



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:21 PM UTC

PDB ID : 3WTT / pdb_00003wtt
Title : Crystal structure of the complex comprised of phosphorylated ETS1, RUNX1, CBFbeta, and the tcralpha gene enhancer DNA
Authors : Shiina, M.; Hamada, K.; Ogata, K.
Deposited on : 2014-04-21
Resolution : 2.35 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

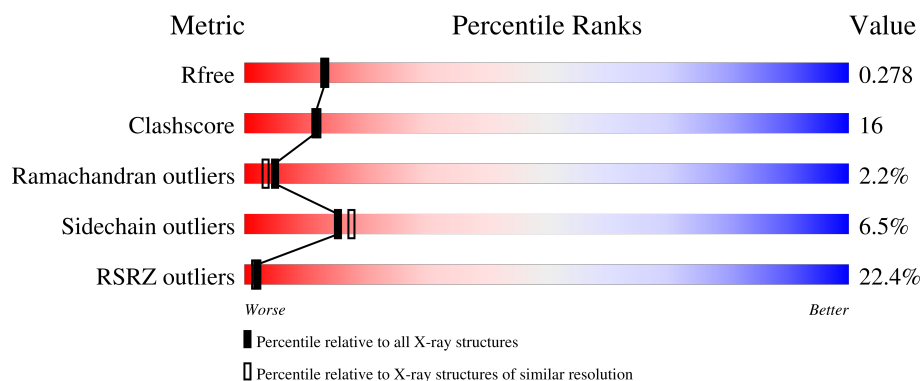
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	
1	F	204	
2	B	142	
2	G	142	
3	C	166	

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Mol	Chain	Length	Quality of chain
3	H	166	40% 30% 24% 44% ..
4	D	15	20% 53% 27%
4	I	15	33% 33% 33%
5	E	15	87% 7% 7%
5	J	15	93% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7083 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	119	Total	C	N	O	S	0	0	0
			919	577	170	168	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	131	Total	C	N	O	S	0	0	0
			1078	675	196	201	6			
2	G	130	Total	C	N	O	S	0	0	0
			1071	671	195	199	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	93	Total	C	N	O	S	0	0	0
			789	512	137	137	3			

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

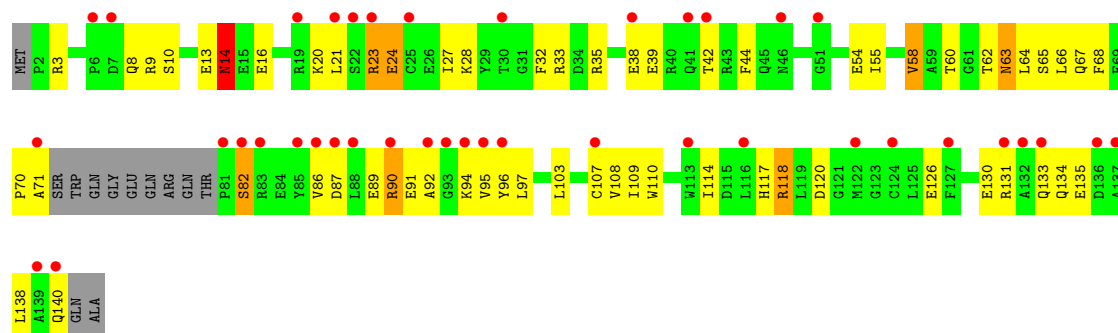
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	15	Total	C	N	O	P	0	0	0
			299	144	54	87	14			
4	I	15	Total	C	N	O	P	0	0	0
			299	144	54	87	14			

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

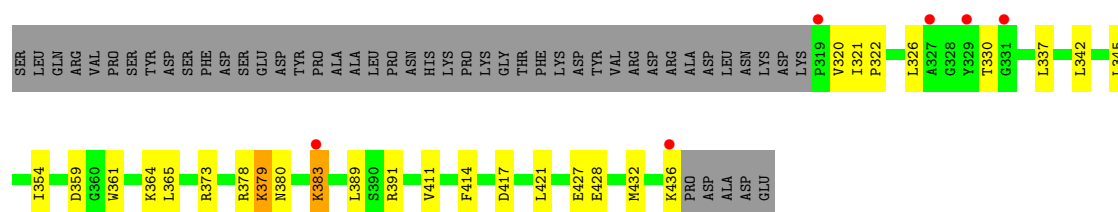
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	15	Total	C	N	O	P	0	0	0
			310	148	59	89	14			
5	J	15	Total	C	N	O	P	0	0	0
			310	148	59	89	14			

- Molecule 6 is water.

