



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:49 AM UTC

PDB ID : 6MD3 / pdb_00006md3
Title : Structure of T. brucei RRP44 PIN domain
Authors : Guimaraes, B.G.; Cesaro, G.
Deposited on : 2018-09-03
Resolution : 2.29 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 types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

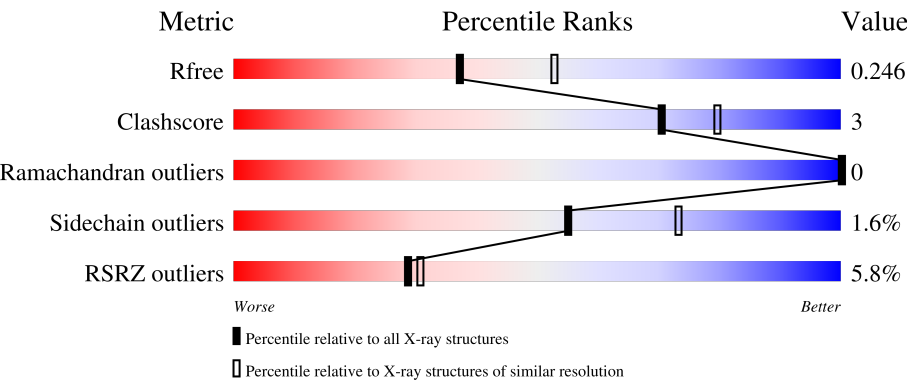
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.29 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 ≥ 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	203	4% 74% 9% 16%
1	B	203	2% 73% 12% 14%
1	C	203	5% 76% 12% 11%
1	D	203	7% 71% 10% 19%
1	E	203	8% 74% 9% 17%

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Mol	Chain	Length	Quality of chain
1	F	203	3% 78% 10% 12%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8635 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 Rrp44p homologue.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	170	Total	C	N	O	S	18	0	0
			1303	813	233	243	14			
1	B	174	Total	C	N	O	S	11	0	0
			1332	828	239	251	14			
1	C	180	Total	C	N	O	S	7	0	0
			1379	856	248	261	14			
1	D	165	Total	C	N	O	S	37	0	0
			1265	793	226	232	14			
1	E	168	Total	C	N	O	S	39	0	0
			1290	806	233	237	14			
1	F	179	Total	C	N	O	S	22	0	0
			1369	849	246	260	14			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	LEU	-	expression tag	UNP Q95Z12
A	220	GLU	-	expression tag	UNP Q95Z12
A	221	HIS	-	expression tag	UNP Q95Z12
A	222	HIS	-	expression tag	UNP Q95Z12
A	223	HIS	-	expression tag	UNP Q95Z12
A	224	HIS	-	expression tag	UNP Q95Z12
A	225	HIS	-	expression tag	UNP Q95Z12
A	226	HIS	-	expression tag	UNP Q95Z12
B	219	LEU	-	expression tag	UNP Q95Z12
B	220	GLU	-	expression tag	UNP Q95Z12
B	221	HIS	-	expression tag	UNP Q95Z12
B	222	HIS	-	expression tag	UNP Q95Z12
B	223	HIS	-	expression tag	UNP Q95Z12
B	224	HIS	-	expression tag	UNP Q95Z12
B	225	HIS	-	expression tag	UNP Q95Z12
B	226	HIS	-	expression tag	UNP Q95Z12
C	219	LEU	-	expression tag	UNP Q95Z12

