Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:43 am BST

PDB ID	:	6G16
Title	:	Structure of the human RBBP4:MTA1(464-546) complex showing loop exchange
Authors	:	Millard, C.J.; Varma, N.; Fairall, L.; Schwabe, J.W.R.
Deposited on	:	2018-03-20
Resolution	:	2.80 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

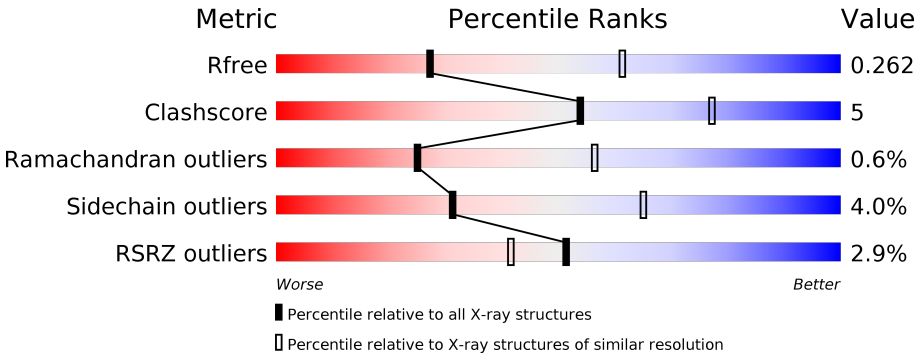
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 >=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 <=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	425	83% 7% • 8%
1	C	425	3% 81% 9% • 8%
1	E	425	3% 79% 12% • 8%
1	G	425	4% 77% 13% • 8%
2	B	85	2% 67% 12% • 19%
2	D	85	2% 65% 13% • 19%

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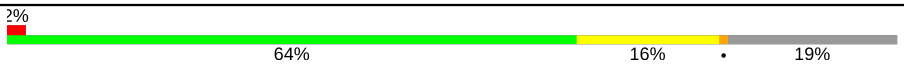
Mol	Chain	Length	Quality of chain
2	F	85	
2	H	85	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14642 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 RBBP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			3091	1950	527	604	10			
1	C	389	Total	C	N	O	S	0	0	0
			3091	1950	527	604	10			
1	E	389	Total	C	N	O	S	0	0	0
			3087	1947	526	604	10			
1	G	389	Total	C	N	O	S	0	0	0
			3087	1947	526	604	10			

- Molecule 2 is a protein called Metastasis-associated protein MTA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	69	Total	C	N	O	S	0	0	0
			570	364	116	88	2			
2	D	69	Total	C	N	O	S	0	0	0
			574	366	116	90	2			
2	F	69	Total	C	N	O	S	0	0	0
			574	366	116	90	2			
2	H	69	Total	C	N	O	S	0	0	0
			568	363	113	90	2			

There are 8 discrepancies between the modelled and reference sequences:

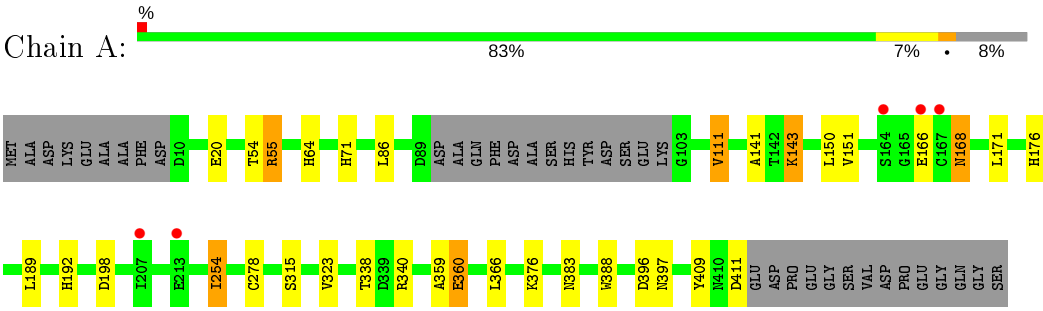
Chain	Residue	Modelled	Actual	Comment	Reference
B	462	GLY	-	expression tag	UNP Q13330
B	463	ALA	-	expression tag	UNP Q13330
D	462	GLY	-	expression tag	UNP Q13330
D	463	ALA	-	expression tag	UNP Q13330
F	462	GLY	-	expression tag	UNP Q13330
F	463	ALA	-	expression tag	UNP Q13330
H	462	GLY	-	expression tag	UNP Q13330
H	463	ALA	-	expression tag	UNP Q13330