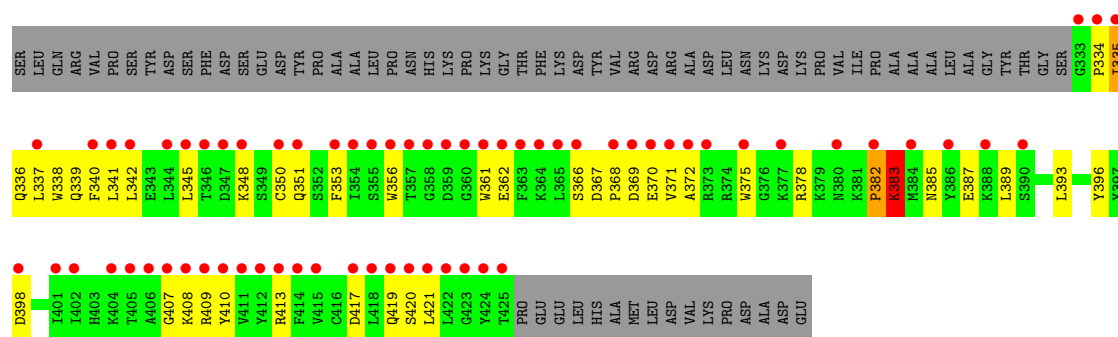
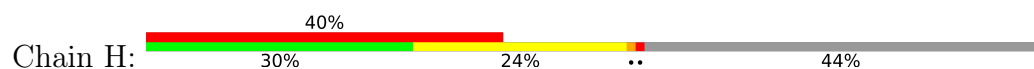
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	19	Total	O	0	0
			19	19		
6	B	5	Total	O	0	0
			5	5		
6	C	18	Total	O	0	0
			18	18		
6	F	24	Total	O	0	0
			24	24		
6	G	11	Total	O	0	0
			11	11		
6	H	2	Total	O	0	0
			2	2		
6	D	9	Total	O	0	0
			9	9		
6	E	18	Total	O	0	0
			18	18		
6	I	4	Total	O	0	0
			4	4		
6	J	17	Total	O	0	0
			17	17		



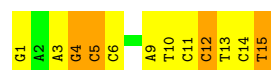
• Molecule 3: Protein C-ets-1



• Molecule 3: Protein C-ets-1



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



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





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

Chain E: 87% 7% 7%



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

Chain J: 93% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.62Å 101.72Å 194.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.68 – 2.35 48.68 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.68-2.35) 98.4 (48.68-2.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.53 (at 2.34Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.241 , 0.277 0.241 , 0.278	Depositor DCC
R_{free} test set	6531 reflections (10.11%)	wwPDB-VP
Wilson B-factor (Å ²)	65.6	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.7	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	0.95	EDS
Total number of atoms	7083	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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	0.78	0/938	1.09	5/1275 (0.4%)
1	F	0.86	0/933	1.18	4/1268 (0.3%)
2	B	0.57	0/1100	0.86	0/1477
2	G	0.67	0/1093	0.92	1/1466 (0.1%)
3	C	0.80	0/994	1.07	2/1342 (0.1%)
3	H	0.49	0/811	0.80	0/1091
4	D	0.51	0/334	1.31	5/512 (1.0%)
4	I	0.49	0/334	1.20	5/512 (1.0%)
5	E	0.49	0/348	0.94	1/537 (0.2%)
5	J	0.45	0/348	0.90	0/537
All	All	0.67	0/7233	1.02	23/10017 (0.2%)

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	4
5	E	0	1
All	All	0	9

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	4	DG	N9-C1'-C2'	-10.32	98.02	113.50
4	I	4	DG	N9-C1'-C2'	-9.40	99.39	113.50
4	D	4	DG	C4'-C3'-O3'	9.07	123.61	110.00
4	I	4	DG	C4'-C3'-O3'	7.41	121.11	110.00
5	E	15	DC	C2'-C3'-O3'	-6.82	101.27	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	ASP	N-CA-C	6.56	120.72	111.92
4	I	4	DG	C5'-C4'-C3'	-6.45	105.22	114.90
4	D	4	DG	C5'-C4'-C3'	-6.15	105.67	114.90
1	F	153	PHE	N-CA-C	5.94	118.83	109.39
4	D	3	DA	N9-C1'-C2'	5.92	122.38	113.50
1	F	133	ASP	N-CA-C	5.87	119.96	111.56
4	D	15	DT	C2'-C3'-O3'	-5.59	103.12	111.50
4	I	15	DT	C4'-C3'-O3'	5.51	118.27	110.00
1	A	128	VAL	N-CA-C	5.47	115.87	107.77
3	C	337	LEU	N-CA-C	5.46	117.94	111.33
2	G	65	SER	N-CA-C	-5.39	99.62	108.41
4	I	11	DC	N1-C1'-C2'	5.38	121.57	113.50
1	A	70	PHE	N-CA-C	5.38	118.20	109.06
3	C	391	ARG	N-CA-C	-5.30	105.62	111.71
1	F	166	ILE	N-CA-C	5.25	114.78	108.06
1	F	154	THR	N-CA-C	-5.21	101.76	109.94
1	A	153	PHE	N-CA-C	5.15	117.58	109.39
1	A	154	THR	N-CA-C	-5.00	102.08	109.94

There are no chirality outliers.

