



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:28 AM UTC

PDB ID : 3WTX / pdb_00003wtx
Title : Crystal structure of the complex comprised of ETS1(Y329A), RUNX1, CBF-BETA, and the tcralpha gene enhancer DNA
Authors : Shiina, M.; Hamada, K.; Ogata, K.
Deposited on : 2014-04-21
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 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

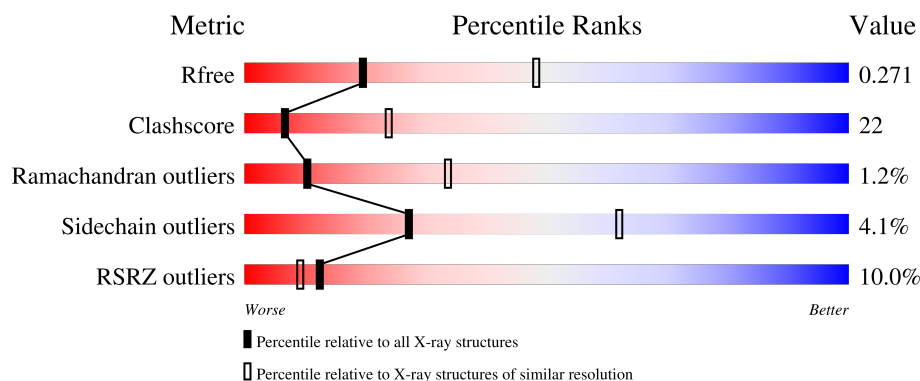
1 Overall quality at a glance

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 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	204	36% 20% • 42%
1	F	204	42% 15% • 42%
2	B	142	11% 50% 41% • 7%
2	G	142	12% 54% 35% • 8%
3	C	166	45% 16% • 38%

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Mol	Chain	Length	Quality of chain
3	H	166	23% 26% 33% 40%
4	D	15	93% 7%
4	I	15	13% 80% 7%
5	E	15	67% 33%
5	J	15	60% 40%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6940 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 Runt-related transcription factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	118	Total	C	N	O	S	0	0	0
			914	574	169	167	4			
1	F	118	Total	C	N	O	S	0	0	0
			914	574	169	167	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	LYS	LEU	engineered mutation	UNP Q03347
F	94	LYS	LEU	engineered mutation	UNP Q03347

- Molecule 2 is a protein called Core-binding factor subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	132	Total	C	N	O	S	0	0	0
			1083	678	197	202	6			
2	G	130	Total	C	N	O	S	0	0	0
			1068	669	194	199	6			

- Molecule 3 is a protein called Protein C-ets-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	103	Total	C	N	O	S	0	0	0
			873	566	150	153	4			
3	H	100	Total	C	N	O	S	0	0	0
			849	551	146	148	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	329	ALA	TYR	engineered mutation	UNP P14921
H	329	ALA	TYR	engineered mutation	UNP P14921

- Molecule 4 is a DNA chain called DNA (5'-D(*GP*AP*AP*GP*CP*CP*AP*CP*AP*TP*CP*CP*TP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	15	Total	C	N	O	P	0	0	0
			299	144	54	87	14			
4	I	15	Total	C	N	O	P	0	0	0
			299	144	54	87	14			

- Molecule 5 is a DNA chain called DNA (5'-D(*AP*GP*AP*GP*GP*AP*TP*GP*TP*GP*GP*CP*TP*TP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	15	Total	C	N	O	P	0	0	0
			310	148	59	89	14			
5	J	15	Total	C	N	O	P	0	0	0
			310	148	59	89	14			

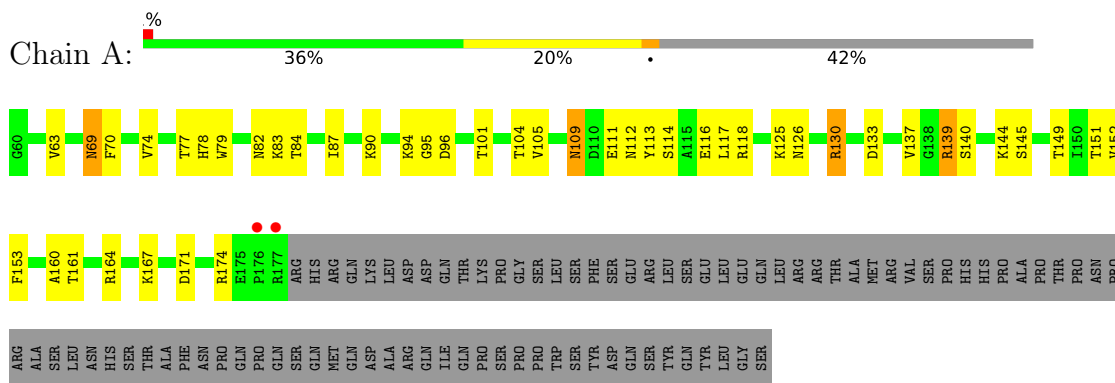
- Molecule 6 is water.