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

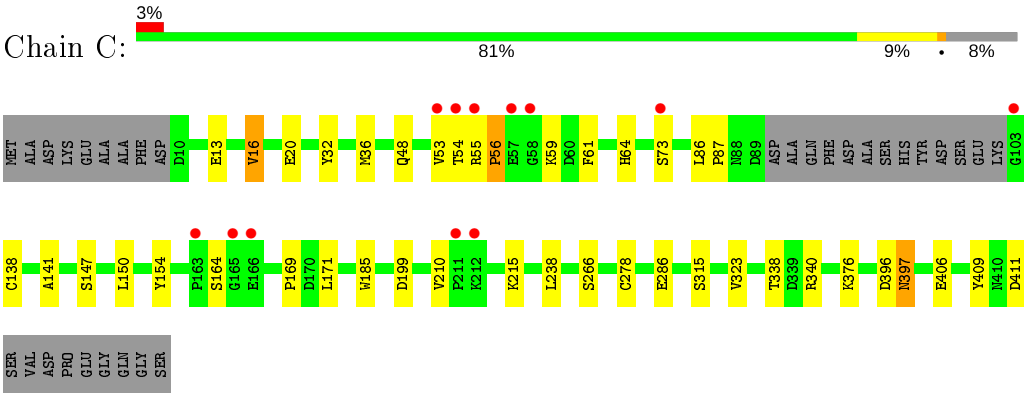
- Molecule 1: Histone-binding protein RBBP4

Chain A:



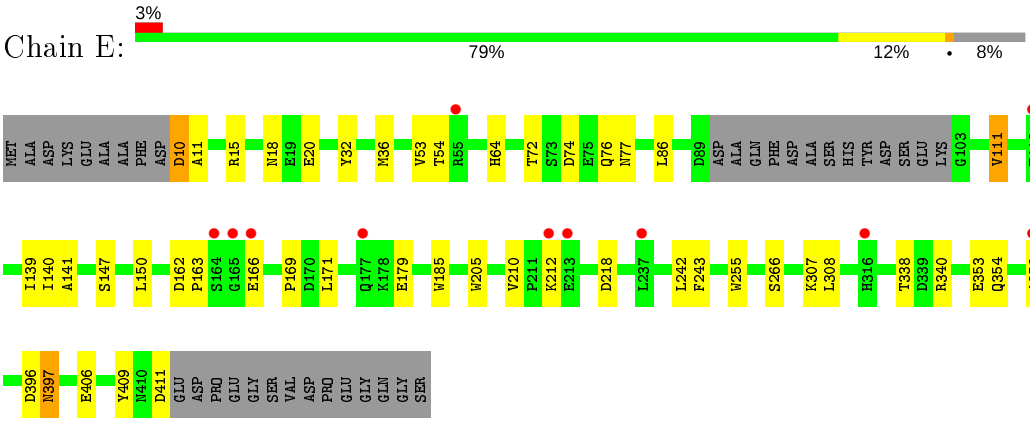
- Molecule 1: Histone-binding protein RBBP4

Chain C:



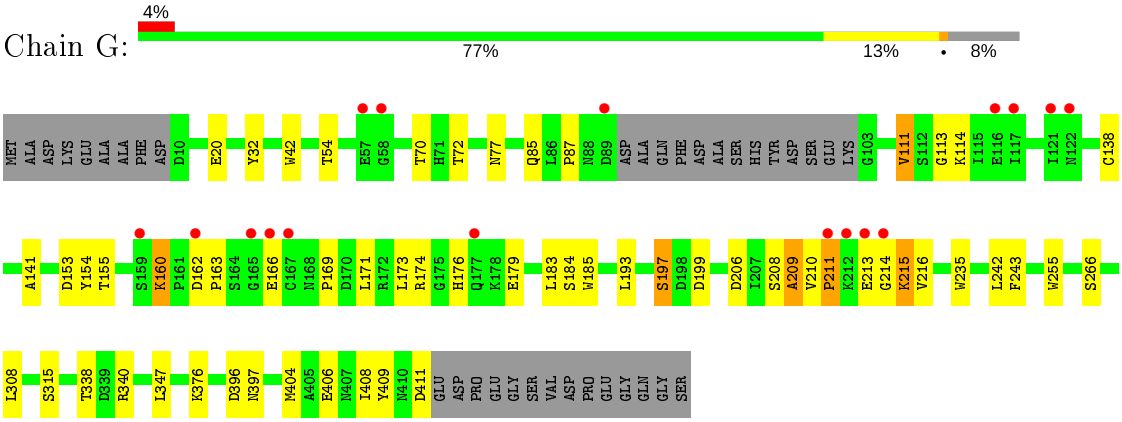
- Molecule 1: Histone-binding protein RBBP4

Chain E:



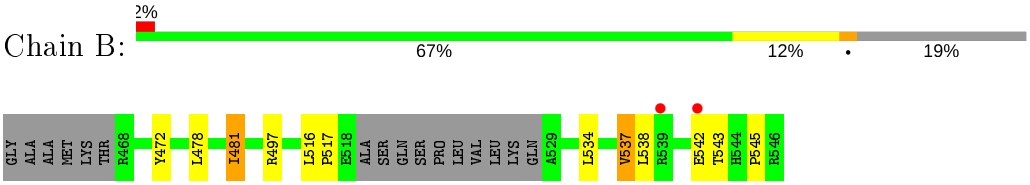
• Molecule 1: Histone-binding protein RBBP4

Chain G:



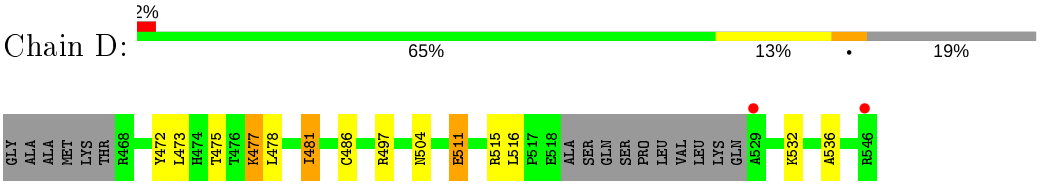
• Molecule 2: Metastasis-associated protein MTA1

Chain B:



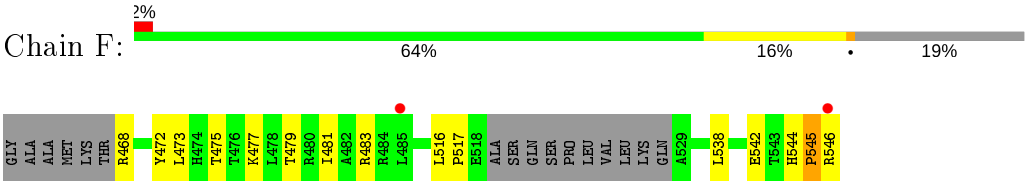
• Molecule 2: Metastasis-associated protein MTA1

Chain D:



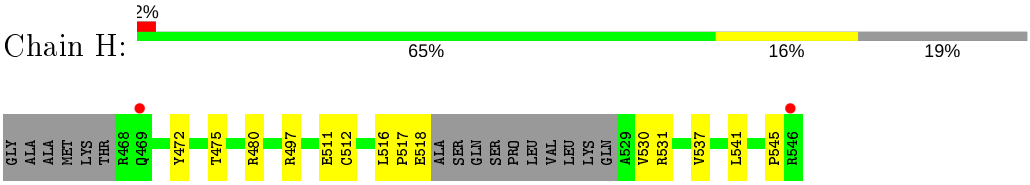
• Molecule 2: Metastasis-associated protein MTA1

Chain F:



• Molecule 2: Metastasis-associated protein MTA1

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.23Å 150.35Å 95.69Å 90.00° 94.99° 90.00°	Depositor
Resolution (Å)	95.33 – 2.80 81.92 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.0 (95.33-2.80) 95.0 (81.92-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.28 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.224 , 0.263 0.227 , 0.262	Depositor DCC
R_{free} test set	2719 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	58.4	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 33.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14642	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.60	0/3176	0.68	0/4328
1	C	0.59	0/3176	0.69	0/4328
1	E	0.64	0/3172	0.74	0/4324
1	G	0.65	0/3172	0.70	0/4324
2	B	0.66	0/584	0.73	0/791
2	D	0.61	0/588	0.76	0/796
2	F	0.67	0/588	0.81	0/796
2	H	0.67	0/582	0.81	0/789
All	All	0.63	0/15038	0.72	0/20476

There are no bond length outliers.

