



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 11:22 AM EDT

PDB ID : 3JU5  
Title : Crystal Structure of Dimeric Arginine Kinase at 1.75-Å Resolution  
Authors : Wu, X.; Ye, S.; Guo, S.; Yan, W.; Bartlam, M.; Rao, Z.  
Deposited on : 2009-09-14  
Resolution : 1.75 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

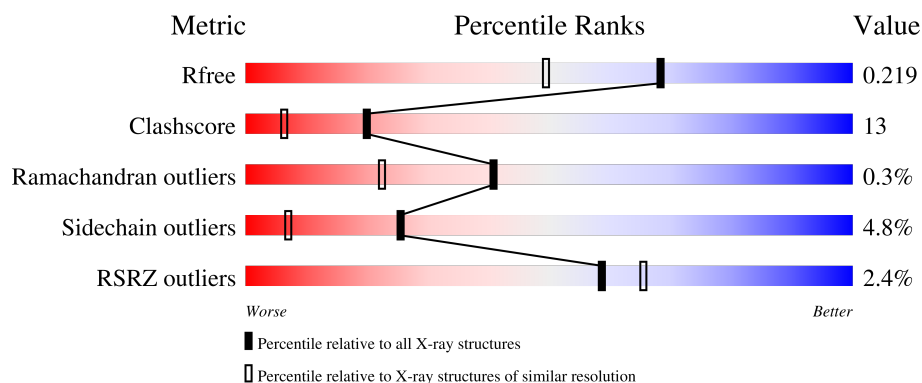
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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))
$R_{free}$	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	370	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>...</div> </div> </div>
1	B	370	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>...</div> </div> </div>
1	C	370	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>5%</div> <div>..</div> </div> </div>
1	D	370	<div> <div></div> <div> <div></div> <div>81%</div> <div>15%</div> <div>..</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13384 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 Arginine kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	Se	0	4	0
			2914	1829	513	551	5	16			
1	B	365	Total	C	N	O	S	Se	0	6	0
			2936	1843	516	555	6	16			
1	C	367	Total	C	N	O	S	Se	0	1	0
			2927	1833	517	558	5	14			
1	D	360	Total	C	N	O	S	Se	0	4	0
			2894	1817	510	545	6	16			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

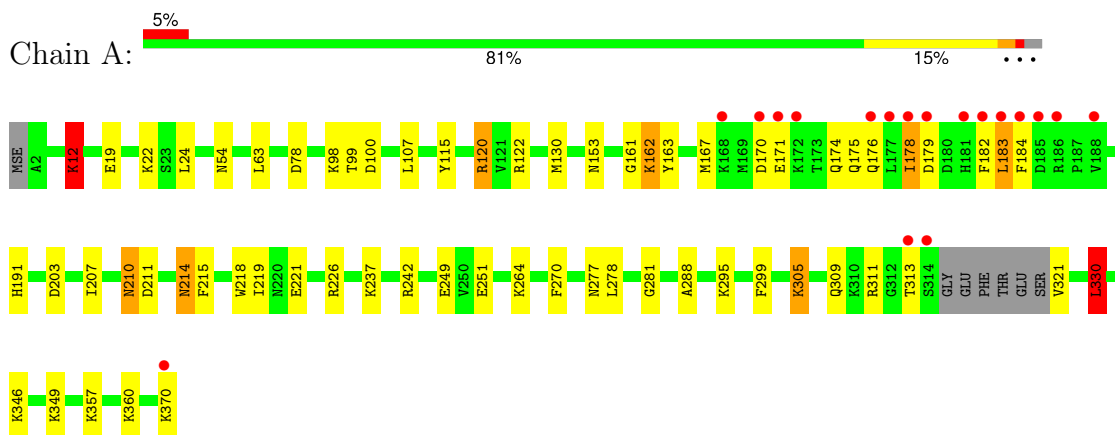
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	413	Total	O	0	0
			413	413		
3	B	496	Total	O	0	0
			496	496		
3	C	416	Total	O	0	0
			416	416		
3	D	386	Total	O	0	0
			386	386		

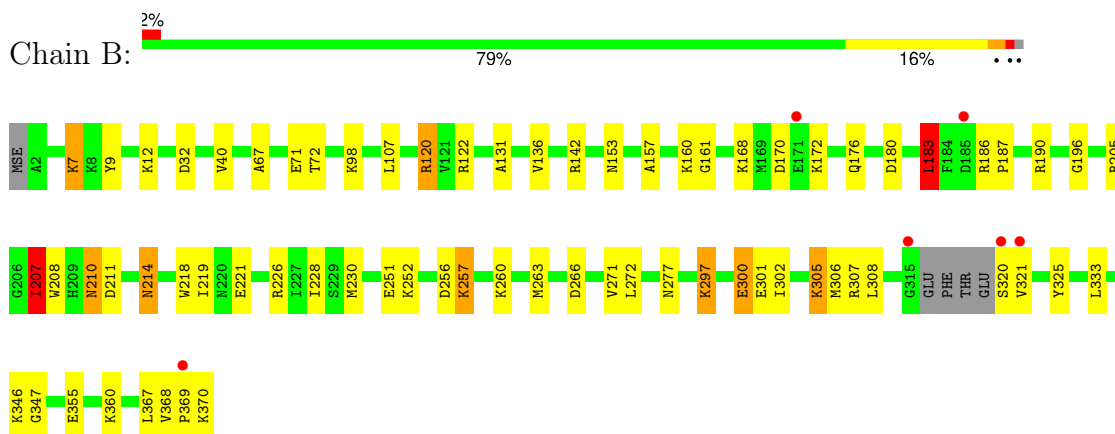
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

