W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:19 PM GMT

PDB ID	:	3WTV
Title	:	Crystal structure of the complex comprised of ETS1(V170G), 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)

The following versions of software and data (see references (i)) were used in the production of this report:

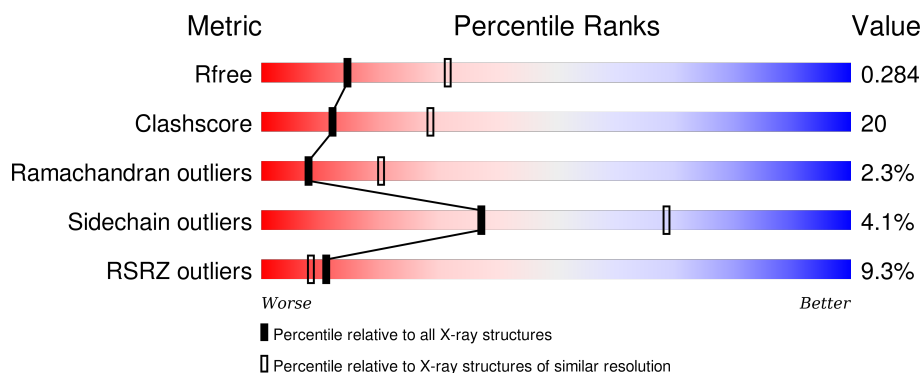|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

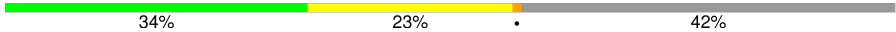The following experimental techniques were used to determine the structure:
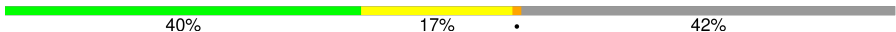*X-RAY DIFFRACTION*

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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	28% / 26% / 30% / 39%
4	D	15	20% / 80%
4	I	15	13% / 80% / 7%
5	E	15	80% / 20%
5	J	15	67% / 33%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 7002 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
			911	571	169	167	4			
1	F	118	Total	C	N	O	S	0	0	0
			911	571	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	GLY	VAL	ENGINEERED MUTATION	UNP Q03347
F	94	LYS	LEU	ENGINEERED MUTATION	UNP Q03347
F	170	GLY	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 299	C 144	N 54	O 87	P 14	0	0	0
4	I	15	Total 299	C 144	N 54	O 87	P 14	0	0	0

- 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 310	C 148	N 59	O 89	P 14	0	0	0
5	J	15	Total 310	C 148	N 59	O 89	P 14	0	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	3	Total 3	O 3	0	0
6	F	4	Total 4	O 4	0	0
6	H	1	Total 1	O 1	0	0
6	J	1	Total 1	O 1	0	0

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 errors 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

Chain G:

6%

51% 37% 9%

MET P2 R3 D7 K11 F12 E15 E16 K20 R23 I27 K28 Y29 D34 R35 F44 Q45 R49 E54 I55 N63 L66 Q67 F68 A71 SER TRP GLN GLY GLU GLN ARG GLN THR P81 S82 Y85 V86 D87 L88 E89 R90 E91 A92 G93 K94

V95 Y96 L97 K98 A99 L103 V106 C107 V108 I109 W110 K111 G112 W113 I114 D115 L116 H117 R118 L119 D120 L125 E126 F127 D128 E129 R130 R131 A132 Q133 Q134 E135 D136 A137 L138 A139 GLN GLN ALA

● Molecule 3: Protein C-ets-1

Chain C:

3%

54% 17% 29%

SER LEU GLN ARG VAL PRO SER TYR ASP PHE ASP SER GLU ASP TYR PRO ALA ALA LEU PRO ASN HIS LYS PRO LYS GLY THR PHE LYS ASP TYR VAL ARG ASP ARG ALA ASP LEU ASN LYS ASP LYS P319 V320 I321 P322 A323 A324 A325 L326 A327 G328 Y329 T330 G331 S332 G333 L341

L345 Q351 I354 K364 L365 M384 N385 Y386 E387 K388 L393 T405 K408 V411 D417 L418 L421 T425 E428 K436 PRO ASP ALA ASP GLU

● Molecule 3: Protein C-ets-1

Chain H:

28%

26% 30% 39%

SER LEU GLN ARG VAL PRO SER TYR ASP PHE ASP SER GLU ASP TYR PRO ALA ALA LEU PRO ASN HIS LYS PRO LYS GLY THR PHE LYS ASP TYR VAL ARG ASP ARG ALA ASP LEU ASN LYS ASP LYS PRO VAL ILE PRO ALA ALA LEU ALA GLY TYR THR GLY SER G333 P334 I335

