



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 09:31 PM BST

PDB ID : 6DVD
Title : Crystal structure of Mycobacterium tuberculosis transcription initiation complex(ECF sigma factor L) with 6 nt spacer and bromine labelled in position "-11
Authors : Lin, W.; Das, K.; Feng, Y.; Ebright, R.H.
Deposited on : 2018-06-23
Resolution : 3.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.13
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

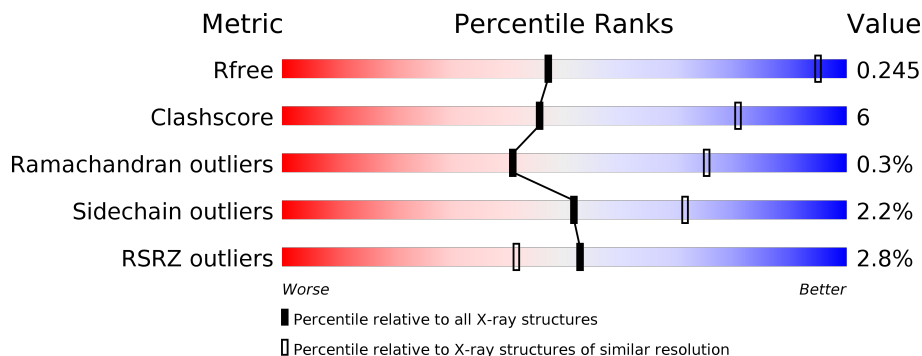
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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}	130704	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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 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	359	
1	B	359	
2	C	1178	
3	D	1316	
4	E	110	
5	F	177	

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Mol	Chain	Length	Quality of chain
6	G	10	 50% 50%
7	H	24	 21% 38% 63%

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 24744 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	225	Total	C	N	O	S	0	0	0
			1716	1080	296	338	2			
1	B	232	Total	C	N	O	S	0	0	0
			1732	1093	296	341	2			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP P9WGZ1
A	-10	GLY	-	expression tag	UNP P9WGZ1
A	-9	HIS	-	expression tag	UNP P9WGZ1
A	-8	HIS	-	expression tag	UNP P9WGZ1
A	-7	HIS	-	expression tag	UNP P9WGZ1
A	-6	HIS	-	expression tag	UNP P9WGZ1
A	-5	HIS	-	expression tag	UNP P9WGZ1
A	-4	HIS	-	expression tag	UNP P9WGZ1
A	-3	HIS	-	expression tag	UNP P9WGZ1
A	-2	HIS	-	expression tag	UNP P9WGZ1
A	-1	HIS	-	expression tag	UNP P9WGZ1
A	0	HIS	-	expression tag	UNP P9WGZ1
B	-11	MET	-	initiating methionine	UNP P9WGZ1
B	-10	GLY	-	expression tag	UNP P9WGZ1
B	-9	HIS	-	expression tag	UNP P9WGZ1
B	-8	HIS	-	expression tag	UNP P9WGZ1
B	-7	HIS	-	expression tag	UNP P9WGZ1
B	-6	HIS	-	expression tag	UNP P9WGZ1
B	-5	HIS	-	expression tag	UNP P9WGZ1
B	-4	HIS	-	expression tag	UNP P9WGZ1
B	-3	HIS	-	expression tag	UNP P9WGZ1
B	-2	HIS	-	expression tag	UNP P9WGZ1
B	-1	HIS	-	expression tag	UNP P9WGZ1
B	0	HIS	-	expression tag	UNP P9WGZ1

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	1126	8724	5459	1531	1695	39	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	1265	9895	6195	1794	1866	40	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	E	81	630	403	106	121	0	0	0

- Molecule 5 is a protein called ECF RNA polymerase sigma factor SigL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	174	1352	840	256	254	2	0	0	0

- Molecule 6 is a DNA chain called DNA (5'-D(*GP*CP*AP*TP*CP*CP*GP*TP*GP*A)-3').

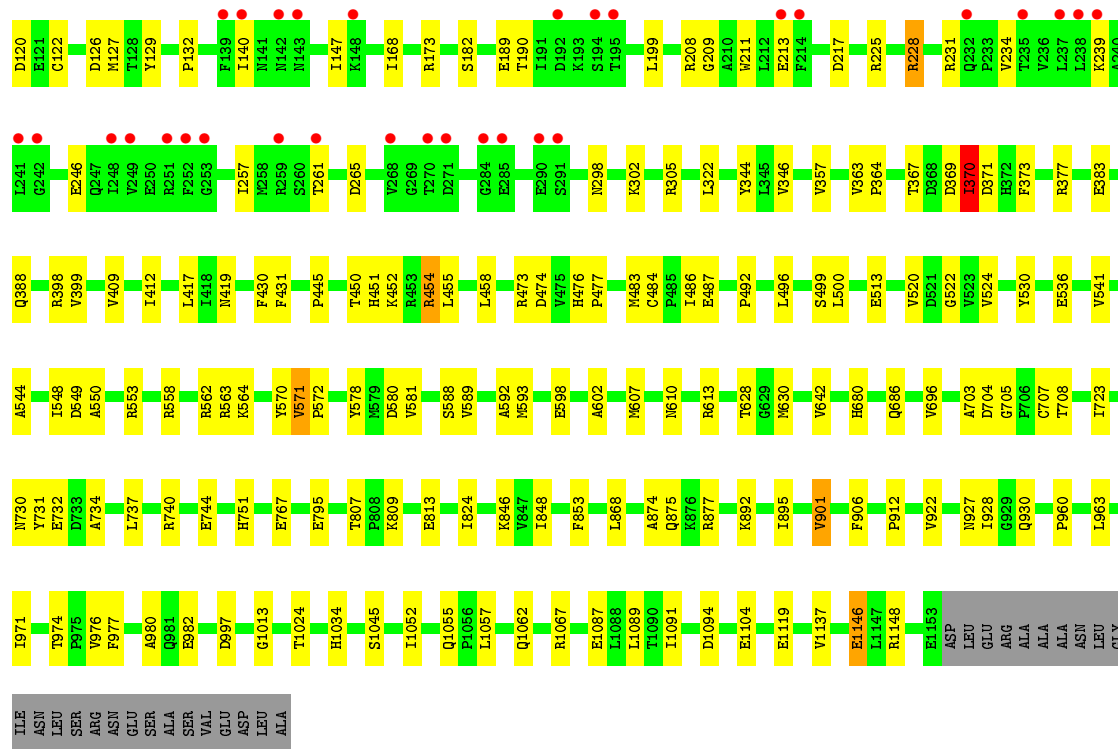
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
6	G	10	202	97	38	58	9	0	0	0