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Chain	Residue	Modelled	Actual	Comment	Reference
C	220	GLU	-	expression tag	UNP Q95Z12
C	221	HIS	-	expression tag	UNP Q95Z12
C	222	HIS	-	expression tag	UNP Q95Z12
C	223	HIS	-	expression tag	UNP Q95Z12
C	224	HIS	-	expression tag	UNP Q95Z12
C	225	HIS	-	expression tag	UNP Q95Z12
C	226	HIS	-	expression tag	UNP Q95Z12
D	219	LEU	-	expression tag	UNP Q95Z12
D	220	GLU	-	expression tag	UNP Q95Z12
D	221	HIS	-	expression tag	UNP Q95Z12
D	222	HIS	-	expression tag	UNP Q95Z12
D	223	HIS	-	expression tag	UNP Q95Z12
D	224	HIS	-	expression tag	UNP Q95Z12
D	225	HIS	-	expression tag	UNP Q95Z12
D	226	HIS	-	expression tag	UNP Q95Z12
E	219	LEU	-	expression tag	UNP Q95Z12
E	220	GLU	-	expression tag	UNP Q95Z12
E	221	HIS	-	expression tag	UNP Q95Z12
E	222	HIS	-	expression tag	UNP Q95Z12
E	223	HIS	-	expression tag	UNP Q95Z12
E	224	HIS	-	expression tag	UNP Q95Z12
E	225	HIS	-	expression tag	UNP Q95Z12
E	226	HIS	-	expression tag	UNP Q95Z12
F	219	LEU	-	expression tag	UNP Q95Z12
F	220	GLU	-	expression tag	UNP Q95Z12
F	221	HIS	-	expression tag	UNP Q95Z12
F	222	HIS	-	expression tag	UNP Q95Z12
F	223	HIS	-	expression tag	UNP Q95Z12
F	224	HIS	-	expression tag	UNP Q95Z12
F	225	HIS	-	expression tag	UNP Q95Z12
F	226	HIS	-	expression tag	UNP Q95Z12

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mn 2 2	0	0
2	B	2	Total Mn 2 2	0	0
2	C	2	Total Mn 2 2	0	0
2	D	2	Total Mn 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	2	Total 2	Mn 2	0	0
2	F	2	Total 2	Mn 2	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Zn 2	0	0
3	B	2	Total 2	Zn 2	0	0
3	C	2	Total 2	Zn 2	0	0
3	D	2	Total 2	Zn 2	0	0
3	E	2	Total 2	Zn 2	0	0
3	F	2	Total 2	Zn 2	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total 3	Cl 3	0	0
4	B	2	Total 2	Cl 2	0	0
4	C	1	Total 1	Cl 1	0	0
4	D	1	Total 1	Cl 1	0	0
4	E	1	Total 1	Cl 1	0	0
4	F	3	Total 3	Cl 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	113	Total 113	O 113	0	0

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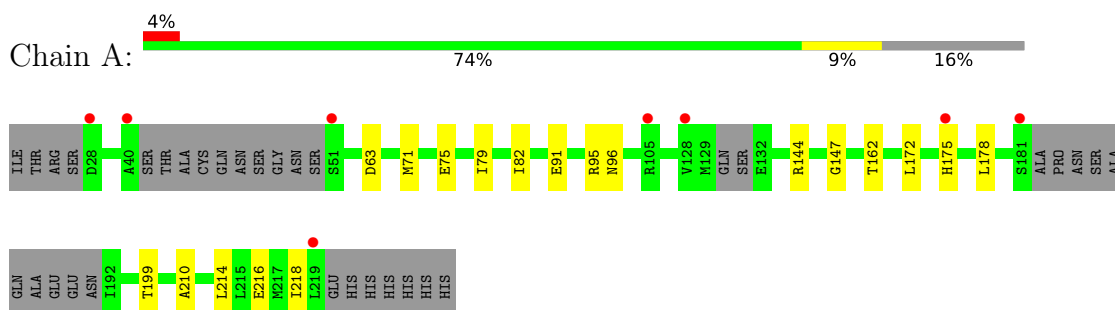
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	160	Total 160	O 160	0	0
5	C	130	Total 130	O 130	0	0
5	D	66	Total 66	O 66	0	0
5	E	64	Total 64	O 64	0	0
5	F	129	Total 129	O 129	0	0

