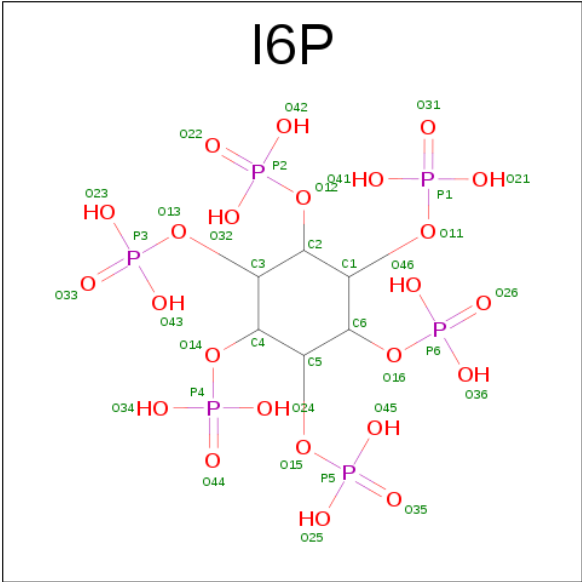
- Molecule 1 is a protein called INOSITOL-PENTAKISPHOSPHATE 2-KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3314	2104	561	636	13			
1	B	426	Total	C	N	O	S	0	0	0
			3380	2146	576	645	13			

There are 16 discrepancies between the modelled and reference sequences:

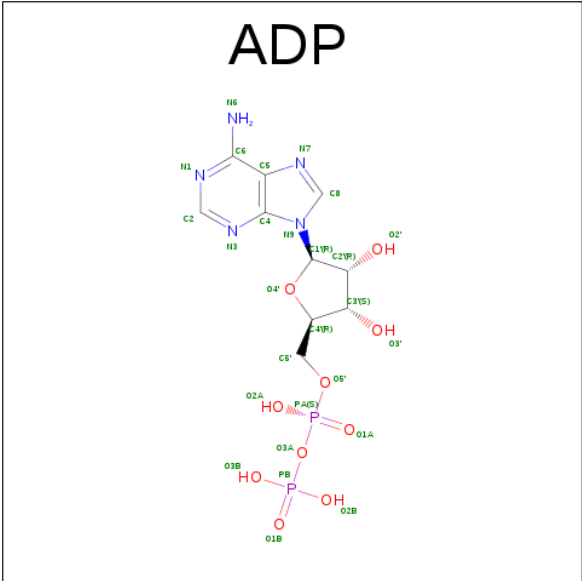
Chain	Residue	Modelled	Actual	Comment	Reference
A	54	SER	ALA	SEE REMARK 999	UNP Q93YN9
A	90	GLN	LYS	SEE REMARK 999	UNP Q93YN9
A	157	THR	SER	SEE REMARK 999	UNP Q93YN9
A	204	ILE	ASN	SEE REMARK 999	UNP Q93YN9
A	224	ARG	SER	SEE REMARK 999	UNP Q93YN9
A	321	CYS	SER	SEE REMARK 999	UNP Q93YN9
A	325	ILE	LEU	SEE REMARK 999	UNP Q93YN9
A	337	ARG	LYS	SEE REMARK 999	UNP Q93YN9
B	54	SER	ALA	SEE REMARK 999	UNP Q93YN9
B	90	GLN	LYS	SEE REMARK 999	UNP Q93YN9
B	157	THR	SER	SEE REMARK 999	UNP Q93YN9
B	204	ILE	ASN	SEE REMARK 999	UNP Q93YN9
B	224	ARG	SER	SEE REMARK 999	UNP Q93YN9
B	321	CYS	SER	SEE REMARK 999	UNP Q93YN9
B	325	ILE	LEU	SEE REMARK 999	UNP Q93YN9
B	337	ARG	LYS	SEE REMARK 999	UNP Q93YN9

- Molecule 2 is INOSITOL 1,2,3,4,5,6-HEXAKISPHOSPHATE (three-letter code: I6P) (formula: C<sub>6</sub>H<sub>18</sub>O<sub>24</sub>P<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			36	6	24	6		
2	B	1	Total	C	O	P	0	0
			36	6	24	6		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

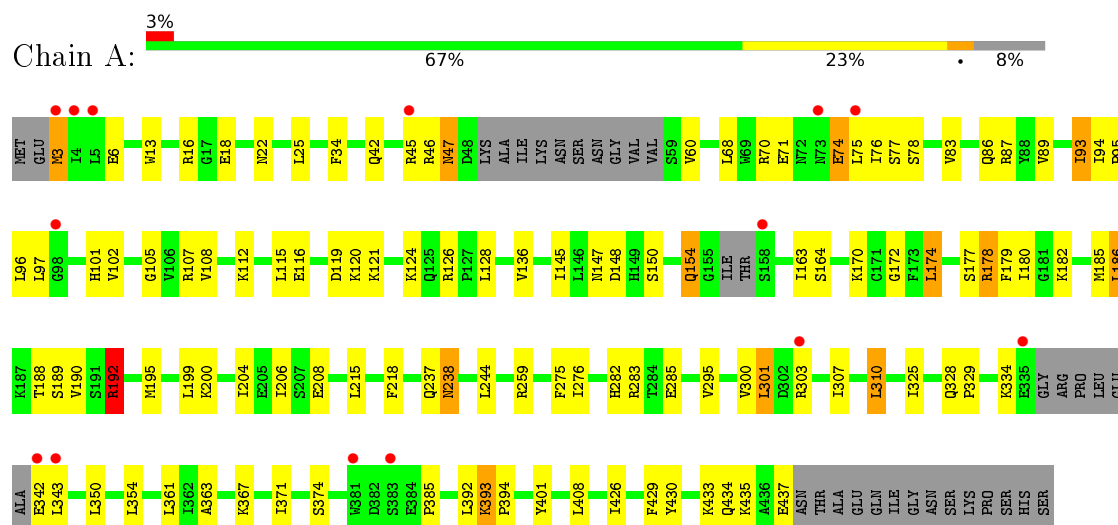