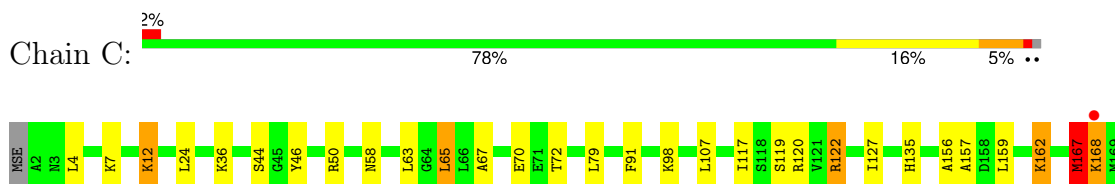
#### • Molecule 1: Arginine kinase

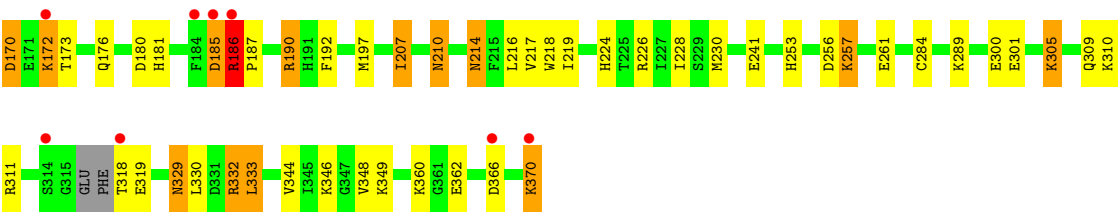


#### • Molecule 1: Arginine kinase

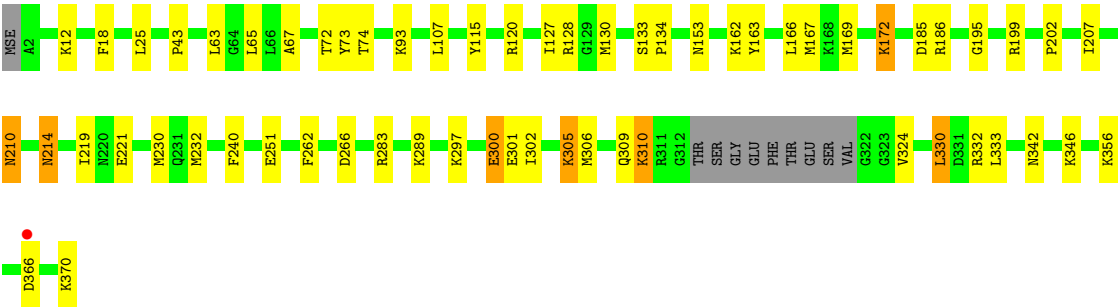
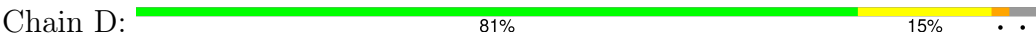


#### • Molecule 1: Arginine kinase





● Molecule 1: Arginine kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.88Å 59.87Å 139.87Å 90.00° 92.72° 90.00°	Depositor
Resolution (Å)	75.34 – 1.75 75.34 – 1.75	Depositor EDS
% Data completeness (in resolution range)	95.9 (75.34-1.75) 95.9 (75.34-1.75)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.75 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.170 , 0.227 0.164 , 0.219	Depositor DCC
$R_{free}$ test set	7021 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.1	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 50.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13384	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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: MG

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	1.05	2/2966 (0.1%)	0.99	7/3958 (0.2%)
1	B	1.13	5/2991 (0.2%)	1.06	8/3992 (0.2%)
1	C	1.06	3/2970 (0.1%)	1.01	4/3965 (0.1%)
1	D	1.04	3/2946 (0.1%)	0.98	3/3930 (0.1%)
All	All	1.07	13/11873 (0.1%)	1.01	22/15845 (0.1%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	71	GLU	CB-CG	7.25	1.66	1.52
1	C	46	TYR	CD2-CE2	6.40	1.49	1.39
1	B	355	GLU	CD-OE1	-6.03	1.19	1.25
1	C	119	SER	CB-OG	5.85	1.49	1.42
1	D	73	TYR	CD1-CE1	5.58	1.47	1.39
1	B	40	VAL	CB-CG2	5.55	1.64	1.52
1	A	12	LYS	CE-NZ	5.45	1.62	1.49
1	D	240	PHE	CE1-CZ	5.40	1.47	1.37
1	B	325	TYR	CD2-CE2	5.31	1.47	1.39
1	B	120	ARG	CG-CD	5.28	1.65	1.51
1	D	18	PHE	CD2-CE2	5.08	1.49	1.39
1	C	70	GLU	CD-OE1	-5.01	1.20	1.25
1	A	12	LYS	CD-CE	5.00	1.63	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	207[A]	ILE	CG1-CB-CG2	-8.15	93.47	111.40
1	B	207[B]	ILE	CG1-CB-CG2	-8.15	93.47	111.40
1	A	242	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	D	199	ARG	NE-CZ-NH1	6.57	123.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	183	LEU	CA-CB-CG	6.30	129.78	115.30
1	A	278	LEU	CB-CG-CD2	-6.25	100.38	111.00
1	C	122	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	D	128	ARG	CG-CD-NE	-5.84	99.54	111.80
1	C	167	MSE	CA-CB-CG	5.83	123.22	113.30
1	C	65	LEU	CB-CA-C	-5.80	99.18	110.20
1	B	32	ASP	CB-CG-OD1	5.74	123.47	118.30
1	A	330	LEU	CB-CG-CD1	5.70	120.69	111.00
1	A	299	PHE	CB-CG-CD2	-5.62	116.86	120.80
1	C	332	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	D	332	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	205	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	A	242	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	78	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	B	211	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	211	ASP	CB-CG-OD1	5.09	122.88	118.30
1	B	180	ASP	CB-CG-OD1	-5.04	113.77	118.30
1	B	142	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	2914	0	2907	77	1
1	B	2936	0	2933	76	0
1	C	2927	0	2906	100	0
1	D	2894	0	2887	47	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	413	0	0	19	2
3	B	496	0	0	27	1
3	C	416	0	0	19	1
3	D	386	0	0	22	1
All	All	13384	0	11633	294	3