- Molecule 7 is a DNA chain called DNA (5'-D(P*CP*GP*TP*GP*TP*CP*AP*GP*TP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*C)-3').

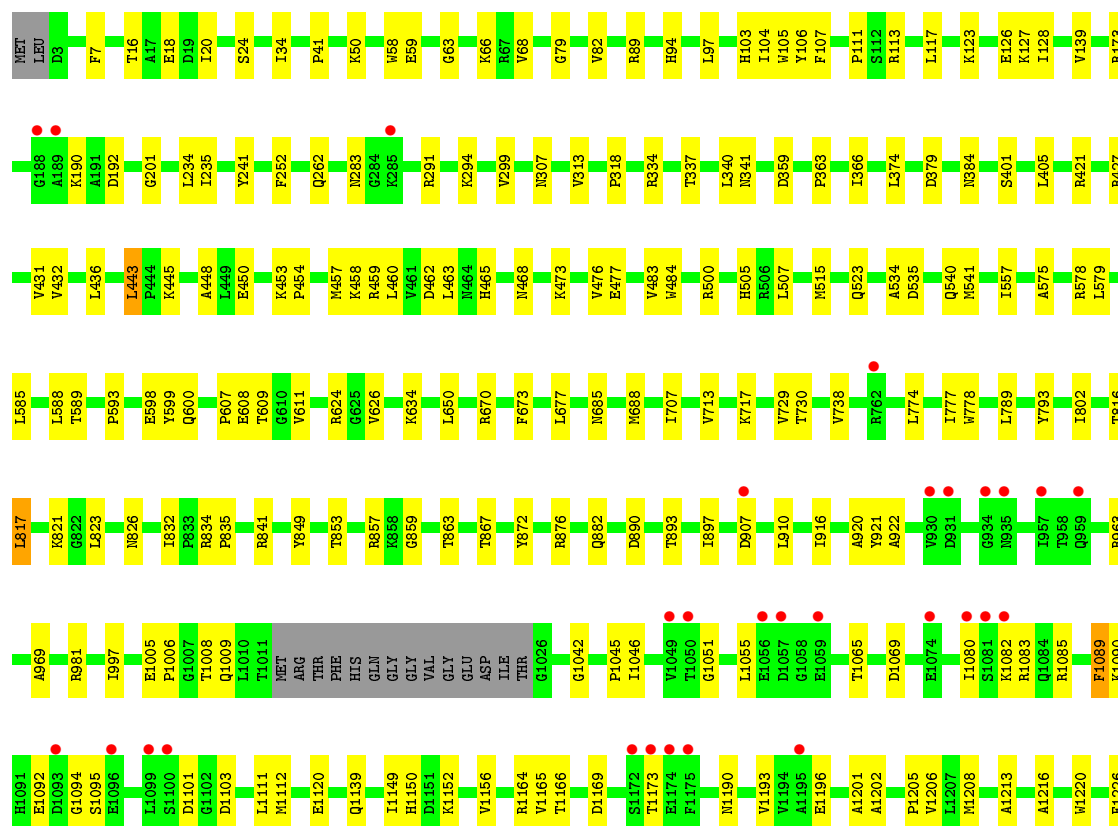
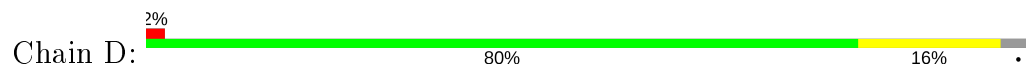
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
7	H	24	491	234	90	144	23	0	0	0

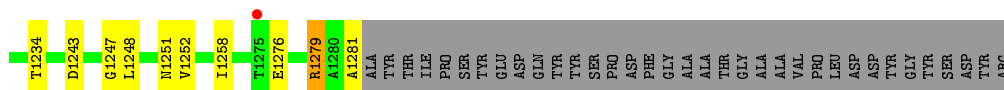
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total	Zn	0	0
			2	2		



• Molecule 3: DNA-directed RNA polymerase subunit beta'

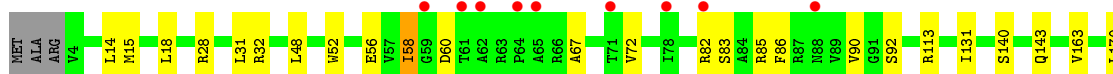
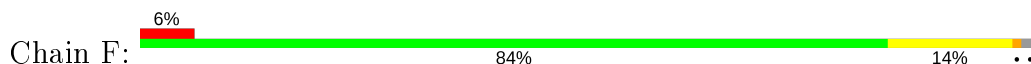




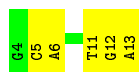
- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: ECF RNA polymerase sigma factor SigL



- Molecule 6: DNA (5'-D(*GP*CP*AP*TP*CP*CP*GP*TP*GP*A)-3')



- Molecule 7: DNA (5'-D(P*CP*GP*TP*GP*TP*CP*AP*GP*TP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	142.13Å 161.49Å 239.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.90 – 3.90 48.73 – 3.90	Depositor EDS
% Data completeness (in resolution range)	73.8 (45.90-3.90) 73.9 (48.73-3.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 3.88Å)	Xtrriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.220 , 0.246 0.220 , 0.245	Depositor DCC
R_{free} test set	2000 reflections (5.31%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtrriage
Anisotropy	0.956	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	24744	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