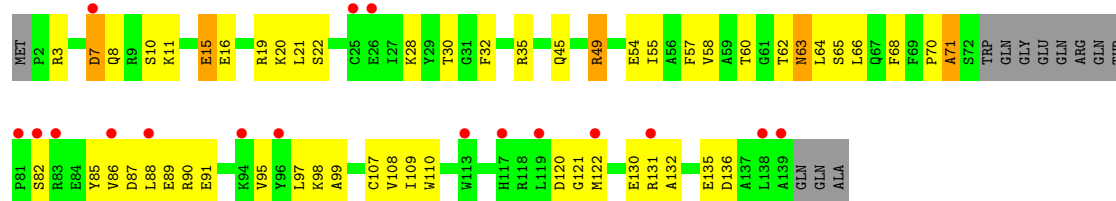
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total	O	0	0
			6	6		
6	B	2	Total	O	0	0
			2	2		
6	C	3	Total	O	0	0
			3	3		
6	F	4	Total	O	0	0
			4	4		
6	G	1	Total	O	0	0
			1	1		
6	E	2	Total	O	0	0
			2	2		
6	I	2	Total	O	0	0
			2	2		
6	J	1	Total	O	0	0
			1	1		

3 Residue-property plots [i](#)

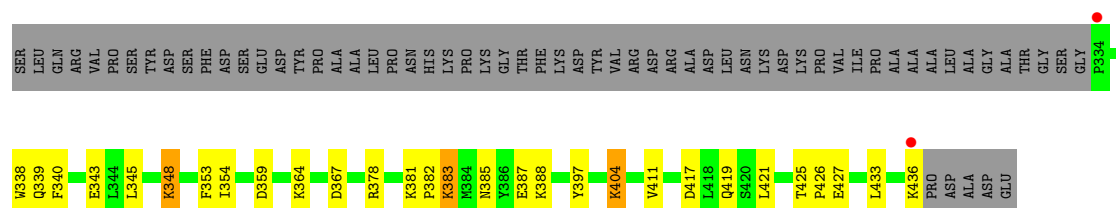
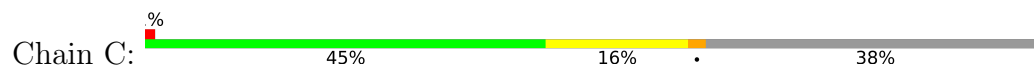
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Runt-related transcription factor 1

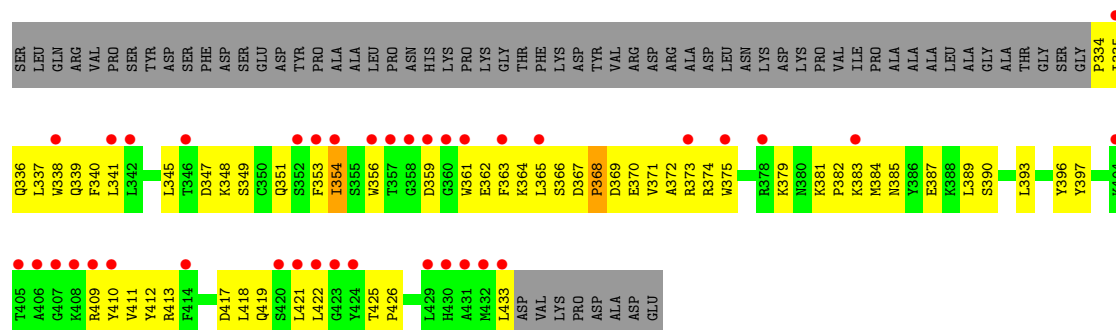
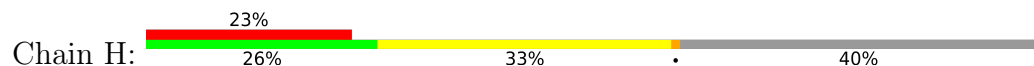




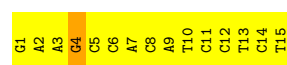
• Molecule 3: Protein C-ets-1



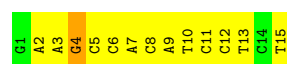
• Molecule 3: Protein C-ets-1



• Molecule 4: DNA (5'-D(*GP*AP*AP*GP*CP*CP*AP*CP*AP*TP*CP*CP*TP*CP*T)-3')



• Molecule 4: DNA (5'-D(*GP*AP*AP*GP*CP*CP*AP*CP*AP*TP*CP*CP*TP*CP*T)-3')



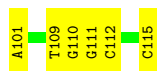
- Molecule 5: DNA (5'-D(*AP*GP*AP*GP*GP*AP*TP*GP*TP*GP*GP*CP*TP*TP*C)-3')

Chain E:  67% 33%



- Molecule 5: DNA (5'-D(*AP*GP*AP*GP*GP*AP*TP*GP*TP*GP*GP*CP*TP*TP*C)-3')

Chain J:  60% 40%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.73Å 101.99Å 194.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.18 – 2.80 45.18 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (45.18-2.80) 98.4 (45.18-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.55 (at 2.81Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.237 , 0.271 0.237 , 0.271	Depositor DCC
R_{free} test set	3891 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å ²)	60.7	Xtriage
Anisotropy	0.868	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6940	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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

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	0.51	0/933	0.84	0/1268
1	F	0.57	0/933	0.93	4/1268 (0.3%)
2	B	0.39	0/1105	0.78	1/1484 (0.1%)
2	G	0.41	0/1090	0.74	1/1462 (0.1%)
3	C	0.50	0/897	0.84	0/1207
3	H	0.35	0/873	0.72	0/1175
4	D	0.38	0/334	0.86	1/512 (0.2%)
4	I	0.38	0/334	0.87	1/512 (0.2%)
5	E	0.36	0/348	0.77	0/537
5	J	0.34	0/348	0.83	1/537 (0.2%)
All	All	0.44	0/7195	0.81	9/9962 (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
4	D	0	1
4	I	0	1
5	E	0	1
All	All	0	3