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 (294) 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:D:366:ASP:HB2	3:D:1414:HOH:O	1.23	1.27
1:A:249:GLU:HG3	3:A:997:HOH:O	1.43	1.18
1:C:309:GLN:NE2	1:C:311:ARG:NE	1.98	1.12
1:C:305:LYS:HE2	3:C:746:HOH:O	1.50	1.10
1:A:19:GLU:OE2	1:B:168:LYS:HE3	1.52	1.09
1:B:252:LYS:HE3	3:B:570:HOH:O	1.53	1.07
1:A:346:LYS:HE3	1:A:346:LYS:HA	1.41	1.02
1:C:122:ARG:HG3	1:C:228:ILE:HD13	1.41	0.99
1:A:167[B]:MSE:HE1	3:A:484:HOH:O	1.62	0.98
1:C:122:ARG:HG3	1:C:228:ILE:CD1	1.94	0.98
1:B:168:LYS:HE2	3:B:1937:HOH:O	1.63	0.97
1:B:307:ARG:CZ	3:B:1060:HOH:O	2.15	0.95
1:A:98:LYS:HD3	3:A:492:HOH:O	1.66	0.94
1:D:301:GLU:HG3	3:D:628:HOH:O	1.65	0.94
1:C:167:MSE:HG3	3:C:900:HOH:O	1.67	0.93
1:B:251:GLU:HG2	3:B:1082:HOH:O	1.70	0.92
1:C:172:LYS:HB2	1:C:172:LYS:NZ	1.86	0.91
1:C:127:ILE:H	1:C:224:HIS:HD2	1.15	0.91
1:C:168:LYS:HG2	1:C:168:LYS:O	1.70	0.89
1:A:167[B]:MSE:CE	3:A:484:HOH:O	2.17	0.88
1:B:256:ASP:OD1	1:B:257:LYS:NZ	2.06	0.88
1:D:186:ARG:HB3	3:D:1844:HOH:O	1.71	0.88
1:C:98:LYS:HD3	3:C:935:HOH:O	1.75	0.86
1:A:210:ASN:HD21	1:A:214:ASN:H	1.24	0.86
1:C:370:LYS:HZ1	1:C:370:LYS:HA	1.39	0.85
1:C:172:LYS:HB2	1:C:172:LYS:HZ3	1.39	0.85
1:B:210:ASN:HD21	1:B:214:ASN:H	1.24	0.84
1:C:309:GLN:HE22	1:C:311:ARG:NE	1.67	0.84
1:B:157:ALA:HB3	3:B:1912:HOH:O	1.76	0.84
1:B:157:ALA:CB	3:B:1912:HOH:O	2.27	0.82
1:A:346:LYS:HE3	1:A:346:LYS:CA	2.07	0.82
1:B:297:LYS:O	1:B:297:LYS:HD3	1.78	0.82
1:C:309:GLN:NE2	1:C:311:ARG:HE	1.79	0.81
1:C:122:ARG:CG	1:C:228:ILE:HD13	2.11	0.80
1:C:370:LYS:HA	1:C:370:LYS:NZ	1.95	0.80
1:A:98:LYS:CD	3:A:492:HOH:O	2.25	0.80
1:A:174:GLN:O	1:A:178:ILE:HG13	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:LYS:NZ	3:B:921:HOH:O	2.04	0.79
1:C:50:ARG:HH22	1:C:135:HIS:HD2	1.31	0.79
1:C:318:THR:HG22	1:C:319:GLU:N	1.98	0.78
1:C:122:ARG:HD3	3:C:1021:HOH:O	1.82	0.78
1:D:153:ASN:OD1	3:D:1170:HOH:O	2.02	0.78
1:D:93:LYS:HE3	3:D:1294:HOH:O	1.83	0.78
1:C:319:GLU:N	3:C:1763:HOH:O	2.17	0.77
1:C:58:ASN:HD22	1:C:190:ARG:HH11	1.30	0.76
1:A:309:GLN:HB2	1:A:330:LEU:HD13	1.68	0.74
1:D:186:ARG:CB	3:D:1844:HOH:O	2.31	0.73
1:C:120:ARG:CZ	1:C:120:ARG:HB2	2.17	0.72
1:A:153:ASN:OD1	3:A:531:HOH:O	2.07	0.72
1:C:210:ASN:HD21	1:C:214:ASN:H	1.37	0.72
1:B:186:ARG:HG3	1:B:186:ARG:HH11	1.54	0.72
1:B:153:ASN:OD1	3:B:516:HOH:O	2.08	0.72
1:A:184:PHE:HD1	1:A:218:TRP:CD1	2.08	0.71
1:C:284:CYS:H	1:C:329:ASN:HD21	1.37	0.71
1:B:190:ARG:HD2	3:B:3046:HOH:O	1.91	0.71
1:C:305:LYS:CE	3:C:746:HOH:O	2.22	0.71
1:B:120:ARG:HD2	3:B:1012:HOH:O	1.90	0.71
1:C:301:GLU:O	1:C:305:LYS:HD2	1.90	0.71
1:C:309:GLN:NE2	1:C:311:ARG:CD	2.53	0.71
1:C:309:GLN:HE22	1:C:311:ARG:CZ	2.04	0.71
1:D:301:GLU:O	1:D:305:LYS:HD2	1.90	0.71
1:B:183:LEU:HD23	1:B:207[B]:ILE:CD1	2.21	0.70
1:D:300:GLU:HB2	3:D:1252:HOH:O	1.91	0.70
1:C:329:ASN:H	1:C:329:ASN:HD22	1.40	0.69
1:D:167[A]:MSE:HG2	1:D:202:PRO:HG2	1.75	0.69
1:A:218:TRP:HE3	1:A:226:ARG:HD2	1.55	0.69
1:C:284:CYS:H	1:C:329:ASN:ND2	1.90	0.69
1:D:162:LYS:CE	3:D:1350:HOH:O	2.39	0.69
1:A:313:THR:OG1	1:A:321:VAL:HG12	1.93	0.69
1:A:251:GLU:OE2	3:A:464:HOH:O	2.12	0.68
1:C:162:LYS:HG2	3:C:379:HOH:O	1.92	0.68
1:D:162:LYS:HE2	3:D:1350:HOH:O	1.93	0.67
1:A:184:PHE:O	3:A:866:HOH:O	2.11	0.67
1:B:122:ARG:HG3	1:B:228:ILE:HG12	1.77	0.66