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	0.23	0/1742	0.44	0/2370
1	B	0.24	0/1758	0.44	0/2397
2	C	0.24	0/8883	0.42	0/12043
3	D	0.23	0/10061	0.40	0/13600
4	E	0.23	0/643	0.38	0/877
5	F	0.23	0/1374	0.39	0/1869
6	G	0.50	0/226	0.84	0/347
7	H	0.58	0/550	1.03	0/848
All	All	0.25	0/25237	0.44	0/34351

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1716	0	1756	29	0
1	B	1732	0	1754	34	0
2	C	8724	0	8651	115	0
3	D	9895	0	9954	137	0
4	E	630	0	622	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	1352	0	1346	20	0
6	G	202	0	114	7	0
7	H	491	0	272	19	0
8	D	2	0	0	0	0
All	All	24744	0	24469	313	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 6.

All (313) 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:40:ARG:HE	1:B:33:THR:HG22	1.46	0.81
3:D:334:ARG:HD3	5:F:90:VAL:HG21	1.63	0.80
1:A:4:SER:HB3	1:B:144:ARG:HH12	1.48	0.76
3:D:363:PRO:HG2	5:F:15:MET:HG3	1.67	0.75
3:D:1090:LYS:HE2	3:D:1103:ASP:HA	1.69	0.74
3:D:454:PRO:HA	3:D:457:MET:HE2	1.69	0.73
2:C:593:MET:HA	2:C:628:THR:HG21	1.70	0.73
3:D:832:ILE:HG22	3:D:834:ARG:H	1.54	0.72
2:C:541:VAL:HG12	2:C:578:TYR:HB2	1.71	0.72
2:C:1024:THR:H	3:D:730:THR:HG21	1.52	0.72
1:B:84:VAL:HG12	1:B:199:LYS:HD2	1.72	0.71
1:B:90:ASP:OD1	1:B:90:ASP:N	2.18	0.71
2:C:558:ARG:HB3	2:C:570:TYR:HB3	1.72	0.70
5:F:14:LEU:HD21	5:F:58:ILE:HG21	1.72	0.70
6:G:12:DG:H2''	6:G:13:DA:H5'	1.74	0.70
3:D:1247:GLY:O	3:D:1251:ASN:ND2	2.23	0.70
2:C:454:ARG:HH12	2:C:487:GLU:HG2	1.58	0.69
3:D:1090:LYS:HB3	3:D:1092:GLU:HG2	1.74	0.68
3:D:1055:LEU:H	3:D:1101:ASP:HB3	1.59	0.67
2:C:928:ILE:HD11	3:D:817:LEU:HD11	1.76	0.66
1:B:81:LYS:HD3	1:B:165:ASP:HB2	1.79	0.65
3:D:1045:PRO:HG2	3:D:1111:LEU:HB2	1.79	0.65
3:D:1248:LEU:HD22	3:D:1258:ILE:HB	1.79	0.65
3:D:882:GLN:HG3	3:D:997:ILE:HD11	1.79	0.64
2:C:536:GLU:OE2	2:C:562:ARG:NH2	2.31	0.64
2:C:104:SER:HB3	2:C:140:ILE:HB	1.80	0.63
3:D:1051:GLY:HA2	3:D:1069:ASP:HB2	1.79	0.63
2:C:122:CYS:HA	2:C:127:MET:HG3	1.79	0.63
3:D:458:LYS:NZ	3:D:462:ASP:OD2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:50:LYS:HE2	3:D:79:GLY:HA3	1.82	0.62
6:G:11:DT:H2'	6:G:12:DG:C8	2.35	0.62
1:B:100:GLN:HG3	1:B:133:LYS:HB2	1.82	0.61
3:D:104:ILE:HD12	3:D:379:ASP:HB3	1.83	0.61
2:C:211:TRP:HZ3	7:H:14:DT:H3'	1.65	0.61
1:A:186:ARG:HG3	1:A:187:THR:HG23	1.84	0.60
2:C:168:ILE:HB	2:C:173:ARG:HD2	1.83	0.60
3:D:436:LEU:HD11	3:D:523:GLN:HB3	1.84	0.59
1:A:40:ARG:NH2	2:C:1013:GLY:O	2.33	0.59
2:C:234:VAL:HG12	2:C:261:THR:HG21	1.84	0.59
1:B:55:ARG:NH2	1:B:137:GLU:OE1	2.36	0.59
3:D:1173:THR:HG22	3:D:1193:VAL:HG21	1.84	0.59
2:C:524:VAL:HG21	2:C:548:ILE:HD13	1.84	0.58
1:A:144:ARG:NH2	1:B:27:GLU:OE2	2.36	0.58
1:B:92:PRO:HB3	1:B:141:GLU:HG2	1.86	0.58
1:B:24:GLU:HB2	1:B:191:LYS:HG3	1.85	0.58
2:C:209:GLY:O	7:H:13:DC:N4	2.37	0.58
5:F:15:MET:HE3	5:F:18:LEU:HD11	1.85	0.58
2:C:571:VAL:HG22	2:C:572:PRO:HD2	1.86	0.58
3:D:1092:GLU:HG3	3:D:1094:GLY:H	1.68	0.58
2:C:824:ILE:HA	5:F:163:VAL:HG13	1.86	0.58
3:D:600:GLN:HB2	3:D:609:THR:HB	1.85	0.57
2:C:32:VAL:HG13	2:C:33:PRO:HD3	1.86	0.57
3:D:337:THR:OG1	3:D:341:ASN:ND2	2.33	0.57
3:D:1165:VAL:HG12	3:D:1205:PRO:HA	1.87	0.57
3:D:1045:PRO:HB2	3:D:1111:LEU:HD12	1.87	0.57
3:D:190:LYS:HE3	3:D:192:ASP:HB3	1.86	0.57
5:F:31:LEU:HD21	7:H:10:DT:C2	2.40	0.57
1:B:147:VAL:HG13	1:B:166:SER:HB2	1.87	0.57
2:C:113:ASP:HB3	2:C:132:PRO:HG2	1.87	0.57
2:C:47:PRO:HG2	2:C:581:VAL:HG13	1.88	0.56
2:C:1087:GLU:HG3	2:C:1091:ILE:HD11	1.85	0.56
1:A:216:VAL:HG13	1:B:216:VAL:HG13	1.88	0.56
2:C:607:MET:SD	2:C:892:LYS:NZ	2.78	0.56
3:D:107:PHE:HZ	3:D:126:GLU:HG2	1.71	0.56
2:C:83:VAL:HG13	2:C:87:GLU:HB2	1.87	0.55
3:D:789:LEU:HD22	3:D:793:TYR:HE2	1.71	0.55
3:D:826:ASN:HB3	3:D:832:ILE:HD11	1.88	0.55
2:C:398:ARG:HH12	5:F:32:ARG:HB3	1.71	0.55