Q336 L337 W338 Q339 F340 L341 I342 E343 L344 L345 T346 K348 S349 C350 Q351 S352 F353 I354 W356 T357 D358 D359 G360 M361 E362 F363 K364 L365 S366 D367 P368 D369 B370 V371 A372 R373 R374 K379 N380 K381 P382 K383 M384 N385 Y386 E387 K388 L389 L393 Y396 Y397 D398 I401

T405 A406 G407 K408 R409 V410 V411 Y412 R413 F414 V415 C416 D417 L418 Q419 S420 L421 L422 G423 Y424 T425 P426 E427 E428 L429 H430 A431 M432 L433 ASP VAL LYS PRO ASP ALA ASP GLU

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

Chain D:

20% 80%

G1 G4 C5 C6 A7 C8 A9 T10 C11 C12 T13 C14 T15

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

Chain I:

13% 80% 7%

G1 A2 A3 G4 C5 C6 A7 C8 A9 T10 C11 C12 T13 C14 T15
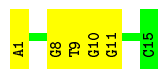
● Molecule 5: DNA (5'-D(*AP*GP*AP*GP*GP*AP*TP*GP*TP*GP*GP*CP*TP*TP*C)-3')

Chain E:

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

Chain J:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.22Å　　102.25Å　　194.59Å 90.00°　　　90.00°　　　90.00°	Depositor
Resolution (Å)	45.26　–　2.70 45.26　–　2.70	Depositor EDS
% Data completeness (in resolution range)	96.4 (45.26-2.70) 96.5 (45.26-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	4.62 (at 2.69Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.242　,　0.284 0.242　,　0.284	Depositor DCC
R_{free} test set	4299 reflections (10.08%)	DCC
Wilson B-factor (Å^2)	76.5	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 57.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.50, <L^2> = 0.33$	Xtriage
Outliers	4 of 42636 reflections (0.009%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7002	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.42	0/930	0.58	0/1263
1	F	0.48	0/930	0.65	0/1263
2	B	0.34	0/1093	0.49	0/1466
2	G	0.37	0/1084	0.50	0/1454
3	C	0.44	0/994	0.56	0/1342
3	H	0.32	0/877	0.45	0/1181
4	D	0.54	0/334	0.87	0/512
4	I	0.57	0/334	0.83	0/512
5	E	0.50	0/348	0.81	0/537
5	J	0.55	0/348	0.85	0/537
All	All	0.43	0/7272	0.62	0/10067

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	2
4	I	0	2
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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 (i)

