



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:33 PM EDT

PDB ID : 3WTU / pdb_00003wtu
Title : Crystal structure of the complex comprised of ETS1 (V170A), 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

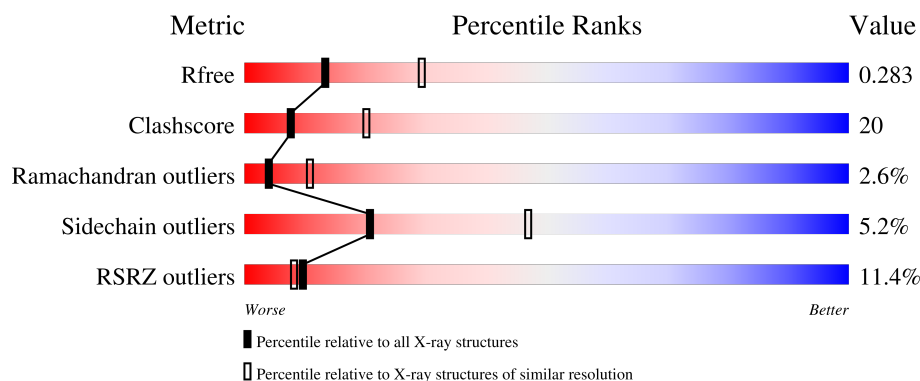
1 Overall quality at a glance

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	35% 21% • 42%
1	F	204	41% 17% • 42%
2	B	142	13% 50% 38% • 8%
2	G	142	11% 46% 39% 5% 9%
3	C	166	46% 24% • 29%

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Mol	Chain	Length	Quality of chain
3	H	166	28% 34% 25% 39%
4	D	15	7% 73% 20%
4	I	15	7% 67% 27%
5	E	15	73% 27%
5	J	15	67% 33%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7030 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
			912	572	169	167	4			
1	F	118	Total	C	N	O	S	0	0	0
			912	572	169	167	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	LYS	LEU	engineered mutation	UNP Q03347
A	170	ALA	VAL	engineered mutation	UNP Q03347
F	94	LYS	LEU	engineered mutation	UNP Q03347
F	170	ALA	VAL	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
			967	627	165	171	4			
3	H	101	Total	C	N	O	S	0	0	0
			853	553	147	149	4			

- 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			

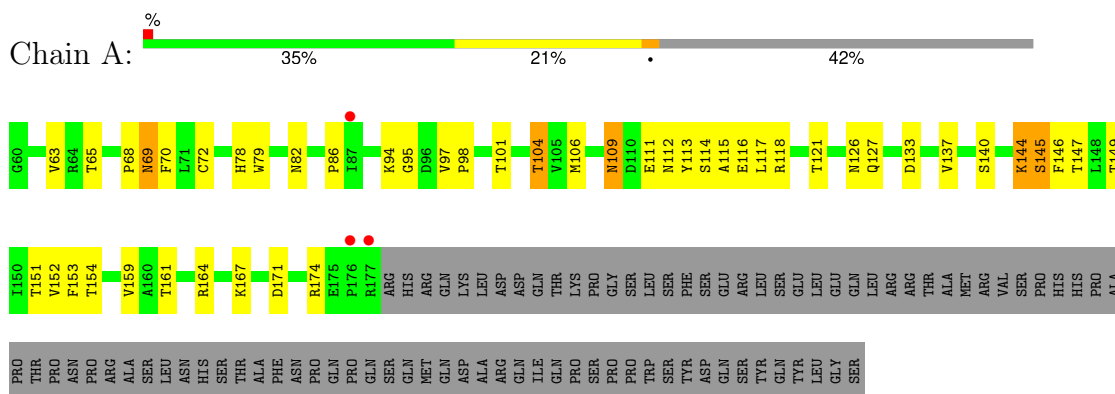
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	5	Total	O	0	0
			5	5		
6	B	4	Total	O	0	0
			4	4		
6	C	7	Total	O	0	0
			7	7		
6	F	6	Total	O	0	0
			6	6		
6	G	2	Total	O	0	0
			2	2		
6	E	7	Total	O	0	0
			7	7		
6	I	1	Total	O	0	0
			1	1		
6	J	3	Total	O	0	0
			3	3		

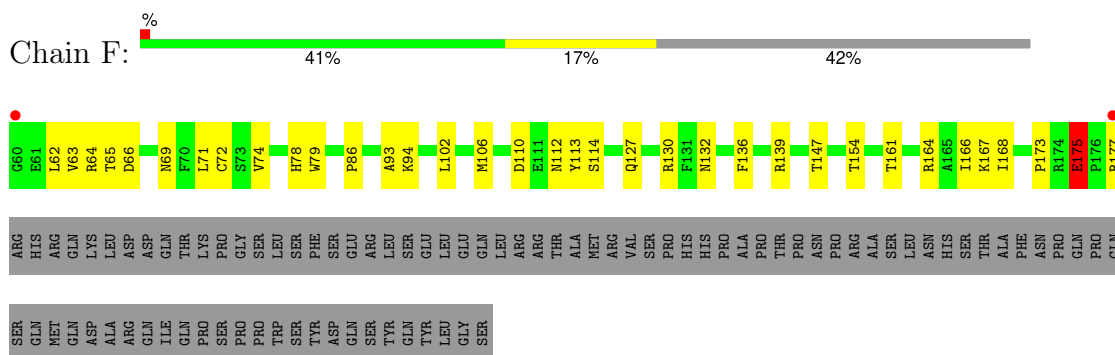
3 Residue-property plots [i](#)

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.