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	90	Total	O	0	0
			90	90		
6	B	97	Total	O	0	0
			97	97		

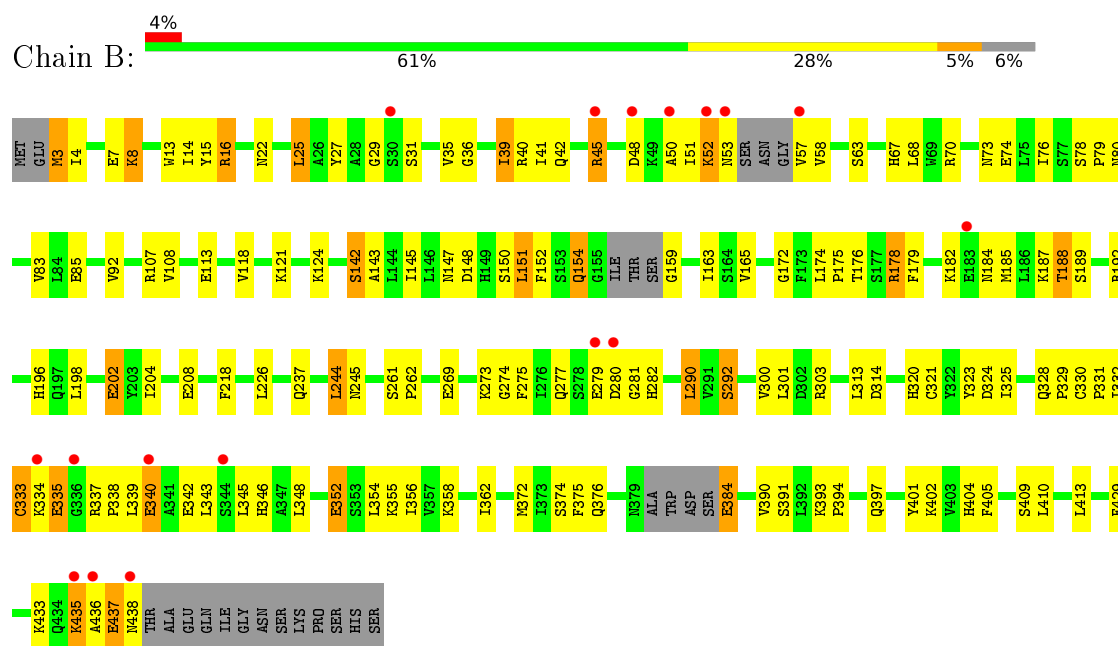
### 3 Residue-property plots

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: INOSITOL-PENTAKISPHOSPHATE 2-KINASE



#### • Molecule 1: INOSITOL-PENTAKISPHOSPHATE 2-KINASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.12Å 113.59Å 142.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.74 – 2.20 71.24 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (88.74-2.20) 99.8 (71.24-2.20)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.227 , 0.270 0.226 , 0.262	Depositor DCC
$R_{free}$ test set	2474 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.9	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7013	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.85% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, I6P, 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	0.36	0/3375	0.54	1/4549 (0.0%)
1	B	0.38	0/3440	0.54	0/4635
All	All	0.37	0/6815	0.54	1/9184 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	ARG	NE-CZ-NH2	-5.20	117.70	120.30

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	3314	0	3312	133	0
1	B	3380	0	3400	167	0
2	A	36	0	6	1	0
2	B	36	0	6	1	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	90	0	0	9	0
6	B	97	0	0	6	0
All	All	7013	0	6748	286	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 21.

