Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 02:28 AM EDT

PDB ID	:	3KNP
Title	:	Crystal structure of DTD from Plasmodium falciparum
Authors	:	Manickam, Y.; Bhatt, T.K.; Sharma, A.
Deposited on	:	2009-11-12
Resolution	:	3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

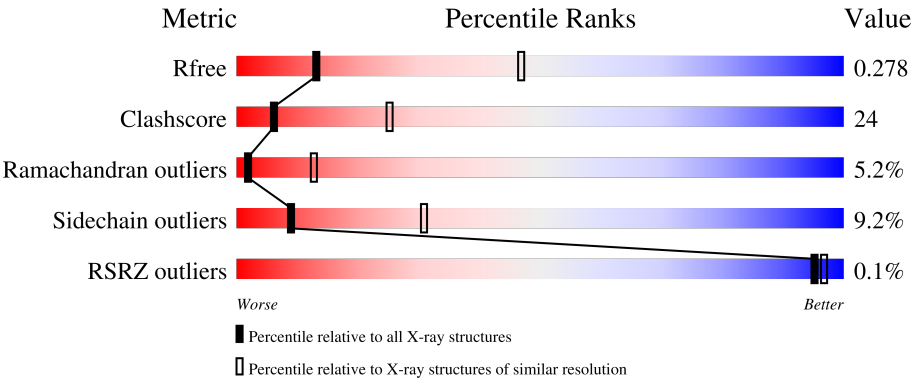
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	164	47% 45%
1	B	164	% 52% 42%
1	C	164	54% 39%
1	D	164	44% 41% 7% 7%
1	E	164	46% 36% 8% 10%

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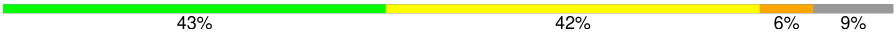
Mol	Chain	Length	Quality of chain
1	F	164	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7387 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 D-tyrosyl-tRNA(Tyr) deacylase.

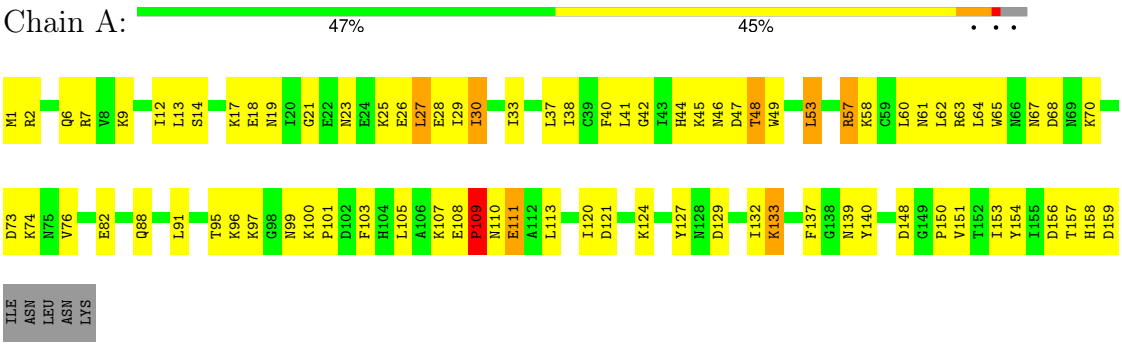
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	0	0	0
			1243	790	216	234	3			
1	B	160	Total	C	N	O	S	0	0	0
			1257	799	220	235	3			
1	C	159	Total	C	N	O	S	0	0	0
			1250	794	219	234	3			
1	D	152	Total	C	N	O	S	0	0	0
			1225	783	212	227	3			
1	E	148	Total	C	N	O	S	0	0	0
			1202	770	208	221	3			
1	F	149	Total	C	N	O	S	0	0	0
			1210	774	209	224	3			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