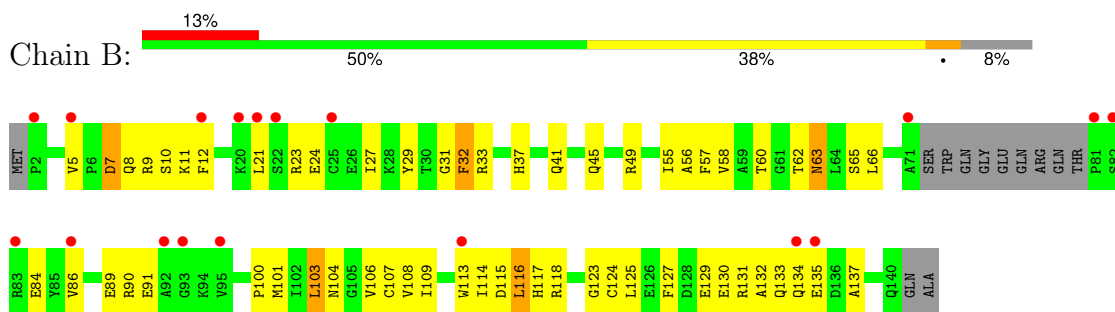
- Molecule 1: Runt-related transcription factor 1



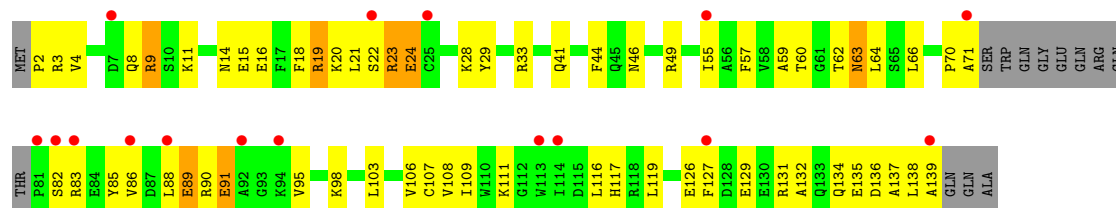
- Molecule 1: Runt-related transcription factor 1



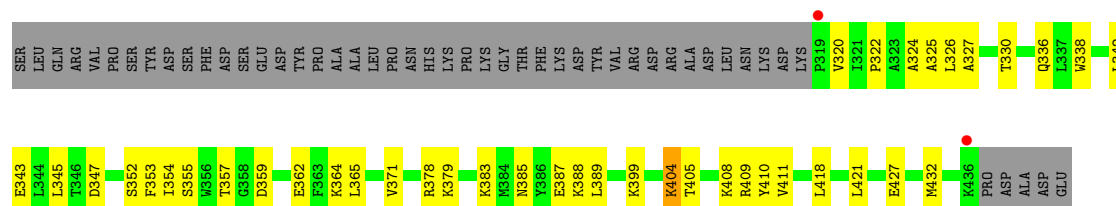
- Molecule 2: Core-binding factor subunit beta



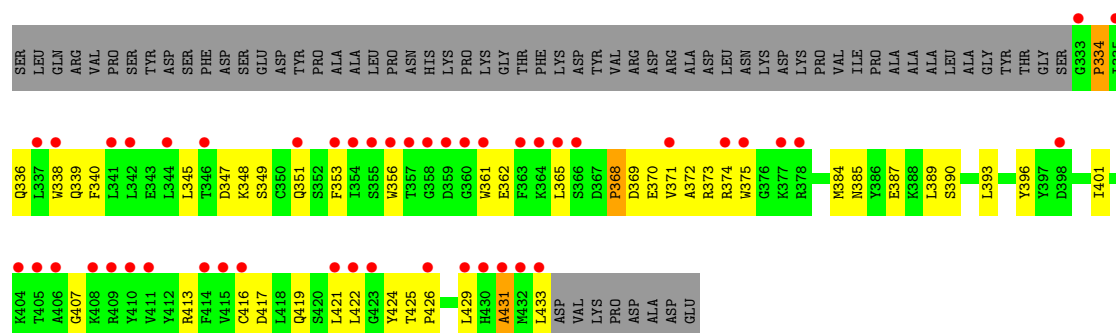
- Molecule 2: Core-binding factor subunit beta



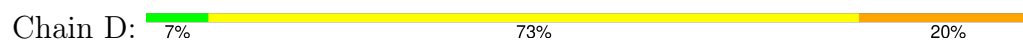
• Molecule 3: Protein C-ets-1



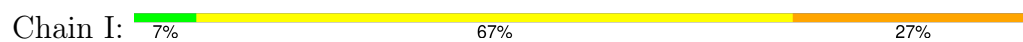
• Molecule 3: Protein C-ets-1



• 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')



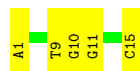
- Molecule 5: DNA (5'-D(*AP*GP*AP*GP*GP*AP*TP*GP*TP*GP*GP*CP*TP*TP*C)-3')