All (9) 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
5	E	13	DT	Sidechain
4	I	12	DC	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	919	0	924	29	0
1	F	914	0	922	13	0
2	B	1078	0	1040	49	0
2	G	1071	0	1034	46	0
3	C	967	0	966	22	0
3	H	789	0	785	41	0
4	D	299	0	170	15	0
4	I	299	0	170	7	0
5	E	310	0	171	1	0
5	J	310	0	171	1	0
6	A	19	0	0	2	0
6	B	5	0	0	0	0
6	C	18	0	0	0	0
6	D	9	0	0	1	0
6	E	18	0	0	0	0
6	F	24	0	0	1	0
6	G	11	0	0	0	0
6	H	2	0	0	0	0
6	I	4	0	0	0	0
6	J	17	0	0	0	0
All	All	7083	0	6353	212	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 16.

All (212) 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:104:THR:HG22	6:A:317:HOH:O	1.69	0.93
1:A:82:ASN:HD21	1:A:118:ARG:HH11	0.96	0.92
3:H:383:LYS:HD2	3:H:383:LYS:H	1.34	0.90
4:I:11:DC:H1'	4:I:12:DC:H5''	1.59	0.82
1:A:87:ILE:O	1:A:87:ILE:HD12	1.81	0.81
1:A:82:ASN:ND2	1:A:118:ARG:HH11	1.79	0.79
2:B:60:THR:HG23	2:B:62:THR:H	1.48	0.78
1:A:82:ASN:HD21	1:A:118:ARG:NH1	1.79	0.77
1:F:161:THR:HG21	1:F:163:HIS:CE1	2.23	0.74
2:B:8:GLN:HE21	2:B:107:CYS:H	1.38	0.72
2:B:82:SER:HB2	2:B:85:TYR:HB2	1.72	0.71
4:D:10:DT:H2''	4:D:11:DC:H5'	1.73	0.71
2:B:108:VAL:HG11	2:B:125:LEU:HB3	1.74	0.70
2:B:136:ASP:HA	2:B:139:ALA:HB3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:383:LYS:NZ	3:C:383:LYS:HB3	2.07	0.69
4:I:14:DC:H2''	4:I:15:DT:H5'	1.75	0.68
2:G:71:ALA:HB3	2:G:131:ARG:HH22	1.60	0.66
3:H:382:PRO:HB2	3:H:383:LYS:HD2	1.78	0.65
3:C:364:LYS:HB2	3:C:411:VAL:HG22	1.78	0.65
2:G:39:GLU:O	2:G:42:THR:HG22	1.97	0.64
2:B:108:VAL:HG12	2:B:109:ILE:N	2.13	0.64
2:G:91:GLU:HG3	2:G:92:ALA:H	1.61	0.64
2:G:60:THR:HG23	2:G:62:THR:H	1.63	0.63
1:F:79:TRP:CZ2	1:F:86:PRO:HD3	2.35	0.62
2:G:71:ALA:HB3	2:G:131:ARG:NH2	2.15	0.61
4:D:11:DC:H2''	4:D:12:DC:C5'	2.30	0.61
1:A:70:PHE:CE2	1:A:152:VAL:HG21	2.36	0.61
3:H:345:LEU:HD22	3:H:356:TRP:NE1	2.15	0.60
1:A:97:VAL:H	1:A:127:GLN:HE22	1.49	0.60
2:G:70:PRO:O	2:G:71:ALA:HB3	2.00	0.60
2:B:106:VAL:O	2:B:108:VAL:HG23	2.02	0.60
2:G:8:GLN:HE21	2:G:107:CYS:H	1.51	0.59
2:G:16:GLU:OE2	2:G:20:LYS:HB2	2.01	0.59
2:B:137:ALA:O	2:B:140:GLN:HG3	2.02	0.59
2:B:5:VAL:HG12	2:B:105:GLY:O	2.02	0.59
3:H:383:LYS:HD2	3:H:383:LYS:N	2.12	0.59
3:H:353:PHE:CD2	3:H:370:GLU:HG2	2.39	0.58
2:B:108:VAL:HG12	2:B:109:ILE:H	1.67	0.58
2:G:86:VAL:O	2:G:86:VAL:HG13	2.04	0.58
2:B:138:LEU:HD12	2:B:138:LEU:H	1.70	0.57
2:G:108:VAL:HG12	2:G:109:ILE:N	2.19	0.57
2:G:9:ARG:O	2:G:13:GLU:HG2	2.04	0.57
4:D:11:DC:C2'	4:D:12:DC:H5''	2.35	0.56
2:B:113:TRP:C	2:B:114:ILE:HD12	2.31	0.56