1:A:22:VAL:HG12	1:A:193:ILE:HG12	1.88	0.55
2:C:1055:GLN:HG2	2:C:1094:ASP:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:458:LEU:HD21	2:C:496:LEU:HD13	1.88	0.55
3:D:1279:ARG:HE	3:D:1281:ALA:H	1.54	0.55
3:D:890:ASP:OD1	3:D:963:ARG:NH2	2.33	0.55
1:B:17:ASN:OD1	1:B:17:ASN:N	2.39	0.54
2:C:982:GLU:HG3	3:D:841:ARG:HH12	1.72	0.54
2:C:642:VAL:HB	2:C:703:ALA:HB3	1.89	0.54
3:D:1042:GLY:O	3:D:1083:ARG:NH2	2.37	0.54
2:C:853:PHE:HD2	2:C:868:LEU:HD23	1.72	0.53
2:C:731:TYR:HE1	3:D:579:LEU:HB2	1.73	0.53
2:C:298:ASN:HA	2:C:302:LYS:HB2	1.91	0.53
2:C:168:ILE:HG12	2:C:431:PHE:HB3	1.91	0.53
3:D:1164:ARG:NH2	3:D:1216:ALA:O	2.42	0.53
3:D:443:LEU:HD13	3:D:448:ALA:HB2	1.90	0.53
3:D:729:VAL:HG11	3:D:802:ILE:HD11	1.91	0.53
3:D:63:GLY:HA2	3:D:66:LYS:HE2	1.91	0.53
2:C:217:ASP:OD2	2:C:231:ARG:NH2	2.42	0.52
3:D:585:LEU:O	3:D:589:THR:OG1	2.27	0.52
1:B:129:ASN:OD1	1:B:130:ASP:N	2.38	0.52
3:D:589:THR:HG21	3:D:688:MET:HG2	1.91	0.52
3:D:34:ILE:HA	3:D:41:PRO:HA	1.91	0.52
5:F:67:ALA:O	7:H:8:DA:N6	2.43	0.52
2:C:960:PRO:HD2	2:C:963:LEU:HD22	1.91	0.52
2:C:190:THR:HG23	2:C:199:LEU:HB2	1.91	0.51
2:C:704:ASP:HB2	2:C:708:THR:HB	1.91	0.51
3:D:117:LEU:HD12	3:D:299:VAL:HG22	1.92	0.51
2:C:257:ILE:HD11	2:C:346:VAL:HG23	1.92	0.51
6:G:12:DG:C2'	6:G:13:DA:H5'	2.40	0.51
1:B:102:PRO:HD3	1:B:131:LYS:H	1.75	0.51
1:A:30:PHE:HE1	1:B:41:THR:HA	1.74	0.51
2:C:1045:SER:HB3	3:D:450:GLU:O	2.10	0.51
1:B:148:PRO:HG3	3:D:626:VAL:HG21	1.93	0.51
2:C:211:TRP:CZ3	7:H:14:DT:H3'	2.45	0.51
1:B:146:TYR:O	3:D:624:ARG:NE	2.44	0.51
2:C:853:PHE:HB2	2:C:868:LEU:HB3	1.93	0.51
1:A:84:VAL:HG13	1:A:119:HIS:HB2	1.93	0.51
1:A:56:ILE:HB	1:A:59:VAL:HG22	1.91	0.51
2:C:740:ARG:NH1	2:C:744:GLU:OE1	2.44	0.51
2:C:451:HIS:HA	2:C:454:ARG:HG2	1.91	0.51
3:D:505:HIS:CD2	3:D:507:LEU:HB2	2.45	0.51
1:A:7:PRO:HA	1:A:25:PRO:HD2	1.93	0.50
2:C:377:ARG:NH2	2:C:383:GLU:OE1	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:182:SER:HB2	2:C:377:ARG:HB2	1.94	0.50
3:D:921:TYR:O	3:D:1150:HIS:NE2	2.41	0.50
5:F:72:VAL:HG22	7:H:4:DT:C2	2.47	0.50
4:E:89:GLU:OE2	4:E:97:ARG:NH1	2.45	0.50
2:C:686:GLN:HA	2:C:705:GLY:HA2	1.94	0.49
3:D:1080:ILE:HG22	3:D:1082:LYS:H	1.76	0.49
3:D:173:ARG:HH21	3:D:201:GLY:HA2	1.78	0.49
6:G:5:DC:H2"	6:G:6:DA:C8	2.47	0.49
1:A:98:ARG:HG3	1:A:135:GLU:HG3	1.95	0.49
1:B:102:PRO:HB3	1:B:130:ASP:HA	1.94	0.49
3:D:460:LEU:HD11	3:D:483:VAL:HG12	1.94	0.49
3:D:778:TRP:CD2	3:D:835:PRO:HG3	2.47	0.49
1:A:89:GLU:HB3	1:A:91:GLU:HG2	1.95	0.49
3:D:500:ARG:HD2	3:D:534:ALA:HB2	1.95	0.49
5:F:140:SER:HB3	5:F:143:GLN:HG3	1.94	0.49
5:F:28:ARG:HB3	7:H:9:DG:H2"	1.94	0.49
2:C:751:HIS:CD2	2:C:877:ARG:HD2	2.48	0.49
2:C:1052:ILE:O	3:D:89:ARG:NH1	2.45	0.49
1:A:217:GLU:HG2	1:B:232:ILE:HD12	1.95	0.48
2:C:1067:ARG:HA	3:D:421:ARG:HA	1.95	0.48
7:H:6:DT:H3'	7:H:7:DC:H5"	1.95	0.48
2:C:62:GLU:OE1	2:C:69:ARG:NE	2.45	0.48
3:D:1220:TRP:CD1	3:D:1243:ASP:HB2	2.48	0.48
4:E:42:GLU:OE1	4:E:100:HIS:NE2	2.43	0.48
1:B:98:ARG:HG2	1:B:135:GLU:HG2	1.96	0.48
2:C:322:LEU:HD23	2:C:357:VAL:HG21	1.95	0.48
3:D:557:ILE:HG23	4:E:40:ILE:HD11	1.96	0.48
2:C:473:ARG:NH2	2:C:492:PRO:O	2.46	0.48
3:D:1139:GLN:NE2	3:D:1149:ILE:O	2.40	0.48
2:C:369:ASP:C	2:C:371:ASP:H	2.16	0.48
5:F:18:LEU:HD13	5:F:48:LEU:HD22	1.95	0.48
2:C:450:THR:HG21	2:C:613:ARG:HD2	1.95	0.48
3:D:1247:GLY:H	3:D:1251:ASN:HD21	1.62	0.48
3:D:366:ILE:HD11	5:F:15:MET:HE2	1.96	0.48
2:C:189:GLU:HB2	2:C:367:THR:HG21	1.96	0.48
2:C:730:ASN:HA	2:C:734:ALA:HB3	1.94	0.48
2:C:848:ILE:HD13	2:C:874:ALA:HB2	1.95	0.48
3:D:505:HIS:ND1	3:D:1005:GLU:HG3	2.29	0.47
2:C:369:ASP:O	2:C:370:ILE:HG12	2.14	0.47
2:C:388:GLN:HG3	2:C:430:PHE:HB2	1.96	0.47
3:D:1169:ASP:H	3:D:1202:ALA:HB3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:549:ASP:OD1	2:C:550:ALA:N	2.47	0.47
