Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:41 pm BST

PDB ID	:	6QCG
Title	:	PCNA complex with Cdt1 N-terminal PIP-box peptide
Authors	:	Perrakis, A.; von Castelmur, E.
Deposited on	:	2018-12-28
Resolution	:	3.40 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 ①) were used in the production of this report:

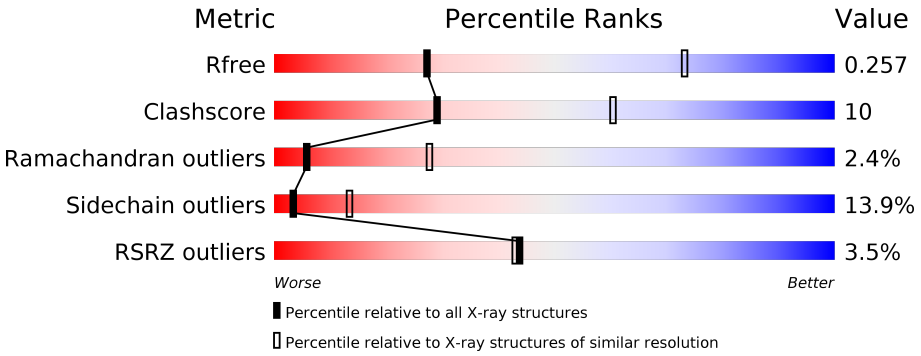
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 <=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	263	7% 65% 24% 5% 5%
1	B	263	% 68% 23% 6% •
1	C	263	3% 67% 24% • 5%
1	D	263	3% 70% 21% • 5%
1	E	263	2% 65% 27% 5% •
1	F	263	3% 68% 24% 5% • •

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Mol	Chain	Length	Quality of chain
2	G	14	21% 36% 14% 29%
2	H	14	29% 43% 14% 14% 29%
2	I	14	43% 7% 21% 29%
2	J	14	29% 29% 36% 7% 29%
2	K	14	7% 29% 43% 29%
2	L	14	43% 29% 29%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12123 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 Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	0	0
			1917	1206	316	379	16			
1	C	250	Total	C	N	O	S	0	0	0
			1905	1200	311	378	16			
1	B	255	Total	C	N	O	S	0	0	0
			1949	1227	322	384	16			
1	E	255	Total	C	N	O	S	0	0	0
			1949	1225	322	386	16			
1	D	250	Total	C	N	O	S	0	0	0
			1894	1195	310	373	16			
1	F	257	Total	C	N	O	S	0	0	0
			1961	1233	324	388	16			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P12004
A	0	PRO	-	expression tag	UNP P12004
C	-1	GLY	-	expression tag	UNP P12004
C	0	PRO	-	expression tag	UNP P12004
B	-1	GLY	-	expression tag	UNP P12004
B	0	PRO	-	expression tag	UNP P12004
E	-1	GLY	-	expression tag	UNP P12004
E	0	PRO	-	expression tag	UNP P12004
D	-1	GLY	-	expression tag	UNP P12004
D	0	PRO	-	expression tag	UNP P12004
F	-1	GLY	-	expression tag	UNP P12004
F	0	PRO	-	expression tag	UNP P12004

- Molecule 2 is a protein called DNA replication factor Cdt1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	10	Total	C	N	O	0	0	0
			91	57	20	14			
2	G	10	Total	C	N	O	0	0	0
			91	57	20	14			
2	H	10	Total	C	N	O	0	0	0
			91	57	20	14			
2	J	10	Total	C	N	O	0	0	0
			91	57	20	14			
2	K	10	Total	C	N	O	0	0	0
			91	57	20	14			
2	L	10	Total	C	N	O	0	0	0
			91	57	20	14			

- Molecule 3 is water.

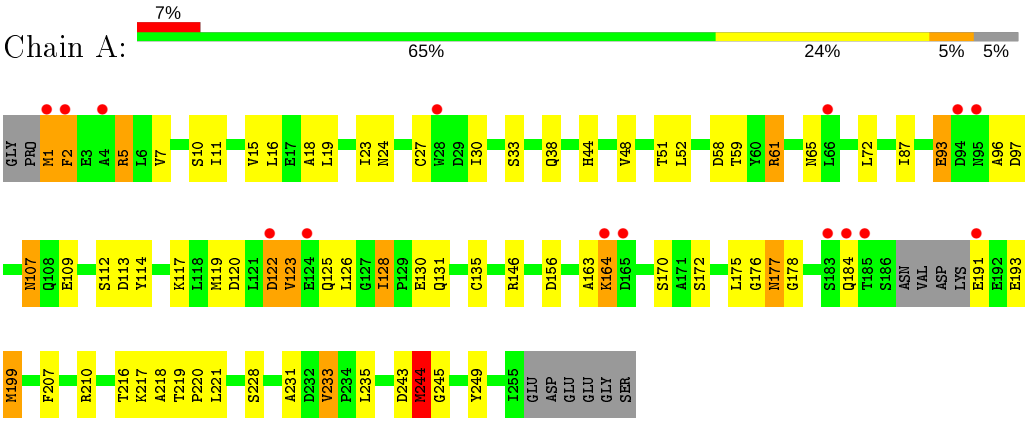
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	O	0	0
			1	1		
3	K	1	Total	O	0	0
			1	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

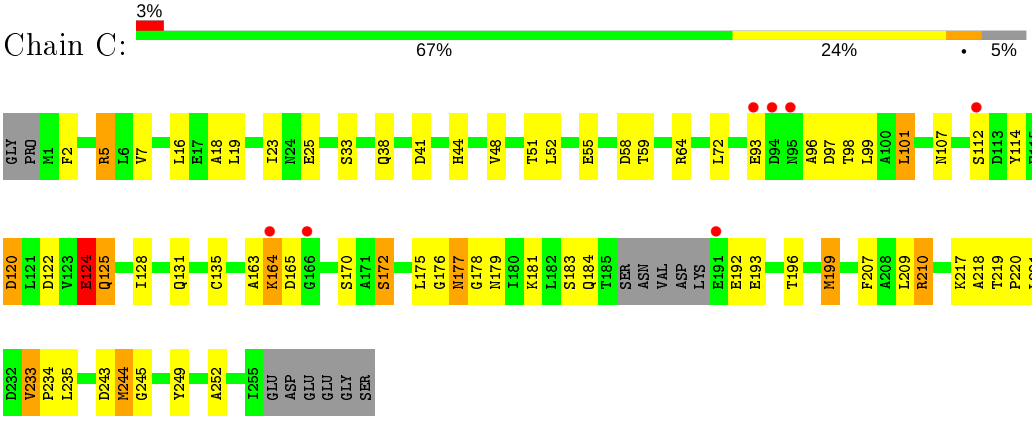
- Molecule 1: Proliferating cell nuclear antigen