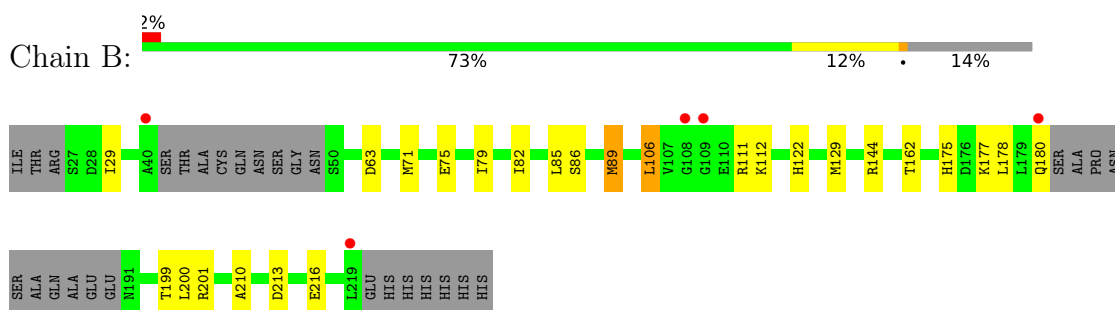
3 Residue-property plots [i](#)

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.

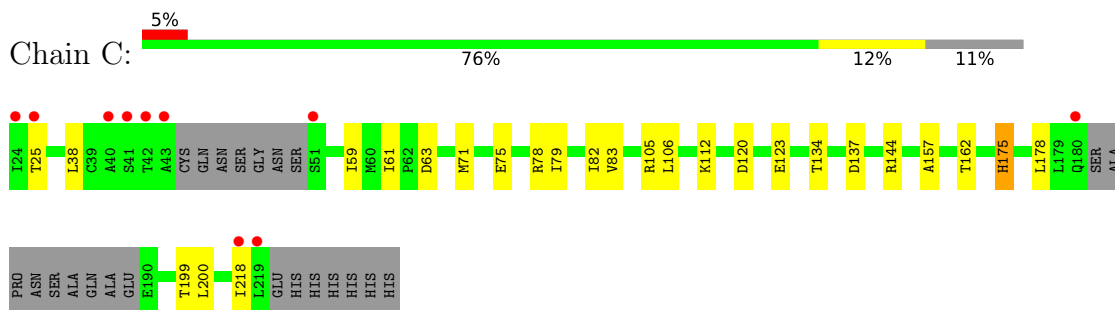
- Molecule 1: Rrp44p homologue



- Molecule 1: Rrp44p homologue

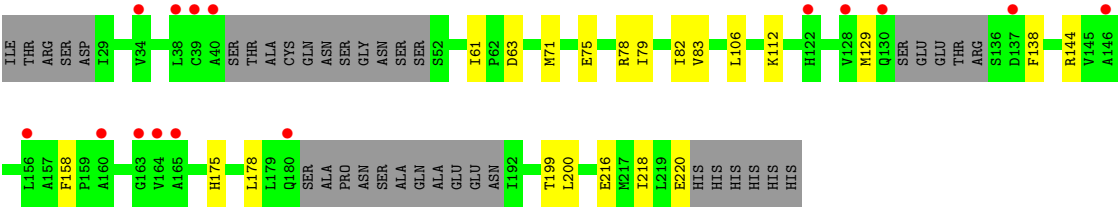


- Molecule 1: Rrp44p homologue

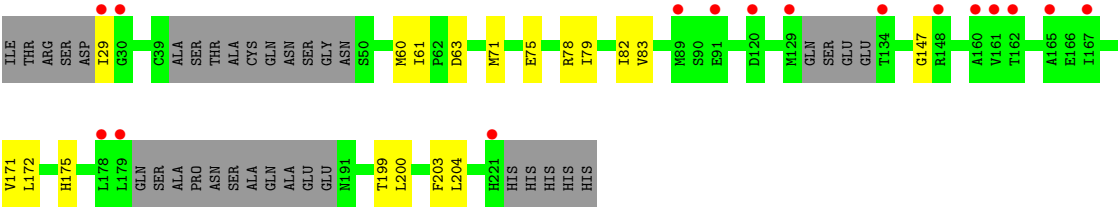


- Molecule 1: Rrp44p homologue

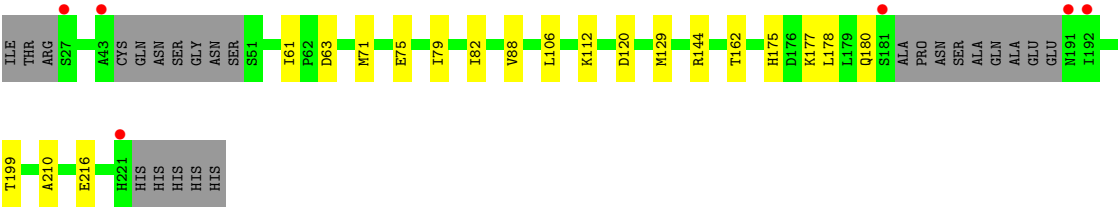
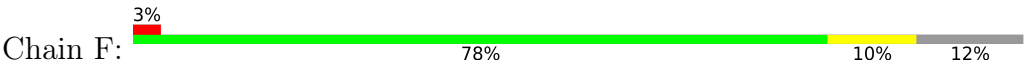