All (286) 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:46:ARG:NH1	1:B:182:LYS:HG3	1.47	1.29
1:B:348:LEU:CD2	1:B:352:GLU:HG2	1.68	1.22
1:A:46:ARG:HH12	1:B:182:LYS:CG	1.56	1.18
1:A:204:ILE:HD12	1:B:345:LEU:HD21	1.24	1.17
1:A:3:MET:CE	1:A:3:MET:HA	1.76	1.14
1:A:178:ARG:HH11	1:A:178:ARG:CG	1.62	1.10
1:A:3:MET:HE2	1:A:3:MET:HA	1.24	1.10
1:B:204:ILE:HG22	1:B:204:ILE:O	1.52	1.10
1:A:204:ILE:CD1	1:B:345:LEU:CD2	2.33	1.06
1:A:178:ARG:HH11	1:A:178:ARG:HG3	1.18	1.04
1:B:178:ARG:CG	1:B:178:ARG:HH11	1.73	1.02
1:A:393:LYS:CA	1:A:393:LYS:HE2	1.86	1.02
1:A:204:ILE:HD13	1:B:345:LEU:HD23	1.39	1.01
1:B:178:ARG:HG3	1:B:178:ARG:HH11	1.21	0.99
1:A:393:LYS:HA	1:A:393:LYS:CE	1.91	0.99
1:A:147:ASN:ND2	1:A:154:GLN:HE21	1.61	0.99
1:A:199:LEU:HD22	1:A:426:ILE:HD13	1.45	0.98
1:A:393:LYS:HE2	1:A:393:LYS:HA	0.99	0.98
1:A:204:ILE:CD1	1:B:345:LEU:HD21	1.94	0.97
1:A:154:GLN:HA	1:A:154:GLN:OE1	1.62	0.96
1:B:340:GLU:HA	1:B:340:GLU:OE1	1.65	0.96
1:B:14:ILE:HD12	1:B:15:TYR:H	1.31	0.95
1:B:348:LEU:CD2	1:B:352:GLU:CG	2.44	0.94
1:A:74:GLU:OE1	1:A:74:GLU:N	2.00	0.93
1:B:348:LEU:CG	1:B:352:GLU:HG2	1.99	0.92
1:B:348:LEU:HD23	1:B:352:GLU:HG2	1.50	0.91
1:B:204:ILE:O	1:B:204:ILE:CG2	2.19	0.90
1:B:39:ILE:HD12	1:B:41:ILE:HG13	1.52	0.89
1:A:393:LYS:HB2	1:A:394:PRO:HD3	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ARG:NH1	1:A:178:ARG:HG3	1.87	0.86
1:B:384:GLU:N	1:B:384:GLU:OE2	2.08	0.86
1:A:275:PHE:HD1	1:A:276:ILE:CD1	1.87	0.86
1:B:348:LEU:HD23	1:B:352:GLU:CG	2.05	0.86
1:B:178:ARG:NH1	1:B:178:ARG:HG3	1.82	0.86
1:A:204:ILE:CD1	1:B:345:LEU:HD23	1.99	0.86
1:A:204:ILE:HD12	1:B:345:LEU:CD2	1.97	0.86
1:A:200:LYS:HE3	6:A:2087:HOH:O	1.77	0.85
1:A:147:ASN:HD22	1:A:154:GLN:HE21	1.25	0.84
1:B:176:THR:HG22	1:B:176:THR:O	1.76	0.83
1:B:39:ILE:HD11	1:B:143:ALA:HB1	1.59	0.83
1:B:8:LYS:HD2	1:B:8:LYS:H	1.44	0.83
1:B:348:LEU:HG	1:B:352:GLU:HG2	1.63	0.81
1:B:52:LYS:HG3	1:B:57:VAL:N	1.95	0.81
1:A:94:ILE:HB	1:A:95:PRO:HD3	1.62	0.81
2:B:500:I6P:O32	2:B:500:I6P:O23	1.97	0.80
1:B:435:LYS:NZ	1:B:438:ASN:HD22	1.78	0.80
1:A:18:GLU:OE1	1:A:126:ARG:HG2	1.80	0.80
1:A:76:ILE:HD12	1:A:77:SER:N	1.96	0.80
1:A:199:LEU:HD22	1:A:426:ILE:CD1	2.12	0.80
1:A:429:PHE:CZ	1:A:433:LYS:HE3	2.17	0.80
1:B:85:GLU:OE2	1:B:409:SER:HA	1.82	0.80
1:A:16:ARG:NH2	1:A:148:ASP:OD1	2.15	0.79
1:B:163:ILE:HD13	1:B:275:PHE:CG	2.18	0.79
1:A:147:ASN:ND2	1:A:154:GLN:NE2	2.30	0.78
1:B:52:LYS:HG2	1:B:53:ASN:N	1.97	0.78
1:A:275:PHE:HD1	1:A:276:ILE:HD12	1.48	0.77
1:B:52:LYS:HB2	1:B:57:VAL:C	2.05	0.77
1:A:393:LYS:HB2	1:A:394:PRO:CD	2.15	0.76
1:A:101:HIS:HD2	1:A:303:ARG:HH22	1.32	0.76
1:B:39:ILE:HD12	1:B:41:ILE:CG1	2.16	0.76
1:B:85:GLU:OE2	1:B:410:LEU:N	2.19	0.75
1:B:337:ARG:HD2	1:B:338:PRO:HD2	1.67	0.75
1:B:39:ILE:HD13	1:B:40:ARG:N	2.02	0.75
