



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:55 PM GMT

PDB ID : 4DU5  
Title : Crystal structure of PfkB protein from Polaromonas sp. JS666  
Authors : Agarwal, R.; Chamala, S.; Evans, B.; Foti, R.; Gizzi, A.; Hellerich, B.; Kar, A.; Lafleur, J.; Siedel, R.; Villigas, G.; Zencheck, W.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYSGRG)  
Deposited on : 2012-02-21  
Resolution : 2.70 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

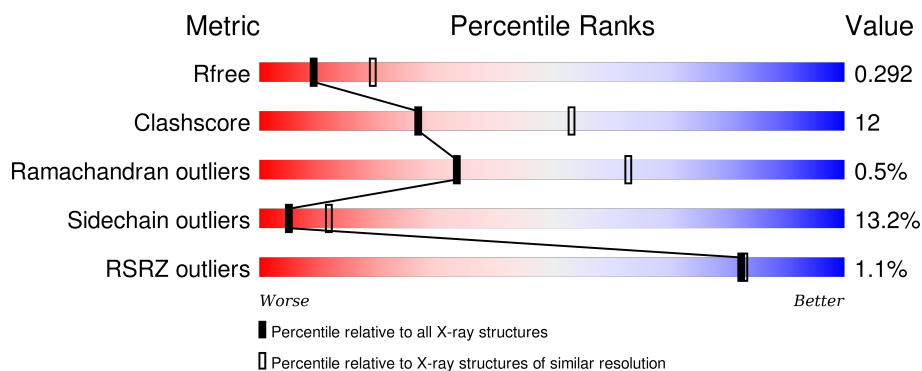
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	336	<div> <div>%</div> <div> <div></div> <div>63%</div> <div>20%</div> <div>•</div> <div>13%</div> </div> </div>
1	B	336	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>17%</div> <div>•</div> <div>12%</div> </div> </div>
1	C	336	<div> <div>%</div> <div> <div></div> <div>65%</div> <div>17%</div> <div>5%</div> <div>13%</div> </div> </div>
1	D	336	<div> <div>%</div> <div> <div></div> <div>64%</div> <div>20%</div> <div>•</div> <div>13%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8654 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 PfkB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	Se	0	0	0
			2128	1344	380	393	2	9			
1	B	295	Total	C	N	O	S	Se	0	0	0
			2135	1348	381	395	2	9			
1	C	294	Total	C	N	O	S	Se	0	0	0
			2133	1348	380	394	2	9			
1	D	294	Total	C	N	O	S	Se	0	0	0
			2130	1347	380	392	2	9			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	EXPRESSION TAG	UNP Q12CR9
A	2	HIS	-	EXPRESSION TAG	UNP Q12CR9
A	3	HIS	-	EXPRESSION TAG	UNP Q12CR9
A	4	HIS	-	EXPRESSION TAG	UNP Q12CR9
A	5	HIS	-	EXPRESSION TAG	UNP Q12CR9
A	6	HIS	-	EXPRESSION TAG	UNP Q12CR9
A	7	HIS	-	EXPRESSION TAG	UNP Q12CR9
A	8	SER	-	EXPRESSION TAG	UNP Q12CR9
A	9	SER	-	EXPRESSION TAG	UNP Q12CR9
A	10	GLY	-	EXPRESSION TAG	UNP Q12CR9
A	11	VAL	-	EXPRESSION TAG	UNP Q12CR9
A	12	ASP	-	EXPRESSION TAG	UNP Q12CR9
A	13	LEU	-	EXPRESSION TAG	UNP Q12CR9
A	14	GLY	-	EXPRESSION TAG	UNP Q12CR9
A	15	THR	-	EXPRESSION TAG	UNP Q12CR9
A	16	GLU	-	EXPRESSION TAG	UNP Q12CR9
A	17	ASN	-	EXPRESSION TAG	UNP Q12CR9
A	18	LEU	-	EXPRESSION TAG	UNP Q12CR9
A	19	TYR	-	EXPRESSION TAG	UNP Q12CR9
A	20	PHE	-	EXPRESSION TAG	UNP Q12CR9
A	21	GLN	-	EXPRESSION TAG	UNP Q12CR9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	22	SER	-	EXPRESSION TAG	UNP Q12CR9
B	1	MSE	-	EXPRESSION TAG	UNP Q12CR9
B	2	HIS	-	EXPRESSION TAG	UNP Q12CR9
B	3	HIS	-	EXPRESSION TAG	UNP Q12CR9