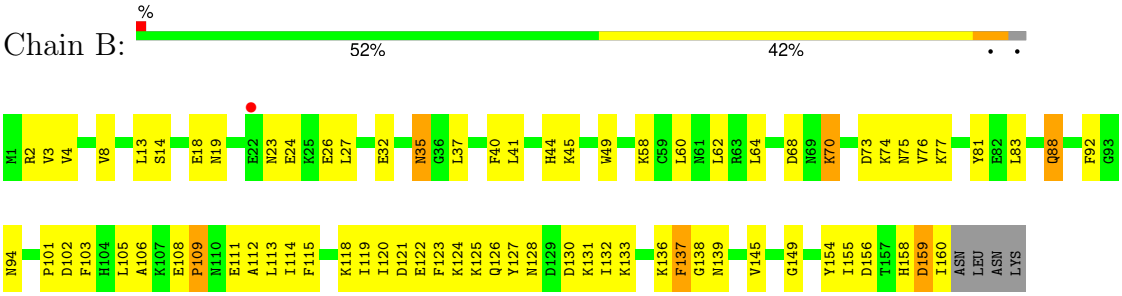
• Molecule 1: D-tyrosyl-tRNA(Tyr) deacylase

Chain A:



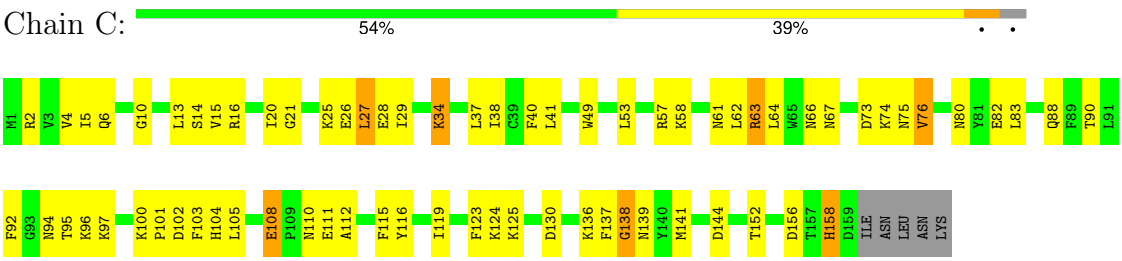
• Molecule 1: D-tyrosyl-tRNA(Tyr) deacylase

Chain B:



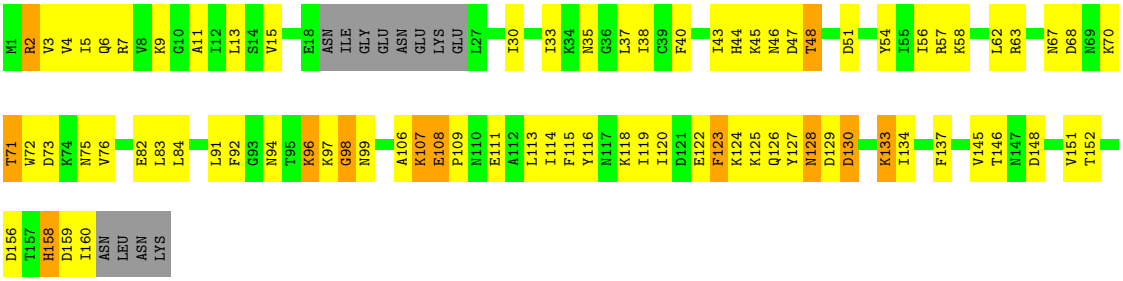
• Molecule 1: D-tyrosyl-tRNA(Tyr) deacylase

Chain C:



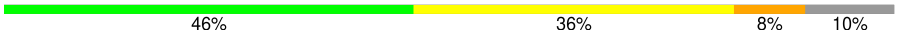
• Molecule 1: D-tyrosyl-tRNA(Tyr) deacylase

Chain D:



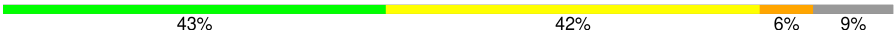
• Molecule 1: D-tyrosyl-tRNA(Tyr) deacylase

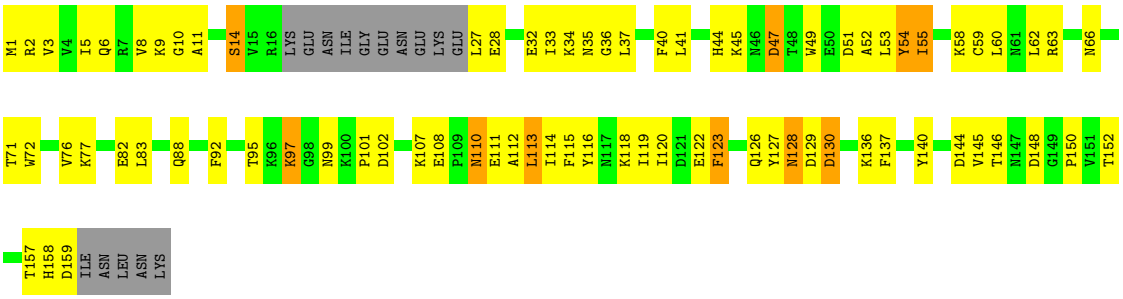
Chain E:



• Molecule 1: D-tyrosyl-tRNA(Tyr) deacylase

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	58.81Å 55.17Å 92.52Å 105.90° 103.10° 98.70°	Depositor
Resolution (Å)	19.87 – 3.30 43.11 – 3.30	Depositor EDS
% Data completeness (in resolution range)	94.6 (19.87-3.30) 94.6 (43.11-3.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 3.32Å)	Xtriage
Refinement program	REFMAC, CNS 1.2	Depositor
R, R_{free}	0.214 , 0.279 0.206 , 0.278	Depositor DCC
R_{free} test set	704 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å^2)	70.9	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 24.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7387	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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	0.44	0/1267	0.72	1/1713 (0.1%)
1	B	0.46	0/1281	0.71	0/1732
1	C	0.44	0/1274	0.70	0/1722
1	D	0.45	0/1248	0.69	0/1689
1	E	0.43	0/1225	0.70	0/1658
1	F	0.44	0/1233	0.71	0/1669
All	All	0.45	0/7528	0.70	1/10183 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	159	ASP	N-CA-C	-7.18	91.62	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1243	0	1154	60	0
1	B	1257	0	1172	55	0
1	C	1250	0	1166	48	0
1	D	1225	0	1161	69	0
1	E	1202	0	1149	74	0
1	F	1210	0	1153	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7387	0	6955	351	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 24.