1:B:348:LEU:HD21	1:B:352:GLU:HG2	1.68	0.75
1:B:39:ILE:CD1	1:B:41:ILE:HG13	2.16	0.75
1:B:163:ILE:HD13	1:B:275:PHE:CD1	2.22	0.74
1:B:108:VAL:HG11	1:B:145:ILE:HD11	1.70	0.73
1:A:178:ARG:HH11	1:A:178:ARG:HG2	1.53	0.73
1:B:108:VAL:HG11	1:B:145:ILE:CD1	2.18	0.72
1:A:147:ASN:HD22	1:A:154:GLN:NE2	1.86	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:LEU:CD1	1:A:354:LEU:HD11	2.20	0.71
1:B:176:THR:CG2	1:B:176:THR:O	2.38	0.71
1:B:184:ASN:O	1:B:187:LYS:HG2	1.90	0.71
1:B:80:ASN:OD1	1:B:83:VAL:HG12	1.91	0.71
1:A:3:MET:CE	1:A:3:MET:CA	2.62	0.71
1:B:277:GLN:H	1:B:397:GLN:HE22	1.38	0.71
1:B:39:ILE:HD11	1:B:143:ALA:CB	2.21	0.70
1:B:3:MET:HA	1:B:3:MET:CE	2.22	0.70
1:A:275:PHE:CD1	1:A:276:ILE:HD12	2.27	0.69
1:B:335:GLU:OE2	1:B:335:GLU:HA	1.91	0.69
1:A:208:GLU:OE1	1:A:259:ARG:NE	2.23	0.69
1:B:178:ARG:CB	1:B:178:ARG:HH11	2.05	0.69
1:A:101:HIS:CD2	1:A:303:ARG:HH22	2.11	0.68
1:A:350:LEU:HD13	1:A:354:LEU:CD1	2.22	0.68
1:A:124:LYS:CB	6:A:2017:HOH:O	2.41	0.68
1:A:47:ASN:HA	1:B:188:THR:CG2	2.24	0.68
1:B:16:ARG:NH2	1:B:148:ASP:OD1	2.27	0.68
1:B:31:SER:O	1:B:35:VAL:HG23	1.94	0.68
1:A:89:VAL:O	1:A:94:ILE:HG12	1.95	0.67
1:B:435:LYS:HZ2	1:B:438:ASN:HD22	1.42	0.67
1:A:192:ARG:NH2	6:A:2030:HOH:O	2.27	0.67
1:B:348:LEU:HD21	1:B:352:GLU:CG	2.23	0.67
1:A:16:ARG:NH2	1:A:150:SER:OG	2.27	0.66
1:A:74:GLU:O	1:A:87:ARG:NH1	2.28	0.66
1:B:404:HIS:HD2	6:B:2081:HOH:O	1.76	0.66
1:B:303:ARG:HB3	6:B:2016:HOH:O	1.95	0.66
1:B:108:VAL:CG1	1:B:145:ILE:CD1	2.73	0.66
1:B:196:HIS:HE1	6:B:2030:HOH:O	1.79	0.66
1:A:385:PRO:HA	6:A:2075:HOH:O	1.95	0.65
1:B:13:TRP:O	1:B:121:LYS:HE2	1.97	0.65
1:B:14:ILE:HD12	1:B:15:TYR:N	2.09	0.65
1:B:25:LEU:HD21	1:B:118:VAL:HG13	1.78	0.64
1:B:384:GLU:CA	1:B:384:GLU:OE2	2.45	0.64
1:A:3:MET:HE3	1:A:3:MET:HA	1.76	0.64
1:A:76:ILE:C	1:A:76:ILE:HD12	2.19	0.64
1:B:45:ARG:HB2	1:B:48:ASP:OD1	1.99	0.63
1:B:79:PRO:HG2	1:B:83:VAL:HG11	1.79	0.63
1:A:74:GLU:CD	1:A:74:GLU:H	2.00	0.63
1:A:328:GLN:HG2	1:A:329:PRO:O	1.99	0.63
1:B:435:LYS:NZ	1:B:438:ASN:ND2	2.47	0.63
1:A:435:LYS:O	1:A:437:GLU:HG3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ASN:HB2	1:B:57:VAL:HB	1.81	0.62
1:A:101:HIS:HD2	1:A:303:ARG:NH2	1.97	0.61
1:A:13:TRP:O	1:A:121:LYS:HE2	2.01	0.61
1:B:50:ALA:O	1:B:51:ILE:HD12	2.01	0.61
1:A:74:GLU:N	1:A:74:GLU:CD	2.54	0.61
1:A:178:ARG:CG	1:A:178:ARG:NH1	2.35	0.60
1:B:178:ARG:HB2	1:B:178:ARG:HH11	1.67	0.60
1:A:199:LEU:CD2	1:A:426:ILE:CD1	2.80	0.60
1:B:14:ILE:CD1	1:B:15:TYR:H	2.11	0.60
1:B:179:PHE:CE2	1:B:345:LEU:HD11	2.37	0.59
1:B:435:LYS:O	1:B:437:GLU:N	2.35	0.59
1:A:350:LEU:CD1	1:A:354:LEU:CD1	2.80	0.58
1:A:128:LEU:HD11	1:B:337:ARG:HG3	1.85	0.58
1:B:277:GLN:H	1:B:397:GLN:NE2	2.00	0.58
1:A:163:ILE:HG13	1:A:275:PHE:CD1	2.38	0.58
1:A:101:HIS:CD2	1:A:303:ARG:NH2	2.72	0.58
1:B:50:ALA:C	1:B:51:ILE:HD12	2.24	0.58