3:H:335:ILE:HD12	3:H:339:GLN:HE21	1.70	0.56
2:B:93:GLY:O	2:B:116:LEU:HB2	2.06	0.56
1:F:63:VAL:HB	1:F:74:VAL:HG22	1.88	0.56
3:H:389:LEU:O	3:H:389:LEU:HD23	2.05	0.56
1:F:114:SER:HB3	2:G:33:ARG:HH12	1.71	0.56
4:D:13:DT:H2''	4:D:14:DC:H5'	1.87	0.56
4:D:11:DC:H2''	4:D:12:DC:H5''	1.88	0.56
2:B:131:ARG:O	2:B:135:GLU:HB2	2.06	0.55
4:I:9:DA:H1'	4:I:10:DT:H5''	1.87	0.55
2:B:81:PRO:HB2	2:B:86:VAL:HG11	1.88	0.55
3:C:345:LEU:HD21	3:C:354:ILE:HG12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:356:TRP:HZ3	3:H:361:TRP:HE3	1.55	0.55
1:A:126:ASN:O	1:A:127:GLN:HB2	2.05	0.55
3:H:417:ASP:OD1	3:H:420:SER:HB3	2.07	0.55
2:G:87:ASP:HB3	2:G:96:TYR:HB2	1.89	0.54
2:B:83:ARG:HG3	2:B:84:GLU:H	1.72	0.54
3:H:345:LEU:HD13	3:H:356:TRP:CZ2	2.42	0.54
1:F:130:ARG:HH12	1:F:132:ASN:HD22	1.54	0.54
2:B:115:ASP:OD1	2:B:118:ARG:HD3	2.08	0.54
2:G:118:ARG:HB3	2:G:120:ASP:OD1	2.08	0.53
2:B:32:PHE:N	2:B:32:PHE:CD2	2.76	0.53
1:F:106:MET:HE1	2:G:64:LEU:C	2.33	0.53
2:B:83:ARG:HG3	2:B:84:GLU:OE2	2.08	0.53
3:H:345:LEU:HD22	3:H:356:TRP:CD1	2.44	0.53
4:I:13:DT:H1'	4:I:14:DC:H5''	1.90	0.53
3:H:342:LEU:HD23	3:H:342:LEU:O	2.08	0.53
4:D:11:DC:H1'	4:D:12:DC:H5''	1.90	0.53
3:C:417:ASP:O	3:C:421:LEU:HD23	2.08	0.52
2:G:68:PHE:CE1	2:G:97:LEU:HB3	2.44	0.52
5:E:15:DC:H2'	5:J:1:DA:O4'	2.09	0.52
3:H:383:LYS:H	3:H:383:LYS:CD	2.16	0.52
3:C:428:GLU:O	3:C:432:MET:HG3	2.09	0.52
3:C:379:LYS:NZ	4:D:9:DA:OP1	2.43	0.52
2:B:23:ARG:HD2	2:B:25:CYS:HB3	1.91	0.52
1:A:74:VAL:O	1:A:87:ILE:HD11	2.09	0.52
1:A:87:ILE:HD12	1:A:87:ILE:C	2.34	0.52
1:A:87:ILE:HG13	6:A:310:HOH:O	2.10	0.52
3:C:373:ARG:HH11	3:C:373:ARG:HG3	1.76	0.51
4:I:14:DC:H2''	4:I:15:DT:C5'	2.40	0.51
2:G:27:ILE:HB	2:G:55:ILE:CG2	2.40	0.51
3:H:367:ASP:O	3:H:370:GLU:HB3	2.11	0.51
2:B:68:PHE:CZ	2:B:97:LEU:HD13	2.46	0.50
2:G:89:GLU:O	2:G:90:ARG:C	2.53	0.50
2:G:118:ARG:HH11	2:G:118:ARG:HB2	1.75	0.50
3:H:393:LEU:HA	3:H:396:TYR:HD2	1.76	0.50
1:F:112:ASN:C	1:F:112:ASN:HD22	2.19	0.50
2:B:8:GLN:NE2	2:B:107:CYS:H	2.08	0.50
2:G:97:LEU:HB2	2:G:110:TRP:HZ3	1.77	0.50
4:D:1:DG:O4'	4:I:15:DT:H2'	2.12	0.50
1:A:66:ASP:OD2	1:A:163:HIS:CD2	2.65	0.49
2:B:14:ASN:HD22	2:B:14:ASN:N	2.09	0.49
2:B:70:PRO:O	2:B:71:ALA:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:5:DC:H2''	4:D:6:DC:H5''	1.94	0.49
2:B:57:PHE:HB2	2:B:60:THR:HG22	1.94	0.49
2:B:138:LEU:HD12	2:B:138:LEU:N	2.28	0.49
2:G:20:LYS:O	2:G:20:LYS:HG3	2.11	0.49
1:A:144:LYS:HE3	3:H:407:GLY:CA	2.43	0.49
3:H:385:ASN:OD1	3:H:387:GLU:HB2	2.13	0.49