1:B:321:VAL:HG13	1:B:321:VAL:O	1.95	0.66
1:D:167[B]:MSE:HG2	1:D:202:PRO:HG2	1.78	0.65
1:C:257:LYS:N	1:C:257:LYS:HD2	2.09	0.65
1:A:19:GLU:OE2	1:B:168:LYS:CE	2.37	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:GLN:HE21	1:C:311:ARG:HD2	1.62	0.65
1:C:122:ARG:HG3	1:C:228:ILE:HD11	1.79	0.65
1:B:160:LYS:HE2	3:B:1073:HOH:O	1.97	0.64
1:D:172:LYS:HD2	3:D:464:HOH:O	1.97	0.64
1:A:176:GLN:O	1:A:179:ASP:HB2	1.96	0.64
1:A:98:LYS:HE2	1:A:99:THR:O	1.97	0.64
1:D:127:ILE:HB	1:D:130[B]:MSE:HG3	1.79	0.64
1:C:127:ILE:H	1:C:224:HIS:CD2	2.07	0.64
1:B:170:ASP:OD1	1:B:170:ASP:O	2.16	0.64
1:D:172:LYS:CD	3:D:464:HOH:O	2.46	0.63
1:B:183:LEU:HD23	1:B:207[B]:ILE:HD13	1.79	0.63
1:B:12:LYS:NZ	1:B:12:LYS:HB3	2.14	0.63
1:C:122:ARG:CG	1:C:228:ILE:CD1	2.72	0.63
1:A:357:LYS:CE	3:A:1237:HOH:O	2.46	0.63
1:A:167[A]:MSE:HE2	1:A:203:ASP:CB	2.28	0.62
1:A:170:ASP:OD1	1:A:171:GLU:N	2.32	0.62
1:C:370:LYS:NZ	1:C:370:LYS:CA	2.63	0.62
1:A:309:GLN:OE1	1:A:311:ARG:NH2	2.33	0.61
1:B:170:ASP:OD1	1:B:170:ASP:C	2.37	0.61
1:C:309:GLN:HE21	1:C:311:ARG:CD	2.11	0.61
1:C:65:LEU:HD21	1:C:79:LEU:HD21	1.82	0.61
1:A:218:TRP:CE3	1:A:226:ARG:HD2	2.35	0.61
1:A:167[A]:MSE:HE2	1:A:203:ASP:CA	2.30	0.60
1:D:166:LEU:CD2	1:D:169:MSE:HE1	2.32	0.60
1:D:166:LEU:HD23	1:D:169:MSE:HE1	1.83	0.60
1:B:307:ARG:NH1	3:B:1060:HOH:O	2.30	0.60
1:C:58:ASN:ND2	1:C:190:ARG:HH11	1.99	0.60
1:D:210:ASN:HD21	1:D:214:ASN:H	1.48	0.60
1:B:260:LYS:HE2	3:B:672:HOH:O	2.01	0.60
1:B:120:ARG:NH1	1:B:122:ARG:HD3	2.17	0.60
1:C:186:ARG:HA	3:C:444:HOH:O	2.02	0.60
1:C:241:GLU:CD	3:C:1093:HOH:O	2.39	0.60
1:C:122:ARG:CB	1:C:228:ILE:HD13	2.32	0.60
1:D:74:THR:HG23	3:D:808:HOH:O	2.01	0.60
1:A:305:LYS:HD3	1:A:370:LYS:OXT	2.02	0.59
1:B:98:LYS:HD2	3:B:1359:HOH:O	2.00	0.59
1:C:122:ARG:NH2	3:C:1321:HOH:O	2.36	0.59
1:C:170:ASP:HB3	1:C:173:THR:HB	1.83	0.58
1:C:98:LYS:NZ	3:C:935:HOH:O	2.27	0.58
1:C:172:LYS:NZ	1:C:172:LYS:CB	2.65	0.58
1:C:185:ASP:O	1:C:186:ARG:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:LYS:NZ	3:D:1350:HOH:O	2.15	0.58
1:C:360:LYS:HE3	3:C:1880:HOH:O	2.03	0.58
1:C:156:ALA:O	1:C:157:ALA:HB3	2.03	0.57
1:D:214:ASN:C	1:D:214:ASN:HD22	2.07	0.57
1:A:360:LYS:NZ	3:A:481:HOH:O	2.13	0.57
1:C:185:ASP:O	1:C:186:ARG:CG	2.52	0.57
1:B:107:LEU:HD11	1:B:346:LYS:HE3	1.86	0.57
1:B:183:LEU:CD2	1:B:207[B]:ILE:HD11	2.35	0.57
1:A:346:LYS:HA	1:A:346:LYS:CE	2.10	0.56
1:C:219:ILE:N	1:C:219:ILE:HD12	2.21	0.56
1:B:214:ASN:C	1:B:214:ASN:HD22	2.07	0.56
1:A:54:ASN:HD21	1:A:191:HIS:CD2	2.23	0.56
1:A:264:LYS:HD2	1:A:270:PHE:CE1	2.41	0.56
1:A:357:LYS:HE3	3:A:1237:HOH:O	2.05	0.56
1:B:186:ARG:HH11	1:B:186:ARG:CG	2.19	0.56
1:D:163:TYR:CE1	1:D:219:ILE:HD12	2.40	0.56
1:B:252:LYS:HE3	3:B:512:HOH:O	2.05	0.55
1:A:313:THR:HG21	1:A:321:VAL:CG1	2.35	0.55
1:B:7:LYS:HB2	1:B:7:LYS:NZ	2.22	0.55
1:A:122:ARG:HD2	3:A:1137:HOH:O	2.06	0.55
1:B:12:LYS:HB3	1:B:12:LYS:HZ3	1.70	0.55
1:C:318:THR:CG2	1:C:319:GLU:N	2.68	0.55
1:C:332:ARG:HD3	3:C:3038:HOH:O	2.06	0.55
1:D:115:TYR:CE2	1:D:356:LYS:HE3	2.42	0.55
1:B:120:ARG:HH12	1:B:122:ARG:HD3	1.71	0.54
1:A:167[A]:MSE:CE	1:A:203:ASP:OD1	2.56	0.54
1:C:180:ASP:O	1:C:181:HIS:HB2	2.08	0.54
1:D:289:LYS:HG2	1:D:324:VAL:HG22	1.90	0.54
1:A:107:LEU:HD13	1:A:346:LYS:HD2	1.89	0.54
