



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:08 PM UTC

PDB ID : 3WTY / pdb_00003wtY
Title : Crystal structure of the complex comprised of ETS1(G333P), RUNX1, CBF-BETA, and the tcralpha gene enhancer DNA
Authors : Shiina, M.; Hamada, K.; Ogata, K.
Deposited on : 2014-04-21
Resolution : 2.70 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

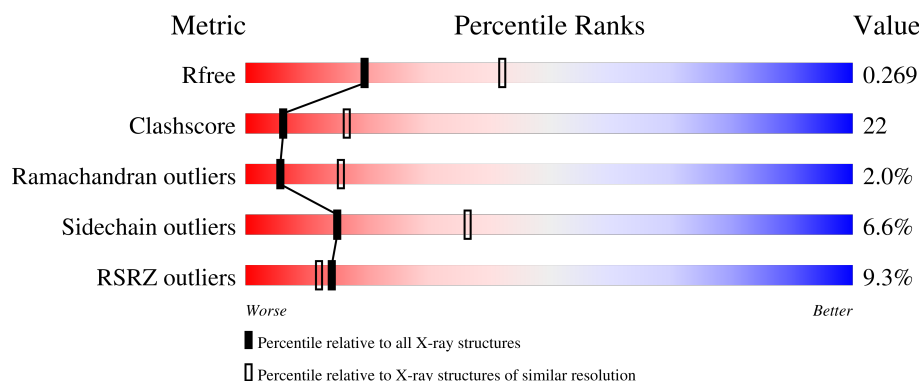
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	40% 14% 42%
1	F	204	42% 15% 42%
2	B	142	11% 40% 44% 7% 8%
2	G	142	11% 55% 32% 9%
3	C	166	4% 47% 22% 29%

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Mol	Chain	Length	Quality of chain
3	H	166	
4	D	15	
4	I	15	
5	E	15	
5	J	15	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7039 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	130	Total	C	N	O	S	0	0	0
			1071	671	195	199	6			
2	G	129	Total	C	N	O	S	0	0	0
			1062	666	193	197	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	118	Total	C	N	O	S	0	0	0
			970	630	165	171	4			
3	H	101	Total	C	N	O	S	0	0	0
			856	556	147	149	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	333	PRO	GLY	engineered mutation	UNP P14921
H	333	PRO	GLY	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').

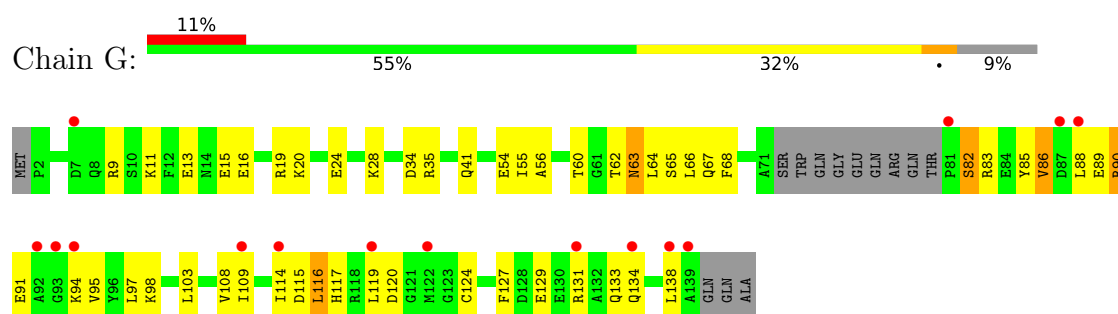
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	15	Total	C	N	O	P	0	0	0
			299	144	54	87	14			
4	I	15	Total	C	N	O	P	0	0	0
			299	144	54	87	14			

- 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').

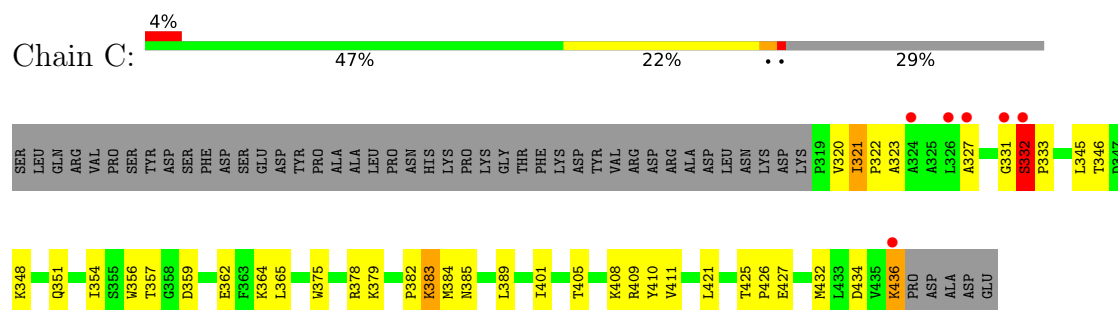
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	15	Total	C	N	O	P	0	0	0
			310	148	59	89	14			
5	J	15	Total	C	N	O	P	0	0	0
			310	148	59	89	14			

- Molecule 6 is water.

