



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 15, 2018 – 12:20 PM EST

PDB ID : 3CFV  
Title : Structural basis of the interaction of RbAp46/RbAp48 with histone H4  
Authors : Pei, X.-Y.; Murzina, N.V.; Zhang, W.; McLaughlin, S.; Verreault, A.; Luisi, B.F.; Laue, E.D.  
Deposited on : 2008-03-04  
Resolution : 2.60 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  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

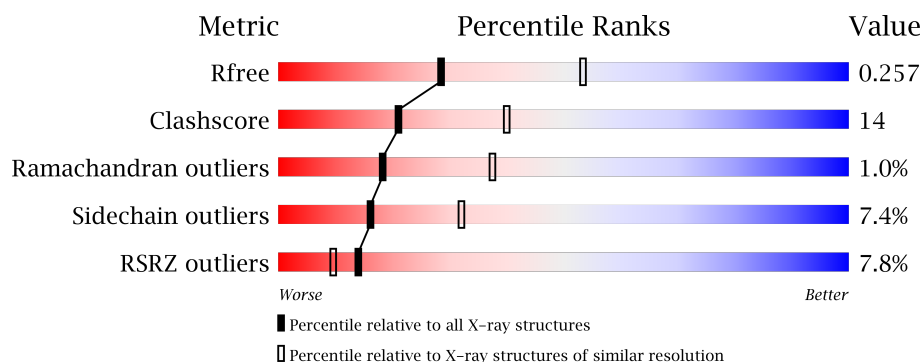
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	414	<div> <div>7%</div> <div>69%</div> <div>23%</div> <div>6%</div> </div>
1	B	414	<div> <div>7%</div> <div>70%</div> <div>21%</div> <div>5%</div> </div>
2	E	18	<div> <div>72%</div> <div>17%</div> <div>11%</div> </div>
2	F	18	<div> <div>17%</div> <div>50%</div> <div>22%</div> <div>6%</div> <div>22%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ARS	A	412	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6782 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 Histone-binding protein RBBP7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	393	Total	C	N	O	S	Se	0	0	0
			3140	1984	538	605	5	8			
1	A	390	Total	C	N	O	S	Se	0	0	0
			3114	1969	533	599	5	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	CLONING ARTIFACT	UNP Q16576
B	-1	MSE	-	CLONING ARTIFACT	UNP Q16576
B	0	ALA	-	CLONING ARTIFACT	UNP Q16576
A	-2	HIS	-	CLONING ARTIFACT	UNP Q16576
A	-1	MSE	-	CLONING ARTIFACT	UNP Q16576
A	0	ALA	-	CLONING ARTIFACT	UNP Q16576

- Molecule 2 is a protein called Histone H4 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	18	Total	C	N	O	0	0	0
			142	86	33	23			
2	F	14	Total	C	N	O	0	0	0
			109	67	27	15			

- Molecule 3 is ARSENIC (three-letter code: ARS) (formula: As).

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

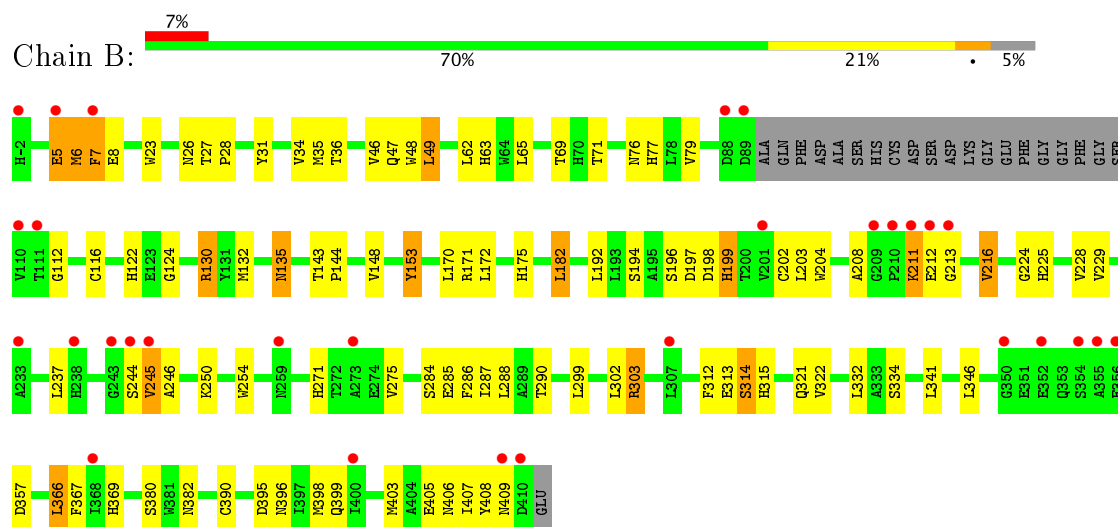
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	125	Total 125	O 125	0	0
4	E	7	Total 7	O 7	0	0
4	A	141	Total 141	O 141	0	0
4	F	2	Total 2	O 2	0	0