There are no bond angle outliers.

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	3091	0	2940	31	0
1	C	3091	0	2940	29	0
1	E	3087	0	2929	36	0
1	G	3087	0	2929	49	0
2	B	570	0	597	8	0
2	D	574	0	601	10	0
2	F	574	0	601	17	0
2	H	568	0	590	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14642	0	14127	153	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 5.

All (153) 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:G:208:SER:O	1:G:210:VAL:HG23	1.63	0.97
1:E:171:LEU:HD21	1:G:211:PRO:HG3	1.63	0.79
1:G:114:LYS:HE3	2:H:472:TYR:CE1	2.19	0.77
1:G:210:VAL:H	1:G:211:PRO:CD	2.02	0.72
1:C:56:PRO:HB2	1:C:59:LYS:HB2	1.70	0.72
1:A:179:GLU:HG2	1:A:198:ASP:HB3	1.72	0.72
1:E:11:ALA:O	1:E:15:ARG:HG3	1.89	0.71
1:G:42:TRP:HB2	1:G:70:THR:HG23	1.72	0.71
1:G:162:ASP:CG	1:G:163:PRO:HD3	2.12	0.70
1:G:174:ARG:HD3	1:G:176:HIS:O	1.91	0.70
1:C:36:MET:CE	1:C:86:LEU:HD23	2.22	0.69
1:G:114:LYS:HE3	2:H:472:TYR:CZ	2.29	0.68
1:G:210:VAL:N	1:G:211:PRO:CD	2.56	0.68
1:E:396:ASP:C	1:E:397:ASN:HD22	1.97	0.67
1:G:206:ASP:O	1:G:210:VAL:HG21	1.94	0.67
1:G:42:TRP:CB	1:G:70:THR:HG23	2.27	0.65
2:B:538:LEU:O	2:B:542:GLU:HG2	1.97	0.63
1:C:396:ASP:C	1:C:397:ASN:HD22	2.02	0.63
1:G:114:LYS:HE3	2:H:472:TYR:CD1	2.33	0.62
1:G:162:ASP:OD1	1:G:163:PRO:HD3	1.99	0.62
1:A:359:ALA:HB1	2:F:545:PRO:CB	2.32	0.60
1:C:13:GLU:HA	1:C:16:VAL:HG23	1.84	0.59
1:C:64:HIS:CD2	1:C:86:LEU:HD12	2.37	0.59
1:G:153:ASP:OD1	1:G:155:THR:HG22	2.03	0.59
2:B:543:THR:OG1	1:E:354:GLN:O	2.21	0.58
1:E:18:ASN:ND2	2:F:468:ARG:HH21	2.01	0.58
1:E:111:VAL:HG13	2:F:472:TYR:HB2	1.85	0.57
1:C:111:VAL:HG13	2:D:472:TYR:HB2	1.85	0.57
1:A:166:GLU:HG3	1:A:168:ASN:ND2	2.20	0.56
1:C:55:ARG:O	1:C:56:PRO:O	2.24	0.56
2:D:486:CYS:SG	2:D:511:GLU:HG2	2.46	0.56
1:G:208:SER:O	1:G:210:VAL:N	2.39	0.56
1:C:20:GLU:OE1	1:C:340:ARG:NH2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:LEU:HD21	1:G:211:PRO:CG	2.33	0.55
2:H:537:VAL:HG12	2:H:541:LEU:HD13	1.89	0.55
1:E:205:TRP:CE2	1:G:173:LEU:HB3	2.41	0.55
1:G:162:ASP:OD1	1:G:162:ASP:N	2.39	0.55
1:C:36:MET:HE1	1:C:86:LEU:HD23	1.89	0.54
1:E:397:ASN:N	1:E:397:ASN:HD22	2.05	0.54
1:G:210:VAL:H	1:G:211:PRO:HD3	1.73	0.54
1:G:111:VAL:HA	1:G:114:LYS:HD2	1.90	0.54
1:E:210:VAL:HG11	1:G:171:LEU:HD21	1.90	0.53
1:G:87:PRO:HG3	2:H:472:TYR:OH	2.08	0.53
1:E:32:TYR:O	2:F:475:THR:HG21	2.08	0.53
1:C:238:LEU:HD12	1:C:286:GLU:HB3	1.90	0.53
1:E:20:GLU:OE1	1:E:340:ARG:NH2	2.41	0.53
1:E:72:THR:H	1:E:77:ASN:HD21	1.56	0.53
1:E:36:MET:CE	1:E:86:LEU:HD23	2.39	0.53