Chain E:  73% 27%



- 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, α , β , γ	78.56Å 102.11Å 194.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.74 – 2.70 48.74 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.74-2.70) 98.9 (48.74-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.25 (at 2.69Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.232 , 0.282 0.233 , 0.283	Depositor DCC
R_{free} test set	4371 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å ²)	71.1	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.7	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	7030	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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	0.63	0/931	1.04	2/1265 (0.2%)
1	F	0.70	0/931	1.10	5/1265 (0.4%)
2	B	0.45	0/1093	0.82	0/1466
2	G	0.53	0/1084	0.89	0/1454
3	C	0.67	0/994	0.97	1/1342 (0.1%)
3	H	0.42	0/877	0.76	0/1181
4	D	0.43	0/334	1.07	2/512 (0.4%)
4	I	0.43	0/334	1.07	3/512 (0.6%)
5	E	0.40	0/348	0.86	0/537
5	J	0.36	0/348	0.83	1/537 (0.2%)
All	All	0.55	0/7274	0.94	14/10071 (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	3
4	I	0	3
5	E	0	1
All	All	0	7

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	4	DG	N9-C1'-C2'	-9.60	99.09	113.50
4	I	4	DG	N9-C1'-C2'	-7.33	102.51	113.50
4	I	4	DG	C4'-C3'-O3'	7.08	120.62	110.00
4	D	4	DG	C4'-C3'-O3'	6.81	120.22	110.00
1	F	154	THR	N-CA-C	-6.54	100.29	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	166	ILE	N-CA-C	6.21	116.01	108.06
1	A	153	PHE	N-CA-C	6.05	119.04	108.52
1	A	133	ASP	N-CA-C	5.55	119.29	111.52
1	F	175	GLU	CA-C-N	5.51	125.46	119.78
1	F	175	GLU	C-N-CA	5.51	125.46	119.78
4	I	14	DC	C5'-C4'-C3'	-5.34	106.89	114.90
3	C	355	SER	N-CA-C	5.31	116.92	108.79
1	F	65	THR	N-CA-C	-5.26	102.21	110.36
5	J	15	DC	C4'-C3'-O3'	5.02	117.53	110.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	4	DG	Sidechain
4	D	5	DC	Sidechain
4	D	9	DA	Sidechain
5	E	13	DT	Sidechain
4	I	4	DG	Sidechain
4	I	5	DC	Sidechain
4	I	9	DA	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	912	0	918	40	0
1	F	912	0	918	25	0
2	B	1071	0	1034	51	0
2	G	1062	0	1026	51	0
3	C	967	0	966	27	0
3	H	853	0	847	50	0
4	D	299	0	170	15	0
4	I	299	0	170	20	0
5	E	310	0	171	2	0
5	J	310	0	171	4	0
6	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	4	0	0	0	0
6	C	7	0	0	0	0
6	E	7	0	0	0	0
6	F	6	0	0	1	0
6	G	2	0	0	0	0
6	I	1	0	0	0	0
6	J	3	0	0	0	0
All	All	7030	0	6391	269	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 (269) 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)
4:I:14:DC:H2''	4:I:15:DT:H5'	1.50	0.94
1:A:82:ASN:HD21	1:A:118:ARG:HH11	1.15	0.93
3:H:419:GLN:HE22	3:H:425:THR:HA	1.28	0.93
2:B:60:THR:HG23	2:B:62:THR:H	1.40	0.84
1:F:64:ARG:HA	1:F:71:LEU:HD23	1.60	0.83
2:G:88:LEU:HD23	2:G:95:VAL:HG22	1.62	0.81
2:G:11:LYS:HG3	2:G:15:GLU:HG3	1.64	0.80
1:A:161:THR:H	2:B:104:ASN:HD21	1.29	0.78
1:F:79:TRP:CZ2	1:F:86:PRO:HD3	2.20	0.77
3:H:362:GLU:HB2	3:H:413:ARG:HH11	1.52	0.74
3:H:375:TRP:CD1	3:H:384:MET:HE2	2.22	0.74
3:C:327:ALA:HA	3:C:421:LEU:HD23	1.70	0.73
1:A:69:ASN:HD21	1:A:95:GLY:H	1.36	0.72
3:H:419:GLN:NE2	3:H:425:THR:HA	2.04	0.72
4:I:14:DC:H2''	4:I:15:DT:C5'	2.19	0.71
3:H:375:TRP:HD1	3:H:384:MET:HE2	1.53	0.71
1:A:109:ASN:ND2	1:A:112:ASN:H	1.90	0.70
1:F:64:ARG:HA	1:F:71:LEU:CD2	2.23	0.69
4:D:10:DT:H2''	4:D:11:DC:H5'	1.75	0.69
1:A:69:ASN:ND2	1:A:95:GLY:H	1.90	0.68
2:G:60:THR:HG23	2:G:62:THR:H	1.59	0.67
2:B:108:VAL:HG12	2:B:109:ILE:N	2.10	0.67
2:G:134:GLN:O	2:G:138:LEU:HG	1.95	0.67
2:G:55:ILE:HD12	2:G:66:LEU:HD12	1.77	0.67