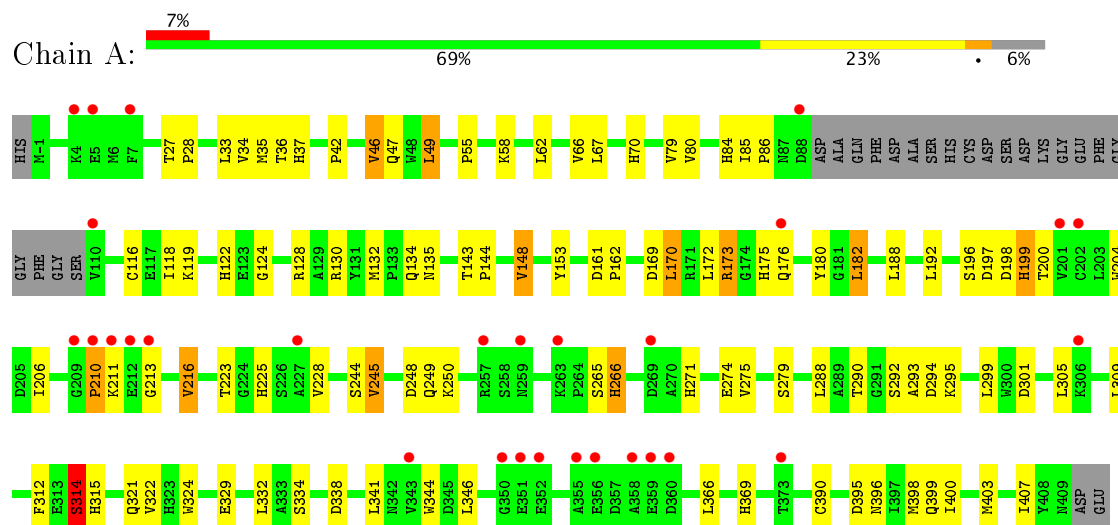
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Histone-binding protein RBBP7



#### • Molecule 1: Histone-binding protein RBBP7



#### • Molecule 2: Histone H4 peptide





● Molecule 2: Histone H4 peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.66Å 44.79Å 109.59Å 90.00° 90.71° 90.00°	Depositor
Resolution (Å)	25.00 – 2.60 24.95 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (25.00-2.60) 99.6 (24.95-2.60)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.02 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.199 , 0.257 0.201 , 0.257	Depositor DCC
$R_{free}$ test set	1577 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.1	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 68.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.074 for l,k,-h 0.022 for h,-k,-l 0.021 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6782	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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: ARS

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	0.23	0/3194	0.42	0/4340
1	B	0.23	0/3220	0.48	2/4374 (0.0%)
2	E	0.24	0/142	0.39	0/188
2	F	0.34	0/109	1.05	2/143 (1.4%)
All	All	0.23	0/6665	0.46	4/9045 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	7	PHE	CB-CA-C	-10.64	89.12	110.40
2	F	30	THR	CB-CA-C	-8.19	89.48	111.60
1	B	7	PHE	N-CA-C	6.93	129.71	111.00
2	F	30	THR	N-CA-C	5.52	125.91	111.00

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	3114	0	2973	77	0
1	B	3140	0	2989	81	0
2	E	142	0	156	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	109	0	127	15	0
3	A	1	0	0	2	0
3	B	1	0	0	1	0
4	A	141	0	0	0	0
4	B	125	0	0	1	0
4	E	7	0	0	0	0
4	F	2	0	0	0	0
All	All	6782	0	6245	175	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 14.