B	4	HIS	-	EXPRESSION TAG	UNP Q12CR9
B	5	HIS	-	EXPRESSION TAG	UNP Q12CR9
B	6	HIS	-	EXPRESSION TAG	UNP Q12CR9
B	7	HIS	-	EXPRESSION TAG	UNP Q12CR9
B	8	SER	-	EXPRESSION TAG	UNP Q12CR9
B	9	SER	-	EXPRESSION TAG	UNP Q12CR9
B	10	GLY	-	EXPRESSION TAG	UNP Q12CR9
B	11	VAL	-	EXPRESSION TAG	UNP Q12CR9
B	12	ASP	-	EXPRESSION TAG	UNP Q12CR9
B	13	LEU	-	EXPRESSION TAG	UNP Q12CR9
B	14	GLY	-	EXPRESSION TAG	UNP Q12CR9
B	15	THR	-	EXPRESSION TAG	UNP Q12CR9
B	16	GLU	-	EXPRESSION TAG	UNP Q12CR9
B	17	ASN	-	EXPRESSION TAG	UNP Q12CR9
B	18	LEU	-	EXPRESSION TAG	UNP Q12CR9
B	19	TYR	-	EXPRESSION TAG	UNP Q12CR9
B	20	PHE	-	EXPRESSION TAG	UNP Q12CR9
B	21	GLN	-	EXPRESSION TAG	UNP Q12CR9
B	22	SER	-	EXPRESSION TAG	UNP Q12CR9
C	1	MSE	-	EXPRESSION TAG	UNP Q12CR9
C	2	HIS	-	EXPRESSION TAG	UNP Q12CR9
C	3	HIS	-	EXPRESSION TAG	UNP Q12CR9
C	4	HIS	-	EXPRESSION TAG	UNP Q12CR9
C	5	HIS	-	EXPRESSION TAG	UNP Q12CR9
C	6	HIS	-	EXPRESSION TAG	UNP Q12CR9
C	7	HIS	-	EXPRESSION TAG	UNP Q12CR9
C	8	SER	-	EXPRESSION TAG	UNP Q12CR9
C	9	SER	-	EXPRESSION TAG	UNP Q12CR9
C	10	GLY	-	EXPRESSION TAG	UNP Q12CR9
C	11	VAL	-	EXPRESSION TAG	UNP Q12CR9
C	12	ASP	-	EXPRESSION TAG	UNP Q12CR9
C	13	LEU	-	EXPRESSION TAG	UNP Q12CR9
C	14	GLY	-	EXPRESSION TAG	UNP Q12CR9
C	15	THR	-	EXPRESSION TAG	UNP Q12CR9
C	16	GLU	-	EXPRESSION TAG	UNP Q12CR9
C	17	ASN	-	EXPRESSION TAG	UNP Q12CR9
C	18	LEU	-	EXPRESSION TAG	UNP Q12CR9
C	19	TYR	-	EXPRESSION TAG	UNP Q12CR9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	20	PHE	-	EXPRESSION TAG	UNP Q12CR9
C	21	GLN	-	EXPRESSION TAG	UNP Q12CR9
C	22	SER	-	EXPRESSION TAG	UNP Q12CR9
D	1	MSE	-	EXPRESSION TAG	UNP Q12CR9
D	2	HIS	-	EXPRESSION TAG	UNP Q12CR9
D	3	HIS	-	EXPRESSION TAG	UNP Q12CR9
D	4	HIS	-	EXPRESSION TAG	UNP Q12CR9
D	5	HIS	-	EXPRESSION TAG	UNP Q12CR9
D	6	HIS	-	EXPRESSION TAG	UNP Q12CR9
D	7	HIS	-	EXPRESSION TAG	UNP Q12CR9
D	8	SER	-	EXPRESSION TAG	UNP Q12CR9
D	9	SER	-	EXPRESSION TAG	UNP Q12CR9
D	10	GLY	-	EXPRESSION TAG	UNP Q12CR9
D	11	VAL	-	EXPRESSION TAG	UNP Q12CR9
D	12	ASP	-	EXPRESSION TAG	UNP Q12CR9
D	13	LEU	-	EXPRESSION TAG	UNP Q12CR9
D	14	GLY	-	EXPRESSION TAG	UNP Q12CR9
D	15	THR	-	EXPRESSION TAG	UNP Q12CR9
D	16	GLU	-	EXPRESSION TAG	UNP Q12CR9
D	17	ASN	-	EXPRESSION TAG	UNP Q12CR9
D	18	LEU	-	EXPRESSION TAG	UNP Q12CR9
D	19	TYR	-	EXPRESSION TAG	UNP Q12CR9
D	20	PHE	-	EXPRESSION TAG	UNP Q12CR9
D	21	GLN	-	EXPRESSION TAG	UNP Q12CR9
D	22	SER	-	EXPRESSION TAG	UNP Q12CR9