Chain A:



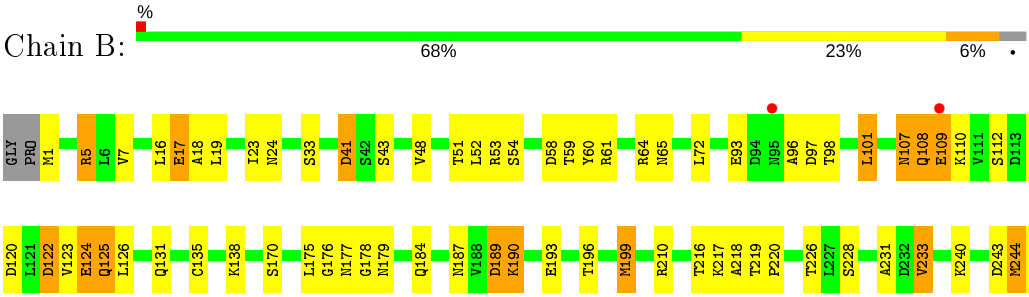
- Molecule 1: Proliferating cell nuclear antigen

Chain C:



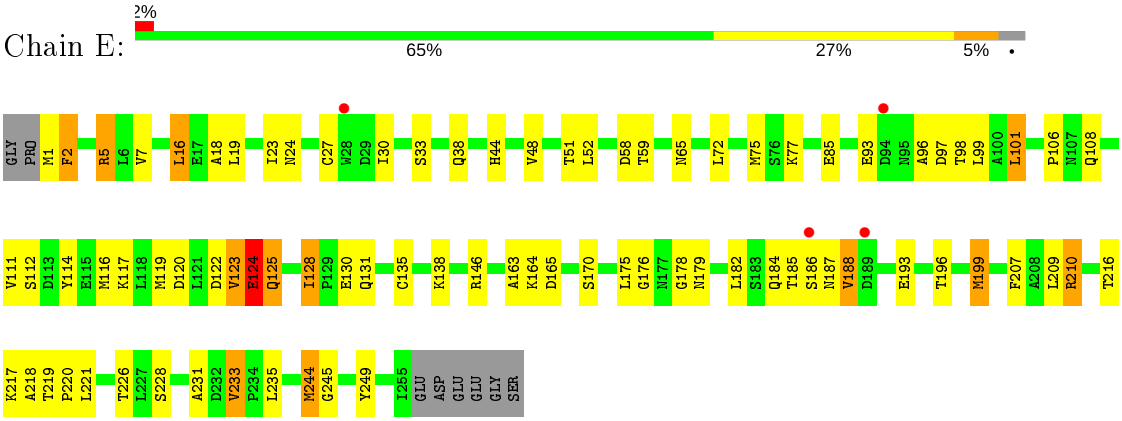
- Molecule 1: Proliferating cell nuclear antigen

Chain B:



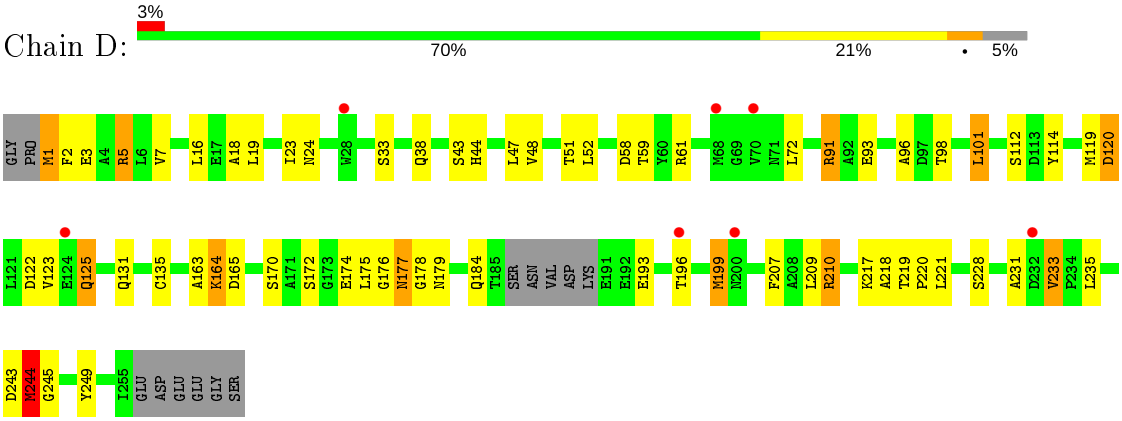
• Molecule 1: Proliferating cell nuclear antigen

Chain E:



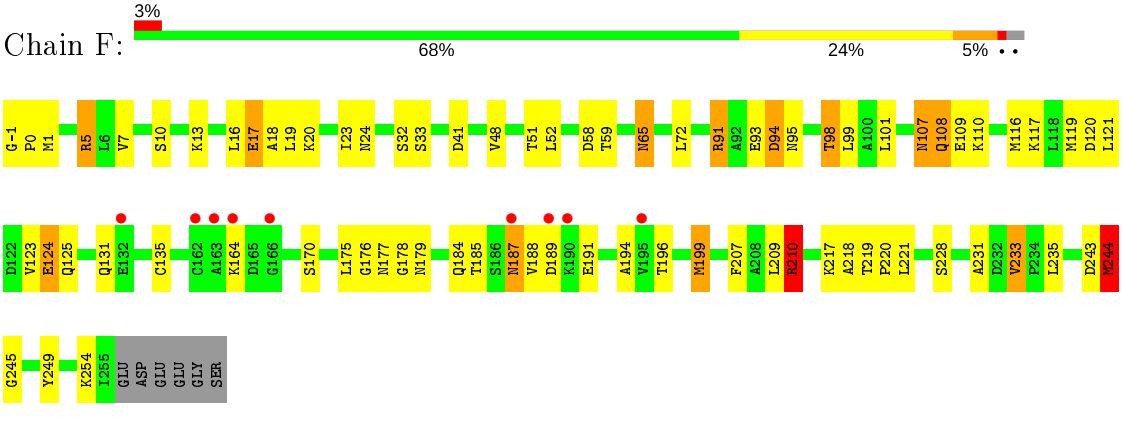
• Molecule 1: Proliferating cell nuclear antigen