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	115	DC	C2'-C3'-O3'	6.31	120.97	111.50
2	B	31	GLY	N-CA-C	5.61	119.17	111.54
4	I	4	DG	N9-C1'-C2'	-5.51	105.23	113.50
1	F	97	VAL	CA-C-N	5.31	125.23	119.76
1	F	97	VAL	C-N-CA	5.31	125.23	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	70	PHE	N-CA-C	5.22	117.12	109.24
2	G	49	ARG	N-CA-C	-5.21	105.77	111.82
1	F	65	THR	N-CA-C	-5.05	103.27	110.59
4	D	4	DG	N9-C1'-C2'	-5.01	105.99	113.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	4	DG	Sidechain
5	E	113	DT	Sidechain
4	I	4	DG	Sidechain

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	914	0	922	40	0
1	F	914	0	922	33	0
2	B	1083	0	1042	58	0
2	G	1068	0	1031	47	0
3	C	873	0	871	21	0
3	H	849	0	845	65	0
4	D	299	0	170	18	0
4	I	299	0	170	15	0
5	E	310	0	171	3	0
5	J	310	0	171	5	0
6	A	6	0	0	0	0
6	B	2	0	0	0	0
6	C	3	0	0	0	0
6	E	2	0	0	0	0
6	F	4	0	0	0	0
6	G	1	0	0	0	0
6	I	2	0	0	0	0
6	J	1	0	0	0	0
All	All	6940	0	6315	285	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 22.