1:A:64:HIS:CE1	1:A:86:LEU:HD12	2.44	0.52
1:C:36:MET:HE2	1:C:86:LEU:HD23	1.89	0.52
1:G:20:GLU:OE1	1:G:340:ARG:NH2	2.41	0.52
1:A:20:GLU:OE1	1:A:340:ARG:NH2	2.42	0.52
1:A:111:VAL:HG13	2:B:472:TYR:HB2	1.91	0.52
1:E:36:MET:HE1	1:E:86:LEU:HD23	1.92	0.52
1:G:210:VAL:H	1:G:211:PRO:HD2	1.73	0.51
2:F:538:LEU:O	2:F:542:GLU:HG2	2.11	0.50
1:G:347:LEU:HB3	2:H:537:VAL:HG11	1.93	0.50
1:C:59:LYS:HD2	1:C:61:PHE:CE1	2.47	0.49
1:A:151:VAL:HB	1:C:171:LEU:HB2	1.94	0.49
1:C:138:CYS:HA	1:C:154:TYR:CE2	2.48	0.49
2:F:545:PRO:O	2:F:545:PRO:HG2	2.12	0.49
1:C:396:ASP:O	1:C:397:ASN:HB2	2.13	0.49
1:A:338:THR:HA	1:A:376:LYS:HG3	1.94	0.48
1:A:64:HIS:ND1	1:A:86:LEU:HD12	2.27	0.48
2:F:479:THR:O	2:F:483:ARG:HG3	2.13	0.48
1:C:55:ARG:O	1:C:56:PRO:C	2.52	0.48
1:G:138:CYS:HA	1:G:154:TYR:CE2	2.47	0.48
1:G:214:GLY:O	1:G:216:VAL:N	2.46	0.48
1:C:199:ASP:OD1	1:C:199:ASP:N	2.39	0.48
1:C:32:TYR:O	2:D:475:THR:HG21	2.14	0.48
1:C:87:PRO:HG3	2:D:472:TYR:OH	2.14	0.48
2:D:515:ARG:O	2:D:515:ARG:HG2	2.14	0.48
1:G:338:THR:HA	1:G:376:LYS:HG3	1.95	0.48
1:A:254:ILE:CD1	1:A:254:ILE:N	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:HIS:ND1	1:C:147:SER:OG	2.45	0.48
1:G:184:SER:HG	1:G:235:TRP:HD1	1.59	0.47
2:H:475:THR:O	2:H:480:ARG:NH1	2.47	0.47
1:A:143:LYS:NZ	1:A:179:GLU:OE1	2.46	0.47
1:A:141:ALA:HB2	1:A:185:TRP:CZ2	2.49	0.47
1:A:359:ALA:HB2	2:F:545:PRO:HG3	1.96	0.47
1:G:214:GLY:C	1:G:216:VAL:N	2.67	0.47
1:A:71:HIS:CD2	1:A:71:HIS:O	2.68	0.47
1:E:406:GLU:HA	1:E:409:TYR:CE2	2.50	0.47
1:A:171:LEU:HD21	1:C:210:VAL:HG11	1.97	0.47
1:G:85:GLN:NE2	1:G:113:GLY:O	2.48	0.47
1:E:141:ALA:HB2	1:E:185:TRP:CZ2	2.50	0.47
1:G:141:ALA:HB2	1:G:185:TRP:CZ2	2.50	0.47
1:G:72:THR:H	1:G:77:ASN:HD21	1.63	0.47
1:G:32:TYR:O	2:H:475:THR:HG21	2.15	0.47
1:E:10:ASP:HB2	1:E:11:ALA:H	1.55	0.46
2:F:516:LEU:N	2:F:517:PRO:HD2	2.30	0.46
2:B:534:LEU:HA	2:B:537:VAL:CG1	2.46	0.46
1:G:160:LYS:HZ3	1:G:160:LYS:CB	2.28	0.46
1:C:397:ASN:HD22	1:C:397:ASN:N	2.13	0.46
2:F:544:HIS:N	2:F:545:PRO:HD3	2.30	0.46
1:A:254:ILE:HD12	1:A:254:ILE:N	2.31	0.46
1:G:160:LYS:HZ3	1:G:160:LYS:HB3	1.81	0.46
1:G:114:LYS:HE3	2:H:472:TYR:CE2	2.50	0.45
1:G:208:SER:O	1:G:209:ALA:C	2.54	0.45
1:G:243:PHE:CE1	1:G:255:TRP:CD1	3.04	0.45
1:E:64:HIS:CE1	1:E:86:LEU:HD12	2.52	0.45
1:G:210:VAL:N	1:G:211:PRO:HD2	2.30	0.45
1:C:278:CYS:SG	1:C:323:VAL:HG12	2.57	0.45
1:C:406:GLU:HA	1:C:409:TYR:CE2	2.52	0.45
1:E:338:THR:HA	1:E:376:LYS:HG3	1.99	0.45
1:E:64:HIS:CD2	1:E:383:ASN:HD21	2.36	0.44