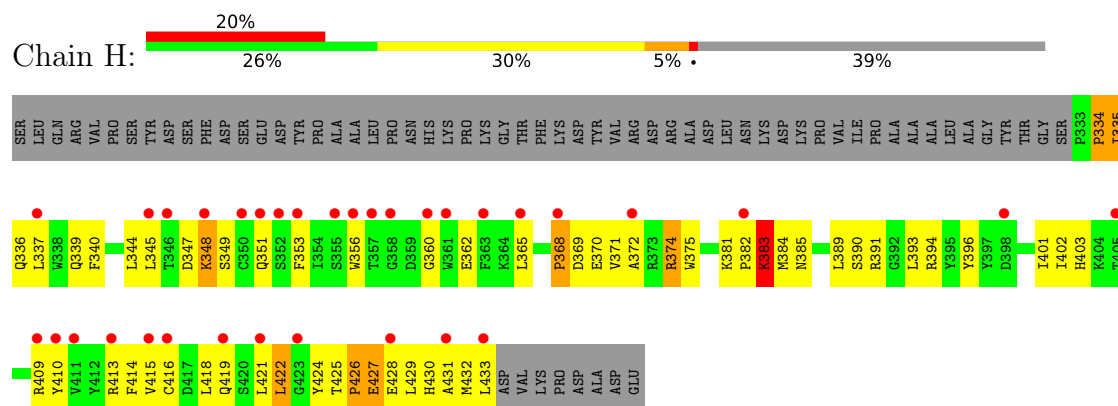
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	O	0	0
			3	3		
6	B	2	Total	O	0	0
			2	2		
6	C	10	Total	O	0	0
			10	10		
6	F	5	Total	O	0	0
			5	5		
6	G	3	Total	O	0	0
			3	3		
6	H	3	Total	O	0	0
			3	3		
6	D	2	Total	O	0	0
			2	2		
6	E	4	Total	O	0	0
			4	4		
6	J	2	Total	O	0	0
			2	2		



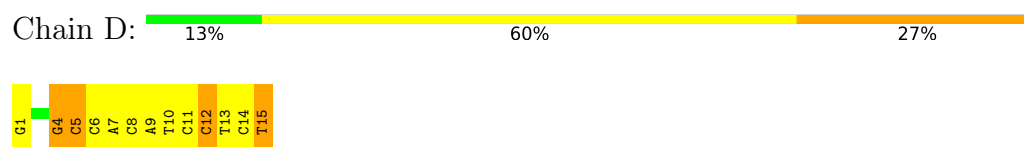
• Molecule 3: Protein C-ets-1



• 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')

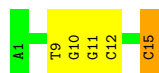


• Molecule 4: DNA (5'-D(*GP*AP*AP*GP*CP*CP*AP*CP*AP*TP*CP*CP*TP*CP*T)-3')



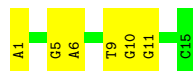
- Molecule 5: DNA (5'-D(*AP*GP*AP*GP*GP*AP*TP*GP*TP*GP*GP*CP*TP*TP*C)-3')

Chain E:  67% 27% 7%



- 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	78.80Å 102.50Å 194.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.69 – 2.70 48.69 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.69-2.70) 98.8 (48.69-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.52 (at 2.69Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.227 , 0.268 0.227 , 0.269	Depositor DCC
R_{free} test set	4390 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å ²)	78.8	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7039	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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	0.67	0/933	0.98	2/1268 (0.2%)
1	F	0.71	0/933	1.07	2/1268 (0.2%)
2	B	0.48	0/1093	0.82	1/1466 (0.1%)
2	G	0.56	0/1084	0.85	0/1454
3	C	0.63	0/998	1.03	3/1349 (0.2%)
3	H	0.41	0/881	0.77	1/1187 (0.1%)
4	D	0.44	0/334	1.16	3/512 (0.6%)
4	I	0.43	0/334	1.00	2/512 (0.4%)
5	E	0.41	0/348	0.87	1/537 (0.2%)
5	J	0.40	0/348	0.84	0/537
All	All	0.56	0/7286	0.94	15/10090 (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	4
4	I	0	2
All	All	0	6

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	ILE	N-CA-C	-10.54	103.27	112.12
4	D	4	DG	N9-C1'-C2'	-8.60	100.61	113.50
4	I	4	DG	N9-C1'-C2'	-7.86	101.71	113.50
4	D	4	DG	C4'-C3'-O3'	7.82	121.73	110.00
3	C	332	SER	CA-C-N	-7.61	112.54	120.38
3	C	332	SER	C-N-CA	-7.61	112.54	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	374	ARG	N-CA-C	-6.33	104.47	111.82
1	A	128	VAL	N-CA-C	5.79	116.20	107.75
5	E	15	DC	C2'-C3'-O3'	-5.79	102.81	111.50
4	I	4	DG	C4'-C3'-O3'	5.74	118.61	110.00
4	D	15	DT	C2'-C3'-O3'	-5.59	103.11	111.50
1	F	70	PHE	N-CA-C	5.43	117.52	108.99
1	A	70	PHE	N-CA-C	5.29	118.06	109.06
2	B	31	GLY	N-CA-C	5.21	117.92	111.93
1	F	154	THR	N-CA-C	-5.13	101.91	109.86