3:H:389:LEU:HD23	3:H:389:LEU:C	2.37	0.49
1:A:113:TYR:CE2	2:B:28:LYS:HD2	2.48	0.48
3:H:368:PRO:C	3:H:370:GLU:H	2.20	0.48
1:A:144:LYS:HE3	3:H:407:GLY:HA3	1.95	0.48
2:B:95:VAL:CG2	2:B:116:LEU:HG	2.43	0.48
3:H:362:GLU:HG3	3:H:413:ARG:HB3	1.95	0.48
1:A:98:PRO:O	1:A:101:THR:OG1	2.27	0.48
3:C:359:ASP:OD2	3:C:359:ASP:C	2.57	0.48
2:G:28:LYS:HG3	2:G:58:VAL:HG21	1.94	0.48
2:G:91:GLU:HB3	2:G:94:LYS:HG2	1.95	0.47
3:C:383:LYS:HB3	3:C:383:LYS:HZ2	1.79	0.47
1:F:114:SER:HB3	2:G:33:ARG:NH1	2.29	0.47
3:H:409:ARG:HG2	3:H:410:TYR:CE2	2.49	0.47
4:D:5:DC:H2''	4:D:6:DC:C5'	2.44	0.47
3:C:326:LEU:O	3:C:421:LEU:HD12	2.14	0.47
1:A:103:VAL:HG21	1:A:129:ALA:HB2	1.96	0.47
3:C:379:LYS:HE3	6:D:107:HOH:O	2.15	0.47
2:G:10:SER:O	2:G:14:ASN:HB2	2.15	0.47
3:H:336:GLN:H	3:H:339:GLN:NE2	2.13	0.47
2:G:108:VAL:CG1	2:G:109:ILE:N	2.79	0.46
1:A:104:THR:HB	1:A:153:PHE:HE1	1.79	0.46
2:B:88:LEU:HD23	2:B:95:VAL:HG22	1.98	0.46
2:B:28:LYS:HE3	2:B:58:VAL:HG21	1.96	0.46
2:G:89:GLU:O	2:G:91:GLU:N	2.49	0.46
3:C:320:VAL:HG11	3:C:432:MET:HE2	1.97	0.46
3:C:383:LYS:HB3	3:C:383:LYS:HZ3	1.81	0.46
1:F:63:VAL:HG22	1:F:64:ARG:N	2.30	0.46
1:F:115:ALA:HB2	1:F:146:PHE:CZ	2.49	0.46
3:C:389:LEU:C	3:C:389:LEU:HD23	2.41	0.46
2:G:3:ARG:HH11	2:G:135:GLU:CD	2.24	0.46
2:G:28:LYS:HG3	2:G:58:VAL:CG2	2.46	0.46
2:G:68:PHE:CZ	2:G:97:LEU:HD13	2.50	0.46
1:A:106:MET:HE1	2:B:65:SER:N	2.32	0.45
2:B:88:LEU:CD2	2:B:95:VAL:HG22	2.47	0.45
2:B:115:ASP:O	2:B:117:HIS:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:64:ARG:HG3	6:F:302:HOH:O	2.16	0.45
1:F:161:THR:HG22	1:F:162:TYR:N	2.30	0.45
2:G:23:ARG:O	2:G:24:GLU:C	2.60	0.45
4:D:10:DT:C2'	4:D:11:DC:H5'	2.45	0.45
2:B:84:GLU:O	2:B:84:GLU:HG2	2.18	0.44
2:G:14:ASN:HD22	2:G:14:ASN:HA	1.65	0.44
2:B:95:VAL:HG21	2:B:116:LEU:HG	1.98	0.44
2:B:115:ASP:C	2:B:117:HIS:H	2.26	0.44
4:D:9:DA:H2''	4:D:10:DT:H5'	2.00	0.44
3:H:335:ILE:HG23	3:H:335:ILE:O	2.16	0.44
4:D:11:DC:H2''	4:D:12:DC:H5'	1.98	0.44
2:G:63:ASN:N	2:G:63:ASN:HD22	2.16	0.44
2:B:98:LYS:HA	2:B:110:TRP:O	2.18	0.44
1:A:87:ILE:O	1:A:87:ILE:CD1	2.59	0.44
3:C:361:TRP:HB3	3:C:414:PHE:HB2	2.00	0.44
1:A:70:PHE:CZ	1:A:152:VAL:HG21	2.53	0.43
1:A:148:LEU:HB2	1:A:162:TYR:HB3	2.00	0.43
3:H:348:LYS:H	3:H:348:LYS:HG2	1.67	0.43
1:A:111:GLU:HG3	1:A:144:LYS:NZ	2.34	0.43
2:B:108:VAL:CG1	2:B:109:ILE:N	2.81	0.43
2:B:27:ILE:HD13	2:B:114:ILE:HD11	1.99	0.43
3:H:350:CYS:HA	3:H:353:PHE:CE1	2.53	0.43
2:B:109:ILE:HD11	2:B:128:ASP:OD2	2.18	0.43
2:G:60:THR:CG2	2:G:62:THR:OG1	2.66	0.43
2:G:134:GLN:O	2:G:138:LEU:HG	2.18	0.43