All (285) 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)
3:H:345:LEU:HB3	3:H:356:TRP:HE1	1.37	0.89
3:H:362:GLU:HB2	3:H:413:ARG:HH11	1.41	0.86
3:H:359:ASP:HB3	3:H:362:GLU:HB3	1.61	0.83
3:H:375:TRP:HD1	3:H:384:MET:HE2	1.44	0.82
3:H:348:LYS:HA	3:H:351:GLN:HE21	1.46	0.81
2:B:60:THR:HG23	2:B:62:THR:H	1.47	0.78
4:I:10:DT:H2''	4:I:11:DC:H5'	1.65	0.77
2:G:35:ARG:HA	2:G:35:ARG:HH11	1.50	0.76
1:A:109:ASN:ND2	1:A:112:ASN:H	1.83	0.76
1:A:104:THR:HG22	1:A:151:THR:HB	1.69	0.74
1:A:90:LYS:HD3	1:A:130:ARG:HG2	1.70	0.73
2:B:7:ASP:HB2	2:B:10:SER:HB3	1.69	0.73
3:H:345:LEU:HD21	3:H:354:ILE:HG12	1.71	0.72
4:D:14:DC:H2''	4:D:15:DT:H5'	1.70	0.72
3:C:383:LYS:H	3:C:383:LYS:HD3	1.53	0.72
4:D:10:DT:H2''	4:D:11:DC:H5'	1.70	0.71
1:A:74:VAL:O	1:A:87:ILE:HD11	1.90	0.71
1:A:69:ASN:ND2	1:A:95:GLY:H	1.88	0.70
1:A:69:ASN:HD21	1:A:95:GLY:H	1.41	0.68
2:G:63:ASN:N	2:G:63:ASN:HD22	1.92	0.67
4:I:11:DC:H1'	4:I:12:DC:H5''	1.75	0.67
2:G:8:GLN:HE21	2:G:107:CYS:H	1.44	0.66
1:F:87:ILE:HD12	1:F:87:ILE:O	1.96	0.66
4:I:9:DA:H1'	4:I:10:DT:H5''	1.76	0.66
2:G:21:LEU:HD22	2:G:57:PHE:CD1	2.31	0.65
2:G:45:GLN:NE2	2:G:49:ARG:HH21	1.94	0.65
3:H:384:MET:HE1	3:H:389:LEU:HB2	1.79	0.65
1:A:109:ASN:C	1:A:109:ASN:HD22	2.05	0.64
2:B:108:VAL:HG11	2:B:125:LEU:HB3	1.80	0.64
2:G:8:GLN:HG2	2:G:132:ALA:HB1	1.78	0.64
3:H:335:ILE:HD12	3:H:339:GLN:NE2	2.13	0.64
1:F:63:VAL:HG22	1:F:64:ARG:N	2.13	0.64
2:G:55:ILE:HD13	2:G:66:LEU:HD12	1.79	0.63
4:D:1:DG:O4'	4:I:15:DT:H2'	1.98	0.63
2:G:35:ARG:HA	2:G:35:ARG:NH1	2.12	0.63
3:C:417:ASP:O	3:C:421:LEU:HD13	1.99	0.62
2:B:15:GLU:O	2:B:19:ARG:HG3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:340:PHE:HZ	3:H:374:ARG:HB3	1.65	0.61
3:H:347:ASP:OD2	3:H:349:SER:HB3	1.99	0.61
4:I:11:DC:H2''	4:I:12:DC:H5''	1.83	0.61
1:F:71:LEU:HD11	1:F:94:LYS:HE3	1.82	0.61
4:I:11:DC:C2'	4:I:12:DC:H5''	2.32	0.60
2:B:84:GLU:HG3	2:B:85:TYR:N	2.15	0.60
1:A:109:ASN:ND2	1:A:111:GLU:H	1.99	0.60
2:B:45:GLN:HB2	2:B:116:LEU:HD21	1.83	0.60
2:B:108:VAL:HG12	2:B:109:ILE:H	1.66	0.60
1:F:81:CYS:HB3	1:F:168:ILE:CG2	2.32	0.59
3:H:334:PRO:HD3	5:J:112:DC:H5'	1.82	0.59
2:B:21:LEU:HD21	2:B:60:THR:HG21	1.84	0.59
3:H:365:LEU:HD21	3:H:368:PRO:CA	2.33	0.59
2:B:20:LYS:HE3	2:B:60:THR:HB	1.85	0.59
3:H:365:LEU:HD21	3:H:368:PRO:HA	1.85	0.58
4:I:8:DC:H2''	4:I:9:DA:C8	2.38	0.58
3:H:381:LYS:O	3:H:384:MET:HB2	2.04	0.58
3:H:393:LEU:HA	3:H:396:TYR:HD2	1.69	0.58
3:H:425:THR:HB	3:H:426:PRO:HD2	1.86	0.58
3:H:345:LEU:HB3	3:H:356:TRP:NE1	2.12	0.58
2:B:8:GLN:HE22	2:B:132:ALA:HA	1.68	0.58
1:F:81:CYS:HB3	1:F:168:ILE:HG23	1.86	0.58
3:C:345:LEU:HD21	3:C:354:ILE:HG12	1.85	0.58
3:H:390:SER:HA	3:H:393:LEU:HD12	1.86	0.58
2:B:106:VAL:O	2:B:108:VAL:HG23	2.04	0.57
1:A:139:ARG:HH11	1:A:139:ARG:HB2	1.69	0.57
3:C:353:PHE:HB2	3:C:367:ASP:HB3	1.84	0.57
1:F:149:THR:HG21	2:G:63:ASN:O	2.04	0.57
2:G:32:PHE:HB3	2:G:35:ARG:CG	2.34	0.57
3:H:365:LEU:HD23	3:H:365:LEU:O	2.04	0.57
3:H:418:LEU:HD22	3:H:422:LEU:HD11	1.87	0.57
4:I:11:DC:H2''	4:I:12:DC:C5'	2.34	0.57
1:A:82:ASN:HD22	1:A:137:VAL:HG22	1.70	0.57
2:B:108:VAL:HG12	2:B:109:ILE:N	2.20	0.57
2:B:93:GLY:O	2:B:116:LEU:HB2	2.04	0.56
2:G:63:ASN:HD22	2:G:63:ASN:H	1.50	0.56
1:F:139:ARG:HH11	1:F:139:ARG:HB2	1.70	0.56
2:G:11:LYS:HE3	2:G:15:GLU:OE1	2.04	0.56
2:B:8:GLN:NE2	2:B:132:ALA:HA	2.21	0.56
1:F:161:THR:HG21	1:F:163:HIS:CE1	2.40	0.56
3:H:375:TRP:CD1	3:H:384:MET:HE2	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:PHE:HB2	2:B:60:THR:HG22	1.86	0.56
1:A:171:ASP:HB3	1:A:174:ARG:HD2	1.87	0.56
1:A:149:THR:HG21	2:B:63:ASN:O	2.06	0.56
2:G:88:LEU:HG	2:G:95:VAL:HG12	1.87	0.56
1:F:148:LEU:HB2	1:F:162:TYR:HB3	1.88	0.56
2:G:16:GLU:OE2	2:G:20:LYS:HB2	2.05	0.56
2:B:68:PHE:CZ	2:B:97:LEU:HD13	2.42	0.55
3:H:409:ARG:O	3:H:411:VAL:HG23	2.05	0.55
3:C:381:LYS:HE2	4:D:9:DA:H4'	1.88	0.55
2:B:100:PRO:HB3	2:B:109:ILE:HD13	1.86	0.55
1:F:75:LEU:HD11	1:F:148:LEU:HD11	1.88	0.55
2:B:115:ASP:HB3	2:B:118:ARG:HB2	1.88	0.55
2:B:41:GLN:HE21	2:B:117:HIS:HA	1.71	0.55
2:G:88:LEU:N	2:G:88:LEU:HD12	2.22	0.55
1:F:177:ARG:NH1	5:J:111:DG:N7	2.55	0.54
2:G:82:SER:OG	2:G:85:TYR:HB2	2.07	0.54
1:A:112:ASN:ND2	2:B:33:ARG:HH12	2.05	0.54
2:G:86:VAL:O	2:G:86:VAL:HG13	2.08	0.54
2:B:63:ASN:N	2:B:63:ASN:HD22	2.05	0.54
3:C:385:ASN:ND2	3:C:387:GLU:HB2	2.21	0.54
1:A:70:PHE:CE2	1:A:152:VAL:HG21	2.43	0.54
3:H:362:GLU:HB2	3:H:413:ARG:HD2	1.90	0.54
4:D:9:DA:H1'	4:D:10:DT:H5''	1.90	0.54