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	34	Total O 34 34	0	0
3	B	21	Total O 21 21	0	0

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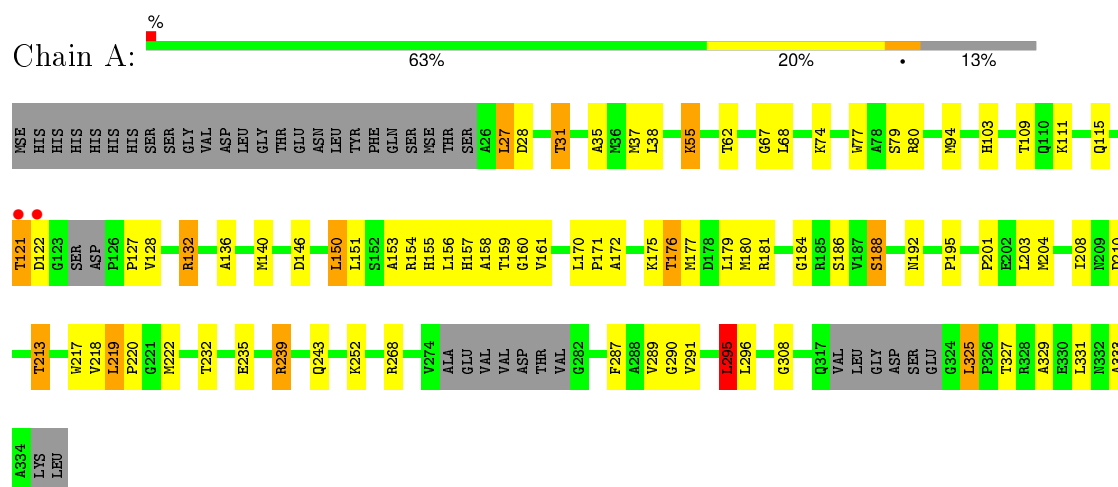
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	24	Total	O	0	0
			24	24		
3	D	47	Total	O	0	0
			47	47		

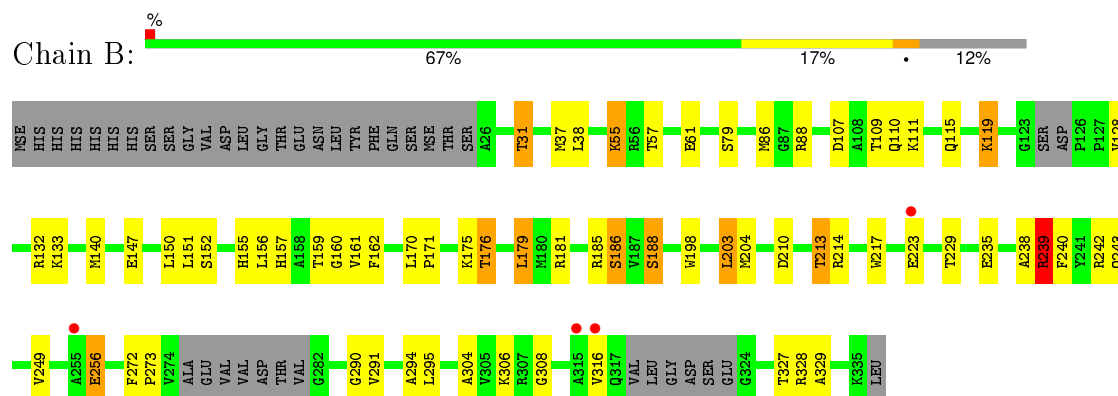
### 3 Residue-property plots

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.