All (351) 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:108:GLU:HG2	1:A:109:PRO:HD2	1.45	0.96
1:C:5:ILE:HG23	1:C:37:LEU:HD21	1.53	0.88
1:E:88:GLN:NE2	1:F:150:PRO:HG2	1.90	0.85
1:E:63:ARG:HB3	1:E:73:ASP:O	1.76	0.84
1:F:111:GLU:O	1:F:115:PHE:HB2	1.80	0.80
1:D:3:VAL:HA	1:D:40:PHE:O	1.81	0.79
1:B:44:HIS:ND1	1:B:45:LYS:N	2.33	0.76
1:E:139:ASN:N	1:E:139:ASN:HD22	1.84	0.76
1:F:9:LYS:HG3	1:F:148:ASP:HB2	1.67	0.75
1:F:66:ASN:HD21	1:F:71:THR:HG22	1.53	0.74
1:F:97:LYS:NZ	1:F:97:LYS:HB3	2.03	0.73
1:B:122:GLU:OE2	1:B:125:LYS:HD3	1.88	0.72
1:C:144:ASP:OD2	1:D:146:THR:HG23	1.91	0.71
1:D:9:LYS:HG3	1:D:148:ASP:HB2	1.71	0.71
1:E:37:LEU:HB2	1:E:83:LEU:HD23	1.74	0.70
1:D:7:ARG:HA	1:D:37:LEU:HD23	1.73	0.69
1:E:87:SER:O	1:E:88:GLN:HG2	1.93	0.69
1:A:150:PRO:HG2	1:B:88:GLN:NE2	2.09	0.68
1:B:62:LEU:HB3	1:B:64:LEU:HD21	1.74	0.68
1:A:13:LEU:HD23	1:A:14:SER:N	2.09	0.68
1:E:144:ASP:OD1	1:F:146:THR:HG23	1.94	0.68
1:A:2:ARG:HG3	1:A:91:LEU:HD23	1.74	0.67
1:B:37:LEU:HB2	1:B:83:LEU:HD23	1.76	0.67
1:E:113:LEU:HD13	1:E:137:PHE:CD2	2.30	0.67
1:F:49:TRP:O	1:F:53:LEU:HG	1.95	0.66
1:C:27:LEU:N	1:C:27:LEU:HD23	2.10	0.66
1:B:45:LYS:HB2	1:B:105:LEU:O	1.96	0.66
1:D:76:VAL:HG21	1:D:83:LEU:HD11	1.77	0.66
1:F:45:LYS:HA	1:F:107:LYS:HB2	1.77	0.66
1:F:14:SER:HB3	1:F:28:GLU:O	1.96	0.65
1:E:144:ASP:HA	1:F:145:VAL:O	1.97	0.65
1:C:37:LEU:HD23	1:C:38:ILE:N	2.12	0.64
1:C:63:ARG:HG2	1:C:73:ASP:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6:GLN:HG3	1:F:152:THR:HG23	1.79	0.64
1:C:67:ASN:HB2	1:C:74:LYS:HG2	1.79	0.64
1:A:41:LEU:HD23	1:A:42:GLY:N	2.13	0.64
1:B:137:PHE:HD2	1:B:138:GLY:N	1.96	0.63
1:D:6:GLN:HB2	1:D:38:ILE:HG22	1.80	0.63
1:D:71:THR:HB	1:D:72:TRP:CD1	2.34	0.63
1:E:7:ARG:HA	1:E:37:LEU:HD23	1.80	0.63
1:B:37:LEU:HB2	1:B:83:LEU:CD2	2.29	0.62
1:E:57:ARG:HD2	1:E:58:LYS:HE2	1.80	0.62
1:E:62:LEU:HD21	1:F:95:THR:HG22	1.80	0.62
1:D:116:TYR:O	1:D:119:ILE:HB	1.99	0.62
1:B:13:LEU:HD23	1:B:14:SER:N	2.16	0.61
1:E:60:LEU:HA	1:E:76:VAL:HG21	1.81	0.61
1:E:116:TYR:O	1:E:119:ILE:HG22	1.99	0.61
1:F:157:THR:O	1:F:158:HIS:ND1	2.33	0.61
1:A:63:ARG:HE	1:A:73:ASP:HA	1.65	0.61
1:F:97:LYS:HB3	1:F:97:LYS:HZ2	1.66	0.61
1:E:45:LYS:HE3	1:E:46:ASN:HD21	1.64	0.61
1:C:15:VAL:HG12	1:C:16:ARG:N	2.17	0.60
1:F:88:GLN:HA	1:F:88:GLN:NE2	2.16	0.60
1:C:58:LYS:HD2	1:C:62:LEU:HD21	1.84	0.60
1:F:11:ALA:HA	1:F:144:ASP:O	2.01	0.60
1:B:76:VAL:HG23	1:B:81:TYR:HB2	1.82	0.60
1:E:149:GLY:HA2	1:F:140:TYR:CE1	2.37	0.60