1:F:167:LYS:C	1:F:168:ILE:HD12	2.33	0.53
3:H:368:PRO:HG2	3:H:369:ASP:H	1.72	0.53
2:B:14:ASN:O	2:B:19:ARG:HD2	2.09	0.53
3:H:348:LYS:O	3:H:351:GLN:HG2	2.07	0.53
3:H:354:ILE:HG13	3:H:365:LEU:HA	1.90	0.53
4:I:2:DA:H1'	4:I:3:DA:H5'	1.91	0.53
3:C:348:LYS:HD3	3:C:433:LEU:O	2.07	0.53
3:H:334:PRO:HD3	5:J:112:DC:C5'	2.38	0.53
4:D:11:DC:H1'	4:D:12:DC:C5'	2.39	0.53
4:D:8:DC:H2''	4:D:9:DA:C8	2.44	0.53
2:B:5:VAL:HG12	2:B:105:GLY:O	2.09	0.53
3:C:382:PRO:HG2	3:C:383:LYS:HD3	1.90	0.52
3:H:417:ASP:O	3:H:421:LEU:HD13	2.09	0.52
3:H:419:GLN:HE22	3:H:425:THR:HA	1.74	0.52
4:D:11:DC:H2''	4:D:12:DC:H5'	1.91	0.52
2:G:70:PRO:HG3	2:G:85:TYR:CE2	2.45	0.52
3:H:356:TRP:O	3:H:364:LYS:HE2	2.09	0.52
2:G:71:ALA:HB1	2:G:131:ARG:HE	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:HIS:CD2	1:A:167:LYS:HE3	2.45	0.52
1:A:112:ASN:HD21	2:B:33:ARG:HH12	1.58	0.52
2:B:4:VAL:HA	2:B:105:GLY:HA2	1.92	0.51
2:B:29:TYR:CE1	2:B:44:PHE:HB2	2.45	0.51
1:F:136:PHE:HB2	1:F:168:ILE:HG12	1.92	0.51
3:C:359:ASP:OD2	3:C:359:ASP:C	2.54	0.51
1:A:161:THR:H	2:B:104:ASN:HD21	1.58	0.51
4:I:11:DC:C1'	4:I:12:DC:H5''	2.39	0.51
2:G:71:ALA:HB2	2:G:131:ARG:HD2	1.92	0.51
2:G:60:THR:HG23	2:G:62:THR:OG1	2.10	0.51
1:A:109:ASN:HD22	1:A:112:ASN:H	1.58	0.51
2:G:3:ARG:HH21	2:G:135:GLU:CD	2.18	0.51
2:G:68:PHE:CZ	2:G:97:LEU:HD13	2.45	0.51
3:H:365:LEU:HD21	3:H:368:PRO:N	2.27	0.50
3:H:369:ASP:O	3:H:373:ARG:HG2	2.10	0.50
2:G:32:PHE:HB3	2:G:35:ARG:HG3	1.94	0.50
3:H:365:LEU:HD22	3:H:410:TYR:CD1	2.47	0.50
1:A:84:THR:HG23	1:A:133:ASP:OD1	2.11	0.50
3:C:383:LYS:HD3	3:C:383:LYS:N	2.21	0.50
3:H:345:LEU:HD22	3:H:356:TRP:CD1	2.45	0.50
2:B:100:PRO:HB3	2:B:109:ILE:CD1	2.42	0.50
1:F:71:LEU:CD1	1:F:94:LYS:HE3	2.42	0.50
4:D:11:DC:H1'	4:D:12:DC:H5'	1.93	0.50
2:G:8:GLN:NE2	2:G:107:CYS:H	2.07	0.49
2:G:21:LEU:HD21	2:G:60:THR:HG21	1.94	0.49
1:A:113:TYR:CZ	2:B:28:LYS:HD2	2.47	0.49
2:G:32:PHE:HB3	2:G:35:ARG:HG2	1.94	0.49
3:H:372:ALA:HB1	3:H:385:ASN:HA	1.95	0.49
2:B:37:HIS:O	2:B:41:GLN:HG3	2.13	0.49
3:C:385:ASN:HD21	3:C:387:GLU:HB2	1.77	0.49
5:E:115:DC:H2'	5:J:101:DA:O4'	2.13	0.49
1:A:69:ASN:HD22	1:A:94:LYS:HB2	1.77	0.49
2:B:95:VAL:O	2:B:113:TRP:HA	2.13	0.49
2:B:113:TRP:O	2:B:114:ILE:HG13	2.13	0.49
2:G:21:LEU:HD22	2:G:57:PHE:CG	2.48	0.48
2:G:131:ARG:CZ	2:G:131:ARG:HB3	2.43	0.48
1:A:82:ASN:HD21	1:A:118:ARG:HH11	1.61	0.48
1:A:109:ASN:ND2	1:A:109:ASN:C	2.72	0.48
1:A:114:SER:O	2:B:33:ARG:NH1	2.46	0.48
2:B:86:VAL:HG23	2:B:97:LEU:CD2	2.44	0.48
3:H:354:ILE:HA	3:H:366:SER:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:7:DA:H2''	4:D:8:DC:O5'	2.14	0.48
1:A:139:ARG:HD3	1:A:139:ARG:N	2.28	0.48
2:B:55:ILE:HG21	2:B:110:TRP:CZ2	2.49	0.48
3:H:353:PHE:C	3:H:366:SER:HB2	2.39	0.48
1:A:112:ASN:C	1:A:112:ASN:HD22	2.22	0.48
3:H:353:PHE:HB3	3:H:370:GLU:HG2	1.95	0.48
1:F:161:THR:HG22	1:F:162:TYR:N	2.29	0.47
1:A:101:THR:HG23	1:A:153:PHE:O	2.15	0.47
1:F:102:LEU:H	1:F:102:LEU:HD22	1.78	0.47
2:G:54:GLU:C	2:G:55:ILE:HD12	2.39	0.47
3:H:393:LEU:HA	3:H:396:TYR:CD2	2.47	0.47
4:D:10:DT:C2'	4:D:11:DC:H5'	2.40	0.47
1:A:69:ASN:HD21	1:A:95:GLY:N	2.12	0.47
2:G:121:GLY:O	2:G:122:MET:HE2	2.15	0.47
3:H:336:GLN:H	3:H:339:GLN:NE2	2.13	0.47
1:A:125:LYS:O	1:A:126:ASN:HB2	2.13	0.47
3:H:354:ILE:HG13	3:H:364:LYS:O	2.14	0.47
4:D:13:DT:H1'	4:D:14:DC:H5''	1.97	0.47
4:I:5:DC:H1'	4:I:6:DC:H5''	1.97	0.47
2:B:57:PHE:HB2	2:B:60:THR:CG2	2.45	0.47
2:B:89:GLU:O	2:B:91:GLU:N	2.47	0.47
2:B:86:VAL:HG13	2:B:86:VAL:O	2.15	0.46
4:I:10:DT:H2''	4:I:11:DC:C5'	2.41	0.46
3:H:361:TRP:CE3	3:H:361:TRP:HA	2.50	0.46
1:A:140:SER:O	1:A:144:LYS:HB2	2.15	0.46
3:C:397:TYR:OH	3:C:404:LYS:HB2	2.16	0.46
3:H:390:SER:O	3:H:393:LEU:HB2	2.15	0.46
4:D:9:DA:H2''	4:D:10:DT:H5'	1.97	0.46
3:H:389:LEU:O	3:H:389:LEU:HD23	2.16	0.46
1:F:102:LEU:HD22	1:F:102:LEU:N	2.31	0.46
1:A:113:TYR:CE2	2:B:28:LYS:HD2	2.51	0.46
2:G:63:ASN:N	2:G:63:ASN:ND2	2.60	0.46
2:B:28:LYS:HE3	2:B:58:VAL:HG21	1.98	0.46
5:J:109:DT:H2''	5:J:110:DG:C8	2.50	0.46
1:F:148:LEU:HD12	1:F:162:TYR:HD1	1.81	0.45
3:H:363:PHE:CZ	3:H:412:TYR:HB2	2.51	0.45
2:B:91:GLU:CD	2:B:94:LYS:HG3	2.42	0.45
1:F:136:PHE:CB	1:F:168:ILE:HG12	2.46	0.45
3:C:404:LYS:HE2	3:C:411:VAL:O	2.17	0.45
1:F:63:VAL:HG12	1:F:72:CYS:O	2.17	0.45
4:D:5:DC:H1'	4:D:6:DC:H5''	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:SER:OG	2:B:30:THR:HB	2.17	0.45
3:C:385:ASN:OD1	3:C:388:LYS:HG3	2.17	0.45