1:A:325:ILE:HD11	1:A:354:LEU:HA	1.85	0.58
1:B:348:LEU:HD23	1:B:352:GLU:HG3	1.84	0.58
1:B:159:GLY:HA2	1:B:376:GLN:NE2	2.19	0.57
1:B:280:ASP:HB3	1:B:282:HIS:HD2	1.69	0.57
1:A:393:LYS:CB	1:A:394:PRO:CD	2.82	0.57
1:B:147:ASN:HD22	1:B:154:GLN:NE2	2.02	0.57
1:A:350:LEU:HD11	1:A:354:LEU:HD11	1.85	0.57
1:A:238:ASN:H	1:A:238:ASN:HD22	1.51	0.57
1:B:196:HIS:HD2	6:B:2091:HOH:O	1.88	0.56
1:B:226:LEU:HA	1:B:292:SER:OG	2.04	0.56
1:A:124:LYS:HB3	6:A:2017:HOH:O	2.03	0.56
1:A:119:ASP:HB2	1:A:136:VAL:CG2	2.35	0.56
1:B:393:LYS:N	1:B:394:PRO:HD2	2.19	0.56
1:B:192:ARG:NH2	6:B:2027:HOH:O	2.39	0.56
1:A:119:ASP:HB2	1:A:136:VAL:HG21	1.87	0.55
1:A:172:GLY:HA3	1:A:218:PHE:CD2	2.41	0.55
1:B:52:LYS:CG	1:B:53:ASN:N	2.69	0.55
1:A:86:GLN:NE2	1:A:105:GLY:O	2.35	0.55
1:B:8:LYS:H	1:B:8:LYS:CD	2.11	0.55
1:B:108:VAL:CG1	1:B:145:ILE:HD13	2.36	0.55
1:B:358:LYS:O	1:B:362:ILE:HG12	2.07	0.55
1:B:27:TYR:CZ	1:B:29:GLY:HA3	2.42	0.54
1:A:94:ILE:C	1:A:96:LEU:H	2.10	0.54
1:A:119:ASP:CG	1:A:136:VAL:HG22	2.27	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:LYS:HZ1	1:B:438:ASN:ND2	2.04	0.54
1:B:202:GLU:OE2	1:B:429:PHE:HZ	1.90	0.54
1:B:269:GLU:OE2	1:B:281:GLY:HA2	2.07	0.53
1:A:46:ARG:HH12	1:B:182:LYS:HG3	0.62	0.53
1:B:340:GLU:OE1	1:B:343:LEU:HD12	2.08	0.53
1:B:321:CYS:O	1:B:325:ILE:HG12	2.08	0.53
1:B:73:ASN:HA	1:B:76:ILE:HG12	1.90	0.53
1:A:124:LYS:HB2	6:A:2017:HOH:O	2.08	0.53
1:A:275:PHE:CD1	1:A:276:ILE:CD1	2.78	0.53
1:A:185:MET:O	1:A:188:THR:HB	2.09	0.52
1:B:348:LEU:HD21	1:B:352:GLU:OE2	2.09	0.52
1:B:300:VAL:HG22	1:B:405:PHE:CZ	2.44	0.52
1:B:320:HIS:CE1	1:B:333:CYS:SG	3.02	0.52
1:A:71:GLU:HA	1:A:71:GLU:OE1	2.10	0.52
1:B:330:CYS:O	1:B:334:LYS:HG3	2.09	0.52
1:A:238:ASN:N	1:A:238:ASN:HD22	2.08	0.52
1:B:147:ASN:HD22	1:B:154:GLN:HE22	1.59	0.51
1:A:128:LEU:HG	6:A:2020:HOH:O	2.10	0.51
1:B:179:PHE:CE2	1:B:345:LEU:CD1	2.93	0.51
1:B:290:LEU:HD11	1:B:375:PHE:CE2	2.46	0.51
1:A:94:ILE:O	1:A:96:LEU:N	2.44	0.51
1:B:159:GLY:CA	1:B:376:GLN:NE2	2.74	0.51
1:B:328:GLN:HG3	1:B:329:PRO:HD2	1.92	0.50
1:A:334:LYS:NZ	6:A:2066:HOH:O	2.43	0.50
1:B:320:HIS:HB3	1:B:346:HIS:NE2	2.27	0.50
1:B:51:ILE:O	1:B:51:ILE:HG22	2.11	0.50
1:A:74:GLU:CD	1:A:75:LEU:H	2.15	0.50
1:A:60:VAL:HG21	1:A:78:SER:O	2.12	0.50
1:A:46:ARG:NH1	1:B:182:LYS:O	2.44	0.50
1:B:124:LYS:O	1:B:124:LYS:HD3	2.10	0.49
1:B:172:GLY:HA3	1:B:218:PHE:CD2	2.46	0.49
1:B:244:LEU:C	1:B:244:LEU:CD2	2.80	0.49
1:B:345:LEU:O	1:B:348:LEU:HB2	2.12	0.49
1:B:67:HIS:CE1	1:B:70:ARG:HH21	2.30	0.49
1:A:393:LYS:CA	1:A:393:LYS:CE	2.67	0.49
1:A:283:ARG:HD3	6:A:2057:HOH:O	2.12	0.49
1:B:435:LYS:HZ1	1:B:438:ASN:HD22	1.57	0.49
1:A:307:ILE:O	1:A:310:LEU:HB2	2.13	0.48
1:A:295:VAL:CG1	1:A:301:LEU:HD22	2.43	0.48
1:B:429:PHE:CZ	1:B:433:LYS:HD2	2.48	0.48