2:C:974:THR:HG23	2:C:980:ALA:H	1.79	0.47
2:C:795:GLU:HG2	2:C:846:LYS:HG2	1.96	0.47
3:D:473:LYS:NZ	3:D:477:GLU:OE2	2.45	0.47
1:A:188:ASP:OD2	1:B:151:GLN:NE2	2.44	0.47
1:B:170:PRO:HB2	1:B:202:ILE:HD11	1.97	0.47
4:E:47:VAL:HG11	4:E:53:LEU:HB2	1.97	0.47
3:D:882:GLN:HG2	3:D:1248:LEU:HB2	1.95	0.47
3:D:500:ARG:HB2	3:D:541:MET:HG2	1.95	0.47
3:D:384:ASN:H	3:D:401:SER:HB3	1.80	0.47
3:D:611:VAL:HG22	3:D:634:LYS:HB2	1.97	0.46
3:D:872:TYR:CD1	6:G:13:DA:H5''	2.51	0.46
2:C:731:TYR:CE1	3:D:579:LEU:HB2	2.49	0.46
7:H:10:DT:H2'	7:H:11:DA:C8	2.50	0.46
2:C:602:ALA:HB2	3:D:853:THR:HG22	1.96	0.46
2:C:1146:GLU:H	2:C:1146:GLU:HG2	1.48	0.46
3:D:1247:GLY:H	3:D:1251:ASN:ND2	2.12	0.46
2:C:1119:GLU:OE2	3:D:89:ARG:NH2	2.48	0.46
1:A:56:ILE:HG12	1:A:136:VAL:HG22	1.98	0.46
3:D:340:LEU:HD11	3:D:405:LEU:HD11	1.98	0.46
3:D:872:TYR:CG	6:G:13:DA:H5''	2.50	0.46
3:D:922:ALA:HB2	3:D:981:ARG:HH21	1.81	0.46
6:G:12:DG:H2'	6:G:13:DA:C8	2.50	0.46
7:H:9:DG:N3	7:H:9:DG:H2'	2.31	0.46
3:D:1085:ARG:HA	3:D:1112:MET:HA	1.98	0.46
3:D:431:VAL:O	3:D:523:GLN:HA	2.15	0.46
7:H:7:DC:OP1	7:H:7:DC:H4'	2.15	0.46
2:C:628:THR:HG23	2:C:630:MET:H	1.80	0.46
2:C:38:ARG:HA	2:C:971:ILE:HG13	1.98	0.46
2:C:588:SER:OG	2:C:589:VAL:N	2.48	0.46
3:D:105:TRP:HB3	3:D:1234:THR:HG22	1.98	0.46
1:A:18:ARG:NH2	2:C:997:ASP:OD1	2.48	0.45
2:C:486:ILE:HD11	3:D:849:TYR:HE2	1.81	0.45
2:C:412:ILE:HD13	2:C:417:LEU:HD21	1.98	0.45
3:D:1166:THR:HB	3:D:1206:VAL:HG21	1.98	0.45
3:D:585:LEU:HD13	3:D:673:PHE:HE2	1.81	0.45
2:C:32:VAL:H	2:C:33:PRO:CD	2.29	0.45
3:D:235:ILE:HD12	3:D:241:TYR:HD1	1.81	0.45
2:C:32:VAL:H	2:C:33:PRO:HD3	1.81	0.45
2:C:115:VAL:HG11	2:C:129:TYR:CZ	2.52	0.45
2:C:522:GLY:O	2:C:553:ARG:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:901:VAL:HG23	2:C:912:PRO:HG3	1.98	0.45
1:A:40:ARG:NE	1:B:33:THR:HG22	2.25	0.45
2:C:544:ALA:HB2	2:C:580:ASP:HB2	1.99	0.44
3:D:1190:ASN:ND2	3:D:1201:ALA:O	2.44	0.44
3:D:463:LEU:HB2	3:D:465:HIS:HD2	1.82	0.44
3:D:589:THR:HG22	3:D:670:ARG:HG2	1.99	0.44
3:D:59:GLU:HG2	3:D:66:LYS:HD3	1.98	0.44
2:C:213:GLU:OE1	2:C:225:ARG:NH1	2.50	0.44
2:C:1089:LEU:HD13	3:D:1252:VAL:HG13	1.99	0.44
3:D:453:LYS:O	3:D:457:MET:HG3	2.17	0.44
3:D:468:ASN:HD22	5:F:175:VAL:HG22	1.82	0.44
3:D:575:ALA:O	3:D:713:VAL:HG21	2.18	0.44
1:B:84:VAL:HG23	1:B:119:HIS:HB2	2.00	0.44
3:D:103:HIS:HB3	3:D:106:TYR:HD2	1.82	0.44
2:C:927:ASN:O	2:C:930:GLN:HG2	2.17	0.44
2:C:680:HIS:O	2:C:1034:HIS:HE1	2.01	0.44
2:C:809:LYS:HE2	2:C:813:GLU:HB2	2.00	0.44
2:C:1104:GLU:OE1	5:F:113:ARG:NH1	2.50	0.44
3:D:588:LEU:HD12	3:D:589:THR:HG23	2.00	0.44
1:A:173:LYS:HE3	1:A:173:LYS:HB2	1.84	0.43
2:C:484:CYS:HB2	2:C:588:SER:HB2	2.00	0.43
3:D:337:THR:O	5:F:92:SER:HA	2.18	0.43
2:C:454:ARG:HH11	2:C:499:SER:HB2	1.82	0.43
3:D:291:ARG:NH2	7:H:24:DG:O6	2.44	0.43
2:C:140:ILE:HA	2:C:147:ILE:HG12	1.99	0.43
2:C:228:ARG:O	2:C:228:ARG:HG3	2.17	0.43
2:C:344:TYR:OH	2:C:364:PRO:O	2.25	0.43
2:C:513:GLU:HB3	2:C:530:TYR:HB3	2.01	0.43
2:C:737:LEU:HG	2:C:895:ILE:HD12	1.99	0.43
2:C:982:GLU:HG3	3:D:841:ARG:NH1	2.32	0.43
1:B:24:GLU:HA	1:B:25:PRO:HA	1.82	0.43
3:D:505:HIS:HD2	3:D:507:LEU:H	1.64	0.43
3:D:445:LYS:HB3	3:D:484:TRP:CZ3	2.53	0.43
1:A:81:LYS:NZ	1:A:165:ASP:HB2	2.34	0.43
1:B:74:THR:HG21	3:D:608:GLU:HB2	2.00	0.43
2:C:455:LEU:HD12	2:C:483:MET:HG3	2.00	0.43
3:D:579:LEU:HD23	3:D:579:LEU:HA	1.88	0.43
3:D:893:THR:HG21	3:D:969:ALA:HB3	2.00	0.43
1:B:28:PRO:HA	1:B:29:GLY:HA2	1.47	0.43
3:D:123:LYS:HE3	3:D:127:LYS:HE2	2.00	0.43
3:D:1279:ARG:HG3	3:D:1279:ARG:H	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:82:ARG:HB3	5:F:83:SER:H	1.67	0.43
3:D:453:LYS:HG3	3:D:476:VAL:HG11	2.00	0.43
2:C:474:ASP:HA	3:D:857:ARG:HD2	2.00	0.43