2:B:103:LEU:O	2:B:104:ASN:C	2.62	0.43
3:H:338:TRP:CE2	3:H:339:GLN:HG3	2.54	0.43
1:A:112:ASN:C	1:A:112:ASN:HD22	2.26	0.43
4:D:5:DC:C2'	4:D:6:DC:H5''	2.49	0.43
1:A:113:TYR:CZ	2:B:28:LYS:HD2	2.53	0.42
2:B:63:ASN:N	2:B:63:ASN:HD22	2.17	0.42
3:H:345:LEU:HB3	3:H:356:TRP:NE1	2.33	0.42
2:G:70:PRO:O	2:G:71:ALA:CB	2.67	0.42
3:H:419:GLN:C	3:H:421:LEU:H	2.27	0.42
1:F:79:TRP:CH2	1:F:86:PRO:HD3	2.55	0.42
1:A:126:ASN:O	1:A:127:GLN:CB	2.68	0.42
3:C:342:LEU:HD12	3:C:342:LEU:HA	1.90	0.42
3:H:341:LEU:HD21	3:H:371:VAL:HG11	2.00	0.42
2:B:28:LYS:O	2:B:55:ILE:HA	2.19	0.42
2:B:86:VAL:HG13	2:B:86:VAL:O	2.20	0.42
2:G:32:PHE:HB3	2:G:35:ARG:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:321:ILE:HB	3:C:322:PRO:HD2	2.01	0.42
4:I:8:DC:OP1	4:I:8:DC:H4'	2.19	0.41
2:G:3:ARG:HD3	2:G:135:GLU:OE2	2.20	0.41
2:G:27:ILE:CD1	2:G:114:ILE:HD11	2.50	0.41
1:A:60:GLY:O	1:A:61:GLU:HB3	2.21	0.41
2:G:44:PHE:CD1	2:G:44:PHE:C	2.96	0.41
3:H:350:CYS:HA	3:H:353:PHE:HE1	1.85	0.41
2:B:131:ARG:HA	2:B:134:GLN:HG2	2.03	0.41
3:C:354:ILE:HG13	3:C:365:LEU:HD23	2.02	0.41
2:G:21:LEU:HD21	2:G:60:THR:HG21	2.02	0.41
3:C:320:VAL:HG12	3:C:321:ILE:HG23	2.03	0.41
2:G:90:ARG:HE	2:G:90:ARG:HB2	1.77	0.41
3:C:379:LYS:O	3:C:380:ASN:HB3	2.20	0.41
2:G:54:GLU:C	2:G:55:ILE:HD12	2.46	0.41
2:B:21:LEU:HD22	2:B:57:PHE:CD1	2.56	0.41
3:C:320:VAL:CG1	3:C:432:MET:HE2	2.50	0.41
2:G:108:VAL:HG13	2:G:126:GLU:O	2.21	0.41
3:H:362:GLU:HA	3:H:413:ARG:CB	2.51	0.41
4:D:11:DC:C1'	4:D:12:DC:H5''	2.50	0.41
1:A:139:ARG:N	1:A:139:ARG:HD3	2.36	0.41
2:B:108:VAL:CG1	2:B:125:LEU:HB3	2.48	0.41
3:C:378:ARG:O	3:C:378:ARG:HG3	2.21	0.41
2:G:91:GLU:HB3	2:G:94:LYS:CG	2.51	0.41
3:H:356:TRP:HZ3	3:H:361:TRP:CE3	2.35	0.41
2:G:55:ILE:HD13	2:G:66:LEU:HD12	2.03	0.40
3:H:340:PHE:CE2	3:H:375:TRP:HB2	2.56	0.40
3:H:345:LEU:HB3	3:H:356:TRP:CZ2	2.56	0.40
3:H:351:GLN:C	3:H:353:PHE:H	2.29	0.40
3:H:362:GLU:HA	3:H:413:ARG:HB3	2.04	0.40
1:A:149:THR:HG21	2:B:63:ASN:O	2.21	0.40
3:H:337:LEU:HA	3:H:375:TRP:CZ3	2.57	0.40
3:H:341:LEU:CD2	3:H:371:VAL:HG11	2.52	0.40
3:H:370:GLU:C	3:H:372:ALA:N	2.78	0.40
3:H:378:ARG:HG3	3:H:378:ARG:HH11	1.86	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	117/204 (57%)	112 (96%)	5 (4%)	0	100	100
1	F	116/204 (57%)	111 (96%)	5 (4%)	0	100	100
2	B	127/142 (89%)	111 (87%)	12 (9%)	4 (3%)	3	2
2	G	126/142 (89%)	106 (84%)	14 (11%)	6 (5%)	2	0
3	C	116/166 (70%)	112 (97%)	4 (3%)	0	100	100
3	H	91/166 (55%)	65 (71%)	21 (23%)	5 (6%)	1	0
All	All	693/1024 (68%)	617 (89%)	61 (9%)	15 (2%)	5	3