1:B:2:ARG:NH1	1:B:92:PHE:HA	2.16	0.60
1:E:116:TYR:HA	1:E:119:ILE:HG22	1.83	0.60
1:A:57:ARG:O	1:A:61:ASN:ND2	2.33	0.59
1:C:15:VAL:HG21	1:C:136:LYS:HD3	1.84	0.59
1:D:113:LEU:HD13	1:D:137:PHE:CD2	2.37	0.59
1:C:67:ASN:HB3	1:C:73:ASP:HB3	1.83	0.59
1:E:100:LYS:HE2	1:F:72:TRP:HB2	1.84	0.59
1:A:29:ILE:HG22	1:A:30:ILE:N	2.17	0.59
1:E:139:ASN:N	1:E:139:ASN:ND2	2.50	0.59
1:C:156:ASP:OD1	1:C:158:HIS:HB2	2.02	0.59
1:F:44:HIS:O	1:F:47:ASP:HB2	2.02	0.59
1:A:63:ARG:HA	1:A:74:LYS:O	2.03	0.58
1:D:7:ARG:HA	1:D:37:LEU:CD2	2.33	0.58
1:F:88:GLN:HA	1:F:88:GLN:HE21	1.69	0.58
1:A:1:MET:H1	1:A:47:ASP:CG	2.06	0.58
1:E:4:VAL:HB	1:E:40:PHE:HB2	1.85	0.58
1:B:156:ASP:HB3	1:B:159:ASP:OD1	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:GLU:OE2	1:C:111:GLU:HB2	2.04	0.58
1:D:94:ASN:OD1	1:D:96:LYS:HG3	2.04	0.58
1:A:40:PHE:HD1	1:A:88:GLN:HE21	1.52	0.58
1:A:1:MET:N	1:A:47:ASP:OD1	2.37	0.57
1:C:14:SER:HB2	1:C:28:GLU:O	2.03	0.57
1:E:6:GLN:HG2	1:E:152:THR:HG23	1.87	0.57
1:A:44:HIS:O	1:A:107:LYS:HE3	2.04	0.57
1:A:45:LYS:HA	1:A:107:LYS:HB2	1.87	0.57
1:A:120:ILE:O	1:A:124:LYS:HG3	2.04	0.57
1:E:94:ASN:HD21	1:E:96:LYS:HD3	1.69	0.57
1:D:13:LEU:HD12	1:D:84:LEU:HD21	1.86	0.57
1:C:4:VAL:HB	1:C:40:PHE:HB2	1.87	0.57
1:C:13:LEU:HD11	1:C:141:MET:SD	2.44	0.57
1:E:108:GLU:HG2	1:E:109:PRO:HD2	1.86	0.57
1:F:58:LYS:O	1:F:62:LEU:HB2	2.04	0.57
1:A:6:GLN:HB2	1:A:38:ILE:CG2	2.33	0.57
1:E:94:ASN:ND2	1:E:96:LYS:HD3	2.20	0.56
1:A:96:LYS:HG2	1:B:160:ILE:HG21	1.87	0.56
1:B:111:GLU:O	1:B:114:ILE:HG22	2.06	0.56
1:C:95:THR:O	1:D:58:LYS:HE2	2.05	0.56
1:D:63:ARG:NE	1:D:73:ASP:O	2.36	0.56
1:E:54:TYR:HE2	1:E:58:LYS:HE3	1.70	0.56
1:A:150:PRO:HG2	1:B:88:GLN:HE22	1.69	0.56
1:C:14:SER:HB3	1:C:29:ILE:HA	1.88	0.56
1:F:5:ILE:HG21	1:F:37:LEU:HD13	1.86	0.56
1:F:116:TYR:O	1:F:119:ILE:HB	2.05	0.56
1:E:97:LYS:HD2	1:E:98:GLY:N	2.21	0.56
1:A:49:TRP:O	1:A:53:LEU:HB2	2.06	0.56
1:B:128:ASN:HB3	1:B:131:LYS:HG2	1.88	0.56
1:C:49:TRP:O	1:C:53:LEU:HD23	2.07	0.55
1:F:128:ASN:O	1:F:130:ASP:N	2.40	0.55
1:F:1:MET:O	1:F:157:THR:N	2.36	0.55
1:D:54:TYR:O	1:D:57:ARG:HB3	2.06	0.55
1:A:57:ARG:C	1:A:61:ASN:HD22	2.10	0.54
1:D:111:GLU:O	1:D:114:ILE:HG23	2.06	0.54
1:D:11:ALA:HB3	1:D:33:ILE:CG1	2.38	0.54
1:F:66:ASN:ND2	1:F:71:THR:HG22	2.20	0.54
1:B:132:ILE:O	1:B:133:LYS:HD2	2.08	0.54
1:A:73:ASP:OD2	1:A:74:LYS:NZ	2.39	0.54
1:D:4:VAL:HB	1:D:40:PHE:HB2	1.90	0.53
1:E:96:LYS:NZ	1:F:159:ASP:HB3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:VAL:HG12	1:C:16:ARG:H	1.73	0.53