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	12	DC	Sidechain
4	D	15	DT	Sidechain
4	D	4	DG	Sidechain
4	D	5	DC	Sidechain
4	I	4	DG	Sidechain
4	I	5	DC	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	43	0
1	F	914	0	922	27	0
2	B	1071	0	1034	58	0
2	G	1062	0	1026	49	0
3	C	970	0	970	34	0
3	H	856	0	852	57	0
4	D	299	0	170	19	0
4	I	299	0	170	17	0
5	E	310	0	171	3	0
5	J	310	0	171	4	0
6	A	3	0	0	0	0
6	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	10	0	0	0	0
6	D	2	0	0	0	0
6	E	4	0	0	0	0
6	F	5	0	0	0	0
6	G	3	0	0	0	0
6	H	3	0	0	0	0
6	J	2	0	0	0	0
All	All	7039	0	6408	300	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 (300) 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:82:ASN:HD21	1:A:118:ARG:HH11	1.07	0.98
1:F:130:ARG:HH12	1:F:132:ASN:HD22	1.04	0.94
3:H:384:MET:HE1	3:H:389:LEU:HB2	1.55	0.88
1:A:82:ASN:HD21	1:A:118:ARG:NH1	1.79	0.81
1:A:82:ASN:ND2	1:A:118:ARG:HH11	1.78	0.81
3:H:348:LYS:HZ2	3:H:348:LYS:HA	1.46	0.81
4:D:10:DT:H2''	4:D:11:DC:H5'	1.64	0.79
3:H:425:THR:HB	3:H:426:PRO:HD2	1.65	0.79
2:G:95:VAL:HG13	2:G:116:LEU:HD21	1.64	0.78
2:G:88:LEU:HG	2:G:95:VAL:HG12	1.65	0.77
4:I:10:DT:H2''	4:I:11:DC:H5''	1.67	0.77
1:A:69:ASN:ND2	1:A:95:GLY:H	1.82	0.76
3:C:383:LYS:H	3:C:383:LYS:HD3	1.50	0.76
1:F:79:TRP:CZ2	1:F:86:PRO:HD3	2.21	0.76
3:H:348:LYS:HA	3:H:351:GLN:HE21	1.51	0.75
1:A:87:ILE:HD13	1:A:87:ILE:H	1.52	0.74
1:A:69:ASN:HD21	1:A:95:GLY:H	1.36	0.73
3:C:332:SER:HB2	3:C:333:PRO:HD3	1.68	0.73
4:I:11:DC:H2''	4:I:12:DC:H5'	1.70	0.73
1:A:104:THR:HG22	1:A:151:THR:HB	1.69	0.73
3:H:383:LYS:HB2	3:H:383:LYS:NZ	2.05	0.72
3:H:345:LEU:HB3	3:H:356:TRP:HE1	1.56	0.71
2:B:8:GLN:HE21	2:B:107:CYS:H	1.38	0.71
2:G:63:ASN:N	2:G:63:ASN:HD22	1.89	0.70
3:H:353:PHE:HB3	3:H:370:GLU:HG2	1.72	0.70
3:H:375:TRP:CD1	3:H:384:MET:HE2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:419:GLN:HE22	3:H:425:THR:HG22	1.54	0.70
2:B:25:CYS:O	2:B:122:MET:HG3	1.91	0.70
2:B:106:VAL:O	2:B:108:VAL:HG23	1.91	0.70
5:E:9:DT:H2''	5:E:10:DG:C8	2.27	0.69
2:B:9:ARG:HA	2:B:127:PHE:CE2	2.28	0.68
2:G:131:ARG:NH1	2:G:131:ARG:HB3	2.07	0.68
1:A:139:ARG:HH11	1:A:139:ARG:HB2	1.59	0.68
3:H:365:LEU:HD21	3:H:368:PRO:HA	1.76	0.67
4:D:11:DC:H2''	4:D:12:DC:C5'	2.24	0.67
4:D:11:DC:H1'	4:D:12:DC:H5''	1.78	0.66
2:B:89:GLU:O	2:B:91:GLU:N	2.28	0.66
1:A:109:ASN:ND2	1:A:111:GLU:H	1.94	0.65
1:A:116:GLU:HG2	1:A:137:VAL:HB	1.78	0.65
3:C:332:SER:CB	3:C:333:PRO:CD	2.74	0.65
2:B:115:ASP:OD1	2:B:118:ARG:HD3	1.96	0.65
1:A:161:THR:H	2:B:104:ASN:HD21	1.43	0.65
1:F:63:VAL:HG22	1:F:64:ARG:N	2.12	0.64
4:I:10:DT:H2''	4:I:11:DC:C5'	2.27	0.64
1:A:80:ARG:HB3	1:A:83:LYS:HD2	1.80	0.64
2:B:108:VAL:HG12	2:B:109:ILE:H	1.62	0.64
3:C:332:SER:HB2	3:C:333:PRO:CD	2.28	0.64
1:A:136:PHE:HB2	1:A:168:ILE:HG12	1.80	0.64
5:E:15:DC:H2'	5:J:1:DA:O4'	1.97	0.63
4:I:10:DT:C2'	4:I:11:DC:H5''	2.28	0.63
3:C:332:SER:O	3:C:333:PRO:C	2.38	0.63
3:H:345:LEU:HD22	3:H:356:TRP:NE1	2.14	0.62
1:A:109:ASN:C	1:A:109:ASN:HD22	2.06	0.62
1:A:159:VAL:HG13	2:B:103:LEU:HA	1.81	0.62
2:B:115:ASP:HB3	2:B:118:ARG:HB2	1.81	0.62
3:C:348:LYS:HZ3	3:C:434:ASP:HB3	1.63	0.62
3:C:327:ALA:HA	3:C:421:LEU:HD23	1.81	0.62
2:B:111:LYS:HD2	2:B:126:GLU:OE2	2.00	0.62
2:B:82:SER:HB2	2:B:86:VAL:HG12	1.81	0.62
4:D:11:DC:C2'	4:D:12:DC:H5''	2.30	0.62
3:H:336:GLN:H	3:H:339:GLN:NE2	1.98	0.61
2:B:34:ASP:O	2:B:35:ARG:HD2	2.01	0.61
3:H:340:PHE:HZ	3:H:374:ARG:HB3	1.66	0.61
3:H:375:TRP:HD1	3:H:384:MET:HE2	1.66	0.61