1:F:175:GLU:OE1	1:F:175:GLU:HA	1.95	0.66
2:G:63:ASN:N	2:G:63:ASN:HD22	1.92	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:GLU:HG3	1:A:144:LYS:HZ2	1.61	0.66
1:A:82:ASN:ND2	1:A:118:ARG:HH11	1.91	0.65
1:A:111:GLU:HG3	1:A:144:LYS:NZ	2.11	0.65
2:B:45:GLN:HE21	2:B:49:ARG:HH12	1.44	0.65
4:I:11:DC:H1'	4:I:12:DC:H5''	1.76	0.65
2:B:129:GLU:O	2:B:133:GLN:HG3	1.97	0.65
3:H:372:ALA:HB1	3:H:385:ASN:HA	1.79	0.64
2:B:108:VAL:HG12	2:B:109:ILE:H	1.61	0.64
3:H:365:LEU:HD21	3:H:368:PRO:CA	2.28	0.63
2:G:90:ARG:O	2:G:91:GLU:HB2	1.98	0.63
4:I:12:DC:H2'	4:I:13:DT:H72	1.81	0.63
2:G:8:GLN:HE21	2:G:107:CYS:H	1.46	0.63
3:C:365:LEU:HD23	3:C:371:VAL:HG21	1.79	0.63
1:A:104:THR:HG22	1:A:151:THR:HB	1.80	0.63
1:F:63:VAL:HG22	1:F:64:ARG:N	2.14	0.63
2:G:9:ARG:HG3	2:G:9:ARG:HH11	1.64	0.62
2:B:55:ILE:HD12	2:B:66:LEU:HD12	1.82	0.62
2:B:108:VAL:HG11	2:B:125:LEU:HB3	1.82	0.61
3:H:365:LEU:HD21	3:H:368:PRO:N	2.15	0.61
1:F:164:ARG:HD2	6:F:306:HOH:O	2.01	0.60
1:A:109:ASN:C	1:A:109:ASN:HD22	2.09	0.60
3:H:347:ASP:OD2	3:H:349:SER:HB3	2.02	0.60
1:A:70:PHE:CE2	1:A:152:VAL:HG21	2.36	0.60
1:A:97:VAL:H	1:A:127:GLN:HE22	1.49	0.60
1:A:159:VAL:HG13	2:B:103:LEU:HA	1.84	0.59
2:G:70:PRO:HG3	2:G:85:TYR:CE2	2.37	0.59
3:C:345:LEU:HD21	3:C:354:ILE:HG12	1.84	0.59
4:D:11:DC:H2''	4:D:12:DC:H5'	1.84	0.59
1:A:82:ASN:HD21	1:A:118:ARG:NH1	1.94	0.59
2:B:9:ARG:HA	2:B:127:PHE:CE2	2.38	0.59
3:H:353:PHE:CG	3:H:370:GLU:HG2	2.38	0.59
1:A:145:SER:HB3	1:A:164:ARG:HA	1.84	0.58
2:B:5:VAL:HG11	2:B:11:LYS:HD2	1.85	0.58
3:H:340:PHE:HZ	3:H:374:ARG:HB3	1.69	0.58
1:A:63:VAL:HG12	1:A:72:CYS:O	2.03	0.58
1:A:112:ASN:C	1:A:112:ASN:HD22	2.12	0.57
2:G:41:GLN:HG2	2:G:119:LEU:HD21	1.86	0.57
4:I:13:DT:H6	4:I:13:DT:H5'	1.69	0.57
1:F:167:LYS:C	1:F:168:ILE:HD12	2.29	0.57
3:C:336:GLN:NE2	3:C:338:TRP:HE1	2.03	0.57
2:G:8:GLN:HE22	2:G:132:ALA:HA	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:VAL:HG12	1:F:72:CYS:O	2.04	0.56
2:G:108:VAL:HG12	2:G:109:ILE:N	2.20	0.56
3:H:385:ASN:OD1	3:H:387:GLU:HB2	2.05	0.56
2:B:134:GLN:O	2:B:137:ALA:HB3	2.05	0.56
3:C:409:ARG:HD2	3:C:410:TYR:CE2	2.40	0.56
2:G:111:LYS:HD2	2:G:126:GLU:OE1	2.05	0.56
4:D:13:DT:H2''	4:D:14:DC:H5'	1.87	0.56
2:B:89:GLU:O	2:B:91:GLU:N	2.39	0.56
3:H:371:VAL:HA	3:H:374:ARG:HB2	1.87	0.56
1:F:78:HIS:HB3	1:F:173:PRO:HG3	1.88	0.55
4:I:9:DA:H1'	4:I:10:DT:H5''	1.87	0.55
3:H:345:LEU:HD13	3:H:356:TRP:CE2	2.42	0.55
3:H:419:GLN:NE2	3:H:426:PRO:HD3	2.22	0.55
2:G:21:LEU:HD21	2:G:60:THR:HG21	1.88	0.55
1:A:68:PRO:O	1:A:94:LYS:HD2	2.07	0.55
4:D:1:DG:O4'	4:I:15:DT:H2'	2.06	0.55
2:G:132:ALA:O	2:G:136:ASP:HB2	2.07	0.54
2:B:63:ASN:N	2:B:63:ASN:HD22	2.06	0.54
2:B:115:ASP:HB3	2:B:118:ARG:HB2	1.88	0.54
3:C:409:ARG:HG3	3:C:410:TYR:CD2	2.43	0.54
1:A:152:VAL:HG12	1:A:154:THR:HG23	1.90	0.54
2:G:8:GLN:HG2	2:G:106:VAL:HA	1.90	0.54
2:G:23:ARG:O	2:G:24:GLU:C	2.50	0.54
2:B:131:ARG:HG2	2:B:131:ARG:HH11	1.73	0.54
3:H:429:LEU:C	3:H:431:ALA:H	2.16	0.54
4:I:12:DC:C2'	4:I:13:DT:H72	2.37	0.53
4:I:13:DT:H5'	4:I:13:DT:C6	2.42	0.53
3:H:365:LEU:HD23	3:H:365:LEU:O	2.08	0.53
2:B:7:ASP:HB2	2:B:10:SER:HB3	1.89	0.53
2:B:21:LEU:HD22	2:B:57:PHE:CD1	2.43	0.53
3:H:348:LYS:HD3	3:H:433:LEU:HD23	1.89	0.53
3:H:368:PRO:HG2	3:H:369:ASP:H	1.74	0.53
4:I:10:DT:H1'	4:I:11:DC:H5'	1.90	0.53
3:H:345:LEU:HD22	3:H:356:TRP:CD1	2.43	0.53
3:H:369:ASP:HB3	3:H:373:ARG:NH2	2.24	0.53
4:D:9:DA:H2''	4:D:10:DT:H5'	1.91	0.53
3:H:353:PHE:HB3	3:H:370:GLU:HG2	1.91	0.52
3:H:419:GLN:HE22	3:H:425:THR:CA	2.11	0.52
2:B:106:VAL:O	2:B:108:VAL:HG23	2.09	0.52
2:G:16:GLU:OE2	2:G:20:LYS:HB2	2.09	0.52