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	911	0	916	41	0
1	F	911	0	916	26	0
2	B	1071	0	1034	45	0
2	G	1062	0	1026	47	0
3	C	967	0	966	23	0
3	H	853	0	847	57	0
4	D	299	0	170	13	0
4	I	299	0	170	20	0
5	E	310	0	171	3	0
5	J	310	0	171	6	0
6	C	3	0	0	0	0
6	F	4	0	0	0	0
6	H	1	0	0	0	0
6	J	1	0	0	0	0
All	All	7002	0	6387	266	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 (266) 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:2:DA:H2"	4:I:3:DA:H5'	1.31	1.10
4:I:9:DA:H2"	4:I:10:DT:H5'	1.36	1.03
4:I:11:DC:H2"	4:I:12:DC:H5'	1.39	1.02
3:H:424:TYR:HB2	3:H:429:LEU:HG	1.53	0.91
1:A:82:ASN:HD21	1:A:118:ARG:HH11	1.19	0.90
4:I:2:DA:H2"	4:I:3:DA:C5'	2.04	0.87
1:A:97:VAL:H	1:A:127:GLN:HE22	1.24	0.84
1:A:87:ILE:HD12	1:A:87:ILE:O	1.80	0.82
1:A:144:LYS:HE3	3:H:407:GLY:HA3	1.62	0.81
2:B:9:ARG:HH11	2:B:9:ARG:HB3	1.48	0.78
2:B:60:THR:HG23	2:B:62:THR:H	1.51	0.74
3:H:367:ASP:HB3	3:H:370:GLU:HB2	1.68	0.73
1:F:71:LEU:HD11	1:F:94:LYS:HE3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:322:PRO:HB2	3:C:325:ALA:HB3	1.70	0.73
4:D:10:DT:H2"	4:D:11:DC:H5'	1.70	0.73
4:I:10:DT:H2"	4:I:11:DC:O5'	1.89	0.72
3:H:372:ALA:HB1	3:H:385:ASN:HA	1.73	0.71
3:H:365:LEU:HD23	3:H:410:TYR:HD2	1.56	0.70
1:A:139:ARG:HG3	1:A:139:ARG:HH11	1.56	0.69
3:H:335:ILE:HD12	3:H:339:GLN:NE2	2.09	0.68
1:F:63:VAL:HB	1:F:74:VAL:HG22	1.75	0.67
2:G:63:ASN:N	2:G:63:ASN:HD22	1.91	0.67
2:B:115:ASP:OD1	2:B:118:ARG:HD3	1.95	0.67
1:F:148:LEU:HB2	1:F:162:TYR:HB3	1.75	0.67
2:G:55:ILE:HD13	2:G:66:LEU:HD12	1.77	0.66
2:B:67:GLN:HA	2:B:67:GLN:HE21	1.61	0.66
1:F:63:VAL:HG22	1:F:64:ARG:H	1.60	0.66
4:I:13:DT:H6	4:I:13:DT:H5'	1.60	0.66
3:H:345:LEU:HB3	3:H:356:TRP:HE1	1.61	0.66
1:A:104:THR:HG22	1:A:151:THR:HB	1.78	0.65
3:H:409:ARG:O	3:H:411:VAL:HG23	1.96	0.65
1:A:109:ASN:ND2	1:A:112:ASN:H	1.94	0.65
1:A:82:ASN:ND2	1:A:118:ARG:HH11	1.92	0.64
2:G:90:ARG:O	2:G:90:ARG:HD3	1.98	0.64
2:G:131:ARG:HB3	2:G:131:ARG:NH1	2.13	0.64
4:I:9:DA:C2'	4:I:10:DT:H5'	2.20	0.63
2:B:106:VAL:O	2:B:108:VAL:HG13	1.99	0.63
3:C:384:MET:SD	3:C:388:LYS:HB2	2.39	0.63
1:A:70:PHE:CE2	1:A:152:VAL:HG21	2.34	0.63
5:J:9:DT:H2'	5:J:10:DG:C8	2.34	0.63
3:C:326:LEU:HB3	3:C:421:LEU:O	2.00	0.62
4:I:11:DC:H2"	4:I:12:DC:C5'	2.23	0.62
1:A:109:ASN:C	1:A:109:ASN:HD22	2.02	0.62
2:G:90:ARG:HD2	2:G:96:TYR:CE2	2.35	0.62
2:B:41:GLN:HE21	2:B:117:HIS:HA	1.65	0.62
4:D:13:DT:H2"	4:D:14:DC:H5'	1.81	0.61
4:I:6:DC:H6	4:I:6:DC:H5'	1.64	0.60