2:C:86:LEU:HA	2:C:86:LEU:HD23	1.90	0.43
3:D:24:SER:HB2	3:D:94:HIS:HB3	2.01	0.43
3:D:262:GLN:HB2	3:D:313:VAL:HG11	2.01	0.42
3:D:859:GLY:O	3:D:863:THR:OG1	2.32	0.42
5:F:170:LEU:HD22	5:F:175:VAL:HG21	2.01	0.42
3:D:294:LYS:NZ	7:H:22:DA:O5'	2.52	0.42
1:B:30:PHE:HA	1:B:33:THR:HG23	2.01	0.42
2:C:592:ALA:HA	2:C:976:VAL:HG21	2.01	0.42
2:C:906:PHE:HA	2:C:912:PRO:HA	2.01	0.42
3:D:16:THR:HG22	3:D:18:GLU:H	1.84	0.42
2:C:731:TYR:HB3	3:D:432:VAL:HG21	2.00	0.42
3:D:867:THR:HG22	3:D:1008:THR:HG23	2.01	0.42
4:E:96:LEU:HD12	4:E:96:LEU:HA	1.86	0.42
3:D:139:VAL:HA	3:D:252:PHE:HA	2.00	0.42
3:D:670:ARG:NH1	3:D:685:ASN:O	2.52	0.42
1:A:3:ILE:HG13	1:A:4:SER:H	1.85	0.42
2:C:57:GLN:HG3	2:C:452:LYS:HB3	2.01	0.42
3:D:128:ILE:HD11	3:D:234:LEU:HD11	2.01	0.42
3:D:427:ARG:NH1	3:D:540:GLN:OE1	2.52	0.42
2:C:610:ASN:OD1	2:C:613:ARG:NH1	2.52	0.42
3:D:598:GLU:HG2	3:D:599:TYR:H	1.84	0.42
3:D:20:ILE:HG23	3:D:318:PRO:HB3	2.02	0.42
3:D:97:LEU:HD22	3:D:374:LEU:HD21	2.00	0.42
1:A:206:ASP:OD1	1:B:226:ASN:ND2	2.52	0.42
2:C:120:ASP:N	2:C:120:ASP:OD1	2.53	0.42
2:C:305:ARG:HA	2:C:305:ARG:HD2	1.83	0.42
2:C:56:VAL:HG21	2:C:500:LEU:HD22	2.02	0.42
2:C:767:GLU:HG2	2:C:807:THR:HG22	2.02	0.42
3:D:897:ILE:HA	3:D:897:ILE:HD12	1.80	0.42
2:C:228:ARG:HH21	7:H:13:DC:H1'	1.83	0.42
1:A:69:VAL:HG12	1:A:128:LEU:HG	2.01	0.42
1:A:3:ILE:HA	1:A:3:ILE:HD12	1.88	0.42
2:C:239:LYS:NZ	2:C:265:ASP:OD2	2.47	0.42
3:D:1101:ASP:OD1	3:D:1101:ASP:N	2.51	0.42
3:D:363:PRO:HD3	5:F:52:TRP:CE2	2.54	0.42
7:H:17:DC:H2''	7:H:18:DA:C8	2.55	0.42
7:H:20:DG:H2''	7:H:21:DG:C8	2.55	0.41
1:B:124:HIS:HE1	1:B:127:THR:HG23	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:228:ARG:NH2	7:H:13:DC:H1'	2.35	0.41
2:C:563:ARG:HG2	2:C:564:LYS:H	1.84	0.41
3:D:1089:PHE:HA	3:D:1095:SER:HA	2.03	0.41
3:D:876:ARG:HG2	3:D:1226:PHE:HZ	1.86	0.41
2:C:58:THR:O	2:C:62:GLU:HG3	2.20	0.41
3:D:58:TRP:CE2	3:D:68:VAL:HG13	2.55	0.41
3:D:823:LEU:HD23	3:D:835:PRO:HB3	2.03	0.41
2:C:399:VAL:HG11	2:C:419:ASN:HB3	2.02	0.41
2:C:445:PRO:HD2	2:C:707:CYS:HB2	2.02	0.41
2:C:476:HIS:CG	2:C:477:PRO:HD2	2.55	0.41
3:D:1046:ILE:HD11	3:D:1120:GLU:HB3	2.01	0.41
7:H:21:DG:H2''	7:H:22:DA:C8	2.55	0.41
2:C:598:GLU:HB3	2:C:977:PHE:HD2	1.85	0.41
1:B:202:ILE:HD13	1:B:207:ALA:HB2	2.02	0.41
2:C:454:ARG:HA	2:C:454:ARG:HD2	1.80	0.41
3:D:816:THR:HG23	3:D:821:LYS:HA	2.01	0.41
2:C:454:ARG:NH1	2:C:499:SER:HB2	2.35	0.41
3:D:111:PRO:O	3:D:113:ARG:NH1	2.51	0.41
3:D:1208:MET:HE3	3:D:1213:ALA:HB2	2.03	0.41
3:D:717:LYS:HE2	3:D:717:LYS:HB3	1.83	0.41
3:D:774:LEU:HD23	3:D:777:ILE:HD12	2.02	0.41
1:A:203:SER:OG	1:A:206:ASP:OD2	2.36	0.41
3:D:1152:LYS:HB2	3:D:1152:LYS:HE3	1.91	0.41
3:D:1152:LYS:O	3:D:1156:VAL:HG23	2.20	0.41
1:A:66:VAL:O	1:A:69:VAL:HG22	2.20	0.41
3:D:123:LYS:HB2	7:H:24:DG:OP1	2.21	0.41
1:A:83:LEU:HA	1:A:123:MET:HE1	2.03	0.40
1:B:42:LEU:HD21	1:B:208:LEU:HA	2.03	0.40
3:D:707:ILE:HD11	4:E:32:PRO:HB3	2.03	0.40
3:D:916:ILE:HG23	3:D:920:ALA:HB3	2.03	0.40
2:C:723:ILE:O	3:D:730:THR:HG23	2.21	0.40
4:E:33:LEU:H	4:E:33:LEU:HD23	1.85	0.40
5:F:131:ILE:HG13	5:F:131:ILE:H	1.69	0.40
3:D:1005:GLU:HB3	3:D:1006:PRO:HD3	2.03	0.40
1:A:83:LEU:HA	1:A:83:LEU:HD23	1.89	0.40
1:A:99:LYS:HG2	1:A:105:VAL:HG22	2.03	0.40
1:B:112:PRO:HA	1:B:113:PRO:HD2	1.96	0.40
3:D:789:LEU:HD22	3:D:793:TYR:CE2	2.53	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	223/359 (62%)	217 (97%)	5 (2%)	1 (0%)	34	71
1	B	230/359 (64%)	213 (93%)	16 (7%)	1 (0%)	34	71
2	C	1124/1178 (95%)	1072 (95%)	47 (4%)	5 (0%)	34	71
3	D	1261/1316 (96%)	1200 (95%)	58 (5%)	3 (0%)	47	79
4	E	79/110 (72%)	76 (96%)	3 (4%)	0	100	100
5	F	172/177 (97%)	168 (98%)	4 (2%)	0	100	100
All	All	3089/3499 (88%)	2946 (95%)	133 (4%)	10 (0%)	41	75