3:H:362:GLU:HB2	3:H:413:ARG:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:ARG:O	2:B:135:GLU:HB2	2.09	0.52
3:C:385:ASN:HD21	3:C:387:GLU:HG3	1.75	0.52
2:G:11:LYS:HG3	2:G:15:GLU:CG	2.37	0.52
3:C:322:PRO:HG2	3:C:326:LEU:HG	1.91	0.51
3:C:405:THR:HG21	3:C:408:LYS:HD2	1.93	0.51
2:G:9:ARG:HH11	2:G:9:ARG:CG	2.22	0.51
3:H:389:LEU:O	3:H:389:LEU:HD23	2.10	0.51
2:B:37:HIS:O	2:B:41:GLN:HG3	2.11	0.51
4:I:2:DA:H1'	4:I:3:DA:H5'	1.93	0.51
2:B:56:ALA:HB2	2:B:63:ASN:HA	1.93	0.51
1:F:106:MET:HE1	2:G:64:LEU:C	2.36	0.50
3:H:384:MET:HE3	3:H:389:LEU:HB2	1.93	0.50
1:F:79:TRP:CH2	1:F:86:PRO:HD3	2.46	0.50
1:F:63:VAL:HB	1:F:74:VAL:HG22	1.92	0.50
2:B:8:GLN:HE22	2:B:132:ALA:HA	1.77	0.50
3:H:369:ASP:HB3	3:H:373:ARG:HH21	1.75	0.50
2:B:57:PHE:HB2	2:B:60:THR:HG22	1.94	0.50
3:H:340:PHE:CZ	3:H:374:ARG:HB3	2.46	0.50
1:F:66:ASP:OD2	1:F:161:THR:OG1	2.29	0.50
3:C:327:ALA:HA	3:C:421:LEU:CD2	2.40	0.50
5:E:15:DC:H2'	5:J:1:DA:O4'	2.12	0.50
3:C:388:LYS:HE2	4:D:10:DT:H2'	1.94	0.49
2:G:19:ARG:HA	2:G:22:SER:OG	2.12	0.49
3:H:431:ALA:C	3:H:433:LEU:H	2.21	0.49
1:A:112:ASN:ND2	1:A:114:SER:H	2.09	0.49
1:A:106:MET:HE1	2:B:65:SER:N	2.28	0.49
4:D:9:DA:H1'	4:D:10:DT:H5''	1.95	0.49
3:H:401:ILE:HA	3:H:416:CYS:HB3	1.94	0.48
5:E:9:DT:H2''	5:E:10:DG:C8	2.48	0.48
1:F:130:ARG:HH12	1:F:132:ASN:HD22	1.60	0.48
1:F:102:LEU:N	1:F:102:LEU:HD22	2.28	0.48
3:H:334:PRO:HG2	5:J:11:DG:H4'	1.94	0.48
4:I:12:DC:H2''	4:I:13:DT:H5'	1.95	0.48
2:G:106:VAL:HG12	2:G:108:VAL:CG2	2.43	0.48
2:G:131:ARG:CZ	2:G:131:ARG:HB3	2.44	0.48
4:D:5:DC:H1'	4:D:6:DC:H5''	1.96	0.48
3:H:422:LEU:C	3:H:424:TYR:H	2.21	0.48
4:I:11:DC:C2'	4:I:12:DC:H5''	2.44	0.48
2:G:82:SER:OG	2:G:85:TYR:HB2	2.13	0.48
4:D:11:DC:H1'	4:D:12:DC:H5''	1.95	0.48
2:G:82:SER:OG	2:G:83:ARG:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1:DG:H2''	4:D:2:DA:OP2	2.13	0.47
2:B:41:GLN:HE21	2:B:117:HIS:HA	1.78	0.47
3:H:347:ASP:CG	3:H:349:SER:HB3	2.38	0.47
1:A:78:HIS:CD2	1:A:167:LYS:HE3	2.49	0.47
3:H:365:LEU:HD21	3:H:368:PRO:HA	1.96	0.47
4:D:14:DC:H2''	4:D:15:DT:H5'	1.95	0.47
4:I:7:DA:H2''	4:I:8:DC:O5'	2.14	0.47
2:B:8:GLN:NE2	2:B:132:ALA:HA	2.30	0.47
2:B:55:ILE:HD12	2:B:66:LEU:CD1	2.44	0.47
1:F:136:PHE:CB	1:F:168:ILE:HG12	2.44	0.47
1:F:69:ASN:HB2	2:G:2:PRO:O	2.15	0.47
2:G:108:VAL:HG12	2:G:109:ILE:H	1.79	0.47
3:H:362:GLU:CB	3:H:413:ARG:HD2	2.45	0.47
2:G:106:VAL:HG12	2:G:108:VAL:HG23	1.97	0.47
1:A:109:ASN:ND2	1:A:109:ASN:C	2.72	0.47
3:H:393:LEU:HA	3:H:396:TYR:HD2	1.79	0.47
2:B:108:VAL:CG1	2:B:109:ILE:N	2.78	0.46
3:H:421:LEU:C	3:H:422:LEU:HD12	2.40	0.46
2:B:29:TYR:CZ	2:B:31:GLY:HA3	2.50	0.46
2:G:16:GLU:OE2	2:G:20:LYS:HD2	2.15	0.46
2:B:45:GLN:HE21	2:B:49:ARG:NH1	2.12	0.46
1:F:112:ASN:C	1:F:112:ASN:HD22	2.23	0.46
3:H:345:LEU:HB3	3:H:356:TRP:HE1	1.81	0.46
1:A:112:ASN:HD21	2:B:33:ARG:HH12	1.64	0.46
2:G:3:ARG:NE	2:G:135:GLU:OE2	2.48	0.46
2:B:27:ILE:HD11	2:B:113:TRP:O	2.15	0.46
2:G:137:ALA:C	2:G:139:ALA:H	2.24	0.45
3:H:338:TRP:CE2	3:H:339:GLN:HG3	2.51	0.45
1:F:177:ARG:NH1	5:J:11:DG:N7	2.63	0.45
1:A:65:THR:HG23	1:A:70:PHE:O	2.16	0.45
5:J:9:DT:H2''	5:J:10:DG:C8	2.52	0.45
3:H:417:ASP:O	3:H:421:LEU:HD13	2.16	0.45
3:C:359:ASP:OD2	3:C:359:ASP:C	2.59	0.45
2:B:32:PHE:CD2	2:B:32:PHE:N	2.84	0.45
3:C:385:ASN:HD21	3:C:387:GLU:CG	2.30	0.45
2:B:57:PHE:HB2	2:B:60:THR:CG2	2.46	0.45
1:A:112:ASN:ND2	2:B:33:ARG:HH12	2.14	0.45
3:C:357:THR:CG2	3:C:362:GLU:HG2	2.47	0.45
1:F:113:TYR:CZ	2:G:28:LYS:HD2	2.52	0.45
3:C:404:LYS:HG3	3:C:405:THR:N	2.31	0.44
2:G:11:LYS:HE3	2:G:15:GLU:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:131:ARG:HB3	2:G:131:ARG:NH1	2.33	0.44