2:B:63:ASN:HD22	2:B:63:ASN:N	1.98	0.60
4:I:13:DT:H5'	4:I:13:DT:C6	2.36	0.60
1:F:149:THR:HG21	2:G:63:ASN:O	2.01	0.60
2:B:113:TRP:C	2:B:114:ILE:HD12	2.22	0.60
1:A:145:SER:HB3	1:A:164:ARG:HA	1.84	0.59
1:F:63:VAL:HG22	1:F:64:ARG:N	2.17	0.59
1:F:157:PRO:HG2	2:G:67:GLN:HG3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:345:LEU:HB3	3:H:356:TRP:NE1	2.17	0.59
4:D:11:DC:H1'	4:D:12:DC:H5"	1.85	0.59
1:A:161:THR:H	2:B:104:ASN:HD21	1.51	0.59
1:A:139:ARG:HG3	1:A:139:ARG:NH1	2.18	0.58
3:H:419:GLN:HE21	3:H:426:PRO:HD3	1.68	0.58
3:H:335:ILE:HD12	3:H:339:GLN:HE21	1.67	0.58
1:F:174:ARG:NH2	5:J:10:DG:N7	2.51	0.58
4:D:11:DC:H2"	4:D:12:DC:H5'	1.86	0.58
1:A:71:LEU:HD11	1:A:94:LYS:HE3	1.85	0.58
4:I:8:DC:OP1	4:I:8:DC:H4'	2.03	0.57
4:D:11:DC:H1'	4:D:12:DC:C5'	2.35	0.57
1:A:149:THR:HG21	2:B:63:ASN:O	2.04	0.57
2:G:108:VAL:HG12	2:G:109:ILE:N	2.20	0.57
1:A:148:LEU:HB2	1:A:162:TYR:HB3	1.87	0.57
3:H:336:GLN:H	3:H:339:GLN:NE2	2.03	0.57
3:H:340:PHE:HZ	3:H:374:ARG:HB3	1.70	0.57
2:G:68:PHE:CZ	2:G:97:LEU:HD13	2.40	0.56
3:H:385:ASN:OD1	3:H:387:GLU:HB2	2.06	0.56
2:G:16:GLU:OE2	2:G:20:LYS:HB2	2.06	0.56
1:A:87:ILE:HD12	1:A:87:ILE:C	2.27	0.55
3:C:417:ASP:O	3:C:421:LEU:HD13	2.07	0.55
2:G:88:LEU:HD23	2:G:95:VAL:HG22	1.87	0.55
2:G:108:VAL:HG11	2:G:125:LEU:HB3	1.87	0.55
3:H:368:PRO:HG2	3:H:369:ASP:H	1.72	0.55
3:H:354:ILE:HD12	3:H:371:VAL:HG11	1.87	0.55
3:H:348:LYS:HE2	3:H:351:GLN:HE22	1.72	0.55
1:F:113:TYR:CE2	2:G:28:LYS:HD2	2.42	0.54
2:B:29:TYR:HA	2:B:55:ILE:HD13	1.89	0.54
1:A:90:LYS:HE3	1:A:130:ARG:HG2	1.90	0.54
1:A:159:VAL:HG13	2:B:103:LEU:HA	1.89	0.54
5:J:8:DG:H2"	5:J:9:DT:O5'	2.08	0.54
3:H:348:LYS:HA	3:H:351:GLN:HE21	1.73	0.53
3:H:353:PHE:C	3:H:366:SER:HB2	2.29	0.53
3:H:354:ILE:O	3:H:354:ILE:HG12	2.07	0.53
2:G:109:ILE:HG13	2:G:128:ASP:HB2	1.91	0.53
3:H:419:GLN:NE2	3:H:425:THR:HA	2.23	0.53
3:H:334:PRO:HG2	3:H:335:ILE:H	1.74	0.53
4:I:2:DA:C2'	4:I:3:DA:C5'	2.85	0.53
3:C:321:ILE:HD13	3:C:321:ILE:N	2.24	0.53
2:G:63:ASN:N	2:G:63:ASN:ND2	2.58	0.53
2:B:98:LYS:HE3	2:B:109:ILE:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:393:LEU:HA	3:H:396:TYR:HD2	1.74	0.53
3:C:425:THR:OG1	3:C:428:GLU:HG3	2.09	0.52
2:B:3:ARG:HH21	2:B:135:GLU:CD	2.12	0.52
1:F:115:ALA:HB2	1:F:146:PHE:CZ	2.45	0.52
2:B:114:ILE:HG23	2:B:120:ASP:N	2.25	0.52
3:H:365:LEU:HD21	3:H:368:PRO:HA	1.90	0.52
1:F:177:ARG:NH1	5:J:11:DG:N7	2.57	0.52
2:G:137:ALA:O	2:G:138:LEU:HD23	2.10	0.52
