



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2017 – 01:47 PM EST

PDB ID : 3WTX  
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 : unknown  
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](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.

---

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-20030345
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-20030345

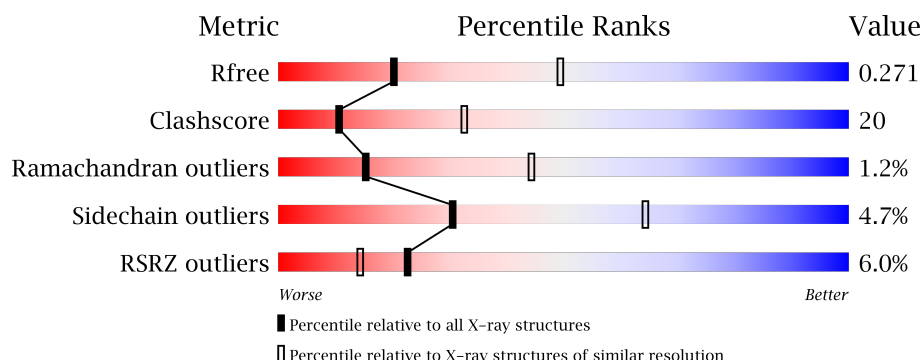
# 1 Overall quality at a glance

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))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (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  $\geq 3$ , 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	204	
1	F	204	
2	B	142	
2	G	142	
3	C	166	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	H	166	<div><div><div></div><div></div><div></div><div></div></div><div>19%27%33%40%</div></div>
4	D	15	<div><div><div></div></div><div>100%</div></div>
4	I	15	<div><div><div></div><div></div></div><div>13%87%</div></div>
5	E	15	<div><div><div></div><div></div></div><div>67%33%</div></div>
5	J	15	<div><div><div></div><div></div></div><div>67%33%</div></div>

## 2 Entry composition [i](#)

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			

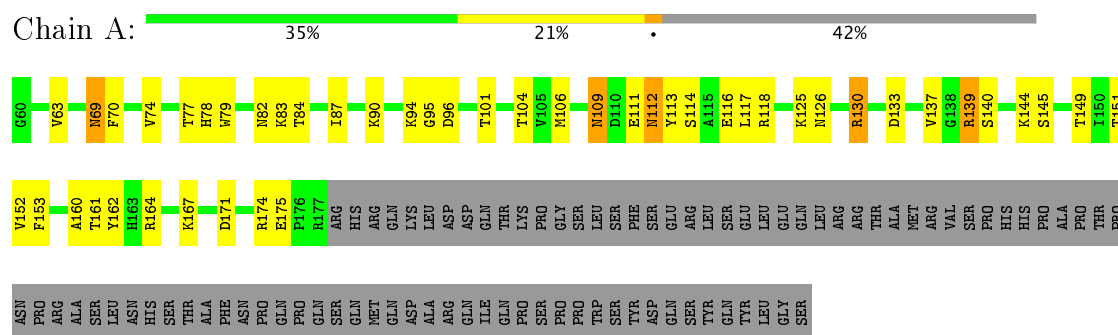
- Molecule 6 is water.

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		

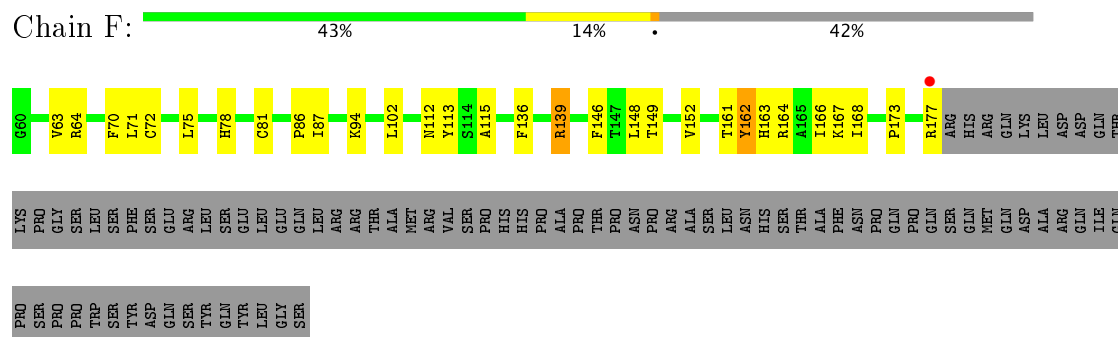
### 3 Residue-property plots

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.