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	81	PRO
2	G	58	VAL
3	H	335	ILE
2	B	116	LEU
2	G	24	GLU
2	G	82	SER
2	G	90	ARG
2	B	91	GLU
2	G	14	ASN
3	H	382	PRO
2	G	130	GLU
3	H	383	LYS
2	B	58	VAL
3	H	334	PRO
3	H	366	SER

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%)	94 (94%)	6 (6%)	17	21
1	F	100/179 (56%)	96 (96%)	4 (4%)	28	37
2	B	114/123 (93%)	105 (92%)	9 (8%)	11	12
2	G	113/123 (92%)	101 (89%)	12 (11%)	6	6
3	C	102/145 (70%)	97 (95%)	5 (5%)	22	28
3	H	84/145 (58%)	80 (95%)	4 (5%)	23	29
All	All	613/894 (69%)	573 (94%)	40 (6%)	15	18

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	THR
1	A	117	LEU
1	A	121	THR
1	A	139	ARG
1	A	155	ASN
1	A	175	GLU
2	B	23	ARG
2	B	48	CYS
2	B	55	ILE
2	B	63	ASN
2	B	94	LYS
2	B	98	LYS
2	B	103	LEU
2	B	116	LEU
2	B	124	CYS
3	C	330	THR
3	C	379	LYS
3	C	383	LYS
3	C	427	GLU
3	C	436	LYS
1	F	87	ILE
1	F	110	ASP

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Mol	Chain	Res	Type
1	F	147	THR
1	F	149	THR
2	G	14	ASN
2	G	23	ARG
2	G	38	GLU
2	G	63	ASN
2	G	67	GLN
2	G	82	SER
2	G	95	VAL
2	G	103	LEU
2	G	117	HIS
2	G	118	ARG
2	G	133	GLN
2	G	140	GLN
3	H	369	ASP
3	H	383	LYS
3	H	398	ASP
3	H	408	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	112	ASN
1	A	119	ASN
1	A	127	GLN
1	A	163	HIS
2	B	8	GLN
2	B	14	ASN
2	B	41	GLN
2	B	134	GLN
2	B	140	GLN
3	C	380	ASN
1	F	112	ASN
1	F	132	ASN
2	G	8	GLN
2	G	14	ASN
2	G	41	GLN
2	G	133	GLN
3	H	339	GLN
3	H	400	ASN

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	119/204 (58%)	0.54	7 (5%)	28 32	42, 58, 84, 96	0
1	F	118/204 (57%)	0.31	8 (6%)	23 26	37, 51, 71, 94	0
2	B	131/142 (92%)	1.78	45 (34%)	1 0	60, 85, 115, 126	0
2	G	130/142 (91%)	1.70	40 (30%)	1 0	56, 77, 107, 119	0
3	C	118/166 (71%)	0.55	6 (5%)	33 39	39, 59, 83, 89	0
3	H	93/166 (56%)	2.64	66 (70%)	0 0	62, 112, 139, 146	0
4	D	15/15 (100%)	-0.17	0	100 100	46, 52, 62, 63	0
4	I	15/15 (100%)	0.34	0	100 100	49, 62, 77, 77	0
5	E	15/15 (100%)	-0.32	0	100 100	43, 49, 60, 65	0
5	J	15/15 (100%)	0.31	0	100 100	47, 57, 71, 73	0
All	All	769/1084 (70%)	1.13	172 (22%)	2 2	37, 67, 119, 146	0