1:D:122:GLU:HG3	1:D:126:GLN:HE21	1.71	0.53
1:A:124:LYS:HB3	1:A:129:ASP:HB3	1.90	0.53
1:B:37:LEU:HD12	1:B:76:VAL:HB	1.91	0.53
1:C:90:THR:HA	1:C:103:PHE:HE1	1.74	0.53
1:B:37:LEU:CD1	1:B:76:VAL:HB	2.38	0.53
1:C:103:PHE:C	1:C:105:LEU:H	2.11	0.53
1:B:136:LYS:O	1:B:139:ASN:HB2	2.07	0.53
1:C:10:GLY:HA2	1:C:34:LYS:O	2.09	0.53
1:E:77:LYS:HG2	1:E:127:TYR:CD1	2.44	0.53
1:B:113:LEU:HA	1:B:137:PHE:CE1	2.44	0.53
1:C:58:LYS:HB3	1:C:62:LEU:HD11	1.91	0.53
1:D:130:ASP:O	1:D:133:LYS:HE3	2.09	0.53
1:E:41:LEU:C	1:E:41:LEU:HD23	2.29	0.53
1:A:103:PHE:C	1:A:105:LEU:H	2.12	0.52
1:B:64:LEU:HD23	1:B:64:LEU:N	2.23	0.52
1:D:44:HIS:ND1	1:D:45:LYS:N	2.57	0.52
1:A:37:LEU:HD21	1:A:65:TRP:CH2	2.45	0.52
1:E:44:HIS:HB3	1:E:47:ASP:OD1	2.09	0.52
1:E:65:TRP:CH2	1:E:76:VAL:HG13	2.44	0.52
1:A:27:LEU:HD12	1:A:27:LEU:H	1.74	0.52
1:D:63:ARG:HB3	1:D:73:ASP:O	2.10	0.52
1:D:56:ILE:HG23	1:D:123:PHE:CE1	2.44	0.52
1:B:75:ASN:OD1	1:B:77:LYS:HB2	2.10	0.51
1:D:2:ARG:HE	1:D:156:ASP:CG	2.14	0.51
1:A:9:LYS:HG2	1:A:148:ASP:HB2	1.92	0.51
1:A:108:GLU:HG2	1:A:109:PRO:CD	2.30	0.51
1:E:37:LEU:HB2	1:E:83:LEU:CD2	2.40	0.51
1:A:99:ASN:HD21	1:E:80:ASN:HD21	1.59	0.51
1:F:76:VAL:HG21	1:F:83:LEU:CD1	2.40	0.51
1:A:33:ILE:HB	1:A:82:GLU:CD	2.31	0.51
1:C:116:TYR:O	1:C:119:ILE:HB	2.10	0.51
1:D:120:ILE:CG2	1:D:124:LYS:HE3	2.40	0.51
1:E:116:TYR:OH	1:E:134:ILE:HB	2.11	0.50
1:E:149:GLY:N	1:E:150:PRO:HA	2.25	0.50
1:E:65:TRP:HH2	1:E:76:VAL:HG13	1.76	0.50
1:D:122:GLU:OE2	1:D:125:LYS:HD3	2.11	0.50
1:B:70:LYS:H	1:B:70:LYS:HD3	1.77	0.50
1:B:3:VAL:HA	1:B:40:PHE:O	2.11	0.50
1:B:49:TRP:CH2	1:B:118:LYS:HG2	2.47	0.50
1:A:29:ILE:HG22	1:A:30:ILE:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:LYS:HD3	1:B:70:LYS:N	2.26	0.50
1:D:56:ILE:HG23	1:D:123:PHE:CD1	2.47	0.49
1:D:156:ASP:HB3	1:D:159:ASP:OD2	2.12	0.49
1:D:62:LEU:O	1:D:75:ASN:HB2	2.12	0.49
1:E:13:LEU:HB3	1:E:31:SER:OG	2.12	0.49
1:C:82:GLU:C	1:C:83:LEU:HD12	2.32	0.49
1:A:113:LEU:HD13	1:A:137:PHE:CG	2.48	0.49
1:C:90:THR:HA	1:C:103:PHE:CE1	2.48	0.49
1:E:77:LYS:HG2	1:E:127:TYR:CE1	2.48	0.49
1:A:67:ASN:ND2	1:A:74:LYS:HE2	2.27	0.49
1:D:2:ARG:NE	1:D:156:ASP:OD2	2.41	0.49
1:F:114:ILE:HG23	1:F:115:PHE:N	2.28	0.49
1:F:54:TYR:HD1	1:F:54:TYR:O	1.94	0.48
1:F:77:LYS:HD2	1:F:127:TYR:CD1	2.48	0.48
1:D:9:LYS:HE3	1:D:35:ASN:HD21	1.77	0.48
1:D:158:HIS:O	1:D:158:HIS:ND1	2.46	0.48
1:E:120:ILE:O	1:E:124:LYS:HG2	2.13	0.48
1:B:4:VAL:HB	1:B:40:PHE:HB2	1.96	0.48
1:F:32:GLU:HG2	1:F:33:ILE:N	2.29	0.48