3:H:338:TRP:CE2	3:H:339:GLN:HG3	2.51	0.45
1:F:63:VAL:CG2	1:F:64:ARG:N	2.79	0.44
2:G:7:ASP:HB2	2:G:10:SER:HB2	1.98	0.44
2:G:108:VAL:HG22	2:G:109:ILE:N	2.31	0.44
3:H:385:ASN:OD1	3:H:387:GLU:HB2	2.18	0.44
1:A:87:ILE:O	1:A:87:ILE:HG13	2.16	0.44
2:B:115:ASP:CG	2:B:118:ARG:HD3	2.42	0.44
1:F:63:VAL:HG22	1:F:64:ARG:H	1.81	0.44
1:F:78:HIS:HB3	1:F:173:PRO:HG3	1.99	0.44
1:A:109:ASN:HD21	1:A:112:ASN:H	1.59	0.44
2:G:132:ALA:O	2:G:136:ASP:HB2	2.17	0.44
3:H:389:LEU:HD23	3:H:389:LEU:C	2.42	0.44
3:H:335:ILE:HG13	3:H:336:GLN:N	2.32	0.44
2:G:85:TYR:HA	2:G:98:LYS:HB3	2.00	0.44
3:H:337:LEU:HD11	3:H:389:LEU:HG	2.00	0.44
2:B:71:ALA:HB1	2:B:131:ARG:NH1	2.32	0.44
3:C:340:PHE:O	3:C:343:GLU:HB3	2.18	0.43
3:H:418:LEU:HD22	3:H:422:LEU:CD1	2.47	0.43
5:E:109:DT:H2''	5:E:110:DG:C8	2.53	0.43
3:H:418:LEU:O	3:H:422:LEU:HB2	2.19	0.43
2:B:113:TRP:C	2:B:114:ILE:HG13	2.44	0.43
2:G:68:PHE:CD1	2:G:99:ALA:HB2	2.54	0.43
3:H:336:GLN:HE21	4:I:7:DA:H3'	1.84	0.43
3:H:359:ASP:HB3	3:H:362:GLU:CB	2.39	0.43
3:H:419:GLN:NE2	3:H:426:PRO:HD3	2.34	0.43
1:F:70:PHE:C	1:F:71:LEU:HD12	2.43	0.43
4:D:13:DT:H2''	4:D:14:DC:C5'	2.48	0.43
1:A:116:GLU:HG2	1:A:137:VAL:HB	2.01	0.43
3:C:419:GLN:CD	3:C:425:THR:HG22	2.44	0.43
2:G:87:ASP:OD2	2:G:90:ARG:HB2	2.19	0.43
3:C:425:THR:HB	3:C:426:PRO:HD2	2.01	0.43
2:B:109:ILE:HD11	2:B:128:ASP:OD1	2.18	0.43
2:G:89:GLU:C	2:G:91:GLU:N	2.77	0.43
3:H:379:LYS:O	3:H:381:LYS:HG2	2.19	0.42
3:C:404:LYS:HG2	5:E:103:DA:OP1	2.19	0.42
1:A:63:VAL:HG23	1:A:74:VAL:HG22	2.02	0.42
1:A:79:TRP:CZ2	1:A:83:LYS:HD3	2.55	0.42
2:B:98:LYS:HE2	2:B:111:LYS:CE	2.50	0.42
1:F:86:PRO:O	1:F:87:ILE:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:113:TYR:CE2	2:G:28:LYS:HD2	2.54	0.42
4:D:1:DG:H2''	4:D:2:DA:OP2	2.19	0.42
1:F:164:ARG:NH1	1:F:164:ARG:HG3	2.35	0.42
2:B:4:VAL:HA	2:B:105:GLY:CA	2.50	0.42
2:B:91:GLU:HB3	2:B:94:LYS:HB2	2.00	0.42
4:D:13:DT:H2''	4:D:14:DC:H5'	2.01	0.42
2:G:98:LYS:HA	2:G:110:TRP:O	2.19	0.42
2:B:128:ASP:CG	2:B:131:ARG:HB2	2.44	0.42
1:F:164:ARG:HG3	1:F:164:ARG:HH11	1.85	0.42
1:F:166:ILE:HG12	1:F:168:ILE:HD12	2.02	0.41
3:H:336:GLN:H	3:H:339:GLN:HE21	1.67	0.41
2:B:71:ALA:CB	2:B:131:ARG:HD3	2.50	0.41
1:F:115:ALA:HB2	1:F:146:PHE:CZ	2.56	0.41
2:G:131:ARG:HB3	2:G:131:ARG:NH1	2.35	0.41
3:H:365:LEU:HD21	3:H:367:ASP:C	2.45	0.41
2:B:12:PHE:CD1	2:B:12:PHE:C	2.98	0.41
1:F:106:MET:HE1	2:G:64:LEU:C	2.44	0.41
2:G:19:ARG:HA	2:G:22:SER:OG	2.21	0.41
3:H:345:LEU:HD13	3:H:356:TRP:NE1	2.35	0.41
4:D:2:DA:H1'	4:D:3:DA:H5'	2.03	0.41
2:B:32:PHE:C	2:B:34:ASP:H	2.28	0.41
1:F:70:PHE:CE2	1:F:152:VAL:HG21	2.55	0.41
2:G:89:GLU:C	2:G:91:GLU:H	2.28	0.41
2:G:108:VAL:HG22	2:G:109:ILE:H	1.86	0.41
3:H:341:LEU:CD2	3:H:371:VAL:HG11	2.51	0.41
3:H:382:PRO:C	3:H:384:MET:H	2.29	0.41
4:I:9:DA:H2''	4:I:10:DT:H5'	2.01	0.41
2:B:32:PHE:CD2	2:B:32:PHE:N	2.89	0.41
4:I:13:DT:H5'	4:I:13:DT:C6	2.56	0.41
2:B:21:LEU:HD22	2:B:57:PHE:CD1	2.56	0.41
3:H:367:ASP:OD2	3:H:368:PRO:HD2	2.21	0.41
3:C:338:TRP:CE2	3:C:339:GLN:HG3	2.56	0.40
3:C:364:LYS:CB	3:C:411:VAL:HG22	2.51	0.40
3:H:335:ILE:HD11	3:H:339:GLN:HB3	2.03	0.40
1:A:63:VAL:CG2	1:A:74:VAL:HG22	2.51	0.40
1:A:145:SER:HB3	1:A:164:ARG:HA	2.03	0.40
3:C:378:ARG:HG3	3:C:378:ARG:HH11	1.86	0.40
1:A:160:ALA:HA	2:B:104:ASN:ND2	2.36	0.40
2:B:98:LYS:HE2	2:B:111:LYS:HE2	2.03	0.40
1:F:139:ARG:N	1:F:139:ARG:HD3	2.36	0.40
2:G:82:SER:OG	2:G:86:VAL:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:348:LYS:HG2	3:H:433:LEU:HD22	2.02	0.40
3:H:419:GLN:NE2	3:H:425:THR:HA	2.34	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	116/204 (57%)	109 (94%)	7 (6%)	0	100	100
1	F	116/204 (57%)	106 (91%)	10 (9%)	0	100	100
2	B	128/142 (90%)	108 (84%)	19 (15%)	1 (1%)	16	44
2	G	126/142 (89%)	109 (86%)	15 (12%)	2 (2%)	7	27
3	C	101/166 (61%)	98 (97%)	2 (2%)	1 (1%)	12	38
3	H	98/166 (59%)	84 (86%)	10 (10%)	4 (4%)	2	8
All	All	685/1024 (67%)	614 (90%)	63 (9%)	8 (1%)	10	34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	71	ALA
2	B	90	ARG
3	C	348	LYS
3	H	383	LYS
2	G	58	VAL
3	H	368	PRO
3	H	397	TYR
3	H	354	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	100/179 (56%)	92 (92%)	8 (8%)	11	34
1	F	100/179 (56%)	99 (99%)	1 (1%)	68	88
2	B	114/123 (93%)	109 (96%)	5 (4%)	25	59
2	G	113/123 (92%)	106 (94%)	7 (6%)	16	45
3	C	94/144 (65%)	90 (96%)	4 (4%)	26	60
3	H	91/144 (63%)	91 (100%)	0	100	100
All	All	612/892 (69%)	587 (96%)	25 (4%)	27	62