● Molecule 1: Rrp44p homologue



● Molecule 1: Rrp44p homologue



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	89.57Å 89.57Å 321.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.91 – 2.29 45.91 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.91-2.29) 99.7 (45.91-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.200 , 0.230 0.208 , 0.246	Depositor DCC
R_{free} test set	3229 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	58.5	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 72.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.148 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8635	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CL, ZN, MN

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	0.87	0/1318	1.45	4/1782 (0.2%)
1	B	0.93	1/1348 (0.1%)	1.46	9/1824 (0.5%)
1	C	0.90	0/1395	1.45	4/1888 (0.2%)
1	D	0.85	0/1280	1.45	5/1731 (0.3%)
1	E	0.84	0/1306	1.43	3/1766 (0.2%)
1	F	0.90	1/1386 (0.1%)	1.42	6/1876 (0.3%)
All	All	0.88	2/8033 (0.0%)	1.44	31/10867 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	129	MET	SD-CE	-5.72	1.65	1.79
1	F	129	MET	SD-CE	-5.63	1.65	1.79

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	63	ASP	CA-CB-CG	7.09	119.69	112.60
1	C	63	ASP	CA-CB-CG	6.76	119.36	112.60
1	B	63	ASP	CA-CB-CG	6.49	119.09	112.60
1	F	63	ASP	CA-CB-CG	6.48	119.08	112.60
1	E	63	ASP	CA-CB-CG	6.44	119.04	112.60
1	F	88	VAL	CA-C-N	6.03	128.28	120.44
1	F	88	VAL	C-N-CA	6.03	128.28	120.44
1	A	63	ASP	CA-CB-CG	5.88	118.48	112.60
1	D	200	LEU	CA-C-N	5.85	128.05	120.44
1	D	200	LEU	C-N-CA	5.85	128.05	120.44
1	A	96	ASN	CA-C-N	5.84	128.37	120.65
1	A	96	ASN	C-N-CA	5.84	128.37	120.65
1	B	89	MET	CA-C-N	5.67	127.87	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	89	MET	C-N-CA	5.67	127.87	120.28
1	C	200	LEU	CA-C-N	5.66	127.80	120.44
1	C	200	LEU	C-N-CA	5.66	127.80	120.44
1	F	216	GLU	CA-C-N	5.52	127.67	120.28
1	F	216	GLU	C-N-CA	5.52	127.67	120.28
1	D	216	GLU	CA-C-N	5.29	127.38	120.28
1	D	216	GLU	C-N-CA	5.29	127.38	120.28
1	B	216	GLU	CB-CG-CD	5.26	121.55	112.60
1	C	120	ASP	CA-CB-CG	5.17	117.77	112.60
1	E	200	LEU	CA-C-N	5.12	127.10	120.44
1	E	200	LEU	C-N-CA	5.12	127.10	120.44
1	B	200	LEU	CA-C-N	5.11	127.09	120.44
1	B	200	LEU	C-N-CA	5.11	127.09	120.44
1	B	106	LEU	CA-C-N	5.11	128.05	120.74
1	B	106	LEU	C-N-CA	5.11	128.05	120.74
1	F	120	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	216	GLU	CB-CG-CD	5.04	121.17	112.60
1	B	213	ASP	CA-CB-CG	5.03	117.63	112.60

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	1303	0	1316	8	0
1	B	1332	0	1341	11	0
1	C	1379	0	1390	13	0
1	D	1265	0	1284	9	0
1	E	1290	0	1306	12	0
1	F	1369	0	1371	7	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	2	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	3	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	3	0	0	0	0
5	A	113	0	0	0	0
5	B	160	0	0	1	0
5	C	130	0	0	0	0
5	D	66	0	0	0	0
5	E	64	0	0	2	0
5	F	129	0	0	0	0
All	All	8635	0	8008	54	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 3.