Chain D:



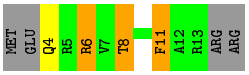
• Molecule 1: Proliferating cell nuclear antigen

Chain F:



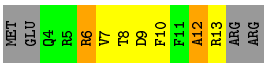
• Molecule 2: DNA replication factor Cdt1

Chain I:



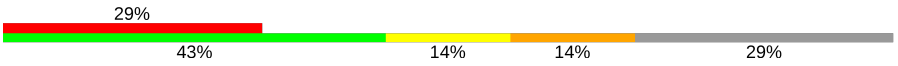
• Molecule 2: DNA replication factor Cdt1

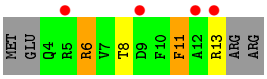
Chain G:



• Molecule 2: DNA replication factor Cdt1

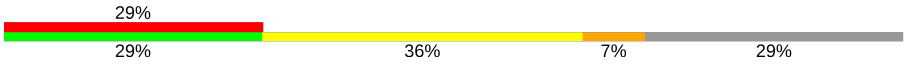
Chain H:

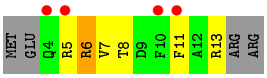




• Molecule 2: DNA replication factor Cdt1

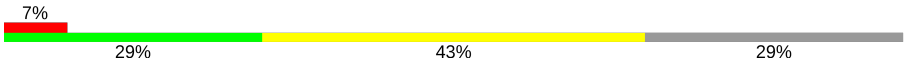
Chain J:

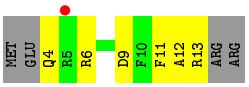




• Molecule 2: DNA replication factor Cdt1

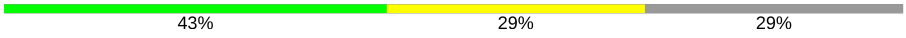
Chain K:

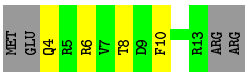




• Molecule 2: DNA replication factor Cdt1

Chain L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	76.58Å 143.17Å 173.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.21 – 3.40 46.17 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.21-3.40) 99.2 (46.17-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.206 , 0.253 0.210 , 0.257	Depositor DCC
R_{free} test set	1333 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	72.4	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12123	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 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.68	0/1942	0.93	2/2623 (0.1%)
1	B	0.71	0/1975	0.95	0/2669
1	C	0.72	0/1930	0.93	1/2608 (0.0%)
1	D	0.70	0/1919	0.89	0/2594
1	E	0.72	0/1975	0.95	1/2669 (0.0%)
1	F	0.72	0/1988	0.96	0/2687
2	G	0.80	0/92	1.40	0/121
2	H	0.87	0/92	1.15	0/121
2	I	1.12	0/92	1.22	0/121
2	J	0.84	0/92	1.05	0/121
2	K	0.78	0/92	1.11	0/121
2	L	0.90	0/92	1.01	0/121
All	All	0.72	0/12281	0.94	4/16576 (0.0%)

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
1	A	0	1
1	B	0	3
1	C	0	1
1	D	0	1
1	E	0	2
1	F	0	1
2	G	0	1
2	K	0	1
All	All	0	11

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	146	ARG	CG-CD-NE	6.43	125.30	111.80
1	A	146	ARG	CG-CD-NE	6.33	125.09	111.80
1	C	55	GLU	CB-CA-C	5.30	121.00	110.40
1	A	156	ASP	CB-CA-C	-5.00	100.39	110.40

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	GLN	Peptide
1	B	107	ASN	Peptide
1	B	109	GLU	Peptide
1	B	131	GLN	Peptide
1	C	131	GLN	Peptide
1	D	131	GLN	Peptide
1	E	131	GLN	Peptide
1	E	185	THR	Peptide
1	F	131	GLN	Peptide
2	G	12	ALA	Peptide
2	K	12	ALA	Peptide

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	1917	0	1921	39	0
1	B	1949	0	1961	42	0
1	C	1905	0	1901	33	0
1	D	1894	0	1891	33	0
1	E	1949	0	1954	44	0
1	F	1961	0	1966	41	0
2	G	91	0	89	4	0
2	H	91	0	89	3	0
2	I	91	0	89	3	0
2	J	91	0	89	6	0
2	K	91	0	89	3	0
2	L	91	0	89	1	0
3	E	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	1	0	0	0	0
All	All	12123	0	12128	232	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 10.