All (175) 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)
2:F:29:ILE:N	2:F:30:THR:HB	1.43	1.32
1:B:6:MSE:HA	1:B:7:PHE:HB3	1.27	1.12
1:B:35:MSE:HE3	1:B:112:GLY:HA3	1.32	1.07
1:B:116:CYS:SG	3:B:412:ARS:AS	2.73	1.06
2:F:29:ILE:H	2:F:30:THR:CB	1.70	1.02
1:A:116:CYS:SG	3:A:412:ARS:AS	2.78	1.02
1:B:143:THR:HG22	1:B:144:PRO:HD2	1.43	1.00
1:B:35:MSE:CE	1:B:112:GLY:HA3	1.93	0.97
1:B:6:MSE:HA	1:B:7:PHE:CB	1.91	0.96
1:A:173:ARG:CG	1:A:173:ARG:HH11	1.78	0.95
1:A:271:HIS:HE1	1:A:290:THR:HG22	1.32	0.95
1:A:403:MSE:HE2	1:A:407:ILE:HB	1.48	0.94
2:F:30:THR:O	2:F:30:THR:CG2	2.10	0.94
1:B:6:MSE:HB3	1:B:8:GLU:HG2	1.50	0.94
2:F:29:ILE:H	2:F:30:THR:HB	0.76	0.87
2:F:30:THR:HG23	2:F:30:THR:O	1.74	0.86
1:B:5:GLU:HA	1:B:7:PHE:HB3	1.57	0.85
2:F:29:ILE:CA	2:F:30:THR:HB	2.09	0.82
1:A:271:HIS:CE1	1:A:290:THR:HG22	2.15	0.81
2:F:29:ILE:HB	2:F:30:THR:OG1	1.80	0.81
1:B:5:GLU:HA	1:B:7:PHE:CB	2.12	0.78
1:B:367:PHE:HB2	1:B:403:MSE:HE3	1.65	0.76
1:B:143:THR:CG2	1:B:144:PRO:HD2	2.12	0.76
1:B:7:PHE:CG	1:B:7:PHE:O	2.38	0.76
1:A:173:ARG:HH11	1:A:173:ARG:HG3	1.48	0.76
1:B:271:HIS:HE1	1:B:290:THR:HG22	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:THR:HG22	1:B:399:GLN:HG2	1.68	0.74
1:A:403:MSE:CE	1:A:407:ILE:HB	2.16	0.74
1:A:33:LEU:HD21	1:A:35:MSE:HE2	1.69	0.74
1:A:173:ARG:HH11	1:A:173:ARG:HG2	1.52	0.73
1:A:172:LEU:HD23	1:A:216:VAL:HG13	1.71	0.73
1:A:36:THR:HG22	1:A:399:GLN:HG2	1.71	0.71
1:B:122:HIS:HD2	1:B:124:GLY:O	1.73	0.71
1:B:6:MSE:CB	1:B:8:GLU:HG2	2.22	0.69
1:B:303:ARG:HB3	1:A:28:PRO:HB2	1.75	0.68
1:A:321:GLN:HE21	1:A:322:VAL:H	1.40	0.67
1:A:49:LEU:HD13	1:A:66:VAL:HG23	1.76	0.67
1:B:143:THR:HG22	1:B:144:PRO:CD	2.24	0.67
2:E:30:THR:O	2:E:34:ILE:HG12	1.94	0.67
1:B:312:PHE:HZ	1:B:346:LEU:HD21	1.61	0.67
1:B:403:MSE:HE2	1:B:407:ILE:CG2	2.25	0.67
1:A:266:HIS:HD2	1:A:305:LEU:HD23	1.59	0.66
1:A:271:HIS:HE1	1:A:290:THR:CG2	2.07	0.66
1:B:245:VAL:HG13	1:B:275:VAL:HB	1.76	0.66
1:B:69:THR:HG22	1:B:76:ASN:OD1	1.95	0.66
1:B:7:PHE:CD2	1:B:7:PHE:O	2.49	0.66
1:A:37:HIS:HD2	1:A:398:MSE:CE	2.09	0.65
1:B:6:MSE:CA	1:B:7:PHE:CB	2.74	0.64
2:F:29:ILE:N	2:F:30:THR:CB	2.40	0.64
1:B:132:MSE:HE2	1:B:135:ASN:HB3	1.79	0.63
1:B:366:LEU:HD22	1:B:403:MSE:HE1	1.81	0.62
1:B:271:HIS:CE1	1:B:290:THR:HG22	2.32	0.61
1:B:321:GLN:HE21	1:B:322:VAL:H	1.49	0.60
2:E:25:ASN:HD22	2:E:25:ASN:H	1.48	0.60
1:B:312:PHE:HZ	1:B:346:LEU:CD2	2.15	0.59
1:B:172:LEU:HD22	1:B:216:VAL:HG22	1.85	0.59
1:A:315:HIS:HE1	1:A:334:SER:OG	1.86	0.59
1:A:122:HIS:HD2	1:A:124:GLY:O	1.85	0.59
1:A:182:LEU:HD22	1:A:192:LEU:HD11	1.85	0.58
1:A:37:HIS:HB3	1:A:398:MSE:HE3	1.85	0.58