3:H:372:ALA:HB1	3:H:385:ASN:HA	1.82	0.61
1:A:149:THR:HG21	2:B:63:ASN:O	2.00	0.60
3:H:401:ILE:HA	3:H:416:CYS:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:60:THR:HG23	2:G:62:THR:H	1.67	0.60
2:B:93:GLY:O	2:B:116:LEU:HB2	2.00	0.60
2:G:89:GLU:O	2:G:91:GLU:N	2.34	0.60
2:G:55:ILE:HD13	2:G:66:LEU:HD12	1.82	0.60
2:B:118:ARG:HB3	2:B:120:ASP:OD2	2.02	0.59
4:I:2:DA:H2''	4:I:3:DA:H5'	1.83	0.59
3:H:409:ARG:HG3	3:H:410:TYR:HD2	1.67	0.59
4:D:9:DA:H1'	4:D:10:DT:H5''	1.84	0.59
3:H:426:PRO:HG2	3:H:427:GLU:OE2	2.03	0.59
1:A:70:PHE:CE2	1:A:152:VAL:HG21	2.38	0.59
2:G:89:GLU:C	2:G:91:GLU:H	2.11	0.59
1:A:112:ASN:C	1:A:112:ASN:HD22	2.11	0.58
2:G:97:LEU:HD12	2:G:114:ILE:HD12	1.87	0.57
2:B:108:VAL:HG12	2:B:109:ILE:N	2.19	0.57
2:B:41:GLN:HE21	2:B:117:HIS:HA	1.69	0.57
3:H:345:LEU:HD22	3:H:356:TRP:CD1	2.40	0.57
2:B:45:GLN:HG3	2:B:116:LEU:HD21	1.87	0.56
2:G:127:PHE:HE1	2:G:129:GLU:HA	1.71	0.56
3:H:337:LEU:HA	3:H:375:TRP:CZ3	2.40	0.56
3:H:347:ASP:OD2	3:H:349:SER:HB3	2.05	0.56
3:H:353:PHE:CB	3:H:370:GLU:HG2	2.35	0.56
2:B:8:GLN:NE2	2:B:107:CYS:H	2.03	0.56
2:B:26:GLU:HA	2:B:122:MET:HE2	1.88	0.56
2:B:130:GLU:O	2:B:133:GLN:HB3	2.06	0.56
2:G:88:LEU:HG	2:G:95:VAL:CG1	2.33	0.56
3:H:348:LYS:HZ2	3:H:348:LYS:CA	2.17	0.56
4:D:11:DC:H2''	4:D:12:DC:H5''	1.87	0.56
2:B:21:LEU:HD22	2:B:57:PHE:CD1	2.41	0.56
3:C:320:VAL:HG11	3:C:432:MET:HB3	1.89	0.55
1:A:87:ILE:H	1:A:87:ILE:CD1	2.18	0.55
3:H:391:ARG:HG3	3:H:391:ARG:HH11	1.71	0.55
2:G:41:GLN:HG2	2:G:119:LEU:HD21	1.89	0.55
2:G:34:ASP:O	2:G:35:ARG:HD2	2.07	0.55
1:A:69:ASN:HD21	1:A:95:GLY:N	2.03	0.54
2:G:94:LYS:HA	2:G:116:LEU:HG	1.89	0.54
3:H:430:HIS:O	3:H:433:LEU:HG	2.07	0.54
3:H:381:LYS:O	3:H:384:MET:HB2	2.07	0.54
4:I:11:DC:H1'	4:I:12:DC:H5''	1.89	0.54
2:B:32:PHE:N	2:B:32:PHE:CD2	2.75	0.54
2:G:16:GLU:OE2	2:G:20:LYS:HB2	2.08	0.54
3:H:345:LEU:HB3	3:H:356:TRP:NE1	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:9:ARG:HG3	2:G:13:GLU:OE2	2.08	0.54
2:B:29:TYR:CZ	2:B:31:GLY:HA3	2.44	0.53
4:D:11:DC:H2''	4:D:12:DC:H5'	1.90	0.53
3:C:332:SER:OG	3:C:333:PRO:HD2	2.08	0.53
1:A:113:TYR:CE2	2:B:28:LYS:HD2	2.44	0.53
3:H:418:LEU:O	3:H:422:LEU:HB2	2.09	0.53
3:H:383:LYS:HB2	3:H:383:LYS:HZ2	1.73	0.53
3:H:391:ARG:HG3	3:H:391:ARG:NH1	2.24	0.53
2:G:108:VAL:HG22	2:G:109:ILE:H	1.73	0.53
2:B:107:CYS:SG	2:B:135:GLU:HG3	2.49	0.53
2:G:41:GLN:OE1	2:G:117:HIS:HA	2.09	0.53
3:H:409:ARG:HG3	3:H:410:TYR:CD2	2.44	0.53
3:H:424:TYR:HB2	3:H:429:LEU:HD13	1.90	0.53
4:D:11:DC:C1'	4:D:12:DC:H5''	2.39	0.53
3:C:331:GLY:O	3:C:332:SER:O	2.25	0.53
2:B:5:VAL:HG12	2:B:105:GLY:O	2.09	0.52
2:G:24:GLU:HA	2:G:124:CYS:HB3	1.90	0.52
3:H:425:THR:OG1	3:H:428:GLU:HB2	2.09	0.52
2:G:11:LYS:O	2:G:15:GLU:HB2	2.10	0.52
3:C:348:LYS:HD2	3:C:351:GLN:NE2	2.24	0.52
3:C:354:ILE:HD12	3:C:365:LEU:CD2	2.40	0.52
2:B:134:GLN:O	2:B:137:ALA:HB3	2.10	0.52
3:C:348:LYS:NZ	3:C:434:ASP:HB3	2.24	0.52
2:G:54:GLU:C	2:G:55:ILE:HD12	2.35	0.52
3:C:357:THR:CG2	3:C:362:GLU:HG2	2.40	0.52
1:F:177:ARG:NH1	5:J:11:DG:N7	2.54	0.52
2:G:134:GLN:O	2:G:138:LEU:HG	2.10	0.52
3:C:364:LYS:HB2	3:C:411:VAL:HG22	1.90	0.51
4:I:9:DA:H1'	4:I:10:DT:H5''	1.92	0.51
1:A:109:ASN:HD22	1:A:111:GLU:H	1.57	0.51
2:B:16:GLU:HG3	2:B:20:LYS:HE3	1.92	0.51
1:F:63:VAL:HG22	1:F:64:ARG:H	1.74	0.51
3:H:362:GLU:HB2	3:H:413:ARG:NH1	2.26	0.51
4:I:2:DA:H1'	4:I:3:DA:H5''	1.92	0.51
3:C:436:LYS:HB2	3:C:436:LYS:NZ	2.26	0.51
1:F:130:ARG:NH1	1:F:132:ASN:HD22	1.89	0.51
4:I:8:DC:H2''	4:I:9:DA:C8	2.45	0.51