All (232) 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:109:GLU:CB	1:C:183:SER:HB2	2.03	0.88
1:E:27:CYS:SG	1:E:123:VAL:HG22	2.20	0.81
1:B:108:GLN:N	1:B:108:GLN:OE1	2.14	0.80
2:K:6:ARG:O	2:K:9:ASP:HB2	1.80	0.80
1:B:52:LEU:HD22	1:B:244:MET:HE3	1.64	0.79
1:C:52:LEU:HD22	1:C:244:MET:HE3	1.64	0.79
1:F:185:THR:OG1	1:F:188:VAL:CG1	2.32	0.78
1:A:27:CYS:SG	1:A:123:VAL:HG13	2.24	0.77
1:D:52:LEU:HD22	1:D:244:MET:HE3	1.67	0.76
1:E:52:LEU:HD22	1:E:244:MET:HE3	1.66	0.75
1:B:52:LEU:HD22	1:B:244:MET:CE	2.18	0.74
1:D:175:LEU:HD12	1:D:176:GLY:N	2.03	0.74
1:A:93:GLU:H	1:A:93:GLU:CD	1.91	0.72
1:A:175:LEU:HD12	1:A:176:GLY:N	2.05	0.72
1:E:175:LEU:HD12	1:E:176:GLY:N	2.04	0.71
1:B:1:MET:HB3	1:B:61:ARG:HH12	1.55	0.71
1:A:52:LEU:HD22	1:A:244:MET:HE3	1.73	0.70
1:B:178:GLY:C	1:B:179:ASN:HD22	1.95	0.70
1:B:17:GLU:OE1	1:B:17:GLU:HA	1.90	0.70
1:F:17:GLU:OE1	1:F:17:GLU:HA	1.91	0.69
1:F:175:LEU:HD12	1:F:176:GLY:N	2.08	0.69
1:F:52:LEU:HD22	1:F:244:MET:CE	2.23	0.69
1:F:52:LEU:HD22	1:F:244:MET:HE3	1.73	0.69
1:A:2:PHE:CD2	1:A:30:ILE:HG21	2.27	0.69
1:F:178:GLY:C	1:F:179:ASN:HD22	1.96	0.69
1:D:178:GLY:C	1:D:179:ASN:HD22	1.96	0.69
1:D:52:LEU:HD22	1:D:244:MET:CE	2.22	0.69
1:A:52:LEU:HD22	1:A:244:MET:CE	2.23	0.68
1:F:185:THR:HG21	1:F:194:ALA:HB1	1.75	0.68
1:C:178:GLY:C	1:C:179:ASN:HD22	1.96	0.68
1:E:178:GLY:C	1:E:179:ASN:HD22	1.96	0.68
1:E:85:GLU:O	1:E:106:PRO:HG3	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:LEU:HD12	1:B:176:GLY:N	2.08	0.67
1:C:164:LYS:HA	1:C:164:LYS:HE3	1.75	0.67
2:I:6:ARG:HB3	2:I:8:THR:HG22	1.76	0.67
1:C:175:LEU:HD12	1:C:176:GLY:N	2.09	0.66
1:E:188:VAL:HG21	1:E:193:GLU:HB3	1.78	0.66
1:E:2:PHE:CD2	1:E:30:ILE:HG21	2.30	0.65
1:E:52:LEU:HD22	1:E:244:MET:CE	2.26	0.65
1:C:52:LEU:HD22	1:C:244:MET:CE	2.26	0.65
1:E:7:VAL:HG23	1:E:58:ASP:HB2	1.79	0.63
1:C:219:THR:N	1:C:220:PRO:HD2	2.15	0.62
1:B:219:THR:N	1:B:220:PRO:HD2	2.15	0.61
1:B:7:VAL:HG23	1:B:58:ASP:HB2	1.81	0.61
1:B:108:GLN:O	1:B:110:LYS:N	2.33	0.60
1:A:38:GLN:HB3	1:A:125:GLN:HE22	1.66	0.60
1:A:219:THR:N	1:A:220:PRO:HD2	2.17	0.60
1:F:188:VAL:HG11	1:F:194:ALA:HB2	1.82	0.60
2:H:6:ARG:HB3	2:H:8:THR:HG22	1.83	0.60
1:C:234:PRO:HG2	2:I:11:PHE:CZ	2.37	0.60
1:D:219:THR:N	1:D:220:PRO:HD2	2.17	0.60
1:A:87:ILE:HB	1:A:104:GLU:HG3	1.84	0.59
1:F:124:GLU:OE2	2:K:13:ARG:HG2	2.02	0.59
1:F:219:THR:N	1:F:220:PRO:HD2	2.17	0.59
1:E:219:THR:N	1:E:220:PRO:HD2	2.17	0.59
1:E:93:GLU:HB2	1:E:96:ALA:HB3	1.84	0.58
1:A:164:LYS:HE3	1:A:164:LYS:HA	1.85	0.58
1:D:1:MET:HB3	1:D:61:ARG:HH12	1.69	0.58
1:C:252:ALA:O	2:I:4:GLN:NE2	2.38	0.56
1:E:188:VAL:HG21	1:E:193:GLU:CB	2.34	0.56
1:E:44:HIS:ND1	3:E:301:HOH:O	2.32	0.56
1:E:111:VAL:O	1:E:111:VAL:HG12	2.06	0.56
1:C:120:ASP:N	1:C:120:ASP:OD1	2.38	0.56
1:E:138:LYS:HG3	1:E:226:THR:HG22	1.88	0.56
1:E:123:VAL:HG12	1:E:125:GLN:HG3	1.88	0.55
1:D:5:ARG:HB3	1:D:59:THR:HB	1.89	0.55
1:F:101:LEU:N	1:F:101:LEU:HD12	2.21	0.55
1:F:185:THR:OG1	1:F:188:VAL:HG12	2.04	0.55
1:A:27:CYS:SG	1:A:123:VAL:CG1	2.94	0.55
1:A:38:GLN:HB3	1:A:125:GLN:NE2	2.22	0.54
1:A:101:LEU:N	1:A:101:LEU:HD12	2.23	0.54
1:F:107:ASN:O	1:F:109:GLU:N	2.40	0.54
1:D:101:LEU:HD12	1:D:101:LEU:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:VAL:HG23	1:A:58:ASP:HB2	1.90	0.54
1:E:5:ARG:HB3	1:E:59:THR:HB	1.90	0.54
1:B:101:LEU:N	1:B:101:LEU:HD12	2.23	0.54
1:D:7:VAL:HG23	1:D:58:ASP:HB2	1.90	0.54
1:B:93:GLU:HB2	1:B:96:ALA:HB3	1.88	0.53
1:C:19:LEU:HD22	1:C:48:VAL:HG11	1.90	0.53
1:C:5:ARG:HB3	1:C:59:THR:HB	1.90	0.53
1:B:5:ARG:HB3	1:B:59:THR:HB	1.91	0.53