2:F:29:ILE:CA	2:F:30:THR:CB	2.80	0.58
1:B:198:ASP:O	1:B:199:HIS:HB2	2.03	0.58
1:B:315:HIS:HE1	1:B:334:SER:OG	1.87	0.57
1:B:48:TRP:HD1	1:B:380:SER:HG	1.52	0.57
1:A:198:ASP:O	1:A:199:HIS:HB2	2.04	0.57
1:A:173:ARG:NH1	1:A:173:ARG:CG	2.50	0.56
1:A:395:ASP:O	1:A:396:ASN:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:VAL:HG22	1:A:172:LEU:HB2	1.89	0.55
1:A:271:HIS:CE1	1:A:290:THR:CG2	2.87	0.54
1:A:37:HIS:HD2	1:A:398:MSE:HE1	1.72	0.54
1:B:367:PHE:HB2	1:B:403:MSE:CE	2.34	0.54
2:F:30:THR:O	2:F:30:THR:HG22	1.89	0.54
1:A:169:ASP:O	1:A:170:LEU:HD13	2.08	0.54
1:A:143:THR:HB	1:A:144:PRO:HD2	1.90	0.53
1:B:366:LEU:HD13	1:B:403:MSE:HE1	1.90	0.53
2:F:31:LYS:N	2:F:32:PRO:HD2	2.24	0.53
1:A:172:LEU:HB3	1:A:204:TRP:CE2	2.44	0.53
1:A:173:ARG:NH1	1:A:173:ARG:HG2	2.22	0.53
1:B:284:SER:HB3	1:B:287:ILE:HG12	1.90	0.53
1:A:35:MSE:HE3	1:A:400:ILE:CG2	2.39	0.53
1:B:35:MSE:HE1	1:B:112:GLY:HA3	1.86	0.53
1:A:197:ASP:HA	1:A:228:VAL:HG13	1.92	0.52
1:B:403:MSE:HE2	1:B:407:ILE:HG22	1.92	0.52
1:A:148:VAL:CG2	1:A:172:LEU:HD12	2.40	0.52
1:A:403:MSE:CE	1:A:407:ILE:CG2	2.88	0.51
1:A:210:PRO:HG2	1:A:213:GLY:HA3	1.91	0.51
2:F:29:ILE:HB	2:F:30:THR:CB	2.41	0.51
2:F:31:LYS:H	2:F:32:PRO:HD2	1.76	0.50
1:B:175:HIS:CD2	1:B:196:SER:HB3	2.46	0.50
1:A:79:VAL:HG22	1:A:119:LYS:HG2	1.92	0.50
1:A:245:VAL:HG13	1:A:275:VAL:HB	1.93	0.50
1:B:5:GLU:N	1:B:7:PHE:HB2	2.26	0.50
1:A:279:SER:HB3	1:A:322:VAL:HG12	1.94	0.50
1:A:35:MSE:HE1	1:A:85:ILE:HG12	1.94	0.50
1:A:37:HIS:CD2	1:A:398:MSE:CE	2.92	0.49
1:A:132:MSE:HE2	1:A:135:ASN:HB3	1.94	0.49
1:A:301:ASP:HB2	1:A:309:LEU:HD11	1.95	0.49
1:B:182:LEU:HD22	1:B:192:LEU:HD11	1.95	0.48
1:A:403:MSE:CE	1:A:407:ILE:CB	2.88	0.48
1:B:405:GLU:HA	1:B:408:TYR:CZ	2.49	0.48
1:B:27:THR:N	1:B:28:PRO:CD	2.77	0.48
1:A:172:LEU:CD2	1:A:216:VAL:HG13	2.42	0.48
1:B:47:GLN:OE1	1:B:130:ARG:HA	2.14	0.47
1:B:224:GLY:HA3	1:B:254:TRP:HH2	1.78	0.47
1:A:173:ARG:NH1	1:A:173:ARG:HG3	2.21	0.47
1:A:403:MSE:HE1	1:A:407:ILE:CG2	2.45	0.47
1:A:132:MSE:HE3	1:A:134:GLN:HB2	1.96	0.47
1:B:132:MSE:HE2	1:B:135:ASN:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:HIS:HE1	1:A:244:SER:OG	1.97	0.47
1:A:265:SER:C	1:A:266:HIS:ND1	2.68	0.47
1:A:42:PRO:HG2	1:A:70:HIS:HB3	1.97	0.47
1:B:69:THR:HB	1:B:77:HIS:H	1.79	0.46
1:B:5:GLU:HA	1:B:7:PHE:HB2	1.97	0.46
1:A:128:ARG:HD2	1:A:180:TYR:O	2.15	0.46
1:A:27:THR:OG1	1:A:28:PRO:HD3	2.16	0.46
1:A:275:VAL:CG1	1:A:290:THR:HG23	2.46	0.46
1:B:23:TRP:HE1	1:B:31:TYR:HH	1.64	0.45
1:B:27:THR:OG1	1:B:28:PRO:HD3	2.16	0.45
1:B:224:GLY:HA3	1:B:254:TRP:CH2	2.51	0.45
2:F:28:GLY:HA2	2:F:29:ILE:HA	1.47	0.45