4:I:11:DC:H2''	4:I:12:DC:C5'	2.40	0.51
3:C:321:ILE:HD13	3:C:321:ILE:N	2.27	0.50
1:F:136:PHE:HB2	1:F:168:ILE:HG12	1.93	0.50
2:G:82:SER:HB2	2:G:86:VAL:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ARG:HH11	1:A:139:ARG:CB	2.24	0.50
3:H:419:GLN:NE2	3:H:425:THR:HA	2.26	0.50
4:I:9:DA:H1'	4:I:10:DT:C5'	2.41	0.50
2:B:27:ILE:HG22	2:B:57:PHE:CD2	2.46	0.50
3:H:348:LYS:O	3:H:351:GLN:HG2	2.12	0.50
2:B:85:TYR:CD1	2:B:98:LYS:HD2	2.46	0.50
1:F:164:ARG:HG3	1:F:164:ARG:HH11	1.76	0.50
2:G:89:GLU:C	2:G:91:GLU:N	2.70	0.49
4:D:10:DT:C2'	4:D:11:DC:H5'	2.39	0.49
1:F:106:MET:HE1	2:G:64:LEU:C	2.37	0.49
2:B:45:GLN:CG	2:B:116:LEU:HD21	2.43	0.49
2:G:63:ASN:N	2:G:63:ASN:ND2	2.59	0.49
4:I:9:DA:H2''	4:I:10:DT:H5'	1.94	0.49
2:G:68:PHE:CE1	2:G:97:LEU:HB3	2.47	0.49
3:C:321:ILE:HB	3:C:322:PRO:HD2	1.94	0.49
1:A:87:ILE:HD13	1:A:87:ILE:O	2.13	0.49
2:B:7:ASP:OD1	2:B:11:LYS:HG2	2.13	0.49
4:D:9:DA:H2''	4:D:10:DT:H5'	1.94	0.49
1:F:166:ILE:HG12	1:F:168:ILE:HD12	1.95	0.48
2:G:85:TYR:HA	2:G:98:LYS:HB3	1.95	0.48
1:F:145:SER:OG	1:F:164:ARG:HA	2.13	0.48
3:H:345:LEU:HD13	3:H:356:TRP:CZ2	2.48	0.48
1:A:86:PRO:HG2	1:A:87:ILE:HD12	1.95	0.48
3:C:359:ASP:OD2	3:C:359:ASP:C	2.56	0.48
3:C:389:LEU:C	3:C:389:LEU:HD23	2.38	0.48
2:G:82:SER:O	2:G:83:ARG:HG2	2.12	0.48
2:B:8:GLN:HE22	2:B:132:ALA:HA	1.77	0.48
2:B:97:LEU:HB2	2:B:110:TRP:HZ3	1.79	0.48
3:H:389:LEU:O	3:H:389:LEU:HD23	2.13	0.48
1:F:113:TYR:CE2	2:G:28:LYS:HD2	2.48	0.48
3:C:320:VAL:HG11	3:C:432:MET:HE2	1.96	0.47
2:B:27:ILE:CD1	2:B:114:ILE:HD11	2.45	0.47
3:H:371:VAL:HA	3:H:374:ARG:HB2	1.94	0.47
3:H:382:PRO:C	3:H:384:MET:H	2.22	0.47
2:B:109:ILE:HD11	2:B:128:ASP:OD1	2.14	0.47
4:D:13:DT:H2''	4:D:14:DC:H5'	1.96	0.47
2:G:55:ILE:HD12	2:G:55:ILE:N	2.30	0.47
5:J:5:DG:H2''	5:J:6:DA:H5'	1.96	0.47
3:H:334:PRO:HG2	3:H:335:ILE:H	1.78	0.47
3:H:362:GLU:HB2	3:H:413:ARG:HH11	1.79	0.47
1:A:87:ILE:CD1	1:A:87:ILE:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:15:GLU:O	2:G:19:ARG:HG2	2.15	0.47
4:I:12:DC:H2''	4:I:13:DT:OP2	2.15	0.47
2:B:7:ASP:HB2	2:B:10:SER:HB2	1.97	0.47
3:C:332:SER:OG	3:C:333:PRO:CD	2.63	0.47
1:A:87:ILE:O	1:A:87:ILE:CG1	2.63	0.46
3:C:320:VAL:CG1	3:C:432:MET:HE2	2.46	0.46
3:H:336:GLN:H	3:H:339:GLN:HE21	1.61	0.46
3:H:421:LEU:O	3:H:422:LEU:HG	2.16	0.46
2:B:95:VAL:O	2:B:113:TRP:HA	2.16	0.46
2:G:131:ARG:HB3	2:G:131:ARG:HH11	1.78	0.46
1:A:113:TYR:CZ	2:B:28:LYS:HD2	2.50	0.46
1:F:79:TRP:CE2	1:F:86:PRO:HD3	2.50	0.46
4:D:5:DC:H1'	4:D:6:DC:H5''	1.96	0.46
3:C:425:THR:HB	3:C:426:PRO:HD2	1.98	0.46
1:A:115:ALA:HB2	1:A:146:PHE:CZ	2.51	0.46
2:B:63:ASN:N	2:B:63:ASN:HD22	2.13	0.46
1:A:139:ARG:HD3	1:A:139:ARG:N	2.31	0.46
3:C:321:ILE:HD13	3:C:321:ILE:H	1.79	0.46
2:G:131:ARG:HA	2:G:134:GLN:CD	2.41	0.46
2:B:71:ALA:HB3	2:B:131:ARG:HD3	1.98	0.46
1:F:136:PHE:CB	1:F:168:ILE:HG12	2.45	0.46
3:H:402:ILE:HD11	3:H:414:PHE:CE1	2.50	0.46
4:I:13:DT:H5'	4:I:13:DT:C6	2.51	0.46
2:G:90:ARG:O	2:G:91:GLU:HB2	2.15	0.45
1:A:136:PHE:CB	1:A:168:ILE:HG12	2.46	0.45
1:F:63:VAL:CG2	1:F:64:ARG:N	2.78	0.45
2:B:130:GLU:O	2:B:134:GLN:HG3	2.17	0.45
3:H:390:SER:HB2	3:H:394:ARG:HH12	1.80	0.45
1:A:91:VAL:HB	1:A:129:ALA:HB3	1.97	0.45
3:H:424:TYR:CB	3:H:429:LEU:HD13	2.47	0.45
2:B:85:TYR:CE1	2:B:98:LYS:HD2	2.52	0.45
3:H:403:HIS:CG	3:H:415:VAL:HG21	2.52	0.45
4:D:1:DG:O4'	4:I:15:DT:H2'	2.17	0.45
1:F:112:ASN:C	1:F:112:ASN:HD22	2.25	0.45
1:F:79:TRP:CH2	1:F:86:PRO:HD3	2.52	0.44
3:H:353:PHE:CG	3:H:370:GLU:HG2	2.51	0.44
1:A:126:ASN:O	1:A:127:GLN:HB2	2.17	0.44