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	77	THR
1	A	96	ASP
1	A	105	VAL
1	A	109	ASN
1	A	117	LEU
1	A	130	ARG
1	A	139	ARG
2	B	63	ASN
2	B	88	LEU
2	B	94	LYS
2	B	103	LEU
2	B	116	LEU
3	C	383	LYS
3	C	404	LYS
3	C	427	GLU
3	C	436	LYS
1	F	139	ARG
2	G	7	ASP
2	G	15	GLU
2	G	30	THR
2	G	63	ASN

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Mol	Chain	Res	Type
2	G	65	SER
2	G	120	ASP
2	G	130	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	82	ASN
1	A	109	ASN
1	A	112	ASN
1	A	119	ASN
1	A	132	ASN
2	B	8	GLN
2	B	104	ASN
2	B	133	GLN
2	B	134	GLN
3	C	380	ASN
1	F	69	ASN
1	F	112	ASN
1	F	126	ASN
1	F	127	GLN
2	G	8	GLN
2	G	41	GLN
2	G	46	ASN
2	G	63	ASN
2	G	67	GLN
2	G	134	GLN
3	H	336	GLN
3	H	339	GLN
3	H	351	GLN
3	H	400	ASN
3	H	419	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	118/204 (57%)	0.14	2 (1%) 69 60	49, 73, 93, 106	0
1	F	118/204 (57%)	0.01	1 (0%) 82 75	47, 63, 87, 103	0
2	B	132/142 (92%)	1.00	16 (12%) 8 6	75, 101, 129, 139	0
2	G	130/142 (91%)	1.08	17 (13%) 7 6	62, 97, 122, 124	0
3	C	103/166 (62%)	0.02	2 (1%) 66 57	47, 69, 84, 93	0
3	H	100/166 (60%)	1.74	38 (38%) 1 0	67, 132, 172, 176	0
4	D	15/15 (100%)	-0.32	0 100 100	56, 62, 74, 77	0
4	I	15/15 (100%)	0.07	0 100 100	57, 70, 87, 91	0
5	E	15/15 (100%)	-0.38	0 100 100	51, 62, 77, 79	0
5	J	15/15 (100%)	-0.04	0 100 100	55, 67, 79, 87	0
All	All	761/1084 (70%)	0.60	76 (9%) 12 9	47, 80, 141, 176	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	81	PRO	6.5
3	H	421	LEU	4.7
2	G	139	ALA	4.7
3	H	356	TRP	4.5
3	H	433	LEU	4.4
3	H	360	GLY	4.3
3	H	342	LEU	3.8
2	B	82	SER	3.7
3	H	346	THR	3.6
1	A	177	ARG	3.5
2	B	72	SER	3.4
3	H	431	ALA	3.4
3	H	405	THR	3.4