3:C:321:ILE:HD13	3:C:321:ILE:H	1.73	0.52
2:G:55:ILE:HG12	2:G:114:ILE:HD11	1.92	0.52
4:D:14:DC:H2"	4:D:15:DT:H5'	1.92	0.52
2:B:5:VAL:HG12	2:B:105:GLY:O	2.09	0.52
2:G:45:GLN:NE2	2:G:49:ARG:HH21	2.07	0.51
1:F:70:PHE:CE2	1:F:152:VAL:HG21	2.45	0.51
3:C:345:LEU:HD21	3:C:354:ILE:HG12	1.93	0.51
4:D:9:DA:H1'	4:D:10:DT:H5"	1.92	0.51
2:G:63:ASN:H	2:G:63:ASN:HD22	1.56	0.51
2:G:87:ASP:OD2	2:G:90:ARG:HB2	2.09	0.51
1:A:70:PHE:O	1:A:71:LEU:HD12	2.11	0.51
3:H:379:LYS:HG3	4:I:9:DA:OP1	2.11	0.51
3:H:419:GLN:HE22	3:H:425:THR:HG22	1.75	0.51
2:G:3:ARG:HD3	2:G:135:GLU:OE1	2.10	0.51
3:H:421:LEU:O	3:H:422:LEU:HG	2.11	0.51
3:H:347:ASP:OD2	3:H:349:SER:HB3	2.11	0.50
3:H:344:LEU:HD23	3:H:371:VAL:HG12	1.93	0.50
3:C:320:VAL:HG12	3:C:321:ILE:HG23	1.93	0.50
4:I:13:DT:H1'	4:I:14:DC:H5'	1.93	0.50
4:D:8:DC:H2"	4:D:9:DA:C8	2.47	0.50
1:A:109:ASN:HD22	1:A:112:ASN:H	1.59	0.50
4:D:6:DC:H6	4:D:6:DC:H5'	1.76	0.50
1:A:109:ASN:ND2	1:A:109:ASN:C	2.66	0.49
3:H:344:LEU:CD2	3:H:371:VAL:HG12	2.43	0.49
2:G:89:GLU:C	2:G:91:GLU:H	2.15	0.49
2:B:70:PRO:HD3	2:B:85:TYR:HE2	1.77	0.49
4:D:13:DT:H1'	4:D:14:DC:H5"	1.95	0.49
1:A:111:GLU:OE1	1:A:144:LYS:HD2	2.13	0.49
3:C:385:ASN:OD1	3:C:388:LYS:HG2	2.13	0.49
3:H:389:LEU:HD23	3:H:389:LEU:O	2.13	0.49
1:F:161:THR:HG22	1:F:162:TYR:N	2.27	0.48
3:H:354:ILE:HD12	3:H:371:VAL:CG1	2.43	0.48
2:B:11:LYS:HE3	2:B:15:GLU:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ASN:HD21	1:A:118:ARG:NH1	2.00	0.48
2:B:32:PHE:CD2	2:B:32:PHE:N	2.80	0.48
3:H:336:GLN:H	3:H:339:GLN:HE21	1.61	0.48
1:F:102:LEU:HD22	1:F:102:LEU:N	2.29	0.48
3:H:365:LEU:HB3	3:H:410:TYR:HB3	1.96	0.48
2:G:108:VAL:HG12	2:G:109:ILE:H	1.78	0.47
1:A:112:ASN:HD22	1:A:112:ASN:C	2.18	0.47
2:B:111:LYS:HD2	2:B:126:GLU:OE2	2.14	0.47
2:B:8:GLN:O	2:B:127:PHE:HE2	1.98	0.47
2:G:90:ARG:HH11	2:G:90:ARG:HG3	1.80	0.47
1:F:87:ILE:HD13	1:F:87:ILE:H	1.79	0.47
2:B:70:PRO:HD3	2:B:85:TYR:CE2	2.50	0.47
4:D:9:DA:H2"	4:D:10:DT:H5'	1.97	0.47
2:B:67:GLN:O	2:B:99:ALA:HB1	2.14	0.47
2:G:68:PHE:CE1	2:G:97:LEU:HB3	2.50	0.47
2:B:29:TYR:CE1	2:B:44:PHE:HB2	2.51	0.46
1:F:105:VAL:HG23	1:F:131:PHE:CZ	2.50	0.46
4:I:6:DC:H5'	4:I:6:DC:C6	2.47	0.46
3:H:361:TRP:CE3	3:H:361:TRP:HA	2.49	0.46
2:G:95:VAL:O	2:G:113:TRP:HA	2.16	0.46
4:D:10:DT:C2'	4:D:11:DC:H5'	2.43	0.46
4:D:7:DA:H2"	4:D:8:DC:O5'	2.15	0.46
3:H:361:TRP:NE1	3:H:426:PRO:HG3	2.30	0.46
2:G:86:VAL:O	2:G:86:VAL:HG13	2.15	0.46
3:C:321:ILE:HB	3:C:322:PRO:HD2	1.97	0.46