2:G:131:ARG:HB3	2:G:131:ARG:CZ	2.48	0.44
4:I:5:DC:H1'	4:I:6:DC:H5''	1.98	0.44
3:H:383:LYS:HB2	3:H:383:LYS:HZ3	1.79	0.44
1:A:109:ASN:ND2	1:A:112:ASN:H	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:GLN:HE21	2:B:140:GLN:HB2	1.51	0.44
2:G:55:ILE:HG22	2:G:56:ALA:N	2.32	0.44
2:G:68:PHE:CZ	2:G:97:LEU:HD13	2.53	0.44
2:G:88:LEU:N	2:G:88:LEU:HD12	2.33	0.44
2:B:66:LEU:CD2	2:B:101:MET:HE1	2.48	0.44
1:F:87:ILE:HD13	1:F:87:ILE:H	1.83	0.43
1:F:166:ILE:HG12	1:F:168:ILE:CD1	2.48	0.43
2:G:115:ASP:O	2:G:117:HIS:N	2.51	0.43
4:D:12:DC:C2'	4:D:13:DT:H71	2.49	0.43
3:C:323:ALA:HB2	3:C:346:THR:HG21	1.99	0.43
1:A:63:VAL:HG12	1:A:72:CYS:O	2.18	0.43
1:F:70:PHE:CE2	1:F:152:VAL:HG21	2.53	0.43
1:A:109:ASN:ND2	1:A:109:ASN:C	2.77	0.43
1:A:87:ILE:O	1:A:87:ILE:HG12	2.19	0.43
4:D:12:DC:H2''	4:D:13:DT:C6	2.54	0.43
2:B:88:LEU:HD23	2:B:95:VAL:HG22	2.00	0.43
4:I:13:DT:H5'	4:I:13:DT:H6	1.84	0.43
1:F:113:TYR:CZ	2:G:28:LYS:HD2	2.54	0.43
3:H:389:LEU:HD23	3:H:389:LEU:C	2.44	0.43
3:H:431:ALA:HB3	3:H:432:MET:HE2	1.99	0.43
2:G:114:ILE:HA	2:G:120:ASP:O	2.18	0.42
3:C:409:ARG:HD2	3:C:410:TYR:CE2	2.55	0.42
1:A:109:ASN:HD22	1:A:112:ASN:H	1.66	0.42
3:C:345:LEU:HB3	3:C:356:TRP:CZ2	2.54	0.42
1:F:78:HIS:HB3	1:F:173:PRO:HG3	2.00	0.42
1:F:148:LEU:HB2	1:F:162:TYR:HB3	2.01	0.42
3:H:382:PRO:O	3:H:384:MET:N	2.53	0.42
2:B:137:ALA:O	2:B:140:GLN:HG3	2.19	0.42
2:G:16:GLU:O	2:G:19:ARG:HG3	2.20	0.42
4:D:5:DC:H2''	4:D:6:DC:C5'	2.49	0.42
2:B:6:PRO:C	2:B:8:GLN:H	2.27	0.42
4:D:12:DC:H2'	4:D:13:DT:H71	2.02	0.42
2:B:45:GLN:HG3	2:B:116:LEU:HD11	2.02	0.42
2:G:55:ILE:HG12	2:G:114:ILE:HD11	2.01	0.42
1:A:112:ASN:C	1:A:112:ASN:ND2	2.76	0.42
3:C:375:TRP:CD1	3:C:384:MET:HE3	2.55	0.41
1:F:63:VAL:HG12	1:F:72:CYS:O	2.20	0.41
2:G:55:ILE:CG2	2:G:56:ALA:N	2.83	0.41
2:G:131:ARG:HA	2:G:134:GLN:CG	2.50	0.41
1:A:166:ILE:HD13	1:A:168:ILE:HD11	2.03	0.41
3:C:382:PRO:HG2	3:C:383:LYS:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:131:ARG:O	2:G:134:GLN:HG2	2.19	0.41
3:H:368:PRO:HG2	3:H:369:ASP:H	1.84	0.41
3:H:393:LEU:HA	3:H:396:TYR:HD2	1.86	0.41
2:B:35:ARG:O	2:B:36:PRO:C	2.62	0.41
3:C:354:ILE:HG13	3:C:365:LEU:HD23	2.03	0.41
3:H:419:GLN:HE21	3:H:425:THR:HA	1.84	0.41
5:J:9:DT:H2''	5:J:10:DG:C8	2.56	0.41
1:A:69:ASN:HD22	1:A:69:ASN:HA	1.70	0.41
2:B:49:ARG:HH11	2:B:49:ARG:HG3	1.86	0.41
3:C:385:ASN:OD1	3:C:385:ASN:C	2.64	0.41
3:C:405:THR:HG21	3:C:408:LYS:HD2	2.03	0.41
1:F:115:ALA:HB2	1:F:146:PHE:CZ	2.56	0.41
3:H:393:LEU:HD22	3:H:402:ILE:HG21	2.03	0.41
2:B:134:GLN:HG3	2:B:134:GLN:H	1.63	0.41
3:C:348:LYS:O	3:C:351:GLN:HG3	2.20	0.41
1:F:63:VAL:CG2	1:F:64:ARG:H	2.34	0.41
4:D:7:DA:H1'	4:D:8:DC:O4'	2.21	0.41
5:E:11:DG:H2''	5:E:12:DC:O5'	2.20	0.41
1:A:79:TRP:CE2	1:A:83:LYS:HD3	2.56	0.41
2:B:89:GLU:C	2:B:91:GLU:N	2.79	0.41
2:B:108:VAL:HG11	2:B:125:LEU:HB3	2.03	0.41
1:A:79:TRP:CZ2	1:A:83:LYS:HD3	2.56	0.40
2:B:8:GLN:O	2:B:127:PHE:HE2	2.05	0.40
2:G:16:GLU:HA	2:G:19:ARG:HD2	2.02	0.40
4:D:8:DC:H2''	4:D:9:DA:C8	2.56	0.40
1:F:105:VAL:HG23	1:F:131:PHE:CZ	2.57	0.40
2:G:115:ASP:C	2:G:117:HIS:H	2.29	0.40
2:B:127:PHE:CD1	2:B:128:ASP:N	2.89	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%)	105 (90%)	10 (9%)	1 (1%)	14	35
2	B	126/142 (89%)	102 (81%)	21 (17%)	3 (2%)	4	12
2	G	125/142 (88%)	111 (89%)	12 (10%)	2 (2%)	7	20
3	C	116/166 (70%)	107 (92%)	8 (7%)	1 (1%)	14	35
3	H	99/166 (60%)	74 (75%)	18 (18%)	7 (7%)	1	1
All	All	698/1024 (68%)	608 (87%)	76 (11%)	14 (2%)	6	16