1:E:101:LEU:HD12	1:E:101:LEU:N	2.23	0.53
1:C:101:LEU:HD12	1:C:101:LEU:N	2.24	0.53
1:B:1:MET:HB3	1:B:61:ARG:NH1	2.22	0.52
1:F:5:ARG:HB3	1:F:59:THR:HB	1.90	0.52
1:D:164:LYS:HA	1:D:164:LYS:HE3	1.91	0.52
1:F:94:ASP:HB2	1:F:98:THR:HG23	1.90	0.52
1:F:219:THR:N	1:F:220:PRO:CD	2.73	0.52
1:D:219:THR:N	1:D:220:PRO:CD	2.73	0.52
1:A:5:ARG:HB3	1:A:59:THR:HB	1.90	0.52
1:B:219:THR:N	1:B:220:PRO:CD	2.73	0.51
1:A:219:THR:N	1:A:220:PRO:CD	2.73	0.51
1:C:219:THR:N	1:C:220:PRO:CD	2.73	0.51
1:E:219:THR:N	1:E:220:PRO:CD	2.73	0.51
1:B:189:ASP:O	1:B:190:LYS:HB2	2.11	0.50
1:A:178:GLY:HA3	1:B:114:TYR:CD2	2.47	0.50
1:C:7:VAL:HG23	1:C:58:ASP:HB2	1.92	0.50
1:F:207:PHE:CE2	1:F:235:LEU:HB2	2.47	0.50
2:J:7:VAL:HG22	2:J:11:PHE:HD2	1.77	0.49
1:A:184:GLN:HG3	1:A:196:THR:HA	1.93	0.49
1:D:47:LEU:HB2	2:J:7:VAL:HG11	1.94	0.49
1:F:188:VAL:HG11	1:F:194:ALA:CB	2.42	0.49
1:F:7:VAL:HG23	1:F:58:ASP:HB2	1.95	0.49
2:H:6:ARG:HB3	2:H:8:THR:CG2	2.43	0.49
1:B:19:LEU:HD22	1:B:48:VAL:HG11	1.95	0.49
1:F:51:THR:O	1:F:245:GLY:HA3	2.13	0.49
1:E:233:VAL:HA	2:L:10:PHE:CE1	2.48	0.48
1:A:126:LEU:HB3	2:H:11:PHE:HB2	1.95	0.48
1:B:51:THR:O	1:B:245:GLY:HA3	2.13	0.48
1:F:65:ASN:HD22	1:F:65:ASN:N	2.10	0.48
1:A:51:THR:O	1:A:245:GLY:HA3	2.13	0.48
1:E:23:ILE:HG13	1:E:72:LEU:CD1	2.43	0.48
1:C:93:GLU:HB3	1:C:96:ALA:HB3	1.96	0.48
1:D:123:VAL:HG13	1:D:123:VAL:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:ASP:O	1:E:124:GLU:N	2.43	0.48
1:E:2:PHE:CD2	1:E:30:ILE:CG2	2.97	0.48
1:A:122:ASP:OD1	2:J:13:ARG:NH2	2.47	0.48
1:A:2:PHE:CD2	1:A:30:ILE:CG2	2.95	0.48
1:B:190:LYS:HB3	1:B:193:GLU:HB2	1.95	0.47
1:F:188:VAL:HG21	1:F:191:GLU:HG3	1.95	0.47
1:B:23:ILE:HG13	1:B:72:LEU:CD1	2.44	0.47
1:D:184:GLN:HG3	1:D:196:THR:HA	1.95	0.47
1:C:38:GLN:OE1	1:C:125:GLN:HB3	2.15	0.47
1:C:184:GLN:HG3	1:C:196:THR:HA	1.96	0.47
1:D:51:THR:O	1:D:245:GLY:HA3	2.15	0.47
1:E:51:THR:O	1:E:245:GLY:HA3	2.15	0.47
1:A:1:MET:CE	1:A:61:ARG:HB3	2.45	0.47
1:C:51:THR:O	1:C:245:GLY:HA3	2.15	0.47
1:E:123:VAL:HG12	1:E:123:VAL:O	2.15	0.47
1:B:65:ASN:N	1:B:65:ASN:HD22	2.14	0.46
1:E:184:GLN:HG3	1:E:196:THR:HA	1.97	0.46
1:D:23:ILE:HG13	1:D:72:LEU:CD1	2.46	0.46
1:C:23:ILE:HG13	1:C:72:LEU:CD1	2.46	0.46
1:D:19:LEU:HD22	1:D:48:VAL:HG11	1.98	0.46
1:F:184:GLN:HG3	1:F:196:THR:HA	1.96	0.46
1:D:1:MET:HB3	1:D:61:ARG:NH1	2.30	0.46
1:E:18:ALA:HB1	1:E:249:TYR:OH	2.16	0.46
1:F:18:ALA:HB1	1:F:249:TYR:OH	2.16	0.46
1:F:19:LEU:HD22	1:F:48:VAL:HG11	1.96	0.46
1:B:41:ASP:OD1	1:B:43:SER:OG	2.27	0.45
1:A:163:ALA:HA	1:A:199:MET:CE	2.47	0.45
1:B:184:GLN:HG3	1:B:196:THR:HA	1.97	0.45
1:B:199:MET:HE3	1:B:199:MET:O	2.16	0.45
1:E:163:ALA:HA	1:E:199:MET:CE	2.46	0.45
1:A:93:GLU:HB2	1:A:96:ALA:HB3	1.98	0.45
1:D:163:ALA:HA	1:D:199:MET:CE	2.46	0.45
1:A:23:ILE:HG13	1:A:72:LEU:CD1	2.46	0.45
1:E:106:PRO:O	1:E:108:GLN:HG3	2.17	0.45
1:B:218:ALA:C	1:B:220:PRO:HD2	2.38	0.45
1:C:18:ALA:HB1	1:C:249:TYR:OH	2.16	0.45
1:D:93:GLU:HB2	1:D:96:ALA:HB3	1.98	0.45
1:C:207:PHE:CZ	1:C:235:LEU:HB2	2.52	0.44
1:A:18:ALA:HB1	1:A:249:TYR:OH	2.17	0.44
1:D:18:ALA:HB1	1:D:249:TYR:OH	2.17	0.44
1:F:107:ASN:CG	1:F:107:ASN:O	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:HIS:O	2:J:6:ARG:HB3	2.17	0.44
1:B:112:SER:HB3	1:B:114:TYR:CE1	2.53	0.44
1:C:218:ALA:C	1:C:220:PRO:HD2	2.38	0.43
1:A:218:ALA:C	1:A:220:PRO:HD2	2.39	0.43
1:A:65:ASN:HD22	1:A:65:ASN:N	2.16	0.43
1:F:-1:GLY:N	1:F:91:ARG:NH1	2.66	0.43
1:E:85:GLU:O	1:E:106:PRO:CG	2.66	0.43
1:F:218:ALA:C	1:F:220:PRO:HD2	2.38	0.43
1:F:23:ILE:HG13	1:F:72:LEU:CD1	2.47	0.43