All (54) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ILE:HG22	1:A:82:ILE:HD11	1.81	0.61
5:B:401:HOH:O	1:C:105:ARG:HG3	2.03	0.58
1:C:25:THR:HB	1:C:123:GLU:HG2	1.86	0.58
1:C:61:ILE:HG12	1:C:83:VAL:HB	1.85	0.57
1:A:71:MET:HE3	1:A:75:GLU:HG3	1.88	0.56
1:B:177:LYS:HB3	1:B:180:GLN:HB2	1.88	0.56
1:B:79:ILE:HG22	1:B:82:ILE:HD11	1.87	0.56
1:C:71:MET:HE3	1:C:75:GLU:HG3	1.88	0.56
1:D:61:ILE:HG12	1:D:83:VAL:HB	1.88	0.55
1:F:71:MET:HE3	1:F:75:GLU:HG3	1.90	0.54
1:F:79:ILE:HG22	1:F:82:ILE:HD11	1.90	0.53
1:A:147:GLY:HA3	1:A:172:LEU:HD21	1.90	0.53
1:E:71:MET:HE3	1:E:75:GLU:HG3	1.91	0.53
1:C:106:LEU:HD22	1:C:112:LYS:HD3	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:177:LYS:HB3	1:F:180:GLN:HB2	1.90	0.52
1:E:60:MET:HE1	1:E:79:ILE:HG23	1.92	0.51
1:C:134:THR:HG22	1:C:137:ASP:CG	2.35	0.51
1:F:106:LEU:HD22	1:F:112:LYS:HD3	1.93	0.51
1:D:106:LEU:HD22	1:D:112:LYS:HD3	1.93	0.51
1:F:144:ARG:HD3	1:F:178:LEU:O	2.12	0.50
1:B:144:ARG:HD3	1:B:178:LEU:O	2.12	0.49
1:C:144:ARG:HD3	1:C:178:LEU:O	2.13	0.49
1:C:79:ILE:HG22	1:C:82:ILE:HD11	1.93	0.49
1:C:78:ARG:HD3	1:F:210:ALA:HB1	1.94	0.48
1:E:79:ILE:HG22	1:E:82:ILE:HD11	1.96	0.48
1:A:144:ARG:HD3	1:A:178:LEU:O	2.14	0.47
1:D:144:ARG:HD3	1:D:178:LEU:O	2.13	0.47
1:E:61:ILE:HG12	1:E:83:VAL:HB	1.96	0.47
1:B:85:LEU:O	1:B:89:MET:HG2	2.14	0.47
1:C:38:LEU:HD22	1:C:157:ALA:HB2	1.96	0.47
1:D:71:MET:HE3	1:D:75:GLU:HG3	1.96	0.46
1:A:91:GLU:O	1:A:95:ARG:HG3	2.16	0.46
1:E:171:VAL:HB	5:E:453:HOH:O	2.17	0.45
1:A:214:LEU:HD21	1:E:79:ILE:HG13	1.99	0.44
1:C:175:HIS:HA	1:C:199:THR:HG22	1.99	0.44
1:F:175:HIS:HA	1:F:199:THR:HG22	1.99	0.44
1:B:29:ILE:HD13	1:B:122:HIS:HA	2.00	0.44
1:C:25:THR:CB	1:C:123:GLU:HG2	2.48	0.44
1:D:79:ILE:HG22	1:D:82:ILE:HD11	2.00	0.44
1:E:60:MET:HG3	5:E:453:HOH:O	2.18	0.43
1:E:147:GLY:HA3	1:E:172:LEU:HD21	2.01	0.43
1:A:175:HIS:HA	1:A:199:THR:HG22	2.01	0.42
1:B:71:MET:HE3	1:B:75:GLU:HG3	2.00	0.42
1:B:111:ARG:HH22	1:D:158:PHE:HB3	1.85	0.42
1:E:60:MET:HE2	1:E:203:PHE:CE2	2.55	0.42
1:D:129:MET:HG2	1:D:138:PHE:CD1	2.55	0.41
1:E:79:ILE:HD11	1:E:204:LEU:HD11	2.01	0.41
1:B:175:HIS:HA	1:B:199:THR:HG22	2.02	0.41
1:A:210:ALA:HB1	1:E:78:ARG:HD3	2.04	0.40
1:B:201:ARG:HG3	1:D:218:ILE:HD12	2.02	0.40
1:C:134:THR:HG22	1:C:137:ASP:OD2	2.22	0.40
1:B:210:ALA:HB1	1:D:78:ARG:HD3	2.03	0.40
1:B:106:LEU:HD11	1:B:112:LYS:HD3	2.02	0.40
1:E:175:HIS:HA	1:E:199:THR:HG22	2.02	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	162/203 (80%)	159 (98%)	3 (2%)	0	100	100
1	B	168/203 (83%)	166 (99%)	2 (1%)	0	100	100
1	C	174/203 (86%)	172 (99%)	2 (1%)	0	100	100
1	D	157/203 (77%)	153 (98%)	4 (2%)	0	100	100
1	E	160/203 (79%)	157 (98%)	3 (2%)	0	100	100
1	F	173/203 (85%)	170 (98%)	3 (2%)	0	100	100
All	All	994/1218 (82%)	977 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	146/174 (84%)	144 (99%)	2 (1%)	59	76
1	B	150/174 (86%)	148 (99%)	2 (1%)	61	77
1	C	155/174 (89%)	151 (97%)	4 (3%)	40	59
1	D	141/174 (81%)	138 (98%)	3 (2%)	47	66
1	E	145/174 (83%)	144 (99%)	1 (1%)	76	87
1	F	154/174 (88%)	152 (99%)	2 (1%)	61	77
All	All	891/1044 (85%)	877 (98%)	14 (2%)	55	73