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Mol	Chain	Res	Type	RSRZ
2	G	138	LEU	3.3
3	H	410	TYR	3.2
2	G	82	SER	3.2
2	B	80	THR	3.2
3	H	423	GLY	3.1
2	G	88	LEU	3.1
3	H	422	LEU	3.0
3	H	365	LEU	3.0
2	B	116	LEU	3.0
3	H	430	HIS	3.0
3	H	359	ASP	2.9
3	H	406	ALA	2.9
3	H	363	PHE	2.9
2	G	86	VAL	2.8
3	H	407	GLY	2.8
2	B	88	LEU	2.8
3	H	409	ARG	2.8
3	H	353	PHE	2.7
2	B	95	VAL	2.7
2	G	83	ARG	2.7
3	H	338	TRP	2.7
3	H	361	TRP	2.6
2	G	26	GLU	2.5
3	H	357	THR	2.5
2	B	16	GLU	2.5
1	F	177	ARG	2.5
2	B	92	ALA	2.4
2	B	93	GLY	2.4
3	H	341	LEU	2.4
2	B	130	GLU	2.4
2	G	113	TRP	2.4
2	G	119	LEU	2.4
3	H	429	LEU	2.4
3	H	358	GLY	2.4
2	B	94	LYS	2.3
2	G	131	ARG	2.3
2	G	94	LYS	2.3
3	C	436	LYS	2.3
2	G	7	ASP	2.3
3	H	352	SER	2.3
3	H	420	SER	2.3
3	H	424	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	176	PRO	2.3
2	G	122	MET	2.3
2	G	117	HIS	2.3
3	H	354	ILE	2.2
3	H	432	MET	2.2
3	H	408	LYS	2.2
2	B	105	GLY	2.2
2	B	96	TYR	2.2
2	B	83	ARG	2.1
3	H	335	ILE	2.1
3	H	414	PHE	2.1
3	H	373	ARG	2.1
3	C	334	PRO	2.1
2	B	86	VAL	2.1
3	H	375	TRP	2.1
3	H	383	LYS	2.0
2	G	96	TYR	2.0
3	H	404	LYS	2.0
2	B	6	PRO	2.0
2	G	25	CYS	2.0
3	H	378	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.