2:D:478:LEU:O	2:D:481:ILE:HG12	2.17	0.44
1:E:18:ASN:ND2	2:F:468:ARG:NH2	2.64	0.44
1:A:278:CYS:SG	1:A:323:VAL:HG12	2.57	0.44
1:G:406:GLU:HA	1:G:409:TYR:CE2	2.53	0.43
1:C:36:MET:CE	1:C:86:LEU:CD2	2.95	0.43
1:E:218:ASP:OD1	1:G:174:ARG:HD2	2.18	0.43
1:G:396:ASP:O	1:G:397:ASN:HB2	2.19	0.43
2:D:515:ARG:HB2	2:D:515:ARG:NH1	2.33	0.43
1:E:162:ASP:HB3	1:E:163:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:545:PRO:HD3	1:E:359:ALA:HB1	2.01	0.43
1:C:141:ALA:HB2	1:C:185:TRP:CZ2	2.54	0.42
1:A:64:HIS:CD2	1:A:383:ASN:HD21	2.36	0.42
2:F:477:LYS:O	2:F:481:ILE:HG12	2.19	0.42
2:H:512:CYS:O	2:H:516:LEU:HB2	2.19	0.42
2:B:516:LEU:N	2:B:517:PRO:HD2	2.35	0.42
1:E:139:ILE:C	1:E:140:ILE:HD12	2.40	0.42
1:E:18:ASN:HD21	2:F:468:ARG:HH21	1.67	0.42
1:G:404:MET:CE	1:G:408:ILE:CG2	2.97	0.42
1:A:189:LEU:HD13	1:A:192:HIS:CE1	2.55	0.42
1:E:76:GLN:HB2	1:E:166:GLU:HG2	2.01	0.42
1:A:360:GLU:HA	1:E:308:LEU:HD13	2.01	0.42
2:D:477:LYS:N	2:D:477:LYS:HD3	2.34	0.42
2:D:532:LYS:HG2	2:D:536:ALA:HB3	2.02	0.42
1:E:243:PHE:CE1	1:E:255:TRP:CD1	3.07	0.42
1:A:360:GLU:OE2	1:E:307:LYS:HE3	2.20	0.42
1:E:396:ASP:O	1:E:397:ASN:HB2	2.20	0.42
1:A:359:ALA:CB	2:F:545:PRO:CB	2.98	0.42
1:G:197:SER:OG	1:G:199:ASP:OD1	2.37	0.42
1:A:396:ASP:O	1:A:397:ASN:HB2	2.20	0.41
1:C:338:THR:HA	1:C:376:LYS:HG3	2.01	0.41
1:E:169:PRO:O	1:G:215:LYS:HD3	2.20	0.41
1:E:64:HIS:ND1	1:E:86:LEU:HD12	2.36	0.41
2:F:544:HIS:N	2:F:545:PRO:CD	2.84	0.41
1:A:359:ALA:HB1	2:F:545:PRO:HB2	2.01	0.41
1:A:150:LEU:HD22	1:C:169:PRO:CB	2.51	0.41
1:A:366:LEU:O	2:B:497:ARG:HD3	2.21	0.41
1:G:183:LEU:HD12	1:G:193:LEU:HD21	2.02	0.41
1:G:214:GLY:C	1:G:216:VAL:H	2.23	0.41
2:D:511:GLU:CD	2:D:515:ARG:HH12	2.24	0.41
1:C:48:GLN:OE1	1:C:131:ARG:HA	2.21	0.41
2:B:478:LEU:HD22	2:B:481:ILE:HD11	2.03	0.40
1:E:140:ILE:HD12	1:E:140:ILE:N	2.36	0.40
1:A:359:ALA:HB1	2:F:545:PRO:HB3	2.03	0.40
1:A:360:GLU:HG3	1:E:308:LEU:HD13	2.03	0.40
1:A:55:ARG:HB3	1:A:55:ARG:CZ	2.52	0.40
1:G:114:LYS:HE3	2:H:472:TYR:CG	2.57	0.40
1:A:388:TRP:CZ2	1:A:409:TYR:HB2	2.57	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	385/425 (91%)	369 (96%)	15 (4%)	1 (0%)	41 72
1	C	385/425 (91%)	367 (95%)	16 (4%)	2 (0%)	29 61
1	E	385/425 (91%)	368 (96%)	17 (4%)	0	100 100
1	G	385/425 (91%)	360 (94%)	21 (6%)	4 (1%)	15 44
2	B	65/85 (76%)	62 (95%)	3 (5%)	0	100 100
2	D	65/85 (76%)	62 (95%)	2 (3%)	1 (2%)	10 33
2	F	65/85 (76%)	61 (94%)	4 (6%)	0	100 100
2	H	65/85 (76%)	62 (95%)	1 (2%)	2 (3%)	4 14
All	All	1800/2040 (88%)	1711 (95%)	79 (4%)	10 (1%)	25 56