1:A:429:PHE:HZ	1:A:433:LYS:HE3	1.74	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:LEU:HB2	1:B:39:ILE:HG22	1.95	0.48
1:A:47:ASN:HA	1:B:188:THR:HG21	1.93	0.48
1:A:68:LEU:HD21	1:A:361:LEU:HD12	1.95	0.47
1:B:244:LEU:CD2	1:B:245:ASN:ND2	2.78	0.47
1:B:85:GLU:OE2	1:B:409:SER:CA	2.59	0.47
1:A:179:PHE:CD2	1:A:342:GLU:OE1	2.67	0.47
1:B:290:LEU:HD11	1:B:375:PHE:CD2	2.50	0.47
1:B:107:ARG:HH11	1:B:142:SER:HB3	1.80	0.47
1:A:70:ARG:HG2	1:A:71:GLU:N	2.28	0.47
1:B:36:GLY:HA2	1:B:151:LEU:HD21	1.97	0.47
1:A:350:LEU:HD13	1:A:354:LEU:HD12	1.96	0.46
1:A:374:SER:O	1:A:401:TYR:HA	2.14	0.46
1:B:107:ARG:HH11	1:B:142:SER:CB	2.28	0.46
1:B:52:LYS:HB2	1:B:58:VAL:N	2.29	0.46
1:B:74:GLU:N	1:B:74:GLU:OE1	2.41	0.46
1:A:154:GLN:CA	1:A:154:GLN:OE1	2.47	0.46
1:A:93:ILE:HG21	1:A:408:LEU:HD13	1.98	0.46
1:A:34:PHE:HE1	1:A:145:ILE:CD1	2.29	0.46
1:A:22:ASN:HD21	1:A:42:GLN:HG2	1.81	0.46
1:B:273:LYS:HG3	1:B:274:GLY:N	2.30	0.46
1:B:78:SER:HB3	1:B:83:VAL:HG13	1.96	0.46
1:A:94:ILE:C	1:A:96:LEU:N	2.68	0.46
1:A:34:PHE:HE1	1:A:145:ILE:HD13	1.80	0.46
1:B:280:ASP:CB	1:B:282:HIS:HD2	2.28	0.46
1:B:108:VAL:HB	1:B:145:ILE:HD13	1.98	0.46
1:B:175:PRO:HB3	6:B:2072:HOH:O	2.15	0.46
1:A:94:ILE:CD1	1:A:102:VAL:HB	2.46	0.46
1:B:435:LYS:C	1:B:437:GLU:H	2.19	0.46
1:B:8:LYS:HD2	1:B:8:LYS:N	2.22	0.45
1:A:45:ARG:HH22	2:A:500:I6P:P3	2.39	0.45
1:B:290:LEU:CD1	1:B:375:PHE:CE2	3.00	0.45
1:A:6:GLU:OE1	1:A:6:GLU:HA	2.15	0.45
1:B:348:LEU:HD21	1:B:352:GLU:CD	2.36	0.45
1:B:22:ASN:HD21	1:B:42:GLN:HG2	1.81	0.45
1:B:332:ILE:HG22	1:B:332:ILE:O	2.15	0.45
1:A:112:LYS:HE3	1:A:116:GLU:OE2	2.17	0.45
1:B:48:ASP:OD1	1:B:48:ASP:N	2.35	0.45
1:B:39:ILE:HD13	1:B:39:ILE:C	2.37	0.44
1:B:152:PHE:CZ	1:B:402:LYS:HE3	2.52	0.44
1:A:115:LEU:HA	1:A:115:LEU:HD23	1.77	0.44
1:B:393:LYS:HB3	1:B:394:PRO:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:VAL:CG1	1:B:391:SER:N	2.80	0.44
1:B:39:ILE:CD1	1:B:41:ILE:CG1	2.86	0.44
1:A:163:ILE:HG13	1:A:275:PHE:CE1	2.53	0.44
1:A:363:ALA:O	1:A:367:LYS:HG3	2.18	0.44
1:A:47:ASN:O	1:B:189:SER:OG	2.36	0.44
1:B:435:LYS:C	1:B:437:GLU:N	2.71	0.44
1:A:182:LYS:HE2	1:A:182:LYS:HB3	1.66	0.44
1:A:310:LEU:HA	1:A:310:LEU:HD12	1.90	0.44
1:B:7:GLU:HG3	1:B:113:GLU:HB3	1.99	0.44
1:A:206:ILE:HD12	1:A:237:GLN:HE22	1.82	0.43
1:A:435:LYS:O	1:A:437:GLU:N	2.47	0.43
1:A:177:SER:HB3	1:A:180:ILE:HG13	2.00	0.43
1:B:313:LEU:O	1:B:314:ASP:HB3	2.18	0.43
1:B:68:LEU:HD22	1:B:413:LEU:HD13	1.99	0.43
1:A:430:TYR:O	1:A:434:GLN:HG2	2.18	0.43
1:A:47:ASN:OD1	1:B:188:THR:HG21	2.19	0.43
1:B:244:LEU:C	1:B:244:LEU:HD23	2.38	0.43
1:A:392:LEU:HA	1:A:392:LEU:HD23	1.89	0.43
1:B:185:MET:O	1:B:188:THR:HG22	2.17	0.43
1:B:323:TYR:CD2	1:B:331:PRO:HD2	2.54	0.43
1:B:92:VAL:HG11	1:B:362:ILE:HD11	2.00	0.43
1:A:238:ASN:ND2	1:A:238:ASN:H	2.16	0.43
1:B:261:SER:HB2	1:B:262:PRO:HD2	2.01	0.43