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	90	ARG
3	C	332	SER
2	G	90	ARG
3	H	334	PRO
3	H	383	LYS
3	H	422	LEU
3	H	426	PRO
2	B	127	PHE
2	G	116	LEU
3	H	335	ILE
2	B	58	VAL
3	H	360	GLY
1	F	143	GLY
3	H	368	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	100/179 (56%)	93 (93%)	7 (7%)	14	34
1	F	100/179 (56%)	95 (95%)	5 (5%)	22	48
2	B	113/123 (92%)	101 (89%)	12 (11%)	6	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	112/123 (91%)	105 (94%)	7 (6%)	16	39
3	C	103/146 (70%)	97 (94%)	6 (6%)	18	42
3	H	92/146 (63%)	88 (96%)	4 (4%)	26	54
All	All	620/896 (69%)	579 (93%)	41 (7%)	15	36

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	87	ILE
1	A	104	THR
1	A	109	ASN
1	A	112	ASN
1	A	130	ARG
1	A	139	ARG
2	B	8	GLN
2	B	20	LYS
2	B	45	GLN
2	B	60	THR
2	B	63	ASN
2	B	67	GLN
2	B	82	SER
2	B	84	GLU
2	B	116	LEU
2	B	122	MET
2	B	136	ASP
2	B	140	GLN
3	C	321	ILE
3	C	378	ARG
3	C	379	LYS
3	C	383	LYS
3	C	427	GLU
3	C	436	LYS
1	F	87	ILE
1	F	96	ASP
1	F	121	THR
1	F	125	LYS
1	F	139	ARG
2	G	63	ASN
2	G	65	SER
2	G	67	GLN