1:C:301:GLU:HG3	1:C:305:LYS:NZ	2.22	0.54
1:A:178:ILE:HG12	1:A:183:LEU:HD23	1.89	0.54
1:A:107:LEU:HD13	1:A:346:LYS:CD	2.38	0.54
1:A:107:LEU:CD1	1:A:346:LYS:CD	2.85	0.53
1:B:207[B]:ILE:HG23	1:B:218:TRP:HD1	1.73	0.53
1:B:306[B]:MSE:HG3	1:B:308:LEU:HD12	1.90	0.53
1:C:117:ILE:HD11	1:C:289:LYS:HG3	1.91	0.53
1:C:170:ASP:HB3	1:C:173:THR:CB	2.38	0.53
1:C:309:GLN:HB2	1:C:330:LEU:HD13	1.89	0.53
1:C:12:LYS:H	1:C:12:LYS:HZ3	1.57	0.53
1:B:183:LEU:HD23	1:B:207[B]:ILE:HD11	1.89	0.53
1:B:302:ILE:HG22	1:B:306[A]:MSE:HE2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:ASN:O	1:D:346:LYS:HE3	2.09	0.53
1:C:261:GLU:HB2	3:C:1901:HOH:O	2.08	0.52
1:D:302:ILE:O	1:D:306[B]:MSE:HG2	2.08	0.52
1:D:232:MSE:HE3	3:D:779:HOH:O	2.09	0.52
1:C:214:ASN:C	1:C:214:ASN:HD22	2.13	0.52
1:D:185:ASP:HA	3:D:936:HOH:O	2.10	0.52
1:D:309:GLN:HB2	1:D:330:LEU:HD13	1.92	0.52
1:B:12:LYS:NZ	1:B:12:LYS:CB	2.72	0.52
1:A:12:LYS:HZ3	1:A:12:LYS:H	1.56	0.52
1:A:167[A]:MSE:HE2	1:A:203:ASP:HA	1.90	0.52
1:A:237:LYS:HE2	3:A:498:HOH:O	2.10	0.52
1:B:306[B]:MSE:HG3	1:B:308:LEU:CD1	2.39	0.52
1:C:187:PRO:O	3:C:2853:HOH:O	2.19	0.52
1:B:367:LEU:O	1:B:369:PRO:HD3	2.11	0.51
1:C:4:LEU:HD12	1:D:43:PRO:O	2.10	0.51
1:B:252:LYS:CE	3:B:512:HOH:O	2.57	0.51
1:C:168:LYS:O	1:C:168:LYS:CG	2.49	0.51
1:D:120:ARG:NE	3:D:455:HOH:O	2.43	0.51
1:A:54:ASN:HD21	1:A:191:HIS:HD2	1.59	0.51
1:D:266:ASP:OD1	3:D:1757:HOH:O	2.19	0.51
1:B:12:LYS:NZ	3:B:771:HOH:O	2.43	0.51
1:B:67:ALA:HA	1:B:72:THR:HG21	1.92	0.51
1:C:176:GLN:NE2	3:C:742:HOH:O	2.31	0.51
1:A:349:LYS:HE2	3:A:1038:HOH:O	2.11	0.51
1:C:360:LYS:HD2	1:C:362:GLU:OE2	2.10	0.50
1:D:309:GLN:HG2	1:D:310:LYS:N	2.26	0.50
1:A:162:LYS:HD2	3:A:1100:HOH:O	2.12	0.50
1:B:207[B]:ILE:HG22	1:B:208:TRP:N	2.27	0.50
1:A:214:ASN:HD22	1:A:214:ASN:C	2.14	0.50
1:A:24:LEU:HD12	1:A:63:LEU:HD12	1.94	0.49
1:A:130:MSE:HE1	1:B:9:TYR:OH	2.12	0.49
1:B:157:ALA:HB1	3:B:1912:HOH:O	2.04	0.49
1:C:366:ASP:CB	3:C:941:HOH:O	2.59	0.49
1:C:329:ASN:H	1:C:329:ASN:ND2	2.08	0.49
1:B:7:LYS:NZ	1:B:7:LYS:CB	2.76	0.49
1:B:183:LEU:CD2	1:B:207[B]:ILE:CD1	2.91	0.49
1:C:305:LYS:HE3	1:C:305:LYS:N	2.28	0.48
1:A:120:ARG:HB2	1:A:120:ARG:CZ	2.43	0.48
1:C:58:ASN:HD22	1:C:190:ARG:NH1	2.04	0.48
1:A:122:ARG:CD	3:A:1137:HOH:O	2.61	0.48
1:C:44:SER:O	1:C:135:HIS:HE1	1.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:PHE:CD2	1:C:333:LEU:HD13	2.49	0.48
1:C:185:ASP:O	1:C:186:ARG:CB	2.62	0.47
1:B:120:ARG:CD	3:B:1012:HOH:O	2.57	0.47
1:A:19:GLU:CD	1:B:168:LYS:HE3	2.30	0.47
1:A:167[A]:MSE:HE2	1:A:203:ASP:HB2	1.94	0.47
1:B:190:ARG:CD	3:B:3046:HOH:O	2.58	0.47
1:C:256:ASP:C	1:C:257:LYS:HD2	2.35	0.47
1:D:134:PRO:HB3	1:D:195:GLY:O	2.15	0.47
1:A:321:VAL:HG13	3:A:1311:HOH:O	2.15	0.46
1:C:370:LYS:CA	1:C:370:LYS:HZ2	2.27	0.46
1:B:307:ARG:NH1	3:B:416:HOH:O	2.44	0.46
1:B:301:GLU:O	1:B:305:LYS:HD3	2.15	0.46
1:B:308:LEU:HD11	1:B:347:GLY:HA3	1.98	0.46
1:C:253:HIS:CE1	1:C:257:LYS:HG2	2.51	0.46
1:B:302:ILE:CG2	1:B:306[A]:MSE:HE2	2.45	0.46
1:A:184:PHE:CD1	1:A:218:TRP:CD1	2.98	0.46
1:B:190:ARG:NH1	3:B:3046:HOH:O	2.48	0.46
1:B:207[A]:ILE:C	1:B:207[A]:ILE:HD13	2.36	0.46
1:C:176:GLN:OE1	1:C:176:GLN:HA	2.15	0.46
1:A:277:ASN:O	1:A:281:GLY:HA2	2.16	0.46
1:D:370:LYS:HE3	3:D:382:HOH:O	2.16	0.46
1:A:175:GLN:HE21	1:A:175:GLN:HA	1.81	0.46