1:F:254:LYS:HE3	2:K:4:GLN:HB2	2.00	0.43
1:B:240:LYS:HD3	1:B:240:LYS:HA	1.91	0.43
1:B:54:SER:HB2	1:B:60:TYR:CD2	2.53	0.43
1:D:218:ALA:O	1:D:221:LEU:HB2	2.19	0.43
1:A:112:SER:HB3	1:A:114:TYR:CE1	2.53	0.43
1:E:218:ALA:C	1:E:220:PRO:HD2	2.39	0.43
1:B:18:ALA:HB1	1:B:249:TYR:OH	2.19	0.43
1:C:124:GLU:HG2	1:C:124:GLU:O	2.19	0.43
1:D:120:ASP:OD1	1:D:120:ASP:N	2.35	0.43
1:D:112:SER:HB3	1:D:114:TYR:CE1	2.53	0.43
1:D:218:ALA:C	1:D:220:PRO:HD2	2.38	0.43
1:E:218:ALA:O	1:E:221:LEU:HB2	2.19	0.43
1:A:19:LEU:HD22	1:A:48:VAL:HG11	2.00	0.42
1:B:138:LYS:HG3	1:B:226:THR:HG22	2.00	0.42
1:D:43:SER:O	2:J:6:ARG:NH2	2.52	0.42
1:B:43:SER:O	2:G:6:ARG:NH2	2.53	0.42
1:D:207:PHE:CZ	1:D:235:LEU:HB2	2.54	0.42
1:D:172:SER:HA	1:D:177:ASN:HB3	2.01	0.42
1:E:19:LEU:HD22	1:E:48:VAL:HG11	2.00	0.42
1:C:231:ALA:O	1:C:233:VAL:HG13	2.19	0.42
1:E:112:SER:HB3	1:E:114:TYR:CE1	2.54	0.42
1:E:16:LEU:HD21	1:E:75:MET:HB3	2.01	0.42
1:C:112:SER:HB3	1:C:114:TYR:CE1	2.55	0.42
1:C:172:SER:HA	1:C:177:ASN:HB3	2.01	0.42
1:C:163:ALA:HA	1:C:199:MET:CE	2.49	0.42
1:E:99:LEU:HD23	1:E:116:MET:CE	2.50	0.42
1:A:218:ALA:O	1:A:221:LEU:HB2	2.19	0.42
1:B:231:ALA:O	1:B:233:VAL:HG13	2.20	0.42
1:F:99:LEU:HD23	1:F:116:MET:CE	2.50	0.42
1:D:3:GLU:OE2	1:D:91:ARG:HD3	2.21	0.41
1:A:207:PHE:CZ	1:A:235:LEU:HB2	2.56	0.41
1:B:216:THR:O	1:B:219:THR:HB	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:GLU:CA	1:C:183:SER:HB2	2.50	0.41
1:A:231:ALA:O	1:A:233:VAL:HG13	2.20	0.41
1:B:123:VAL:O	1:B:123:VAL:HG13	2.20	0.41
1:C:218:ALA:O	1:C:221:LEU:HB2	2.20	0.41
1:E:209:LEU:O	1:E:210:ARG:C	2.58	0.41
1:B:233:VAL:HA	2:G:10:PHE:CE1	2.55	0.41
1:B:123:VAL:HG13	1:B:125:GLN:NE2	2.35	0.41
1:B:122:ASP:OD2	1:F:124:GLU:CD	2.59	0.41
1:F:199:MET:O	1:F:199:MET:CE	2.69	0.41
1:E:207:PHE:CZ	1:E:235:LEU:HB2	2.55	0.41
1:F:93:GLU:O	1:F:95:ASN:N	2.54	0.41
1:B:124:GLU:OE2	2:G:13:ARG:HG2	2.21	0.41
1:B:199:MET:O	1:B:199:MET:CE	2.69	0.41
1:B:126:LEU:HA	2:G:12:ALA:O	2.21	0.41
1:C:209:LEU:O	1:C:210:ARG:C	2.59	0.41
1:E:124:GLU:O	1:E:124:GLU:HG2	2.21	0.41
1:D:209:LEU:O	1:D:210:ARG:C	2.59	0.41
1:C:114:TYR:CD2	1:B:178:GLY:HA3	2.56	0.41
1:E:65:ASN:N	1:E:65:ASN:HD22	2.17	0.41
1:A:172:SER:HA	1:A:177:ASN:HB3	2.03	0.41
1:C:99:LEU:HD23	1:C:116:MET:CE	2.51	0.41
1:D:231:ALA:O	1:D:233:VAL:HG13	2.21	0.41
1:F:231:ALA:O	1:F:233:VAL:HG13	2.20	0.41
1:F:218:ALA:O	1:F:221:LEU:HB2	2.20	0.41
1:A:11:ILE:O	1:A:15:VAL:HG23	2.22	0.40
1:E:38:GLN:NE2	1:E:128:ILE:HD11	2.36	0.40
1:F:188:VAL:CG2	1:F:191:GLU:OE2	2.69	0.40
1:F:209:LEU:O	1:F:210:ARG:C	2.58	0.40
2:J:7:VAL:HG22	2:J:11:PHE:CD2	2.55	0.40
1:E:231:ALA:O	1:E:233:VAL:HG13	2.20	0.40
1:F:207:PHE:CZ	1:F:235:LEU:HB2	2.57	0.40
1:A:216:THR:O	1:A:219:THR:HB	2.22	0.40
1:E:182:LEU:HD23	1:F:110:LYS:HB2	2.03	0.40
1:D:38:GLN:CD	1:D:125:GLN:HG2	2.42	0.40
1:E:216:THR:O	1:E:219:THR:HB	2.21	0.40
1:F:10:SER:HA	1:F:13:LYS:HD3	2.04	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	247/263 (94%)	220 (89%)	21 (8%)	6 (2%)	6 28
1	B	253/263 (96%)	222 (88%)	23 (9%)	8 (3%)	4 22
1	C	246/263 (94%)	221 (90%)	20 (8%)	5 (2%)	7 30
1	D	246/263 (94%)	220 (89%)	23 (9%)	3 (1%)	13 41
1	E	253/263 (96%)	223 (88%)	25 (10%)	5 (2%)	7 30
1	F	255/263 (97%)	224 (88%)	22 (9%)	9 (4%)	3 21
2	G	8/14 (57%)	5 (62%)	2 (25%)	1 (12%)	0 2
2	H	8/14 (57%)	6 (75%)	2 (25%)	0	100 100
2	I	8/14 (57%)	8 (100%)	0	0	100 100
2	J	8/14 (57%)	8 (100%)	0	0	100 100
2	K	8/14 (57%)	7 (88%)	1 (12%)	0	100 100
2	L	8/14 (57%)	6 (75%)	2 (25%)	0	100 100
All	All	1548/1662 (93%)	1370 (88%)	141 (9%)	37 (2%)	6 28