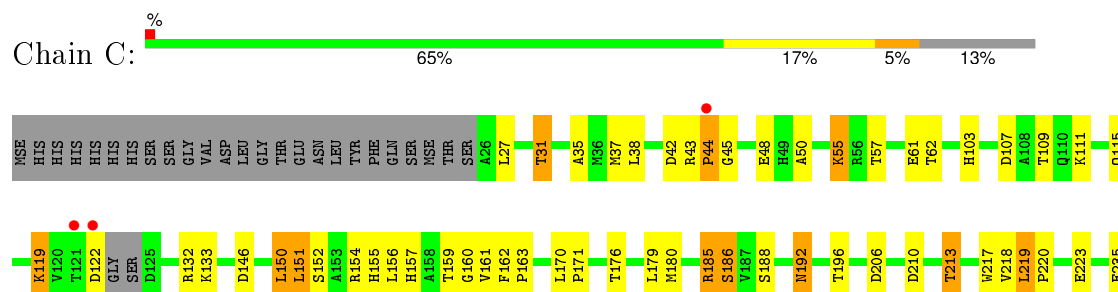
#### • Molecule 1: PfkB

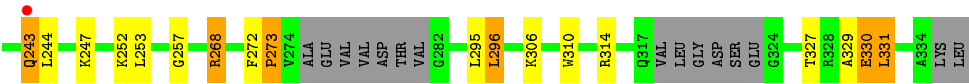


#### • Molecule 1: PfkB

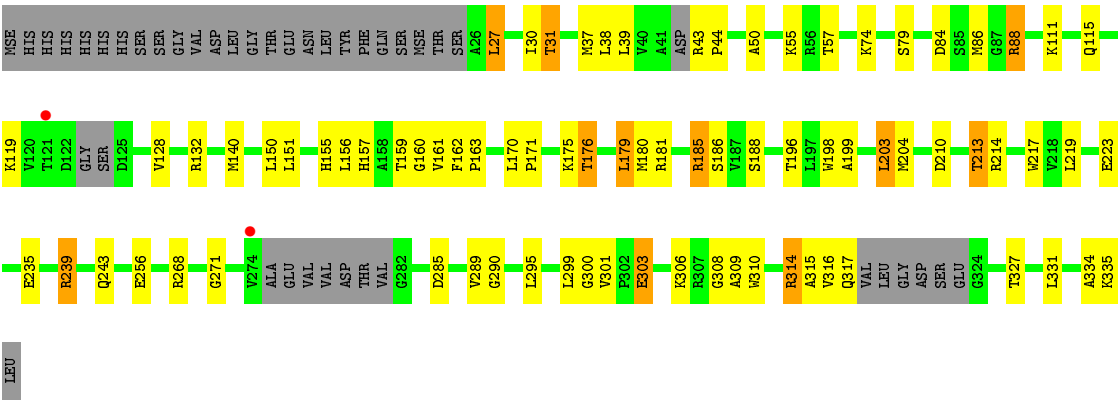


#### • Molecule 1: PfkB





• Molecule 1: PfkB





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.92Å 83.08Å 196.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.68 – 2.70 43.68 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (43.68-2.70) 98.9 (43.68-2.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.87 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.226 , 0.296 0.225 , 0.292	Depositor DCC
$R_{free}$ test set	1904 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.1	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 36.9	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	2 of 37682 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8654	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.36 % 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 6.5393e-05. 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, 0.375 respectively for untwinned datasets, and 0.333, 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:  
CL

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	0.72	0/2161	0.83	3/2915 (0.1%)
1	B	0.80	0/2168	0.82	1/2925 (0.0%)
1	C	0.78	1/2166 (0.0%)	0.87	3/2924 (0.1%)
1	D	0.76	0/2162	0.82	2/2917 (0.1%)
All	All	0.77	1/8657 (0.0%)	0.84	9/11681 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	44	PRO	N-CD	5.02	1.54	1.47

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	LEU	CA-CB-CG	5.80	128.64	115.30
1	D	301	VAL	C-N-CD	5.75	140.48	128.40
1	C	151	LEU	CA-CB-CG	5.70	128.40	115.30
1	C	45	GLY	C-N-CD	5.58	140.11	128.40
1	C	43	ARG	C-N-CD	5.52	139.99	128.40
1	A	122	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	132	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	D	27	LEU	CA-CB-CG	5.13	127.10	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	239	ARG	NE-CZ-NH1	5.09	122.84	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	THR	Peptide

## 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	2128	0	2082	52	0
1	B	2135	0	2089	50	0
1	C	2133	0	2092	49	0
1	D	2130	0	2089	55	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	34	0	0	0	0
3	B	21	0	0	0	0
3	C	24	0	0	0	0
3	D	47	0	0	5	0
All	All	8654	0	8352	202	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 12.