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	81	PRO	7.5
3	H	425	THR	6.6
2	B	82	SER	5.6
2	G	82	SER	5.4
2	B	137	ALA	5.3
3	H	356	TRP	5.1
3	H	357	THR	5.0
2	B	71	ALA	4.7
2	B	86	VAL	4.7
3	H	360	GLY	4.7
2	B	93	GLY	4.6
3	H	353	PHE	4.6
2	G	7	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
2	B	70	PRO	4.6
3	C	319	PRO	4.6
3	H	365	LEU	4.5
3	H	421	LEU	4.4
2	G	137	ALA	4.3
3	H	368	PRO	4.2
3	H	351	GLN	4.2
3	H	420	SER	4.0
3	H	364	LYS	4.0
3	H	337	LEU	4.0
2	B	80	THR	4.0
2	B	10	SER	4.0
3	H	344	LEU	3.9
3	H	354	ILE	3.9
3	H	375	TRP	3.9
3	H	363	PHE	3.8
3	H	355	SER	3.8
2	G	86	VAL	3.8
2	G	87	ASP	3.8
2	G	127	PHE	3.8
2	B	95	VAL	3.8
1	A	178	ARG	3.7
3	H	423	GLY	3.7
2	B	7	ASP	3.7
2	B	96	TYR	3.6
1	F	60	GLY	3.6
3	H	405	THR	3.6
3	H	377	LYS	3.6
1	F	175	GLU	3.6
3	H	404	LYS	3.5
3	H	361	TRP	3.5
3	H	335	ILE	3.5
2	B	81	PRO	3.4
2	B	83	ARG	3.4
3	H	345	LEU	3.4
1	F	176	PRO	3.4
2	G	139	ALA	3.4
2	B	138	LEU	3.3
3	H	373	ARG	3.3
3	H	348	LYS	3.3
2	B	94	LYS	3.3
3	H	341	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
3	H	333	GLY	3.2
3	H	350	CYS	3.1
3	H	340	PHE	3.1
2	G	132	ALA	3.1
2	G	83	ARG	3.1
2	B	114	ILE	3.0
3	H	419	GLN	3.0
2	B	92	ALA	3.0
2	B	116	LEU	3.0
2	G	131	ARG	3.0
3	H	347	ASP	3.0
3	H	407	GLY	3.0
3	H	406	ALA	3.0
3	H	411	VAL	3.0
3	H	410	TYR	3.0
2	G	94	LYS	3.0
2	G	93	GLY	3.0
2	B	21	LEU	2.9
2	B	140	GLN	2.9
1	F	155	ASN	2.9
2	G	140	GLN	2.9
3	H	362	GLU	2.9
2	G	90	ARG	2.9
2	G	71	ALA	2.9
3	H	414	PHE	2.9
2	G	38	GLU	2.9
3	H	346	THR	2.9
2	B	108	VAL	2.8
3	H	398	ASP	2.8
2	B	6	PRO	2.8
2	G	116	LEU	2.8
2	G	122	MET	2.8
1	F	177	ARG	2.8
2	G	22	SER	2.8
3	H	358	GLY	2.8
3	H	402	ILE	2.7
2	B	132	ALA	2.7
2	G	23	ARG	2.7
2	B	17	PHE	2.7
2	G	25	CYS	2.7
2	B	20	LYS	2.6
2	B	5	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	G	95	VAL	2.6
2	B	2	PRO	2.6
2	B	107	CYS	2.6
2	B	119	LEU	2.6
2	G	46	ASN	2.6
3	C	436	LYS	2.6
2	G	19	ARG	2.6
2	G	6	PRO	2.6
3	H	372	ALA	2.6
3	H	369	ASP	2.6
3	H	424	TYR	2.6
1	A	132	ASN	2.5
2	G	42	THR	2.5
3	H	384	MET	2.5
3	C	383	LYS	2.5
2	B	117	HIS	2.5
2	G	30	THR	2.5
3	H	390	SER	2.5
2	G	21	LEU	2.5
3	H	388	LYS	2.5
3	H	417	ASP	2.5
2	B	25	CYS	2.4
2	G	113	TRP	2.4
2	G	136	ASP	2.4
3	H	371	VAL	2.4
2	G	88	LEU	2.4
2	G	96	TYR	2.4
3	H	359	ASP	2.4
3	H	366	SER	2.3
3	H	386	TYR	2.3
3	H	334	PRO	2.3
2	B	85	TYR	2.3
3	C	331	GLY	2.3
1	A	64	ARG	2.3
3	H	370	GLU	2.3
3	H	342	LEU	2.3
3	H	422	LEU	2.3
2	B	121	GLY	2.3
2	B	22	SER	2.3
3	H	415	VAL	2.3
2	G	92	ALA	2.2
3	C	329	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
3	H	382	PRO	2.2
2	B	24	GLU	2.2
2	G	133	GLN	2.2
1	A	62	LEU	2.2
3	H	409	ARG	2.1
2	B	124	CYS	2.1
2	G	107	CYS	2.1
2	B	42	THR	2.1
3	C	327	ALA	2.1
3	H	401	ILE	2.1
3	H	418	LEU	2.1
2	B	4	VAL	2.1
2	G	41	GLN	2.1
2	B	105	GLY	2.1
2	B	139	ALA	2.1
2	B	122	MET	2.1
2	B	135	GLU	2.1
2	G	85	TYR	2.1
3	H	412	TYR	2.1
1	F	163	HIS	2.1
1	A	60	GLY	2.1
2	G	51	GLY	2.1
1	F	161	THR	2.1
3	H	380	ASN	2.1
3	H	413	ARG	2.1
2	B	16	GLU	2.0
2	G	124	CYS	2.0
1	A	176	PRO	2.0
1	A	63	VAL	2.0
1	F	95	GLY	2.0
3	H	408	LYS	2.0
2	B	125	LEU	2.0
2	B	90	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.