1:B:212:GLU:HA	1:B:213:GLY:HA2	1.64	0.44
1:A:279:SER:HG	1:A:324:TRP:HD1	1.65	0.44
1:A:314:SER:HB2	1:A:344:TRP:HH2	1.82	0.44
1:B:6:MSE:HB2	1:B:8:GLU:H	1.83	0.44
2:E:26:ILE:H	2:E:26:ILE:HG12	1.41	0.44
1:B:395:ASP:O	1:B:396:ASN:HB2	2.18	0.44
1:A:341:LEU:HB3	1:A:369:HIS:HB3	2.01	0.43
1:A:175:HIS:CD2	1:A:196:SER:CB	3.01	0.43
1:B:5:GLU:CA	1:B:7:PHE:CB	2.91	0.43
1:B:225:HIS:CD2	1:B:246:ALA:HB3	2.54	0.43
1:B:211:LYS:HE3	1:B:211:LYS:HA	2.00	0.43
1:A:292:SER:OG	1:A:293:ALA:N	2.52	0.42
1:B:313:GLU:O	1:B:314:SER:CB	2.66	0.42
1:B:172:LEU:HD22	1:B:216:VAL:CG2	2.49	0.42
1:A:315:HIS:HD2	1:A:338:ASP:OD2	2.02	0.42
1:A:46:VAL:CG1	1:A:67:LEU:HD23	2.49	0.42
1:A:46:VAL:HG13	1:A:67:LEU:HD23	2.00	0.42
1:B:5:GLU:CA	1:B:7:PHE:HB2	2.49	0.42
1:A:37:HIS:CD2	1:A:398:MSE:HE1	2.53	0.42
1:B:194:SER:HB3	1:B:204:TRP:HZ3	1.85	0.42
1:B:341:LEU:HB3	1:B:369:HIS:HB3	2.01	0.42
1:A:248:ASP:O	1:A:249:GLN:HB2	2.20	0.42
1:B:182:LEU:HD23	1:B:182:LEU:HA	1.93	0.42
1:B:6:MSE:CB	1:B:8:GLU:H	2.33	0.42
1:B:405:GLU:HA	1:B:408:TYR:CE2	2.55	0.41
1:B:26:ASN:HA	1:B:26:ASN:HD22	1.70	0.41
1:B:237:LEU:HD13	1:B:285:GLU:HB3	2.02	0.41
1:B:286:PHE:O	1:B:302:LEU:HG	2.20	0.41
1:A:49:LEU:HD12	1:A:49:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ASP:HA	1:B:228:VAL:HG13	2.02	0.41
1:B:390:CYS:SG	1:B:398:MSE:HE2	2.60	0.41
1:A:312:PHE:HZ	1:A:346:LEU:CD2	2.34	0.41
1:B:312:PHE:CZ	1:B:346:LEU:CD2	3.01	0.41
1:B:171:ARG:HD2	4:B:518:HOH:O	2.19	0.41
1:A:55:PRO:HB2	1:A:58:LYS:CG	2.51	0.41
1:B:357:ASP:OD1	2:E:36:ARG:HD3	2.20	0.41
1:A:175:HIS:CD2	1:A:196:SER:HB3	2.56	0.41
1:B:225:HIS:HE1	1:B:244:SER:OG	2.04	0.41
1:A:85:ILE:HA	1:A:86:PRO:HD3	1.94	0.41
1:B:63:HIS:CD2	1:B:382:ASN:HD21	2.39	0.41
1:A:116:CYS:HG	3:A:412:ARS:AS	2.62	0.41
1:A:47:GLN:OE1	1:A:130:ARG:HA	2.21	0.41
1:A:294:ASP:O	1:A:295:LYS:HB2	2.20	0.40
1:B:153:TYR:C	1:B:153:TYR:CD2	2.94	0.40
1:B:202:CYS:HB2	1:B:204:TRP:CH2	2.56	0.40
1:A:80:VAL:HB	1:A:118:ILE:HG22	2.03	0.40
1:A:161:ASP:HA	1:A:162:PRO:HD3	1.88	0.40
1:A:390:CYS:HA	1:A:399:GLN:O	2.21	0.40
1:B:175:HIS:CD2	1:B:196:SER:CB	3.04	0.40
1:B:312:PHE:CZ	1:B:346:LEU:HD21	2.50	0.40
2:F:29:ILE:HB	2:F:30:THR:HG1	1.84	0.40
1:A:200:THR:HG22	1:A:223:THR:HG22	2.03	0.40
1:B:49:LEU:HA	1:B:49:LEU:HD12	1.85	0.40
1:A:188:LEU:HA	1:A:188:LEU:HD12	1.90	0.40
1:B:271:HIS:HE1	1:B:290:THR:CG2	2.29	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	386/414 (93%)	368 (95%)	15 (4%)	3 (1%)	22	44
1	B	389/414 (94%)	370 (95%)	15 (4%)	4 (1%)	18	37
2	E	16/18 (89%)	16 (100%)	0	0	100	100
2	F	12/18 (67%)	10 (83%)	1 (8%)	1 (8%)	1	1
All	All	803/864 (93%)	764 (95%)	31 (4%)	8 (1%)	18	37