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	370	ILE
1	B	159	ILE
2	C	732	GLU
1	A	184	GLU
2	C	32	VAL
3	D	593	PRO
3	D	1089	PHE
2	C	520	VAL
2	C	922	VAL
3	D	607	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	194/308 (63%)	190 (98%)	4 (2%)	53	73
1	B	191/308 (62%)	186 (97%)	5 (3%)	46	68
2	C	950/998 (95%)	929 (98%)	21 (2%)	52	71
3	D	1050/1095 (96%)	1029 (98%)	21 (2%)	55	74
4	E	66/90 (73%)	65 (98%)	1 (2%)	65	80
5	F	134/136 (98%)	129 (96%)	5 (4%)	34	60
All	All	2585/2935 (88%)	2528 (98%)	57 (2%)	52	71

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	18	ARG
1	A	111	VAL
1	A	116	VAL
1	B	79	ASN
1	B	90	ASP
1	B	147	VAL
1	B	184	GLU
1	B	188	ASP
2	C	32	VAL
2	C	39	VAL
2	C	80	VAL
2	C	126	ASP
2	C	208	ARG
2	C	228	ARG
2	C	246	GLU
2	C	363	VAL
2	C	370	ILE
2	C	373	PHE
2	C	409	VAL
2	C	454	ARG
2	C	571	VAL
2	C	696	VAL
2	C	875	GLN
2	C	901	VAL
2	C	1057	LEU
2	C	1062	GLN
2	C	1137	VAL
2	C	1146	GLU
2	C	1148	ARG