All (202) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance ( $\text{\AA}$ )	Clash overlap ( $\text{\AA}$ )
1:D:159:THR:HG22	1:D:161:VAL:H	1.15	1.10
1:C:155:HIS:ND1	1:C:186:SER:HB3	1.66	1.08
1:B:159:THR:HG22	1:B:161:VAL:H	1.17	1.07
1:A:159:THR:HG23	1:A:192:ASN:HD22	1.18	1.04
1:D:155:HIS:HE2	1:D:188:SER:HB2	1.20	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:HIS:ND1	1:B:186:SER:HB3	1.74	1.01
1:B:155:HIS:HE2	1:B:188:SER:HB2	1.28	0.99
1:D:155:HIS:ND1	1:D:186:SER:HB3	1.82	0.94
1:B:327:THR:HG22	1:B:329:ALA:H	1.30	0.94
1:C:42:ASP:O	1:C:119:LYS:HE2	1.69	0.93
1:C:38:LEU:HD13	1:C:115:GLN:HE21	1.34	0.92
1:D:155:HIS:NE2	1:D:188:SER:HB2	1.85	0.92
1:C:155:HIS:NE2	1:C:188:SER:HB2	1.87	0.90
1:C:210:ASP:O	1:C:213:THR:HB	1.74	0.87
1:A:159:THR:CG2	1:A:192:ASN:HD22	1.87	0.86
1:B:239:ARG:HH11	1:B:239:ARG:HG3	1.41	0.85
1:C:107:ASP:OD1	1:C:109:THR:HG22	1.76	0.85
1:D:303:GLU:HG3	3:D:435:HOH:O	1.76	0.84
1:C:272:PHE:HB3	1:C:273:PRO:HD3	1.61	0.83
1:C:155:HIS:HE2	1:C:188:SER:HB2	1.43	0.81
1:B:107:ASP:OD1	1:B:109:THR:HG22	1.81	0.81
1:A:235:GLU:O	1:A:239:ARG:HG2	1.81	0.79
1:B:198:TRP:CD1	1:B:204:MSE:HG2	2.17	0.79
1:C:38:LEU:HD13	1:C:115:GLN:HG3	1.65	0.79
1:B:210:ASP:O	1:B:213:THR:HB	1.83	0.78
1:D:159:THR:HG22	1:D:161:VAL:N	1.97	0.78
1:A:159:THR:HG22	1:A:160:GLY:N	1.98	0.77
1:B:155:HIS:NE2	1:B:188:SER:HB2	2.00	0.76
1:A:31:THR:HG22	1:A:157:HIS:O	1.86	0.75
1:D:210:ASP:O	1:D:213:THR:HB	1.87	0.74
1:C:180:MSE:HG3	1:C:185:ARG:HB3	1.70	0.74
1:A:150:LEU:HD22	1:A:180:MSE:SE	2.40	0.72
1:A:210:ASP:O	1:A:213:THR:HB	1.90	0.71
1:C:155:HIS:CE1	1:C:188:SER:HB2	2.25	0.71
1:C:159:THR:CG2	1:C:192:ASN:HD21	2.04	0.70
1:B:198:TRP:CG	1:B:204:MSE:HG2	2.26	0.70
1:A:27:LEU:O	1:A:153:ALA:HA	1.90	0.70
1:C:327:THR:HG22	1:C:329:ALA:H	1.56	0.70
1:D:38:LEU:HD13	1:D:115:GLN:HG3	1.75	0.69
1:A:159:THR:HG23	1:A:192:ASN:ND2	2.02	0.68
1:A:38:LEU:HD13	1:A:115:GLN:HG3	1.76	0.68
1:A:235:GLU:OE2	1:A:268:ARG:NH2	2.26	0.67
1:D:37:MSE:SE	1:D:55:LYS:HD3	2.45	0.67
1:C:150:LEU:HD22	1:C:180:MSE:SE	2.46	0.66
1:B:272:PHE:HB3	1:B:273:PRO:CD	2.26	0.66
1:C:180:MSE:HE3	1:C:185:ARG:HG2	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:LEU:HD13	1:C:115:GLN:NE2	2.09	0.65
1:B:88:ARG:HH11	1:C:48:GLU:HG2	1.62	0.64
1:A:158:ALA:HB1	1:A:177:MSE:HE2	1.78	0.64
1:B:155:HIS:HE2	1:B:188:SER:CB	2.08	0.64
1:B:327:THR:HG22	1:B:329:ALA:N	2.09	0.64
1:C:155:HIS:HE2	1:C:188:SER:CB	2.11	0.63
1:D:37:MSE:HE2	1:D:86:MSE:CE	2.29	0.63
1:A:290:GLY:HA3	1:A:308:GLY:HA2	1.81	0.62
1:C:159:THR:HG22	1:C:192:ASN:HD21	1.63	0.62
1:C:37:MSE:SE	1:C:55:LYS:HD3	2.50	0.61
1:A:159:THR:HG22	1:A:161:VAL:H	1.66	0.61
1:A:159:THR:CG2	1:A:160:GLY:N	2.64	0.61
1:A:158:ALA:CB	1:A:177:MSE:HE2	2.30	0.61
1:D:155:HIS:HE2	1:D:188:SER:CB	2.05	0.60
1:D:213:THR:HG22	1:D:214:ARG:HG3	1.82	0.60
1:A:37:MSE:SE	1:A:55:LYS:HD3	2.51	0.60
1:D:180:MSE:HG3	1:D:185:ARG:HB3	1.82	0.60
1:A:35:ALA:HB2	1:A:62:THR:HG21	1.83	0.60
1:C:38:LEU:CD1	1:C:115:GLN:HG3	2.31	0.60
1:A:181:ARG:O	1:A:184:GLY:N	2.26	0.60
1:C:35:ALA:HB2	1:C:62:THR:HG21	1.84	0.60