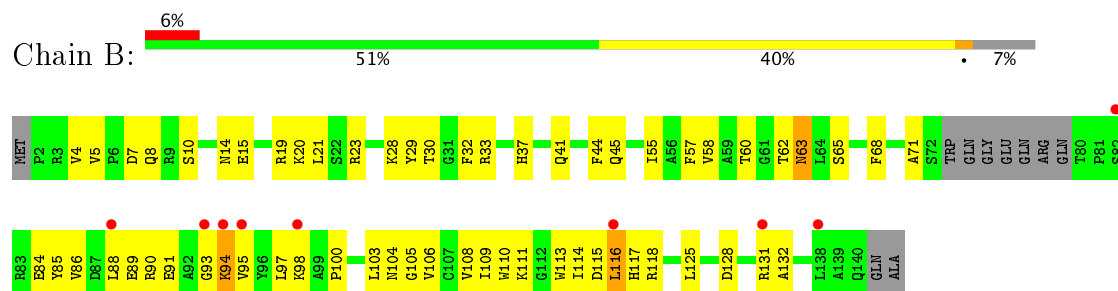
#### • Molecule 1: Runt-related transcription factor 1



#### • Molecule 1: Runt-related transcription factor 1

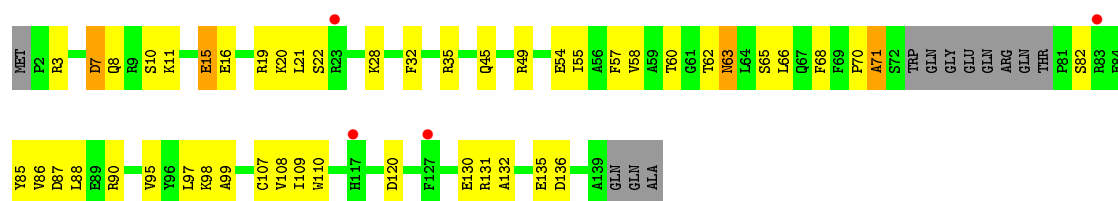


#### • Molecule 2: Core-binding factor subunit beta

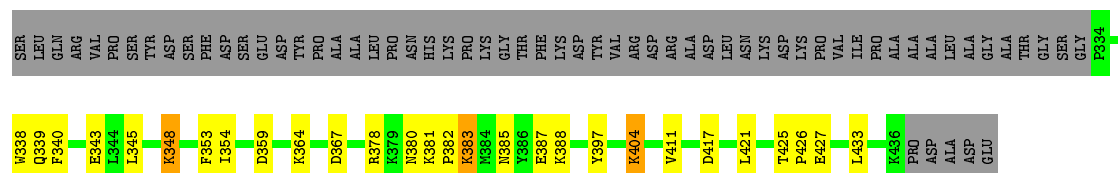


#### • Molecule 2: Core-binding factor subunit beta

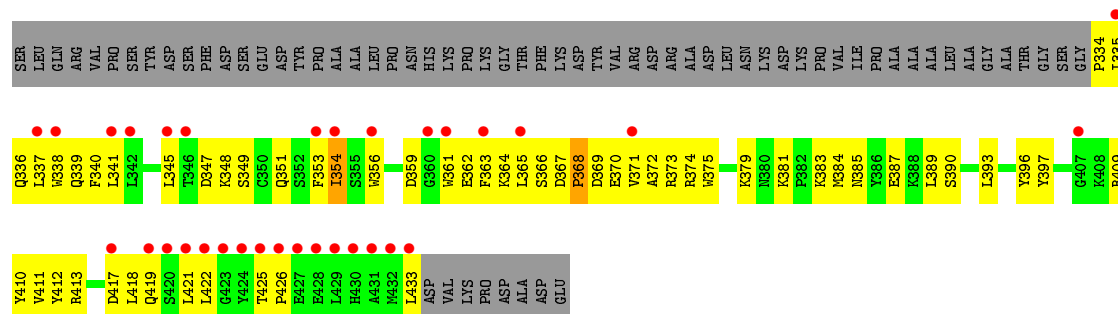
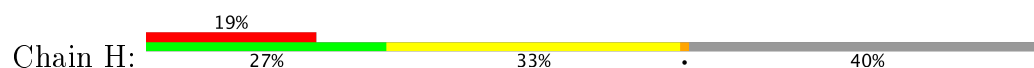