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Mol	Chain	Res	Type
2	G	82	SER
2	G	86	VAL
2	G	103	LEU
2	G	133	GLN
3	H	344	LEU
3	H	348	LYS
3	H	383	LYS
3	H	427	GLU

Sometimes 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	163	HIS
2	B	8	GLN
2	B	41	GLN
2	B	63	ASN
2	B	67	GLN
2	B	104	ASN
2	B	140	GLN
3	C	380	ASN
1	F	112	ASN
1	F	127	GLN
1	F	132	ASN
1	F	158	GLN
2	G	45	GLN
2	G	46	ASN
2	G	63	ASN
2	G	67	GLN
3	H	339	GLN
3	H	351	GLN
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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.17	2 (1%) 69 67	54, 71, 94, 104	0
1	F	118/204 (57%)	0.08	1 (0%) 82 81	50, 64, 84, 104	0
2	B	130/142 (91%)	0.99	15 (11%) 9 8	70, 98, 129, 136	0
2	G	129/142 (90%)	1.00	15 (11%) 9 8	70, 91, 117, 122	0
3	C	118/166 (71%)	0.29	6 (5%) 33 29	51, 71, 104, 109	0
3	H	101/166 (60%)	1.65	33 (32%) 1 1	74, 123, 164, 167	0
4	D	15/15 (100%)	-0.20	0 100 100	58, 62, 72, 78	0
4	I	15/15 (100%)	0.38	0 100 100	62, 70, 84, 87	0
5	E	15/15 (100%)	-0.24	0 100 100	54, 61, 75, 77	0
5	J	15/15 (100%)	0.13	0 100 100	56, 68, 85, 88	0
All	All	774/1084 (71%)	0.63	72 (9%) 14 12	50, 81, 130, 167	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	353	PHE	6.7
2	G	139	ALA	4.5
3	H	431	ALA	4.2
3	H	433	LEU	4.2
3	C	331	GLY	3.7
2	G	81	PRO	3.7
2	G	7	ASP	3.4
3	H	360	GLY	3.3
3	H	365	LEU	3.3
3	H	351	GLN	3.3
3	H	357	THR	3.3
3	H	358	GLY	3.2
3	H	421	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
3	H	416	CYS	3.2
3	C	332	SER	3.1
2	B	83	ARG	3.0
3	H	423	GLY	3.0
3	H	356	TRP	3.0
2	G	87	ASP	3.0
1	F	176	PRO	2.9
2	B	22	SER	2.9
2	B	81	PRO	2.9
2	B	107	CYS	2.9
3	H	409	ARG	2.8
3	H	410	TYR	2.8
3	H	361	TRP	2.8
2	B	7	ASP	2.8
3	H	363	PHE	2.7
3	H	398	ASP	2.7
2	B	71	ALA	2.6
3	H	355	SER	2.6
2	B	93	GLY	2.6
3	H	411	VAL	2.6
3	H	346	THR	2.5
3	H	415	VAL	2.5
2	G	109	ILE	2.4
1	A	67	SER	2.4
2	G	88	LEU	2.4
3	C	326	LEU	2.4
2	G	122	MET	2.4
1	A	177	ARG	2.4
3	H	368	PRO	2.4
3	H	419	GLN	2.4
3	H	413	ARG	2.4
3	H	352	SER	2.4
3	C	436	LYS	2.3
2	B	86	VAL	2.3
2	G	131	ARG	2.3
3	H	350	CYS	2.3
2	B	10	SER	2.3
3	H	345	LEU	2.3
2	B	85	TYR	2.2
3	C	324	ALA	2.2
2	B	96	TYR	2.2
2	G	134	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
3	H	348	LYS	2.2
3	H	428	GLU	2.2
2	G	138	LEU	2.2
2	G	92	ALA	2.1
2	B	132	ALA	2.1
3	C	327	ALA	2.1
2	G	94	LYS	2.1
3	H	382	PRO	2.1
2	G	93	GLY	2.1
2	B	5	VAL	2.1
2	B	6	PRO	2.1
2	B	25	CYS	2.1
3	H	405	THR	2.1
3	H	337	LEU	2.1
3	H	372	ALA	2.0
2	G	119	LEU	2.0
2	G	114	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.