2:G:71:ALA:HB1	2:G:131:ARG:HE	1.80	0.46
3:H:348:LYS:HA	3:H:351:GLN:HB2	1.97	0.46
2:B:98:LYS:CE	2:B:111:LYS:HE2	2.46	0.46
2:B:134:GLN:O	2:B:137:ALA:HB3	2.16	0.46
2:G:27:ILE:HB	2:G:55:ILE:CG2	2.45	0.46
2:B:11:LYS:HD2	2:B:106:VAL:HG21	1.98	0.46
3:C:364:LYS:CB	3:C:411:VAL:HG22	2.45	0.46
1:A:97:VAL:H	1:A:127:GLN:NE2	2.03	0.46
3:C:385:ASN:HD21	3:C:387:GLU:HB2	1.81	0.46
5:E:15:DC:H2'	5:J:1:DA:O4'	2.16	0.46
2:B:95:VAL:O	2:B:113:TRP:HA	2.16	0.46
1:A:115:ALA:HB2	1:A:146:PHE:CZ	2.51	0.46
3:C:324:ALA:O	3:C:329:TYR:HB3	2.16	0.46
1:A:71:LEU:CD1	1:A:94:LYS:HE3	2.46	0.46
2:G:85:TYR:HA	2:G:98:LYS:HB3	1.98	0.46
3:H:362:GLU:HB2	3:H:413:ARG:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:424:TYR:CD2	3:H:429:LEU:HD21	2.52	0.45
3:H:353:PHE:HB3	3:H:370:GLU:HG2	1.98	0.45
1:A:65:THR:HG23	1:A:71:LEU:HA	1.98	0.45
5:J:9:DT:OP1	5:J:9:DT:H4'	2.16	0.45
2:B:4:VAL:HA	2:B:105:GLY:HA2	1.98	0.45
1:A:78:HIS:CD2	1:A:167:LYS:HE3	2.51	0.45
4:I:11:DC:C2'	4:I:12:DC:H5'	2.28	0.45
2:G:29:TYR:CD2	2:G:44:PHE:HD2	2.34	0.45
2:B:21:LEU:HD21	2:B:60:THR:HG21	1.97	0.45
2:G:45:GLN:HG2	2:G:49:ARG:HE	1.82	0.45
1:F:66:ASP:OD2	1:F:161:THR:HB	2.17	0.45
2:B:114:ILE:HA	2:B:120:ASP:O	2.16	0.45
2:B:67:GLN:HE21	2:B:67:GLN:CA	2.26	0.44
2:B:98:LYS:HA	2:B:110:TRP:O	2.18	0.44
2:B:130:GLU:O	2:B:134:GLN:HG3	2.17	0.44
2:G:68:PHE:CD1	2:G:99:ALA:HB2	2.52	0.44
1:F:145:SER:OG	1:F:164:ARG:HA	2.18	0.44
3:H:418:LEU:O	3:H:422:LEU:HB2	2.17	0.44
3:H:338:TRP:NE1	3:H:339:GLN:HG3	2.32	0.44
3:H:348:LYS:HA	3:H:351:GLN:NE2	2.32	0.44
3:H:430:HIS:O	3:H:433:LEU:HG	2.18	0.44
4:I:7:DA:H2"	4:I:8:DC:O5'	2.17	0.44
2:B:5:VAL:CG2	2:B:6:PRO:HD2	2.47	0.44
1:F:78:HIS:CD2	1:F:167:LYS:HG2	2.52	0.44
2:G:71:ALA:CB	2:G:131:ARG:HE	2.30	0.44
5:E:9:DT:H2"	5:E:10:DG:C8	2.53	0.44
3:H:419:GLN:HE22	3:H:425:THR:HA	1.83	0.43
2:G:106:VAL:O	2:G:108:VAL:HG23	2.18	0.43
3:H:422:LEU:HD13	3:H:429:LEU:HD11	2.01	0.43
3:C:327:ALA:HA	3:C:421:LEU:HD23	1.99	0.43
3:H:373:ARG:NH1	3:H:373:ARG:HB2	2.32	0.43
3:H:350:CYS:O	3:H:354:ILE:HG22	2.19	0.43
2:G:11:LYS:HE3	2:G:15:GLU:OE2	2.18	0.43
3:H:381:LYS:O	3:H:384:MET:HB2	2.18	0.43
1:F:157:PRO:CG	2:G:67:GLN:HG3	2.47	0.43
1:A:101:THR:HG23	1:A:153:PHE:O	2.18	0.43
2:G:12:PHE:HB2	2:G:106:VAL:HG11	2.01	0.43
1:A:75:LEU:HD21	1:A:89:PHE:CD2	2.54	0.43
2:G:134:GLN:O	2:G:138:LEU:HG	2.19	0.43
1:A:144:LYS:CE	3:H:407:GLY:HA3	2.43	0.43
2:B:98:LYS:HE3	2:B:111:LYS:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:393:LEU:HA	3:H:396:TYR:CD2	2.53	0.43