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	209	ALA
1	C	56	PRO
2	D	504	ASN
1	G	215	LYS
1	A	315	SER
1	C	315	SER
1	G	315	SER
2	H	545	PRO
1	G	211	PRO
2	H	517	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	347/375 (92%)	338 (97%)	9 (3%)	46 79
1	C	347/375 (92%)	336 (97%)	11 (3%)	39 73
1	E	346/375 (92%)	330 (95%)	16 (5%)	27 60
1	G	346/375 (92%)	334 (96%)	12 (4%)	36 70
2	B	58/71 (82%)	56 (97%)	2 (3%)	37 71
2	D	59/71 (83%)	53 (90%)	6 (10%)	7 22
2	F	59/71 (83%)	56 (95%)	3 (5%)	24 55
2	H	58/71 (82%)	53 (91%)	5 (9%)	10 30
All	All	1620/1784 (91%)	1556 (96%)	64 (4%)	31 65

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	THR
1	A	55	ARG
1	A	111	VAL
1	A	143	LYS
1	A	168	ASN
1	A	179	GLU
1	A	254	ILE
1	A	360	GLU
1	A	411	ASP
2	B	481	ILE
2	B	537	VAL
1	C	16	VAL
1	C	53	VAL
1	C	54	THR
1	C	73	SER
1	C	111	VAL
1	C	150	LEU
1	C	164	SER
1	C	215	LYS
1	C	266	SER
1	C	397	ASN
1	C	411	ASP
2	D	473	LEU
2	D	477	LYS