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	THR
1	A	218	ILE
1	B	86	SER
1	B	162	THR
1	C	59	ILE
1	C	162	THR
1	C	175	HIS
1	C	218	ILE
1	D	175	HIS
1	D	199	THR
1	D	220	GLU
1	E	29	ILE
1	F	61	ILE
1	F	162	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	93	GLN
1	A	175	HIS
1	B	175	HIS
1	C	70	ASN
1	C	72	ASN
1	C	113	GLN
1	D	70	ASN
1	D	72	ASN
1	D	93	GLN
1	D	104	GLN
1	D	113	GLN
1	D	153	HIS
1	E	72	ASN
1	E	96	ASN
1	E	139	ASN
1	E	175	HIS
1	F	72	ASN
1	F	175	HIS
1	F	202	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 35 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, 95th 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	170/203 (83%)	0.54	8 (4%)	36 38	44, 63, 100, 114	4 (2%)
1	B	174/203 (85%)	0.28	5 (2%)	53 56	36, 52, 85, 119	3 (1%)
1	C	180/203 (88%)	0.37	10 (5%)	30 32	45, 55, 100, 114	2 (1%)
1	D	165/203 (81%)	0.85	15 (9%)	15 16	48, 74, 108, 132	9 (5%)
1	E	168/203 (82%)	0.87	16 (9%)	14 15	39, 77, 116, 148	10 (5%)
1	F	179/203 (88%)	0.33	6 (3%)	48 50	25, 57, 91, 121	6 (3%)
All	All	1036/1218 (85%)	0.53	60 (5%)	29 31	25, 62, 106, 148	34 (3%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	43	ALA	4.5
1	D	40	ALA	4.2
1	F	221	HIS	3.9
1	E	29	ILE	3.9
1	B	219	LEU	3.9
1	E	134	THR	3.7
1	D	180	GLN	3.6
1	D	164	VAL	3.5
1	A	219	LEU	3.5
1	A	105	ARG	3.3
1	A	40	ALA	3.2
1	E	160	ALA	3.2
1	E	221	HIS	3.1
1	C	43	ALA	3.1
1	C	219	LEU	3.0
1	F	181	SER	3.0
1	E	120	ASP	3.0
1	D	163	GLY	2.9
1	D	128	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	42	THR	2.9
1	D	38	LEU	2.9
1	D	156	LEU	2.9
1	C	24	ILE	2.9
1	D	130	GLN	2.7
1	D	165	ALA	2.7
1	F	27	SER	2.7
1	D	34	VAL	2.7
1	D	39	CYS	2.6
1	E	165	ALA	2.6
1	E	129	MET	2.6
1	E	162	THR	2.6
1	C	41	SER	2.6
1	B	40	ALA	2.5
1	C	25	THR	2.5
1	F	192	ILE	2.5
1	E	148	ARG	2.4
1	E	91	GLU	2.4
1	E	30	GLY	2.3
1	D	160	ALA	2.3
1	B	180	GLN	2.3
1	A	181	SER	2.3
1	E	161	VAL	2.3
1	F	191	ASN	2.3
1	B	108	GLY	2.3
1	D	122	HIS	2.2
1	C	40	ALA	2.2
1	C	51	SER	2.2
1	E	179	LEU	2.2