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	314	SER
1	B	5	GLU
1	B	406	ASN
1	A	314	SER
2	F	30	THR
1	B	208	ALA
1	A	210	PRO
1	A	206	ILE

### 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	345/356 (97%)	321 (93%)	24 (7%)	18	35
1	B	348/356 (98%)	321 (92%)	27 (8%)	15	29
2	E	14/14 (100%)	12 (86%)	2 (14%)	4	6
2	F	10/14 (71%)	10 (100%)	0	100	100
All	All	717/740 (97%)	664 (93%)	53 (7%)	16	32

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

Mol	Chain	Res	Type
1	B	6	MSE
1	B	34	VAL
1	B	46	VAL

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Mol	Chain	Res	Type
1	B	49	LEU
1	B	62	LEU
1	B	65	LEU
1	B	71	THR
1	B	79	VAL
1	B	130	ARG
1	B	135	ASN
1	B	148	VAL
1	B	153	TYR
1	B	170	LEU
1	B	182	LEU
1	B	199	HIS
1	B	203	LEU
1	B	211	LYS
1	B	216	VAL
1	B	229	VAL
1	B	245	VAL
1	B	250	LYS
1	B	288	LEU
1	B	299	LEU
1	B	303	ARG
1	B	332	LEU
1	B	366	LEU
1	B	409	ASN
2	E	25	ASN
2	E	26	ILE
1	A	34	VAL
1	A	46	VAL
1	A	49	LEU
1	A	62	LEU
1	A	84	HIS
1	A	148	VAL
1	A	153	TYR
1	A	170	LEU
1	A	173	ARG
1	A	176	GLN
1	A	182	LEU
1	A	199	HIS
1	A	211	LYS
1	A	216	VAL
1	A	245	VAL
1	A	250	LYS