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Mol	Chain	Res	Type
3	D	7	PHE
3	D	82	VAL
3	D	283	ASN
3	D	307	ASN
3	D	359	ASP
3	D	443	LEU
3	D	459	ARG
3	D	515	MET
3	D	535	ASP
3	D	578	ARG
3	D	650	LEU
3	D	677	LEU
3	D	738	VAL
3	D	817	LEU
3	D	907	ASP
3	D	910	LEU
3	D	1009	GLN
3	D	1065	THR
3	D	1196	GLU
3	D	1276	GLU
3	D	1279	ARG
4	E	84	GLU
5	F	56	GLU
5	F	58	ILE
5	F	60	ASP
5	F	85	ARG
5	F	86	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	225/359 (62%)	-0.34	1 (0%) 92 87	16, 39, 97, 148	0
1	B	232/359 (64%)	-0.27	2 (0%) 84 77	26, 63, 111, 150	0
2	C	1126/1178 (95%)	-0.17	33 (2%) 51 40	12, 48, 141, 173	0
3	D	1265/1316 (96%)	-0.16	30 (2%) 59 48	9, 61, 159, 205	0
4	E	81/110 (73%)	0.35	6 (7%) 14 11	49, 72, 145, 166	0
5	F	174/177 (98%)	0.24	10 (5%) 23 19	39, 86, 136, 162	0
6	G	10/10 (100%)	-0.02	0 100 100	115, 135, 171, 178	0
7	H	24/24 (100%)	1.13	5 (20%) 1 1	125, 155, 191, 206	0
All	All	3137/3533 (88%)	-0.14	87 (2%) 53 41	9, 58, 150, 206	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	252	PHE	5.5
3	D	1093	ASP	4.8
2	C	251	ARG	3.8
2	C	104	SER	3.6
2	C	253	GLY	3.5
3	D	1081	SER	3.4
7	H	15	DG	3.4
5	F	61	THR	3.3
2	C	248	ILE	3.3
7	H	6	DT	3.3
3	D	1175	PHE	3.2
3	D	1099	LEU	3.2
4	E	78	TYR	3.2
5	F	62	ALA	3.1
3	D	1059	GLU	3.1
1	B	157	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	284	GLY	2.9
2	C	99	PHE	2.9
2	C	195	THR	2.8
4	E	68	TYR	2.8
2	C	268	VAL	2.8
2	C	192	ASP	2.8
2	C	285	GLU	2.8
2	C	241	LEU	2.8
3	D	930	VAL	2.7
2	C	242	GLY	2.7
3	D	1056	GLU	2.7
2	C	194	SER	2.6
2	C	271	ASP	2.6
2	C	237	LEU	2.6
2	C	249	VAL	2.6
5	F	177	ARG	2.6
2	C	140	ILE	2.6
5	F	59	GLY	2.6
2	C	239	LYS	2.6
2	C	261	THR	2.6
3	D	957	ILE	2.6
2	C	290	GLU	2.5
3	D	1049	VAL	2.5
2	C	238	LEU	2.5
3	D	1172	SER	2.5
1	B	156	GLY	2.5
3	D	959	GLN	2.4
2	C	214	PHE	2.4
2	C	259	ARG	2.3
2	C	213	GLU	2.3
3	D	935	ASN	2.3
3	D	1096	GLU	2.3
2	C	291	SER	2.3
3	D	189	ALA	2.3
5	F	64	PRO	2.3
3	D	188	GLY	2.3
1	A	226	ASN	2.2
2	C	235	THR	2.2
2	C	270	THR	2.2
3	D	1195	ALA	2.2
2	C	139	PHE	2.2
3	D	1082	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
5	F	65	ALA	2.2
3	D	934	GLY	2.2
4	E	72	GLY	2.2
3	D	1174	GLU	2.2
3	D	1050	THR	2.2
3	D	285	LYS	2.2
2	C	232	GLN	2.2
3	D	931	ASP	2.2
2	C	143	ASN	2.2
3	D	1173	THR	2.2
3	D	1100	SER	2.2
7	H	5	DG	2.2
3	D	1057	ASP	2.1
7	H	14	DT	2.1
3	D	1275	THR	2.1
3	D	1074	GLU	2.1
7	H	7	DC	2.1
2	C	148	LYS	2.1
3	D	762	ARG	2.1
2	C	142	ASN	2.1
4	E	79	VAL	2.1
3	D	1080	ILE	2.1
5	F	71	THR	2.0
5	F	78	ILE	2.0
5	F	82	ARG	2.0
4	E	28	GLY	2.0
4	E	71	LEU	2.0
5	F	88	ASN	2.0
3	D	907	ASP	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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	ZN	D	2001	1/1	0.95	0.11	60,60,60,60	0
8	ZN	D	2002	1/1	0.99	0.05	68,68,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.