1	A	128	VAL	2.2
1	B	109	GLY	2.2
1	A	28	ASP	2.1
1	E	167	ILE	2.1
1	D	137	ASP	2.1
1	C	180	GLN	2.1
1	E	89	MET	2.1
1	E	178	LEU	2.1
1	A	51	SER	2.0
1	D	146	ALA	2.0
1	A	175	HIS	2.0
1	C	218	ILE	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 oligosaccharides 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, 95th 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	MN	E	301	1/1	0.80	0.13	167,167,167,167	0
3	ZN	F	304	1/1	0.82	0.23	178,178,178,178	0
3	ZN	C	304	1/1	0.83	0.24	147,147,147,147	0
2	MN	D	301	1/1	0.84	0.18	163,163,163,163	0
2	MN	F	301	1/1	0.84	0.15	131,131,131,131	0
3	ZN	D	303	1/1	0.85	0.18	253,253,253,253	0
3	ZN	D	304	1/1	0.86	0.21	143,143,143,143	0
4	CL	F	307	1/1	0.86	0.31	94,94,94,94	0
2	MN	E	302	1/1	0.87	0.24	132,132,132,132	0
4	CL	B	305	1/1	0.87	0.15	85,85,85,85	0
3	ZN	E	304	1/1	0.87	0.15	131,131,131,131	0
2	MN	B	301	1/1	0.89	0.17	96,96,96,96	0
4	CL	A	306	1/1	0.89	0.17	100,100,100,100	0
4	CL	A	307	1/1	0.90	0.12	97,97,97,97	0
2	MN	A	301	1/1	0.91	0.10	139,139,139,139	0
4	CL	B	306	1/1	0.92	0.14	96,96,96,96	0
4	CL	E	305	1/1	0.92	0.12	90,90,90,90	0
2	MN	C	301	1/1	0.92	0.10	135,135,135,135	0
2	MN	D	302	1/1	0.93	0.34	78,78,78,78	0
2	MN	A	302	1/1	0.94	0.25	102,102,102,102	0
4	CL	F	305	1/1	0.94	0.11	82,82,82,82	0
4	CL	F	306	1/1	0.94	0.10	79,79,79,79	0
4	CL	D	305	1/1	0.94	0.13	112,112,112,112	0
4	CL	C	305	1/1	0.95	0.10	73,73,73,73	0
3	ZN	B	304	1/1	0.95	0.14	111,111,111,111	0
3	ZN	A	304	1/1	0.95	0.14	133,133,133,133	0
3	ZN	A	303	1/1	0.97	0.16	60,60,60,60	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	F	302	1/1	0.97	0.20	89,89,89,89	0
3	ZN	C	303	1/1	0.98	0.14	60,60,60,60	1
3	ZN	E	303	1/1	0.98	0.08	132,132,132,132	0
2	MN	C	302	1/1	0.98	0.11	94,94,94,94	0
2	MN	B	302	1/1	0.98	0.08	68,68,68,68	0
4	CL	A	305	1/1	0.98	0.13	76,76,76,76	0
3	ZN	B	303	1/1	0.99	0.11	70,70,70,70	0
3	ZN	F	303	1/1	0.99	0.10	75,75,75,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.