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Mol	Chain	Res	Type
2	D	481	ILE
2	D	497	ARG
2	D	511	GLU
2	D	516	LEU
1	E	10	ASP
1	E	53	VAL
1	E	54	THR
1	E	74	ASP
1	E	111	VAL
1	E	124	GLU
1	E	126	GLU
1	E	147	SER
1	E	150	LEU
1	E	179	GLU
1	E	212	LYS
1	E	242	LEU
1	E	266	SER
1	E	353	GLU
1	E	397	ASN
1	E	411	ASP
2	F	473	LEU
2	F	545	PRO
2	F	546	ARG
1	G	54	THR
1	G	111	VAL
1	G	160	LYS
1	G	166	GLU
1	G	169	PRO
1	G	179	GLU
1	G	197	SER
1	G	213	GLU
1	G	242	LEU
1	G	266	SER
1	G	308	LEU
1	G	411	ASP
2	H	497	ARG
2	H	511	GLU
2	H	518	GLU
2	H	530	VAL
2	H	531	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	71	HIS
1	A	168	ASN
1	A	177	GLN
1	A	200	HIS
2	B	498	HIS
1	C	397	ASN
1	E	18	ASN
1	E	64	HIS
1	E	76	GLN
1	E	77	ASN
1	E	272	HIS
1	E	397	ASN
1	G	18	ASN
1	G	64	HIS
1	G	71	HIS
1	G	77	ASN
1	G	88	ASN
1	G	239	HIS
1	G	272	HIS
1	G	328	HIS
1	G	385	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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^{th} 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^2)	Q<0.9
1	A	389/425 (91%)	0.25	5 (1%)	77	72	38, 54, 83, 110	0
1	C	389/425 (91%)	0.19	12 (3%)	49	39	40, 57, 83, 105	0
1	E	389/425 (91%)	0.32	11 (2%)	53	43	34, 52, 88, 120	0
1	G	389/425 (91%)	0.29	17 (4%)	34	24	37, 57, 86, 109	0
2	B	69/85 (81%)	0.15	2 (2%)	51	41	43, 58, 77, 89	0
2	D	69/85 (81%)	0.04	2 (2%)	51	41	41, 57, 91, 108	0
2	F	69/85 (81%)	0.16	2 (2%)	51	41	36, 58, 87, 119	0
2	H	69/85 (81%)	0.19	2 (2%)	51	41	30, 52, 79, 99	0
All	All	1832/2040 (89%)	0.25	53 (2%)	51	41	30, 56, 86, 120	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	57	GLU	5.9
2	F	546	ARG	5.5
1	G	89	ASP	5.4
1	C	58	GLY	5.3
1	G	211	PRO	4.8
1	E	165	GLY	4.8
1	G	213	GLU	4.6
1	G	165	GLY	4.5
1	E	212	LYS	4.3
2	H	546	ARG	4.1
1	G	167	CYS	3.9
1	A	166	GLU	3.8
1	G	166	GLU	3.5
1	C	73	SER	3.4
1	G	212	LYS	3.2
2	B	542	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	212	LYS	3.1
1	C	211	PRO	3.1
1	G	162	ASP	3.0
1	G	57	GLU	3.0
1	G	58	GLY	3.0
1	C	53	VAL	2.9
1	G	214	GLY	2.9
1	E	166	GLU	2.8
1	C	54	THR	2.8
1	E	55	ARG	2.8
1	E	213	GLU	2.8
2	D	546	ARG	2.6
1	E	316	HIS	2.6
2	D	529	ALA	2.6
1	E	164	SER	2.5
1	C	166	GLU	2.5
1	C	103	GLY	2.5
1	E	118	GLU	2.5
1	E	177	GLN	2.5
1	A	164	SER	2.5
1	G	121	ILE	2.5
1	A	207	ILE	2.4
1	E	237	LEU	2.3
2	H	469	GLN	2.3
1	G	122	ASN	2.3
1	G	177	GLN	2.3
1	C	163	PRO	2.3
2	F	485	LEU	2.3
1	C	55	ARG	2.3
1	G	117	ILE	2.2
1	C	165	GLY	2.2
1	G	159	SER	2.1
1	A	167	CYS	2.1
1	A	213	GLU	2.1
1	E	359	ALA	2.0
1	G	116	GLU	2.0
2	B	539	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.