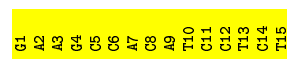
• Molecule 3: Protein C-ets-1



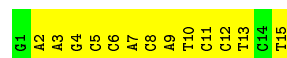
• Molecule 3: Protein C-ets-1



• 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')





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

Chain J: 67% 33%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.7	Xtriage
Anisotropy	0.868	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 53.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<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

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	0.43	0/933	0.60	0/1268
1	F	0.47	0/933	0.64	0/1268
2	B	0.36	0/1105	0.50	0/1484
2	G	0.37	0/1090	0.50	0/1462
3	C	0.47	0/897	0.58	0/1207
3	H	0.32	0/873	0.47	0/1175
4	D	0.54	0/334	0.81	0/512
4	I	0.52	0/334	0.82	0/512
5	E	0.52	0/348	0.77	0/537
5	J	0.51	0/348	0.78	0/537
All	All	0.43	0/7195	0.61	0/9962

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.

There are no bond angle outliers.

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	41	0
1	F	914	0	922	31	0
2	B	1083	0	1042	54	0
2	G	1068	0	1031	43	0
3	C	873	0	871	20	0
3	H	849	0	845	61	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	271	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 20.

All (271) 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: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:HH11	2:G:35:ARG:HA	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD3	3:C:383:LYS:H	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:HD22	2:G:63:ASN:N	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:O	1:F:87:ILE:HD12	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
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
4:D:1:DG:O4'	4:I:15:DT:H2'	1.98	0.63
2:G:55:ILE:HD13	2:G:66:LEU:HD12	1.79	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
3:H:347:ASP:OD2	3:H:349:SER:HB3	1.99	0.61
3:H:340:PHE:HZ	3:H:374:ARG:HB3	1.65	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:108:VAL:HG12	2:B:109:ILE:H	1.66	0.60
2:B:45:GLN:HB2	2:B:116:LEU:HD21	1.83	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
1:A:109:ASN:C	1:A:109:ASN:HD22	2.05	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HB2	1:A:139:ARG:HH11	1.69	0.57
3:C:353:PHE:HB2	3:C:367:ASP:HB3	1.84	0.57
2:G:32:PHE:HB3	2:G:35:ARG:CG	2.34	0.57
1:F:149:THR:HG21	2:G:63:ASN:O	2.04	0.57
3:H:365:LEU:O	3:H:365:LEU:HD23	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
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:HD12	2:G:88:LEU:N	2.22	0.55
2:G:82:SER:OG	2:G:85:TYR:HB2	2.07	0.54
1:F:177:ARG:NH1	5:J:111:DG:N7	2.55	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD22	2:B:63:ASN:N	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
4:D:9:DA:H1'	4:D:10:DT:H5''	1.90	0.54
3:H:362:GLU:HB2	3:H:413:ARG:HD2	1.90	0.54
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
4:D:11:DC:H2''	4:D:12:DC:H5'	1.91	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
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
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:29:TYR:CE1	2:B:44:PHE:HB2	2.45	0.51
2:B:4:VAL:HA	2:B:105:GLY:HA2	1.92	0.51
1:F:136:PHE:HB2	1:F:168:ILE:HG12	1.92	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: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:11:DC:H1'	4:D:12:DC:H5'	1.93	0.50