1:D:310:TRP:O	1:D:314:ARG:HB3	2.02	0.60
1:A:155:HIS:NE2	1:A:188:SER:HB2	2.18	0.59
1:B:256:GLU:CD	1:B:256:GLU:N	2.55	0.59
1:A:109:THR:O	1:A:109:THR:HG22	2.02	0.59
1:D:84:ASP:OD2	1:D:86:MSE:HB2	2.02	0.59
1:D:37:MSE:HE3	1:D:39:LEU:HD21	1.85	0.58
1:A:159:THR:HG22	1:A:160:GLY:H	1.67	0.58
1:B:156:LEU:HD21	1:B:176:THR:HG22	1.85	0.58
1:C:272:PHE:HB3	1:C:273:PRO:CD	2.33	0.57
1:C:159:THR:HG22	1:C:161:VAL:H	1.71	0.56
1:D:303:GLU:CG	3:D:435:HOH:O	2.44	0.56
1:D:155:HIS:CE1	1:D:217:TRP:CZ3	2.93	0.56
1:D:156:LEU:HD21	1:D:176:THR:CG2	2.35	0.56
1:D:79:SER:HA	1:D:140:MSE:SE	2.56	0.56
1:D:198:TRP:NE1	1:D:204:MSE:HG3	2.21	0.56
1:A:55:LYS:NZ	1:D:50:ALA:O	2.35	0.55
1:B:107:ASP:CG	1:B:109:THR:HG22	2.27	0.55
1:B:88:ARG:NH1	1:C:48:GLU:HG2	2.22	0.55
1:B:290:GLY:HA3	1:B:308:GLY:HA2	1.89	0.55
1:D:37:MSE:SE	1:D:86:MSE:HE2	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:LYS:NZ	1:C:50:ALA:O	2.31	0.54
1:B:159:THR:CG2	1:B:161:VAL:H	2.06	0.54
1:C:159:THR:HG22	1:C:160:GLY:N	2.23	0.54
1:B:256:GLU:CD	1:B:256:GLU:H	2.10	0.54
1:D:31:THR:HG23	1:D:157:HIS:HB3	1.88	0.54
1:D:88:ARG:CB	1:D:88:ARG:HH11	2.20	0.54
1:B:157:HIS:HA	1:B:188:SER:HB3	1.90	0.53
1:D:300:GLY:HA3	3:D:435:HOH:O	2.08	0.53
1:D:37:MSE:CE	1:D:86:MSE:CE	2.86	0.53
1:A:218:VAL:HG12	1:A:220:PRO:HD3	1.91	0.53
1:D:37:MSE:HE3	1:D:39:LEU:CD2	2.38	0.53
1:A:159:THR:CG2	1:A:160:GLY:H	2.22	0.53
1:B:31:THR:HG23	1:B:157:HIS:HB3	1.89	0.53
1:D:155:HIS:ND1	1:D:186:SER:CB	2.64	0.52
1:C:154:ARG:NH2	1:C:296:LEU:O	2.43	0.52
1:D:27:LEU:HD12	1:D:74:LYS:HB3	1.90	0.52
1:A:67:GLY:HA3	1:A:325:LEU:HD23	1.92	0.52
1:A:31:THR:CG2	1:A:157:HIS:O	2.56	0.52
1:B:155:HIS:CE1	1:B:217:TRP:CZ3	2.98	0.52
1:D:88:ARG:HB2	1:D:88:ARG:HH11	1.75	0.52
1:C:150:LEU:HD11	1:C:176:THR:HG23	1.91	0.52
1:B:61:GLU:OE1	1:B:159:THR:HB	2.10	0.51
1:D:198:TRP:CD1	1:D:204:MSE:HG3	2.46	0.51
1:C:310:TRP:CZ3	1:C:331:LEU:HD23	2.46	0.51
1:D:299:LEU:HD22	1:D:303:GLU:OE2	2.11	0.51
1:A:156:LEU:HD21	1:A:176:THR:HG22	1.92	0.51
1:D:38:LEU:HD13	1:D:115:GLN:HE21	1.76	0.50
1:C:103:HIS:HE1	1:C:146:ASP:OD2	1.95	0.50
1:B:159:THR:CG2	1:B:160:GLY:N	2.74	0.50
1:B:38:LEU:HD13	1:B:115:GLN:HE21	1.76	0.50
1:B:37:MSE:HE2	1:B:86:MSE:SE	2.61	0.49
1:C:219:LEU:O	1:C:252:LYS:CE	2.61	0.49
1:B:213:THR:HG22	1:B:214:ARG:HG3	1.95	0.49
1:A:77:TRP:CE3	1:A:94:MSE:HG2	2.48	0.49
1:C:253:LEU:N	1:C:257:GLY:O	2.43	0.49
1:C:156:LEU:HD22	1:C:176:THR:HG22	1.95	0.48
1:C:243:GLN:HE21	1:C:244:LEU:HG	1.79	0.48
1:B:109:THR:HG23	1:B:110:GLN:HG3	1.96	0.48
1:C:61:GLU:OE1	1:C:159:THR:HB	2.14	0.48
1:B:294:ALA:CB	1:B:304:ALA:HA	2.43	0.48
1:A:109:THR:O	1:A:109:THR:CG2	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:HIS:CE1	1:A:217:TRP:CZ3	3.03	0.47
1:B:79:SER:HA	1:B:140:MSE:SE	2.64	0.47
1:C:31:THR:HG22	1:C:157:HIS:O	2.15	0.47
1:D:285:ASP:O	1:D:289:VAL:HG23	2.15	0.47
1:A:80:ARG:HG3	1:A:140:MSE:HG2	1.96	0.47
1:C:314:ARG:HH12	1:C:330:GLU:HG2	1.79	0.47
1:B:272:PHE:HB3	1:B:273:PRO:HD2	1.95	0.47
1:A:219:LEU:O	1:A:252:LYS:HE3	2.15	0.47
1:C:235:GLU:OE2	1:C:268:ARG:NH2	2.47	0.46
1:D:334:ALA:O	1:D:335:LYS:CB	2.63	0.46