2:B:108:VAL:CG1	2:B:109:ILE:H	2.28	0.44
2:B:45:GLN:OE1	2:B:116:LEU:HD22	2.18	0.44
2:G:71:ALA:HB3	2:G:131:ARG:NE	2.33	0.44
4:D:11:DC:H1'	4:D:12:DC:C5'	2.46	0.44
2:B:115:ASP:O	2:B:117:HIS:N	2.50	0.44
1:F:63:VAL:CG2	1:F:64:ARG:N	2.79	0.44
3:H:390:SER:O	3:H:393:LEU:HB2	2.18	0.44
3:C:404:LYS:HE2	3:C:411:VAL:O	2.17	0.44
4:I:8:DC:H2''	4:I:9:DA:C8	2.53	0.44
1:A:69:ASN:HD21	1:A:95:GLY:N	2.12	0.43
1:A:126:ASN:O	1:A:127:GLN:HB2	2.17	0.43
2:G:8:GLN:HB3	2:G:127:PHE:HE2	1.83	0.43
1:A:149:THR:HG21	2:B:63:ASN:O	2.17	0.43
2:B:56:ALA:CB	2:B:63:ASN:HA	2.48	0.43
4:D:10:DT:C2'	4:D:11:DC:H5'	2.47	0.43
1:A:109:ASN:HD21	1:A:112:ASN:H	1.64	0.43
1:A:116:GLU:HG2	1:A:137:VAL:HB	2.00	0.43
2:G:46:ASN:O	2:G:49:ARG:HB2	2.18	0.43
1:A:79:TRP:CZ2	1:A:86:PRO:HD3	2.53	0.43
1:A:115:ALA:HB2	1:A:146:PHE:CZ	2.52	0.43
2:B:21:LEU:HD21	2:B:60:THR:HG21	2.01	0.43
1:F:63:VAL:HG22	1:F:64:ARG:H	1.82	0.43
1:A:140:SER:O	1:A:144:LYS:HB3	2.19	0.43
3:C:353:PHE:CD2	3:C:353:PHE:N	2.87	0.43
3:H:429:LEU:O	3:H:429:LEU:HD23	2.18	0.43
4:I:11:DC:C1'	4:I:12:DC:H5''	2.47	0.43
2:B:131:ARG:HG2	2:B:131:ARG:NH1	2.34	0.43
2:G:63:ASN:HD22	2:G:63:ASN:H	1.63	0.43
3:C:324:ALA:HB2	3:C:343:GLU:HG3	2.02	0.42
3:C:364:LYS:HB3	3:C:411:VAL:HG22	2.01	0.42
2:B:86:VAL:HG13	2:B:86:VAL:O	2.19	0.42
1:F:168:ILE:HD12	1:F:168:ILE:N	2.34	0.42
2:G:29:TYR:CD2	2:G:44:PHE:HD2	2.38	0.42
1:A:144:LYS:HE2	3:H:407:GLY:HA2	2.01	0.42
3:C:347:ASP:OD1	3:C:347:ASP:C	2.62	0.42
4:D:6:DC:H2''	4:D:7:DA:C8	2.54	0.42
2:B:115:ASP:C	2:B:117:HIS:H	2.28	0.42
2:G:9:ARG:CG	2:G:9:ARG:NH1	2.78	0.42
1:A:171:ASP:HB3	1:A:174:ARG:HD2	2.02	0.42
2:G:18:PHE:C	2:G:20:LYS:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:320:VAL:HG11	3:C:432:MET:HB3	2.01	0.42
2:G:18:PHE:O	2:G:20:LYS:N	2.53	0.41
2:G:63:ASN:N	2:G:63:ASN:ND2	2.60	0.41
4:D:8:DC:H2''	4:D:9:DA:C8	2.55	0.41
3:C:336:GLN:HE21	3:C:338:TRP:HE1	1.67	0.41
2:B:113:TRP:C	2:B:114:ILE:HG13	2.45	0.41
1:A:112:ASN:C	1:A:112:ASN:ND2	2.78	0.41
2:G:9:ARG:NH1	2:G:129:GLU:OE1	2.53	0.41
3:H:353:PHE:CB	3:H:370:GLU:HG2	2.50	0.41
3:C:364:LYS:CB	3:C:411:VAL:HG22	2.50	0.41
3:H:393:LEU:HA	3:H:396:TYR:CD2	2.55	0.41
4:I:11:DC:H2''	4:I:12:DC:H5''	2.03	0.41
2:B:100:PRO:O	2:B:101:MET:HB3	2.21	0.41
3:H:336:GLN:H	3:H:339:GLN:HE21	1.68	0.41
3:H:361:TRP:HZ2	3:H:419:GLN:HE21	1.67	0.41
3:H:396:TYR:HB3	3:H:401:ILE:HB	2.02	0.41
1:F:93:ALA:O	1:F:127:GLN:NE2	2.50	0.41
3:C:322:PRO:HB2	3:C:325:ALA:HB3	2.02	0.41
3:C:342:LEU:HD12	3:C:342:LEU:HA	1.94	0.41
2:G:4:VAL:HG13	2:G:135:GLU:HG2	2.03	0.41
1:A:69:ASN:HD22	1:A:94:LYS:HB2	1.85	0.41
3:C:389:LEU:C	3:C:389:LEU:HD23	2.45	0.41
1:A:98:PRO:HG2	1:A:101:THR:OG1	2.21	0.41
1:A:112:ASN:HD22	1:A:113:TYR:N	2.18	0.41
2:G:21:LEU:HD22	2:G:57:PHE:CD1	2.56	0.41
2:G:23:ARG:H	2:G:23:ARG:HD3	1.86	0.41
2:G:85:TYR:HA	2:G:98:LYS:HB3	2.03	0.41
3:H:389:LEU:HD23	3:H:389:LEU:C	2.45	0.40
4:I:5:DC:H1'	4:I:6:DC:H5''	2.03	0.40
4:I:14:DC:C2'	4:I:15:DT:C5'	2.95	0.40
2:B:12:PHE:CD1	2:B:12:PHE:C	2.99	0.40
2:B:8:GLN:HE21	2:B:107:CYS:H	1.68	0.40
2:B:123:GLY:O	2:B:124:CYS:HB3	2.21	0.40
1:F:114:SER:HB3	2:G:33:ARG:HH11	1.87	0.40
4:I:6:DC:H2''	4:I:7:DA:C8	2.57	0.40
3:C:418:LEU:HD23	3:C:418:LEU:HA	1.79	0.40
3:H:348:LYS:HA	3:H:351:GLN:CG	2.51	0.40
2:B:100:PRO:HA	2:B:109:ILE:HA	2.04	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%)	110 (95%)	5 (4%)	1 (1%)	14	35
2	B	126/142 (89%)	105 (83%)	14 (11%)	7 (6%)	1	2
2	G	125/142 (88%)	109 (87%)	9 (7%)	7 (6%)	1	2
3	C	116/166 (70%)	111 (96%)	5 (4%)	0	100	100
3	H	99/166 (60%)	82 (83%)	14 (14%)	3 (3%)	3	8
All	All	698/1024 (68%)	626 (90%)	54 (8%)	18 (3%)	4	11