1:F:71:LEU:CD1	1:F:94:LYS:HE3	2.42	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:F:167:LYS:C	1:F:168:ILE:HD12	2.33	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: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
4:D:7:DA:H2''	4:D:8:DC:O5'	2.14	0.48
3:H:354:ILE:HA	3:H:366:SER:H	1.79	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: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
4:D:10:DT:C2'	4:D:11:DC:H5'	2.40	0.47
1:F:102:LEU:H	1:F:102:LEU:HD22	1.78	0.47
3:H:393:LEU:HA	3:H:396:TYR:CD2	2.47	0.47
1:A:69:ASN:HD21	1:A:95:GLY:N	2.12	0.47
2:G:3:ARG:HH21	2:G:135:GLU:CD	2.18	0.47
3:H:336:GLN:H	3:H:339:GLN:NE2	2.13	0.47
4:D:13:DT:H1'	4:D:14:DC:H5''	1.97	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: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
3:C:359:ASP:OD2	3:C:359:ASP:C	2.54	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:9:DA:H2"	4:D:10:DT:H5'	1.97	0.46
3:H:390:SER:O	3:H:393:LEU:HB2	2.15	0.46
3:H:389:LEU:HD23	3:H:389:LEU:O	2.16	0.46
1:F:102:LEU:N	1:F:102:LEU:HD22	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:A:87:ILE:O	1:A:87:ILE:HG13	2.16	0.45
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
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
4:D:5:DC:H1'	4:D:6:DC:H5"	1.99	0.45
1:F:63:VAL:HG12	1:F:72:CYS:O	2.17	0.45
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:108:VAL:HG22	2:G:109:ILE:N	2.31	0.44
2:G:7:ASP:HB2	2:G:10:SER:HB2	1.98	0.44
3:H:385:ASN:OD1	3:H:387:GLU:HB2	2.18	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: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
1:A:109:ASN:ND2	1:A:109:ASN:C	2.72	0.43
3:H:418:LEU:O	3:H:422:LEU:HB2	2.19	0.43
1:A:112:ASN:HD22	1:A:112:ASN:C	2.22	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:MET:HE1	2:B:65:SER:HB2	2.00	0.43
2:G:68:PHE:CD1	2:G:99:ALA:HB2	2.54	0.43
3:H:353:PHE:C	3:H:366:SER:HB2	2.39	0.43
3:H:359:ASP:HB3	3:H:362:GLU:CB	2.39	0.43
3:H:336:GLN:HE21	4:I:7:DA:H3'	1.84	0.43
3:H:419:GLN:NE2	3:H:426:PRO:HD3	2.34	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
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
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
4:D:1:DG:H2''	4:D:2:DA:OP2	2.19	0.42
1:F:86:PRO:O	1:F:87:ILE:HG23	2.20	0.42
1:F:113:TYR:CE2	2:G:28:LYS:HD2	2.54	0.42
1:F:164:ARG:HG3	1:F:164:ARG:NH1	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
1:F:164:ARG:HG3	1:F:164:ARG:HH11	1.85	0.42
2:G:54:GLU:C	2:G:55:ILE:HD12	2.39	0.42
3:H:375:TRP:HD1	3:H:384:MET:CE	2.33	0.41
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:NH1	2:G:131:ARG:HB3	2.35	0.41
4:D:2:DA:H1'	4:D:3:DA:H5'	2.03	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
1:F:70:PHE:CE2	1:F:152:VAL:HG21	2.55	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
4:I:9:DA:H2''	4:I:10:DT:H5'	2.01	0.41
4:I:13:DT:H5'	4:I:13:DT:C6	2.56	0.41
2:B:32:PHE:CD2	2:B:32:PHE:N	2.89	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:LEU:HD22	2:B:57:PHE:CD1	2.56	0.41
2:B:91:GLU:CD	2:B:94:LYS:HG3	2.42	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
3:H:389:LEU:HD23	3:H:389:LEU:C	2.42	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
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 ⓘ

### 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	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%)	22	55
2	G	126/142 (89%)	109 (86%)	15 (12%)	2 (2%)	11	36
3	C	101/166 (61%)	98 (97%)	2 (2%)	1 (1%)	18	50
3	H	98/166 (59%)	84 (86%)	10 (10%)	4 (4%)	3	11
All	All	685/1024 (67%)	614 (90%)	63 (9%)	8 (1%)	15	44