1:A:120:LYS:HD2	1:A:120:LYS:O	2.18	0.42
1:A:186:LEU:HD12	1:A:186:LEU:HA	1.88	0.42
1:A:301:LEU:HD11	1:A:371:ILE:HD13	2.01	0.42
1:B:3:MET:HA	1:B:3:MET:HE2	2.01	0.42
1:A:108:VAL:HB	1:A:145:ILE:CD1	2.49	0.42
1:A:174:LEU:HD13	1:A:215:LEU:HD21	2.01	0.42
1:B:16:ARG:NH2	1:B:150:SER:OG	2.53	0.42
1:B:374:SER:O	1:B:401:TYR:HA	2.19	0.42
1:A:83:VAL:HG22	1:A:107:ARG:NE	2.35	0.41
1:B:325:ILE:CD1	1:B:354:LEU:HG	2.50	0.41
1:B:329:PRO:HB2	1:B:334:LYS:HZ2	1.85	0.41
1:B:339:LEU:O	1:B:342:GLU:HB2	2.20	0.41
1:A:328:GLN:HG3	1:A:329:PRO:HD2	2.01	0.41
1:A:16:ARG:HH22	1:A:148:ASP:CG	2.23	0.41
1:A:282:HIS:O	1:A:285:GLU:HG2	2.20	0.41
1:B:324:ASP:CG	1:B:346:HIS:HD1	2.24	0.41
1:A:76:ILE:C	1:A:76:ILE:CD1	2.86	0.41
1:A:94:ILE:HB	1:A:95:PRO:CD	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LEU:HG	1:A:307:ILE:CD1	2.51	0.41
1:B:39:ILE:HD12	1:B:41:ILE:CD1	2.50	0.41
1:A:190:VAL:HB	1:A:195:MET:HE2	2.02	0.41
1:B:3:MET:HA	1:B:3:MET:HE1	1.98	0.41
1:B:325:ILE:HD12	1:B:354:LEU:CD2	2.51	0.41
1:B:352:GLU:O	1:B:355:LYS:HB2	2.21	0.41
1:B:165:VAL:O	1:B:372:MET:HA	2.21	0.41
1:B:435:LYS:HD2	1:B:435:LYS:N	2.35	0.41
1:B:325:ILE:HD12	1:B:354:LEU:HD23	2.02	0.40
1:B:390:VAL:HG12	1:B:391:SER:N	2.36	0.40
1:B:338:PRO:HA	1:B:342:GLU:OE1	2.22	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	409/451 (91%)	393 (96%)	14 (3%)	2 (0%)	34	35
1	B	418/451 (93%)	401 (96%)	16 (4%)	1 (0%)	52	59
All	All	827/902 (92%)	794 (96%)	30 (4%)	3 (0%)	39	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	436	ALA
1	A	170	LYS
1	A	393	LYS



### 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	371/399 (93%)	353 (95%)	18 (5%)	31	36
1	B	378/399 (95%)	346 (92%)	32 (8%)	13	13
All	All	749/798 (94%)	699 (93%)	50 (7%)	20	21

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	MET
1	A	25	LEU
1	A	47	ASN
1	A	74	GLU
1	A	93	ILE
1	A	154	GLN
1	A	164	SER
1	A	174	LEU
1	A	178	ARG
1	A	186	LEU
1	A	189	SER
1	A	192	ARG
1	A	238	ASN
1	A	244	LEU
1	A	300	VAL
1	A	301	LEU
1	A	310	LEU
1	A	343	LEU
1	B	3	MET
1	B	4	ILE
1	B	8	LYS
1	B	16	ARG
1	B	25	LEU
1	B	39	ILE
1	B	45	ARG
1	B	52	LYS
1	B	63	SER

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Mol	Chain	Res	Type
1	B	142	SER
1	B	151	LEU
1	B	154	GLN
1	B	174	LEU
1	B	178	ARG
1	B	188	THR
1	B	198	LEU
1	B	202	GLU
1	B	208	GLU
1	B	237	GLN
1	B	244	LEU
1	B	279	GLU
1	B	290	LEU
1	B	292	SER
1	B	301	LEU
1	B	333	CYS
1	B	335	GLU
1	B	340	GLU
1	B	352	GLU
1	B	356	ILE
1	B	384	GLU
1	B	435	LYS
1	B	437	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	66	GLN
1	A	91	ASN
1	A	101	HIS
1	A	147	ASN
1	A	149	HIS
1	A	238	ASN
1	A	404	HIS
1	B	22	ASN
1	B	72	ASN
1	B	91	ASN
1	B	147	ASN
1	B	149	HIS
1	B	196	HIS
1	B	376	GLN

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Mol	Chain	Res	Type
1	B	379	ASN
1	B	397	GLN
1	B	404	HIS