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	90	ARG
2	G	91	GLU
2	G	19	ARG
3	H	334	PRO
2	B	32	PHE
2	B	116	LEU
2	B	130	GLU
2	G	116	LEU
3	H	431	ALA
2	B	58	VAL
2	G	14	ASN
2	G	24	GLU
2	G	59	ALA
2	G	89	GLU
2	B	7	ASP
2	B	24	GLU
1	F	110	ASP
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	99/178 (56%)	91 (92%)	8 (8%)	11	27
1	F	99/178 (56%)	94 (95%)	5 (5%)	21	48
2	B	113/123 (92%)	109 (96%)	4 (4%)	32	61
2	G	112/123 (91%)	105 (94%)	7 (6%)	16	39
3	C	102/145 (70%)	94 (92%)	8 (8%)	11	29
3	H	91/145 (63%)	91 (100%)	0	100	100
All	All	616/892 (69%)	584 (95%)	32 (5%)	21	47

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	104	THR
1	A	109	ASN
1	A	117	LEU
1	A	121	THR
1	A	144	LYS
1	A	145	SER
1	A	147	THR
2	B	23	ARG
2	B	63	ASN
2	B	84	GLU
2	B	103	LEU
3	C	330	THR
3	C	352	SER
3	C	378	ARG
3	C	379	LYS
3	C	383	LYS
3	C	399	LYS
3	C	404	LYS
3	C	427	GLU
1	F	62	LEU
1	F	94	LYS