2:G:44:PHE:C	2:G:44:PHE:CD1	2.92	0.43
1:A:144:LYS:NZ	3:H:408:LYS:HE3	2.34	0.43
3:H:362:GLU:HB2	3:H:413:ARG:HH11	1.84	0.43
2:B:9:ARG:HA	2:B:127:PHE:CE2	2.54	0.42
2:G:54:GLU:C	2:G:55:ILE:HD12	2.40	0.42
2:G:131:ARG:HB3	2:G:131:ARG:HH11	1.82	0.42
1:A:126:ASN:O	1:A:127:GLN:HB2	2.20	0.42
3:H:345:LEU:HD22	3:H:356:TRP:NE1	2.35	0.42
2:B:86:VAL:HG13	2:B:86:VAL:O	2.19	0.42
1:F:79:TRP:CZ2	1:F:86:PRO:HD3	2.54	0.42
4:I:5:DC:H2"	4:I:6:DC:H5'	2.01	0.42
1:F:82:ASN:OD1	1:F:118:ARG:NH1	2.45	0.42
1:F:111:GLU:OE2	1:F:141:GLY:HA3	2.19	0.42
3:C:405:THR:HG21	3:C:408:LYS:HD2	2.01	0.42
2:G:115:ASP:O	2:G:117:HIS:N	2.53	0.42
3:C:364:LYS:HB2	3:C:411:VAL:HG22	2.01	0.42
1:A:62:LEU:HD21	1:A:92:VAL:HG21	2.01	0.42
4:I:8:DC:H2"	4:I:9:DA:C8	2.55	0.42
3:C:330:THR:C	3:C:332:SER:H	2.23	0.42
2:G:118:ARG:HB3	2:G:120:ASP:OD2	2.20	0.42
2:B:29:TYR:CZ	2:B:31:GLY:HA3	2.55	0.41
3:H:383:LYS:HG3	3:H:383:LYS:O	2.19	0.41
1:A:80:ARG:HG3	1:A:170:GLY:O	2.20	0.41
2:B:68:PHE:HA	2:B:99:ALA:HB2	2.02	0.41
1:A:174:ARG:NH2	5:E:10:DG:N7	2.65	0.41
1:A:79:TRP:CZ2	1:A:86:PRO:HD3	2.56	0.41
4:I:12:DC:H2"	4:I:13:DT:OP2	2.21	0.41
2:B:130:GLU:H	2:B:130:GLU:HG2	1.57	0.41
1:F:87:ILE:HD13	1:F:87:ILE:N	2.36	0.41
3:C:418:LEU:HD23	3:C:418:LEU:HA	1.82	0.41
2:B:27:ILE:HD12	2:B:114:ILE:HD11	2.02	0.41
3:H:354:ILE:O	3:H:354:ILE:HG23	2.20	0.41
1:A:105:VAL:HG23	1:A:131:PHE:CZ	2.56	0.41
2:B:68:PHE:CZ	2:B:97:LEU:HD13	2.56	0.41
1:F:175:GLU:HA	1:F:175:GLU:OE1	2.20	0.41
1:F:75:LEU:HD11	1:F:148:LEU:HD11	2.03	0.40
3:H:361:TRP:HB3	3:H:414:PHE:HB2	2.03	0.40
3:C:354:ILE:HD12	3:C:365:LEU:HD22	2.01	0.40
2:G:34:ASP:O	2:G:35:ARG:HD2	2.20	0.40
3:C:322:PRO:HG2	3:C:326:LEU:HG	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:ASP:O	2:B:117:HIS:N	2.54	0.40
2:G:98:LYS:HA	2:G:110:TRP:O	2.20	0.40
2:B:37:HIS:O	2:B:41:GLN:HG3	2.21	0.40
2:G:136:ASP:C	2:G:138:LEU:H	2.25	0.40
3:C:385:ASN:ND2	3:C:387:GLU:HB2	2.36	0.40
3:C:341:LEU:HD11	3:C:393:LEU:HD21	2.04	0.40
1:A:99:ASP:OD1	1:A:125:LYS:HD2	2.22	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%)	6 (5%)	1 (1%)	21	49
1	F	116/204 (57%)	109 (94%)	6 (5%)	1 (1%)	21	49
2	B	126/142 (89%)	98 (78%)	26 (21%)	2 (2%)	12	30
2	G	125/142 (88%)	103 (82%)	19 (15%)	3 (2%)	7	19
3	C	116/166 (70%)	112 (97%)	4 (3%)	0	100	100
3	H	99/166 (60%)	68 (69%)	22 (22%)	9 (9%)	1	1
All	All	698/1024 (68%)	599 (86%)	83 (12%)	16 (2%)	8	20