1:B:156:LEU:HD21	1:B:176:THR:CG2	2.45	0.46
1:A:77:TRP:CE2	1:A:79:SER:HB2	2.51	0.45
1:B:170:LEU:HB3	1:B:171:PRO:HD3	1.98	0.45
1:D:290:GLY:HA3	1:D:308:GLY:HA2	1.98	0.45
1:D:170:LEU:HB3	1:D:171:PRO:HD3	1.99	0.45
1:C:162:PHE:N	1:C:163:PRO:HD2	2.32	0.45
1:B:238:ALA:O	1:B:242:ARG:HG2	2.17	0.45
1:D:156:LEU:CD2	1:D:176:THR:HG23	2.47	0.45
1:B:161:VAL:O	1:B:162:PHE:C	2.55	0.45
1:A:28:ASP:HA	1:A:154:ARG:HG3	1.99	0.44
1:A:201:PRO:O	1:A:204:MSE:HB3	2.17	0.44
1:A:291:VAL:O	1:A:295:LEU:HD22	2.17	0.44
1:D:162:PHE:N	1:D:163:PRO:HD2	2.32	0.44
1:B:238:ALA:HA	1:B:249:VAL:HG11	1.99	0.44
1:D:199:ALA:HB3	1:D:203:LEU:HD23	1.99	0.44
1:B:31:THR:HG22	1:B:157:HIS:O	2.17	0.44
1:A:235:GLU:O	1:A:239:ARG:CG	2.61	0.44
1:C:219:LEU:O	1:C:252:LYS:HE2	2.17	0.43
1:B:119:LYS:HA	1:B:119:LYS:HD3	1.67	0.43
1:C:159:THR:HG23	1:C:192:ASN:HD21	1.81	0.43
1:A:172:ALA:O	1:A:176:THR:HB	2.17	0.43
1:B:203:LEU:HA	1:B:203:LEU:HD12	1.67	0.43
1:B:155:HIS:ND1	1:B:186:SER:CB	2.65	0.43
1:D:271:GLY:HA2	1:D:309:ALA:HB1	1.99	0.43
1:D:235:GLU:OE2	1:D:268:ARG:NH2	2.52	0.43
1:A:170:LEU:HB3	1:A:171:PRO:CD	2.48	0.43
1:D:159:THR:CG2	1:D:160:GLY:N	2.82	0.43
1:B:229:THR:HG22	1:B:240:PHE:CD1	2.53	0.43
1:C:170:LEU:HB3	1:C:171:PRO:HD3	2.01	0.43
1:C:107:ASP:CG	1:C:109:THR:HG22	2.39	0.43
1:D:30:ILE:O	1:D:156:LEU:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:ARG:NH1	1:B:239:ARG:HG3	2.18	0.43
1:A:103:HIS:HE1	1:A:146:ASP:OD2	2.02	0.43
1:A:156:LEU:HD21	1:A:176:THR:CG2	2.49	0.42
1:B:37:MSE:SE	1:B:55:LYS:HD3	2.69	0.42
1:A:80:ARG:HD3	1:A:136:ALA:O	2.19	0.42
1:D:43:ARG:HA	1:D:44:PRO:HD3	1.84	0.42
1:C:159:THR:CG2	1:C:160:GLY:N	2.83	0.42
1:D:37:MSE:CE	1:D:39:LEU:HD21	2.48	0.42
1:A:27:LEU:HA	1:A:74:LYS:HB3	2.02	0.42
1:A:155:HIS:HD1	1:A:186:SER:CB	2.33	0.42
1:C:272:PHE:CB	1:C:273:PRO:HD3	2.41	0.42
1:D:239:ARG:CZ	3:D:414:HOH:O	2.67	0.41
1:D:155:HIS:CE1	1:D:188:SER:HB2	2.51	0.41
1:C:154:ARG:O	1:C:185:ARG:HG3	2.20	0.41
1:D:315:ALA:C	1:D:317:GLN:H	2.23	0.41
1:A:208:ILE:HA	1:A:208:ILE:HD13	1.90	0.41
1:D:196:THR:HB	3:D:412:HOH:O	2.19	0.41
1:B:327:THR:HG22	1:B:328:ARG:N	2.35	0.41
1:C:218:VAL:HG12	1:C:220:PRO:HD3	2.02	0.41
1:B:159:THR:HG22	1:B:161:VAL:N	2.02	0.41
1:A:287:PHE:CE2	1:A:291:VAL:HG11	2.55	0.41
1:A:327:THR:HG22	1:A:329:ALA:H	1.85	0.41
1:D:256:GLU:OE2	1:D:256:GLU:N	2.54	0.41
1:A:157:HIS:ND1	1:A:188:SER:HB3	2.36	0.40
1:D:203:LEU:HD12	1:D:203:LEU:HA	1.87	0.40
1:D:175:LYS:HE2	1:D:179:LEU:HD13	2.02	0.40
1:B:38:LEU:HD13	1:B:115:GLN:HG3	2.04	0.40
1:B:147:GLU:HG2	1:B:179:LEU:HD21	2.04	0.40
1:A:68:LEU:HD23	1:A:289:VAL:HG13	2.04	0.40
1:D:119:LYS:HD3	1:D:119:LYS:HA	1.86	0.40
1:A:203:LEU:HD12	1:A:203:LEU:O	2.21	0.40
1:C:192:ASN:H	1:C:192:ASN:ND2	2.19	0.40
1:A:67:GLY:CA	1:A:325:LEU:HD23	2.50	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	286/336 (85%)	267 (93%)	16 (6%)	3 (1%)	19	45
1	B	287/336 (85%)	273 (95%)	13 (4%)	1 (0%)	46	75
1	C	286/336 (85%)	273 (96%)	12 (4%)	1 (0%)	46	75
1	D	284/336 (84%)	273 (96%)	10 (4%)	1 (0%)	39	69
All	All	1143/1344 (85%)	1086 (95%)	51 (4%)	6 (0%)	34	63