1:A:182:PHE:O	1:A:218:TRP:NE1	2.40	0.46
1:C:346:LYS:HA	1:C:349:LYS:HE3	1.97	0.46
1:C:318:THR:HG22	1:C:319:GLU:CB	2.47	0.45
1:A:163:TYR:CE1	1:A:219:ILE:HD12	2.51	0.45
1:C:50:ARG:HH22	1:C:135:HIS:CD2	2.21	0.45
1:C:120:ARG:CZ	1:C:120:ARG:CB	2.82	0.45
1:D:93:LYS:CE	3:D:1294:HOH:O	2.54	0.45
1:A:107:LEU:CD1	1:A:346:LYS:HD3	2.46	0.45
1:C:309:GLN:NE2	1:C:311:ARG:HD2	2.25	0.44
1:B:252:LYS:CG	3:B:570:HOH:O	2.65	0.44
1:C:186:ARG:CA	3:C:444:HOH:O	2.64	0.44
1:D:370:LYS:HE3	1:D:370:LYS:HB2	1.78	0.44
1:A:210:ASN:HD21	1:A:214:ASN:N	2.04	0.44
1:C:122:ARG:HB2	1:C:228:ILE:HD13	1.99	0.44
1:B:186:ARG:CG	1:B:186:ARG:NH1	2.78	0.44
1:A:305:LYS:CD	1:A:370:LYS:OXT	2.66	0.43
1:C:366:ASP:HB2	3:C:941:HOH:O	2.17	0.43
1:D:107:LEU:CD1	1:D:346:LYS:HG3	2.48	0.43
1:B:266:ASP:OD2	1:C:36:LYS:NZ	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:LEU:CD1	1:C:346:LYS:HG3	2.49	0.43
1:B:263:MSE:HG2	1:B:271:VAL:HB	1.99	0.43
1:C:349:LYS:HE3	1:C:349:LYS:HB2	1.73	0.43
1:A:24:LEU:HD12	1:A:63:LEU:CD1	2.49	0.43
1:A:175:GLN:HA	1:A:175:GLN:NE2	2.33	0.43
1:C:346:LYS:HB2	1:C:346:LYS:HE2	1.59	0.43
1:B:219:ILE:HD13	1:B:219:ILE:HG21	1.61	0.43
1:C:216:LEU:HD21	1:C:218:TRP:CE2	2.53	0.43
1:A:115:TYR:O	1:A:288:ALA:HA	2.19	0.42
1:A:167[A]:MSE:HE3	1:A:203:ASP:OD1	2.18	0.42
1:C:346:LYS:HA	1:C:349:LYS:CE	2.49	0.42
1:D:133:SER:HB3	3:D:786:HOH:O	2.19	0.42
1:C:50:ARG:NH2	1:C:135:HIS:HD2	2.09	0.42
1:D:166:LEU:HA	1:D:169:MSE:HE3	2.01	0.42
1:D:283:ARG:NH2	3:D:1002:HOH:O	2.52	0.42
1:C:24:LEU:HA	1:C:24:LEU:HD23	1.81	0.42
1:D:67:ALA:HA	1:D:72:THR:HG21	2.00	0.42
1:A:357:LYS:NZ	3:A:1237:HOH:O	2.39	0.42
1:D:342:ASN:C	1:D:346:LYS:HE3	2.40	0.42
1:B:218:TRP:CE3	1:B:226:ARG:HD2	2.55	0.42
1:A:161:GLY:HA3	1:A:210:ASN:HA	2.02	0.41
1:B:176:GLN:HG2	3:B:971:HOH:O	2.20	0.41
1:D:25:LEU:HD13	1:D:65:LEU:HD21	2.02	0.41
1:C:207:ILE:HD13	1:C:207:ILE:C	2.41	0.41
1:C:301:GLU:HG3	1:C:305:LYS:HZ3	1.84	0.41
1:A:313:THR:HG21	1:A:321:VAL:HG13	2.02	0.41
1:C:192:PHE:HA	1:C:197:MSE:HE3	2.01	0.41
1:D:251:GLU:HB2	1:D:262:PHE:CE2	2.55	0.41
1:B:131:ALA:HB3	1:B:136:VAL:HA	2.03	0.41
1:B:300:GLU:O	1:B:300:GLU:HG3	2.12	0.41
1:B:321:VAL:O	1:B:321:VAL:CG1	2.66	0.41
1:A:184:PHE:HD1	1:A:218:TRP:CG	2.36	0.41
1:A:178:ILE:HG12	1:A:183:LEU:CD2	2.51	0.41
1:A:346:LYS:HE3	3:A:388:HOH:O	2.21	0.41
1:C:67:ALA:HA	1:C:72:THR:HG21	2.03	0.41
1:A:98:LYS:HE2	1:A:100:ASP:HB2	2.02	0.41
1:B:161:GLY:HA3	1:B:210:ASN:HA	2.03	0.41
1:A:210:ASN:ND2	1:A:215:PHE:H	2.19	0.41
1:C:159:LEU:HA	1:C:159:LEU:HD23	1.77	0.41
1:C:217:VAL:HA	1:C:226:ARG:O	2.21	0.41
1:A:170:ASP:CG	1:A:171:GLU:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:LEU:HD22	1:B:277:ASN:HB3	2.02	0.41
1:D:306[B]:MSE:HE2	1:D:306[B]:MSE:HB3	1.89	0.41
1:A:98:LYS:CE	1:A:99:THR:O	2.68	0.40
1:A:63:LEU:HD12	1:A:63:LEU:HA	1.92	0.40
1:B:307:ARG:NH2	3:B:416:HOH:O	2.51	0.40
1:D:186:ARG:HB2	3:D:1844:HOH:O	2.11	0.40
1:B:196:GLY:HA2	3:B:1720:HOH:O	2.21	0.40
1:C:344:VAL:O	1:C:348:VAL:HG23	2.21	0.40
1:A:12:LYS:H	1:A:12:LYS:NZ	2.19	0.40
1:B:176:GLN:CG	3:B:971:HOH:O	2.68	0.40
1:B:368:VAL:O	1:B:369:PRO:C	2.56	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:LYS:NZ	3:A:1217:HOH:O[2_545]	2.17	0.03
3:A:3052:HOH:O	3:B:3062:HOH:O[2_555]	2.17	0.03
3:C:1760:HOH:O	3:D:1872:HOH:O[2_646]	2.17	0.03