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	23	ARG
3	H	354	ILE
3	H	359	ASP
3	H	361	TRP
2	B	70	PRO

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Mol	Chain	Res	Type
1	F	111	GLU
3	H	370	GLU
2	B	116	LEU
2	G	116	LEU
3	H	355	SER
3	H	368	PRO
3	H	422	LEU
1	A	95	GLY
2	G	130	GLU
3	H	358	GLY
3	H	334	PRO

5.3.2 Protein sidechains (i)

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%)	94 (95%)	5 (5%)	29	59
1	F	99/178 (56%)	95 (96%)	4 (4%)	38	69
2	B	113/123 (92%)	108 (96%)	5 (4%)	35	65
2	G	112/123 (91%)	107 (96%)	5 (4%)	34	65
3	C	102/145 (70%)	100 (98%)	2 (2%)	63	87
3	H	91/145 (63%)	87 (96%)	4 (4%)	35	65
All	All	616/892 (69%)	591 (96%)	25 (4%)	37	69

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

Mol	Chain	Res	Type
1	A	77	THR
1	A	96	ASP
1	A	109	ASN
1	A	112	ASN
1	A	145	SER
2	B	9	ARG
2	B	63	ASN

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Mol	Chain	Res	Type
2	B	67	GLN
2	B	103	LEU
2	B	130	GLU
3	C	321	ILE
3	C	351	GLN
1	F	83	LYS
1	F	87	ILE
1	F	96	ASP
1	F	112	ASN
2	G	7	ASP
2	G	63	ASN
2	G	90	ARG
2	G	103	LEU
2	G	120	ASP
3	H	361	TRP
3	H	373	ARG
3	H	384	MET
3	H	398	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	109	ASN
1	A	112	ASN
1	A	119	ASN
1	A	127	GLN
1	A	132	ASN
1	A	155	ASN
2	B	8	GLN
2	B	41	GLN
2	B	63	ASN
2	B	67	GLN
2	B	104	ASN
2	B	134	GLN
3	C	380	ASN
1	F	112	ASN
1	F	132	ASN
1	F	163	HIS
2	G	8	GLN
2	G	46	ASN
2	G	63	ASN

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Mol	Chain	Res	Type
2	G	67	GLN
3	H	339	GLN
3	H	351	GLN
3	H	380	ASN
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 (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(Å²)	Q<0.9
1	A	118/204 (57%)	0.35	1 (0%)	87	88	50, 72, 95, 110	0
1	F	118/204 (57%)	0.28	1 (0%)	87	88	47, 62, 82, 103	0
2	B	130/142 (91%)	0.84	11 (8%)	13	10	77, 101, 128, 135	0
2	G	129/142 (90%)	0.71	8 (6%)	24	23	63, 88, 115, 120	0
3	C	118/166 (71%)	0.45	5 (4%)	40	39	46, 69, 100, 111	0
3	H	101/166 (60%)	2.01	46 (45%)	0	0	71, 131, 173, 179	0
4	D	15/15 (100%)	-0.13	0	100	100	57, 60, 76, 78	0
4	I	15/15 (100%)	-0.11	0	100	100	57, 69, 84, 85	0
5	E	15/15 (100%)	-0.18	0	100	100	50, 61, 73, 77	0
5	J	15/15 (100%)	-0.01	0	100	100	54, 66, 79, 87	0
All	All	774/1084 (71%)	0.68	72 (9%)	11	8	46, 80, 143, 179	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	426	PRO	6.3
3	H	421	LEU	5.9
3	H	346	THR	5.6
3	H	423	GLY	5.6
3	H	416	CYS	5.0
3	H	417	ASP	4.9
3	H	357	THR	4.8
3	H	424	TYR	4.8
3	H	431	ALA	4.8
3	H	335	ILE	4.6
3	H	361	TRP	4.3
3	C	332	SER	4.2
3	H	425	THR	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	96	TYR	4.2
3	H	422	LEU	3.8
3	H	345	LEU	3.8
3	H	364	LYS	3.8
3	C	327	ALA	3.7
3	H	334	PRO	3.4
3	H	353	PHE	3.4
3	H	418	LEU	3.3
3	H	419	GLN	3.2
3	H	427	GLU	3.2
2	G	133	GLN	3.1
1	A	60	GLY	3.1
3	H	354	ILE	3.0
3	H	356	TRP	3.0
3	H	420	SER	2.9
3	H	333	GLY	2.9
3	H	342	LEU	2.9
3	H	379	LYS	2.9
3	H	371	VAL	2.8
3	H	429	LEU	2.8
3	H	363	PHE	2.7
2	B	93	GLY	2.7
2	B	82	SER	2.7
2	B	94	LYS	2.7
2	G	82	SER	2.7
3	H	414	PHE	2.6
3	H	432	MET	2.6
3	H	409	ARG	2.6
3	H	359	ASP	2.6
3	H	355	SER	2.6
2	G	109	ILE	2.6
2	B	98	LYS	2.5
3	H	383	LYS	2.5
3	H	348	LYS	2.4
3	H	415	VAL	2.4
3	H	341	LEU	2.4
1	F	177	ARG	2.3
2	B	86	VAL	2.3
3	H	428	GLU	2.3
3	C	421	LEU	2.3
2	G	127	PHE	2.3
3	C	333	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	G	93	GLY	2.2
2	B	116	LEU	2.2
3	C	320	VAL	2.2
3	H	338	TRP	2.2
2	B	5	VAL	2.1
3	H	401	ILE	2.1
3	H	398	ASP	2.1
2	B	95	VAL	2.1
3	H	366	SER	2.1
2	G	7	ASP	2.1
2	G	111	LYS	2.1
2	G	131	ARG	2.1
3	H	405	THR	2.1
2	B	15	GLU	2.0
2	B	105	GLY	2.0
3	H	337	LEU	2.0
3	H	350	CYS	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 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.