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	THR
1	A	333	ALA
1	D	316	VAL
1	C	273	PRO
1	A	127	PRO
1	B	316	VAL

### 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	200/238 (84%)	177 (88%)	23 (12%)	7	16
1	B	201/238 (84%)	173 (86%)	28 (14%)	4	10
1	C	202/238 (85%)	171 (85%)	31 (15%)	3	8
1	D	201/238 (84%)	177 (88%)	24 (12%)	6	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	804/952 (84%)	698 (87%)	106 (13%)	5 12

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	31	THR
1	A	55	LYS
1	A	111	LYS
1	A	121	THR
1	A	128	VAL
1	A	132	ARG
1	A	150	LEU
1	A	151	LEU
1	A	175	LYS
1	A	176	THR
1	A	179	LEU
1	A	188	SER
1	A	195	PRO
1	A	219	LEU
1	A	222	MSE
1	A	232	THR
1	A	239	ARG
1	A	243	GLN
1	A	295	LEU
1	A	296	LEU
1	A	325	LEU
1	A	331	LEU
1	B	31	THR
1	B	55	LYS
1	B	57	THR
1	B	111	LYS
1	B	119	LYS
1	B	128	VAL
1	B	132	ARG
1	B	133	LYS
1	B	150	LEU
1	B	151	LEU
1	B	152	SER
1	B	175	LYS
1	B	176	THR
1	B	179	LEU

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Mol	Chain	Res	Type
1	B	181	ARG
1	B	185	ARG
1	B	186	SER
1	B	188	SER
1	B	203	LEU
1	B	213	THR
1	B	223	GLU
1	B	235	GLU
1	B	239	ARG
1	B	243	GLN
1	B	256	GLU
1	B	291	VAL
1	B	295	LEU
1	B	306	LYS
1	C	27	LEU
1	C	31	THR
1	C	44	PRO
1	C	55	LYS
1	C	57	THR
1	C	111	LYS
1	C	119	LYS
1	C	122	ASP
1	C	132	ARG
1	C	133	LYS
1	C	150	LEU
1	C	151	LEU
1	C	152	SER
1	C	179	LEU
1	C	185	ARG
1	C	186	SER
1	C	192	ASN
1	C	196	THR
1	C	206	ASP
1	C	213	THR
1	C	217	TRP
1	C	219	LEU
1	C	223	GLU
1	C	243	GLN
1	C	247	LYS
1	C	268	ARG
1	C	295	LEU
1	C	296	LEU

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Mol	Chain	Res	Type
1	C	306	LYS
1	C	330	GLU
1	C	331	LEU
1	D	31	THR
1	D	57	THR
1	D	88	ARG
1	D	111	LYS
1	D	128	VAL
1	D	132	ARG
1	D	150	LEU
1	D	151	LEU
1	D	176	THR
1	D	179	LEU
1	D	181	ARG
1	D	185	ARG
1	D	203	LEU
1	D	213	THR
1	D	219	LEU
1	D	223	GLU
1	D	239	ARG
1	D	243	GLN
1	D	295	LEU
1	D	303	GLU
1	D	306	LYS
1	D	314	ARG
1	D	327	THR
1	D	331	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	HIS
1	A	115	GLN
1	A	139	HIS
1	A	192	ASN
1	B	103	HIS
1	B	115	GLN
1	B	192	ASN
1	C	103	HIS
1	C	115	GLN
1	C	192	ASN
1	C	243	GLN

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Mol	Chain	Res	Type
1	D	103	HIS
1	D	115	GLN

### 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 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	285/336 (84%)	-0.05	2 (0%) 89 90	21, 35, 49, 64	0
1	B	286/336 (85%)	-0.20	4 (1%) 78 77	12, 29, 49, 65	0
1	C	285/336 (84%)	-0.10	4 (1%) 78 77	15, 30, 48, 71	0
1	D	285/336 (84%)	-0.19	2 (0%) 89 90	15, 28, 51, 66	0
All	All	1141/1344 (84%)	-0.14	12 (1%) 82 83	12, 30, 49, 71	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	122	ASP	3.6
1	C	121	THR	3.3
1	C	122	ASP	3.0
1	B	316	VAL	2.9
1	A	121	THR	2.5
1	B	223	GLU	2.4
1	B	255	ALA	2.4
1	C	243	GLN	2.3
1	D	121	THR	2.2
1	B	315	ALA	2.2
1	D	274	VAL	2.1
1	C	44	PRO	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [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( $\text{\AA}^2$ )	Q<0.9
2	CL	C	401	1/1	0.98	0.10	-	27,27,27,27	0
2	CL	A	401	1/1	0.95	0.07	-	29,29,29,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.