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Mol	Chain	Res	Type
1	A	266	HIS
1	A	274	GLU
1	A	288	LEU
1	A	299	LEU
1	A	314	SER
1	A	329	GLU
1	A	332	LEU
1	A	366	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	26	ASN
1	B	63	HIS
1	B	75	GLN
1	B	84	HIS
1	B	87	ASN
1	B	122	HIS
1	B	175	HIS
1	B	176	GLN
1	B	225	HIS
1	B	249	GLN
1	B	271	HIS
1	B	304	ASN
1	B	315	HIS
1	B	321	GLN
1	B	342	ASN
1	B	353	GLN
1	B	399	GLN
1	B	409	ASN
2	E	25	ASN
1	A	26	ASN
1	A	37	HIS
1	A	75	GLN
1	A	87	ASN
1	A	122	HIS
1	A	135	ASN
1	A	137	HIS
1	A	175	HIS
1	A	176	GLN
1	A	225	HIS
1	A	249	GLN

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Mol	Chain	Res	Type
1	A	271	HIS
1	A	315	HIS
1	A	321	GLN
1	A	342	ASN
1	A	384	ASN
1	A	399	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 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 ⓘ

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	382/414 (92%)	0.17	29 (7%) 15 10	17, 47, 84, 120	1 (0%)
1	B	385/414 (92%)	0.27	30 (7%) 14 9	14, 47, 86, 120	7 (1%)
2	E	18/18 (100%)	0.49	0 100 100	46, 77, 96, 99	0
2	F	14/18 (77%)	0.60	3 (21%) 1 0	46, 63, 94, 94	0
All	All	799/864 (92%)	0.23	62 (7%) 14 9	14, 48, 89, 120	8 (1%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	212	GLU	6.7
1	B	89	ASP	5.6
1	B	400	ILE	5.5
1	B	368	ILE	5.4
1	B	211	LYS	5.0
1	A	210	PRO	5.0
1	B	212	GLU	4.9
1	A	355	ALA	4.9
1	A	259	ASN	4.9
1	B	213	GLY	4.6
1	A	211	LYS	4.6
1	B	410	ASP	4.5
1	B	354	SER	4.3
1	A	110	VAL	4.2
1	B	7	PHE	4.0
1	B	210	PRO	3.9
1	B	209	GLY	3.6
1	B	355	ALA	3.6
1	A	352	GLU	3.5
1	A	213	GLY	3.4
1	A	373	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	7	PHE	3.4
1	B	88	ASP	3.3
1	B	356	GLU	3.3
1	B	110	VAL	3.2
1	B	409	ASN	3.2
1	A	356	GLU	3.1
1	A	358	ALA	3.0
2	F	29	ILE	2.9
1	A	4	LYS	2.9
1	A	88	ASP	2.9
2	F	30	THR	2.8
1	B	350	GLY	2.7
1	B	201	VAL	2.6
1	A	5	GLU	2.6
1	B	243	GLY	2.6
1	B	352	GLU	2.6
1	A	306	LYS	2.5
1	A	269	ASP	2.5
1	B	273	ALA	2.5
1	A	359	GLU	2.4
1	B	259	ASN	2.4
1	B	244	SER	2.4
2	F	40	ARG	2.3
1	A	263	LYS	2.3
1	A	227	ALA	2.3
1	A	209	GLY	2.2
1	B	-2	HIS	2.2
1	B	238	HIS	2.2
1	A	351	GLU	2.2
1	B	233	ALA	2.2
1	A	176	GLN	2.2
1	A	360	ASP	2.1
1	B	111	THR	2.1
1	B	245	VAL	2.1
1	A	201	VAL	2.1
1	A	350	GLY	2.1
1	A	202	CYS	2.1
1	B	307	LEU	2.0
1	A	343	VAL	2.0
1	A	257	ARG	2.0
1	B	5	GLU	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( $\text{\AA}^2$ )	Q<0.9
3	ARS	B	412	1/1	0.96	0.21	0.09	99,99,99,99	0
3	ARS	A	412	1/1	0.99	0.12	-0.80	80,80,80,80	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.