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	B	109	GLU
1	E	123	VAL
1	F	94	ASP
1	F	108	GLN
1	F	124	GLU
1	A	123	VAL
1	A	210	ARG
1	B	124	GLU
1	B	187	ASN
1	B	190	LYS
1	E	187	ASN

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Mol	Chain	Res	Type
1	F	1	MET
1	F	107	ASN
1	F	210	ARG
1	C	124	GLU
1	C	210	ARG
1	B	107	ASN
1	B	122	ASP
1	B	210	ARG
1	E	210	ARG
1	D	122	ASP
1	D	210	ARG
1	F	0	PRO
1	F	187	ASN
2	G	8	THR
1	A	122	ASP
1	A	244	MET
1	C	122	ASP
1	B	244	MET
1	E	124	GLU
1	E	244	MET
1	D	244	MET
1	F	244	MET
1	A	128	ILE
1	C	107	ASN
1	C	244	MET

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	215/229 (94%)	183 (85%)	32 (15%)	3 12
1	B	219/229 (96%)	193 (88%)	26 (12%)	5 19
1	C	213/229 (93%)	182 (85%)	31 (15%)	3 12
1	D	210/229 (92%)	185 (88%)	25 (12%)	5 19
1	E	219/229 (96%)	192 (88%)	27 (12%)	4 17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	220/229 (96%)	189 (86%)	31 (14%)	3 13
2	G	9/13 (69%)	6 (67%)	3 (33%)	0 1
2	H	9/13 (69%)	6 (67%)	3 (33%)	0 1
2	I	9/13 (69%)	6 (67%)	3 (33%)	0 1
2	J	9/13 (69%)	6 (67%)	3 (33%)	0 1
2	K	9/13 (69%)	8 (89%)	1 (11%)	6 22
2	L	9/13 (69%)	6 (67%)	3 (33%)	0 1
All	All	1350/1452 (93%)	1162 (86%)	188 (14%)	3 13

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	PHE
1	A	5	ARG
1	A	10	SER
1	A	16	LEU
1	A	24	ASN
1	A	33	SER
1	A	44	HIS
1	A	61	ARG
1	A	93	GLU
1	A	97	ASP
1	A	98	THR
1	A	104	GLU
1	A	107	ASN
1	A	113	ASP
1	A	117	LYS
1	A	119	MET
1	A	120	ASP
1	A	128	ILE
1	A	130	GLU
1	A	135	CYS
1	A	164	LYS
1	A	170	SER
1	A	177	ASN
1	A	191	GLU
1	A	193	GLU
1	A	199	MET
1	A	217	LYS

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Mol	Chain	Res	Type
1	A	228	SER
1	A	233	VAL
1	A	243	ASP
1	A	244	MET
1	C	2	PHE
1	C	5	ARG
1	C	16	LEU
1	C	25	GLU
1	C	33	SER
1	C	41	ASP
1	C	44	HIS
1	C	64	ARG
1	C	97	ASP
1	C	98	THR
1	C	101	LEU
1	C	117	LYS
1	C	119	MET
1	C	120	ASP
1	C	124	GLU
1	C	125	GLN
1	C	128	ILE
1	C	135	CYS
1	C	164	LYS
1	C	165	ASP
1	C	170	SER
1	C	172	SER
1	C	177	ASN
1	C	181	LYS
1	C	192	GLU
1	C	193	GLU
1	C	199	MET
1	C	217	LYS
1	C	228	SER
1	C	233	VAL
1	C	243	ASP
1	B	5	ARG
1	B	16	LEU
1	B	17	GLU
1	B	24	ASN
1	B	33	SER
1	B	41	ASP
1	B	53	ARG

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Mol	Chain	Res	Type
1	B	64	ARG
1	B	97	ASP
1	B	98	THR
1	B	101	LEU
1	B	108	GLN
1	B	117	LYS
1	B	119	MET
1	B	120	ASP
1	B	125	GLN
1	B	135	CYS
1	B	170	SER
1	B	177	ASN
1	B	189	ASP
1	B	199	MET
1	B	217	LYS
1	B	228	SER
1	B	233	VAL
1	B	243	ASP
1	B	255	ILE
1	E	1	MET
1	E	2	PHE
1	E	5	ARG
1	E	16	LEU
1	E	24	ASN
1	E	33	SER
1	E	77	LYS
1	E	97	ASP
1	E	98	THR
1	E	101	LEU
1	E	117	LYS
1	E	119	MET
1	E	120	ASP
1	E	124	GLU
1	E	125	GLN
1	E	128	ILE
1	E	130	GLU
1	E	135	CYS
1	E	164	LYS
1	E	165	ASP
1	E	170	SER
1	E	186	SER
1	E	188	VAL