1	B	438	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 10 ligands modelled in this entry, 6 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	$\# Z  > 2$
2	I6P	A	500	5	30,36,36	0.74	0	60,60,60	1.13	4 (6%)
3	ADP	A	600	5	24,29,29	0.99	1 (4%)	23,45,45	1.88	3 (13%)
2	I6P	B	500	5	30,36,36	0.73	0	60,60,60	1.21	5 (8%)
3	ADP	B	600	5	24,29,29	0.99	1 (4%)	23,45,45	1.75	2 (8%)

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	I6P	A	500	5	-	0/30/54/54	0/1/1/1
3	ADP	A	600	5	-	0/12/32/32	0/3/3/3
2	I6P	B	500	5	-	0/30/54/54	0/1/1/1
3	ADP	B	600	5	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	ADP	C5-C4	2.79	1.46	1.40
3	B	600	ADP	C5-C4	3.13	1.47	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	ADP	N3-C2-N1	-7.10	123.30	128.87
3	B	600	ADP	N3-C2-N1	-6.73	123.58	128.87
3	A	600	ADP	C1'-N9-C4	-3.19	123.24	126.81
2	A	500	I6P	O14-P4-O44	-2.60	101.27	107.48
3	B	600	ADP	C1'-N9-C4	-2.18	124.37	126.81
3	A	600	ADP	C2'-C1'-N9	-2.16	107.68	113.47
2	B	500	I6P	O34-P4-O14	-2.00	100.64	106.62
2	A	500	I6P	O23-P3-O43	2.03	114.90	107.44
2	B	500	I6P	O36-P6-O46	2.12	115.21	107.44
2	A	500	I6P	O21-P1-O41	2.20	115.54	107.44
2	A	500	I6P	O12-C2-C1	2.32	113.28	108.54
2	B	500	I6P	O23-P3-O43	2.32	115.97	107.44
2	B	500	I6P	O25-P5-O45	2.41	116.27	107.44
2	B	500	I6P	O12-C2-C3	2.52	113.70	108.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	I6P	1	0
2	B	500	I6P	1	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	417/451 (92%)	-0.02	14 (3%) 49 47	11, 22, 38, 53	0
1	B	426/451 (94%)	0.10	17 (3%) 42 41	11, 21, 40, 63	0
All	All	843/902 (93%)	0.04	31 (3%) 45 44	11, 22, 39, 63	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	343	LEU	5.9
1	B	336	GLY	5.8
1	A	383	SER	5.5
1	B	50	ALA	4.9
1	B	436	ALA	4.8
1	B	280	ASP	4.3
1	B	48	ASP	4.1
1	A	342	GLU	4.0
1	B	334	LYS	3.5
1	A	3	MET	3.4
1	A	73	ASN	3.3
1	B	435	LYS	3.2
1	B	57	VAL	3.1
1	A	335	GLU	3.1
1	B	438	ASN	3.1
1	B	53	ASN	2.8
1	A	5	LEU	2.7
1	B	52	LYS	2.6
1	A	158	SER	2.5
1	A	75	LEU	2.5
1	A	98	GLY	2.5
1	B	30	SER	2.3
1	B	340	GLU	2.3
1	A	45	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	381	TRP	2.2
1	A	4	ILE	2.2
1	B	279	GLU	2.2
1	B	45	ARG	2.1
1	B	183	GLU	2.0
1	B	344	SER	2.0
1	A	303	ARG	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
5	MG	B	1031	1/1	0.87	0.11	0.10	43,43,43,43	0
2	I6P	B	500	36/36	0.97	0.12	-0.25	18,21,33,35	0
2	I6P	A	500	36/36	0.98	0.12	-0.28	16,20,27,30	0
4	ZN	A	700	1/1	0.98	0.12	-0.48	33,33,33,33	0
3	ADP	B	600	27/27	0.98	0.10	-0.77	16,17,22,23	0
3	ADP	A	600	27/27	0.98	0.10	-1.00	14,21,27,27	0
5	MG	A	1128	1/1	0.87	0.10	-1.14	44,44,44,44	0
5	MG	B	1030	1/1	0.89	0.07	-	23,23,23,23	0
5	MG	A	1129	1/1	0.96	0.06	-	27,27,27,27	0
4	ZN	B	700	1/1	0.98	0.07	-	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.