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Mol	Chain	Res	Type
1	F	139	ARG
1	F	147	THR
1	F	175	GLU
2	G	9	ARG
2	G	23	ARG
2	G	63	ASN
2	G	86	VAL
2	G	89	GLU
2	G	103	LEU
2	G	117	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) 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	127	GLN
2	B	8	GLN
2	B	41	GLN
2	B	45	GLN
2	B	46	ASN
2	B	104	ASN
2	B	117	HIS
2	B	133	GLN
2	B	134	GLN
2	B	140	GLN
3	C	336	GLN
3	C	380	ASN
3	C	385	ASN
1	F	112	ASN
1	F	126	ASN
1	F	127	GLN
1	F	132	ASN
2	G	8	GLN
2	G	46	ASN
2	G	63	ASN
2	G	67	GLN
2	G	117	HIS
2	G	134	GLN

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Mol	Chain	Res	Type
3	H	336	GLN
3	H	339	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 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	3 (2%) 58 55	44, 63, 90, 101	0
1	F	118/204 (57%)	-0.05	2 (1%) 69 67	43, 54, 74, 101	0
2	B	130/142 (91%)	1.18	18 (13%) 6 5	65, 90, 118, 130	0
2	G	129/142 (90%)	0.96	16 (12%) 8 7	62, 80, 110, 115	0
3	C	118/166 (71%)	0.21	2 (1%) 69 67	40, 62, 91, 101	0
3	H	101/166 (60%)	2.05	47 (46%) 0 0	62, 120, 166, 171	0
4	D	15/15 (100%)	-0.27	0 100 100	51, 55, 68, 69	0
4	I	15/15 (100%)	0.21	0 100 100	53, 63, 82, 87	0
5	E	15/15 (100%)	-0.41	0 100 100	46, 54, 65, 71	0
5	J	15/15 (100%)	0.01	0 100 100	51, 61, 76, 81	0
All	All	774/1084 (71%)	0.66	88 (11%) 10 8	40, 71, 125, 171	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	81	PRO	6.6
3	H	433	LEU	6.6
2	G	139	ALA	5.3
3	C	319	PRO	5.2
3	H	431	ALA	4.9
3	H	421	LEU	4.8
3	H	356	TRP	4.6
3	H	357	THR	4.5
3	H	429	LEU	4.4
3	H	364	LYS	4.4
2	G	82	SER	4.1
3	H	430	HIS	4.0
3	H	358	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	81	PRO	3.7
2	G	22	SER	3.4
3	H	409	ARG	3.3
3	H	360	GLY	3.3
3	H	432	MET	3.3
3	H	411	VAL	3.2
2	G	88	LEU	3.2
3	H	375	TRP	3.2
3	H	353	PHE	3.1
3	H	355	SER	3.1
1	F	177	ARG	3.0
2	B	134	GLN	3.0
3	H	346	THR	3.0
3	H	363	PHE	3.0
3	H	354	ILE	3.0
3	H	415	VAL	3.0
3	H	377	LYS	2.9
3	H	365	LEU	2.9
2	B	71	ALA	2.9
3	H	406	ALA	2.9
3	H	405	THR	2.8
3	H	351	GLN	2.8
3	H	335	ILE	2.8
3	H	361	TRP	2.7
2	B	95	VAL	2.7
3	H	410	TYR	2.7
2	B	12	PHE	2.6
2	B	86	VAL	2.6
2	B	21	LEU	2.6
2	G	7	ASP	2.6
3	H	342	LEU	2.6
3	H	404	LYS	2.6
3	H	359	ASP	2.5
3	H	333	GLY	2.5
2	B	2	PRO	2.5
2	G	86	VAL	2.5
2	B	82	SER	2.5
3	H	337	LEU	2.5
2	B	20	LYS	2.5
3	H	423	GLY	2.5
2	B	93	GLY	2.4
2	G	25	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
3	H	426	PRO	2.4
2	B	83	ARG	2.3
2	G	94	LYS	2.3
3	C	436	LYS	2.3
2	G	83	ARG	2.3
3	H	416	CYS	2.3
3	H	414	PHE	2.3
2	B	22	SER	2.3
2	B	25	CYS	2.3
3	H	398	ASP	2.3
3	H	408	LYS	2.2
2	B	113	TRP	2.2
3	H	338	TRP	2.2
2	G	114	ILE	2.2
2	G	127	PHE	2.2
1	F	60	GLY	2.2
2	G	113	TRP	2.1
2	B	92	ALA	2.1
2	G	71	ALA	2.1
2	B	135	GLU	2.1
3	H	366	SER	2.1
3	H	344	LEU	2.1
2	G	55	ILE	2.1
3	H	371	VAL	2.1
1	A	177	ARG	2.1
3	H	378	ARG	2.1
3	H	341	LEU	2.1
2	B	5	VAL	2.1
1	A	176	PRO	2.0
3	H	422	LEU	2.0
1	A	87	ILE	2.0
3	H	374	ARG	2.0
2	G	92	ALA	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 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.