## 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	363/370 (98%)	360 (99%)	2 (1%)	1 (0%)	41	22
1	B	367/370 (99%)	361 (98%)	4 (1%)	2 (0%)	29	12
1	C	364/370 (98%)	358 (98%)	5 (1%)	1 (0%)	41	22
1	D	360/370 (97%)	354 (98%)	5 (1%)	1 (0%)	41	22
All	All	1454/1480 (98%)	1433 (99%)	16 (1%)	5 (0%)	41	22

All (5) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	221	GLU
1	B	221	GLU
1	C	186	ARG
1	D	221	GLU
1	B	187	PRO

### 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	323/311 (104%)	312 (97%)	11 (3%)	37	14
1	B	326/311 (105%)	310 (95%)	16 (5%)	25	7
1	C	323/311 (104%)	301 (93%)	22 (7%)	16	3
1	D	320/311 (103%)	307 (96%)	13 (4%)	30	10
All	All	1292/1244 (104%)	1230 (95%)	62 (5%)	25	7

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	22	LYS
1	A	120	ARG
1	A	162	LYS
1	A	178	ILE
1	A	183	LEU
1	A	207	ILE
1	A	210	ASN
1	A	214	ASN
1	A	305	LYS
1	A	330	LEU
1	B	7	LYS
1	B	172	LYS
1	B	183	LEU
1	B	207[A]	ILE
1	B	207[B]	ILE
1	B	210	ASN