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Mol	Chain	Res	Type
1	E	199	MET
1	E	217	LYS
1	E	228	SER
1	E	233	VAL
1	D	1	MET
1	D	2	PHE
1	D	5	ARG
1	D	16	LEU
1	D	24	ASN
1	D	33	SER
1	D	91	ARG
1	D	98	THR
1	D	101	LEU
1	D	119	MET
1	D	120	ASP
1	D	125	GLN
1	D	135	CYS
1	D	164	LYS
1	D	165	ASP
1	D	170	SER
1	D	174	GLU
1	D	177	ASN
1	D	193	GLU
1	D	199	MET
1	D	217	LYS
1	D	228	SER
1	D	233	VAL
1	D	243	ASP
1	D	244	MET
1	F	5	ARG
1	F	16	LEU
1	F	17	GLU
1	F	20	LYS
1	F	24	ASN
1	F	32	SER
1	F	33	SER
1	F	41	ASP
1	F	65	ASN
1	F	91	ARG
1	F	98	THR
1	F	108	GLN
1	F	117	LYS

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Mol	Chain	Res	Type
1	F	119	MET
1	F	120	ASP
1	F	121	LEU
1	F	123	VAL
1	F	125	GLN
1	F	135	CYS
1	F	164	LYS
1	F	170	SER
1	F	177	ASN
1	F	187	ASN
1	F	189	ASP
1	F	199	MET
1	F	210	ARG
1	F	217	LYS
1	F	228	SER
1	F	233	VAL
1	F	243	ASP
1	F	244	MET
2	I	6	ARG
2	I	8	THR
2	I	11	PHE
2	G	6	ARG
2	G	7	VAL
2	G	9	ASP
2	H	6	ARG
2	H	11	PHE
2	H	13	ARG
2	J	5	ARG
2	J	6	ARG
2	J	8	THR
2	K	11	PHE
2	L	4	GLN
2	L	6	ARG
2	L	8	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	125	GLN
1	A	177	ASN
1	A	179	ASN

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Mol	Chain	Res	Type
1	A	184	GLN
1	C	125	GLN
1	C	177	ASN
1	C	179	ASN
1	C	184	GLN
1	C	200	ASN
1	B	8	GLN
1	B	44	HIS
1	B	65	ASN
1	B	125	GLN
1	B	177	ASN
1	B	179	ASN
1	B	184	GLN
1	E	8	GLN
1	E	65	ASN
1	E	125	GLN
1	E	179	ASN
1	E	184	GLN
1	D	8	GLN
1	D	44	HIS
1	D	65	ASN
1	D	177	ASN
1	D	179	ASN
1	D	184	GLN
1	F	65	ASN
1	F	177	ASN
1	F	179	ASN
1	F	184	GLN
1	F	200	ASN
2	L	4	GLN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	251/263 (95%)	0.48	18 (7%) 15 17	60, 89, 129, 174	0
1	B	255/263 (96%)	0.12	2 (0%) 86 85	44, 71, 121, 141	0
1	C	250/263 (95%)	0.21	7 (2%) 53 51	51, 76, 118, 146	0
1	D	250/263 (95%)	0.36	7 (2%) 53 51	64, 91, 121, 161	0
1	E	255/263 (96%)	0.20	4 (1%) 72 70	46, 75, 118, 149	0
1	F	257/263 (97%)	0.29	9 (3%) 44 43	58, 80, 124, 185	0
2	G	10/14 (71%)	0.78	0 100 100	84, 96, 109, 134	0
2	H	10/14 (71%)	1.98	4 (40%) 0 0	121, 135, 136, 140	0
2	I	10/14 (71%)	0.56	0 100 100	98, 108, 114, 115	0
2	J	10/14 (71%)	2.00	4 (40%) 0 0	121, 125, 132, 132	0
2	K	10/14 (71%)	0.60	1 (10%) 7 8	83, 92, 98, 116	0
2	L	10/14 (71%)	0.96	0 100 100	87, 93, 100, 112	0
All	All	1578/1662 (94%)	0.31	56 (3%) 44 43	44, 82, 127, 185	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	166	GLY	4.0
2	J	11	PHE	3.7
1	F	187	ASN	3.5
1	D	28	TRP	3.5
2	J	5	ARG	3.4
1	F	190	LYS	3.4
1	A	195	VAL	3.3
1	E	189	ASP	3.2
1	E	94	ASP	3.1
1	C	95	ASN	3.1
1	A	1	MET	3.1

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Mol	Chain	Res	Type	RSRZ
2	J	10	PHE	3.0
2	H	5	ARG	3.0
1	A	94	ASP	2.9
1	F	189	ASP	2.8
1	C	164	LYS	2.8
2	J	4	GLN	2.8
1	D	124	GLU	2.7
1	C	166	GLY	2.7
1	A	197	ILE	2.7
1	F	163	ALA	2.6
1	A	164	LYS	2.6
2	K	5	ARG	2.6
1	C	94	ASP	2.5
1	A	28	TRP	2.5
1	C	191	GLU	2.5
1	A	184	GLN	2.5
1	A	191	GLU	2.4
1	A	183	SER	2.4
1	B	95	ASN	2.4
1	D	70	VAL	2.3
1	F	195	VAL	2.3
1	A	95	ASN	2.3
1	A	185	THR	2.3
1	F	132	GLU	2.3
1	D	196	THR	2.3
1	A	165	ASP	2.2
1	E	28	TRP	2.2
1	F	162	CYS	2.2
1	A	4	ALA	2.2
2	H	9	ASP	2.2
1	C	93	GLU	2.1
1	C	112	SER	2.1
1	D	68	MET	2.1
1	A	196	THR	2.1
1	B	109	GLU	2.1
1	E	186	SER	2.1
2	H	12	ALA	2.1
1	D	200	ASN	2.1
1	A	66	LEU	2.1
2	H	13	ARG	2.1
1	D	232	ASP	2.1
1	A	122	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	164	LYS	2.0
1	A	2	PHE	2.0
1	A	124	GLU	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.