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%)	90 (90%)	10 (10%)	9	26
1	F	100/179 (56%)	97 (97%)	3 (3%)	46	80
2	B	114/123 (93%)	108 (95%)	6 (5%)	26	59
2	G	113/123 (92%)	107 (95%)	6 (5%)	26	59
3	C	94/144 (65%)	90 (96%)	4 (4%)	33	67
3	H	91/144 (63%)	91 (100%)	0	100	100
All	All	612/892 (69%)	583 (95%)	29 (5%)	30	64

All (29) 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	109	ASN
1	A	112	ASN
1	A	117	LEU
1	A	130	ARG
1	A	139	ARG
1	A	162	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	175	GLU
2	B	23	ARG
2	B	63	ASN
2	B	88	LEU
2	B	94	LYS
2	B	103	LEU
2	B	116	LEU
3	C	380	ASN
3	C	383	LYS
3	C	404	LYS
3	C	427	GLU
1	F	112	ASN
1	F	139	ARG
1	F	162	TYR
2	G	7	ASP
2	G	15	GLU
2	G	63	ASN
2	G	65	SER
2	G	120	ASP
2	G	130	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) 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	41	GLN
2	B	104	ASN
2	B	133	GLN
2	B	134	GLN
3	C	380	ASN
3	C	400	ASN
1	F	112	ASN
1	F	127	GLN
2	G	8	GLN
2	G	41	GLN
2	G	45	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	G	67	GLN
2	G	134	GLN
3	H	339	GLN
3	H	351	GLN
3	H	419	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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, 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	118/204 (57%)	0.15	0 100 100	49, 73, 93, 106	0
1	F	118/204 (57%)	0.03	1 (0%) 86 81	47, 63, 87, 103	0
2	B	132/142 (92%)	0.52	9 (6%) 18 10	75, 101, 129, 139	0
2	G	130/142 (91%)	0.52	4 (3%) 49 38	62, 97, 122, 124	0
3	C	103/166 (62%)	0.12	0 100 100	47, 69, 84, 93	0
3	H	100/166 (60%)	1.51	32 (32%) 0 0	67, 132, 172, 176	0
4	D	15/15 (100%)	-0.13	0 100 100	56, 62, 74, 77	0
4	I	15/15 (100%)	-0.19	0 100 100	57, 70, 87, 91	0
5	E	15/15 (100%)	-0.22	0 100 100	51, 62, 77, 79	0
5	J	15/15 (100%)	-0.23	0 100 100	55, 67, 79, 87	0
All	All	761/1084 (70%)	0.41	46 (6%) 23 14	47, 80, 141, 176	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	424	TYR	6.1
3	H	346	THR	5.8
3	H	421	LEU	5.7
3	H	423	GLY	5.3
3	H	422	LEU	4.6
3	H	429	LEU	4.4
3	H	426	PRO	4.4
3	H	342	LEU	4.0
3	H	361	TRP	3.5
3	H	341	LEU	3.5
3	H	360	GLY	3.3
3	H	335	ILE	3.3
3	H	425	THR	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	H	433	LEU	3.2
3	H	432	MET	3.1
2	B	94	LYS	2.9
3	H	356	TRP	2.8
3	H	345	LEU	2.8
3	H	420	SER	2.8
3	H	428	GLU	2.7
2	B	98	LYS	2.7
3	H	407	GLY	2.7
3	H	353	PHE	2.6
2	B	95	VAL	2.6
2	B	82	SER	2.5
3	H	419	GLN	2.4
3	H	337	LEU	2.4
1	F	177	ARG	2.4
2	B	116	LEU	2.3
3	H	371	VAL	2.3
2	G	83	ARG	2.3
3	H	417	ASP	2.2
2	B	88	LEU	2.2
3	H	430	HIS	2.2
3	H	338	TRP	2.2
3	H	427	GLU	2.2
3	H	354	ILE	2.2
3	H	363	PHE	2.1
2	G	127	PHE	2.1
2	G	117	HIS	2.1
2	B	93	GLY	2.1
2	B	138	LEU	2.1
2	G	23	ARG	2.1
3	H	431	ALA	2.0
3	H	365	LEU	2.0
2	B	131	ARG	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.