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Mol	Chain	Res	Type
1	B	214	ASN
1	B	230	MSE
1	B	257	LYS
1	B	297	LYS
1	B	300	GLU
1	B	305	LYS
1	B	320	SER
1	B	333	LEU
1	B	360	LYS
1	B	370	LYS
1	C	7	LYS
1	C	12	LYS
1	C	63	LEU
1	C	162	LYS
1	C	167	MSE
1	C	168	LYS
1	C	170	ASP
1	C	172	LYS
1	C	185	ASP
1	C	186	ARG
1	C	190	ARG
1	C	207	ILE
1	C	210	ASN
1	C	214	ASN
1	C	230	MSE
1	C	257	LYS
1	C	300	GLU
1	C	305	LYS
1	C	310	LYS
1	C	329	ASN
1	C	333	LEU
1	C	370	LYS
1	D	12	LYS
1	D	63	LEU
1	D	172	LYS
1	D	207	ILE
1	D	210	ASN
1	D	214	ASN
1	D	230	MSE
1	D	297	LYS
1	D	300	GLU
1	D	305	LYS

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Mol	Chain	Res	Type
1	D	310	LYS
1	D	330	LEU
1	D	333	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	6	GLN
1	A	153	ASN
1	A	174	GLN
1	A	175	GLN
1	A	191	HIS
1	A	210	ASN
1	A	214	ASN
1	A	277	ASN
1	B	153	ASN
1	B	210	ASN
1	B	214	ASN
1	B	277	ASN
1	C	58	ASN
1	C	135	HIS
1	C	210	ASN
1	C	214	ASN
1	C	224	HIS
1	C	277	ASN
1	C	309	GLN
1	C	329	ASN
1	D	5	ASN
1	D	6	GLN
1	D	54	ASN
1	D	175	GLN
1	D	210	ASN
1	D	214	ASN
1	D	277	ASN

### 5.3.3 RNA ⓘ

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	350/370 (94%)	-0.24	18 (5%) 28 34	8, 14, 42, 61	0
1	B	352/370 (95%)	-0.36	6 (1%) 70 77	7, 13, 32, 44	0
1	C	354/370 (95%)	-0.29	9 (2%) 57 63	7, 16, 34, 46	0
1	D	347/370 (93%)	-0.38	1 (0%) 94 95	7, 16, 33, 38	0
All	All	1403/1480 (94%)	-0.32	34 (2%) 59 65	7, 15, 33, 61	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	318	THR	9.9
1	A	184	PHE	8.2
1	A	172	LYS	6.2
1	A	170	ASP	5.7
1	A	314	SER	5.2
1	A	178	ILE	4.2
1	B	369	PRO	4.1
1	A	171	GLU	3.9
1	A	181	HIS	3.7
1	C	168	LYS	3.4
1	A	186	ARG	3.3
1	B	315	GLY	3.3
1	C	184	PHE	3.1
1	C	370	LYS	3.0
1	C	185	ASP	2.9
1	A	370	LYS	2.9
1	A	183	LEU	2.8
1	C	314	SER	2.8
1	A	182	PHE	2.8
1	C	172	LYS	2.7
1	B	185	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	320	SER	2.7
1	B	171	GLU	2.6
1	A	188	VAL	2.6
1	A	179	ASP	2.6
1	A	176	GLN	2.6
1	A	168	LYS	2.4
1	B	321	VAL	2.1
1	A	313	THR	2.1
1	C	186	ARG	2.1
1	A	177	LEU	2.1
1	C	366	ASP	2.1
1	A	185	ASP	2.1
1	D	366	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 monosaccharides 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	C	371	1/1	0.99	0.07	12,12,12,12	0
2	MG	A	371	1/1	1.00	0.08	13,13,13,13	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.