1:F:60:LEU:O	1:F:76:VAL:HG12	2.14	0.48
1:F:113:LEU:O	1:F:116:TYR:HB3	2.13	0.48
1:A:41:LEU:HD23	1:A:41:LEU:C	2.33	0.48
1:F:3:VAL:HA	1:F:40:PHE:O	2.13	0.48
1:F:44:HIS:ND1	1:F:158:HIS:NE2	2.59	0.48
1:B:60:LEU:O	1:B:77:LYS:HE2	2.13	0.48
1:B:127:TYR:HA	1:E:35:ASN:ND2	2.29	0.48
1:C:63:ARG:HH11	1:D:99:ASN:HB2	1.78	0.48
1:F:9:LYS:HA	1:F:35:ASN:OD1	2.14	0.48
1:D:118:LYS:NZ	1:D:118:LYS:HB3	2.29	0.48
1:D:54:TYR:HD1	1:D:57:ARG:NH2	2.11	0.47
1:D:82:GLU:C	1:D:83:LEU:HD12	2.34	0.47
1:D:6:GLN:CG	1:D:152:THR:HG23	2.45	0.47
1:A:6:GLN:O	1:A:38:ILE:HG22	2.13	0.47
1:E:60:LEU:HD23	1:E:83:LEU:HD11	1.96	0.47
1:E:142:ASN:OD1	1:F:146:THR:HG22	2.14	0.47
1:A:62:LEU:HB3	1:A:64:LEU:HD21	1.95	0.47
1:D:106:ALA:O	1:D:107:LYS:O	2.32	0.47
1:F:10:GLY:HA2	1:F:33:ILE:O	2.14	0.47
1:D:5:ILE:CG2	1:D:37:LEU:HD13	2.44	0.47
1:E:48:THR:OG1	1:E:50:GLU:HB2	2.15	0.47
1:E:57:ARG:HG3	1:E:58:LYS:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:LEU:HB3	1:C:57:ARG:HH22	1.80	0.46
1:F:3:VAL:HG23	1:F:41:LEU:HA	1.96	0.46
1:F:157:THR:C	1:F:158:HIS:HD1	2.19	0.46
1:D:108:GLU:HB2	1:D:111:GLU:CD	2.35	0.46
1:F:44:HIS:HD1	1:F:158:HIS:CE1	2.33	0.46
1:B:2:ARG:O	1:B:41:LEU:HD12	2.15	0.46
1:B:122:GLU:C	1:B:124:LYS:H	2.18	0.46
1:D:76:VAL:HG21	1:D:83:LEU:CD1	2.45	0.46
1:E:9:LYS:HE2	1:E:148:ASP:OD1	2.16	0.46
1:E:108:GLU:HG2	1:E:109:PRO:CD	2.45	0.46
1:D:44:HIS:HB3	1:D:47:ASP:CG	2.36	0.46
1:A:17:LYS:O	1:A:19:ASN:N	2.45	0.46
1:F:54:TYR:O	1:F:54:TYR:CD1	2.69	0.46
1:D:63:ARG:HA	1:D:75:ASN:HA	1.98	0.46
1:E:48:THR:C	1:E:50:GLU:N	2.66	0.46
1:E:61:ASN:HB3	1:F:99:ASN:ND2	2.31	0.46
1:F:76:VAL:HG21	1:F:83:LEU:HD11	1.97	0.46
1:C:58:LYS:O	1:C:62:LEU:HG	2.16	0.45
1:E:82:GLU:HA	1:E:131:LYS:HB3	1.97	0.45
1:A:38:ILE:HG23	1:A:38:ILE:O	2.17	0.45
1:A:124:LYS:HD3	1:A:129:ASP:HB2	1.98	0.45
1:D:15:VAL:HG22	1:D:30:ILE:HG21	1.96	0.45
1:B:101:PRO:HB2	1:B:103:PHE:CZ	2.52	0.45
1:E:37:LEU:HD12	1:E:76:VAL:HG11	1.99	0.45
1:E:45:LYS:CE	1:E:46:ASN:HD21	2.30	0.45
1:E:57:ARG:CB	1:E:57:ARG:HH11	2.30	0.45
1:B:8:VAL:HG11	1:B:145:VAL:HG13	1.99	0.45
1:E:60:LEU:HA	1:E:76:VAL:CG2	2.47	0.45
1:B:114:ILE:CG2	1:B:115:PHE:N	2.79	0.45
1:D:7:ARG:HB3	1:D:151:VAL:HB	1.98	0.45
1:A:124:LYS:HE2	1:A:132:ILE:HG22	1.98	0.45
1:B:13:LEU:HD23	1:B:13:LEU:C	2.36	0.45
1:D:54:TYR:HD1	1:D:57:ARG:HH21	1.65	0.45
1:E:45:LYS:HG3	1:E:46:ASN:CG	2.37	0.45
1:F:34:LYS:HB3	1:F:35:ASN:H	1.60	0.45
1:B:109:PRO:O	1:B:112:ALA:N	2.49	0.45
1:F:2:ARG:NH1	1:F:92:PHE:CD1	2.85	0.45
1:F:52:ALA:O	1:F:55:ILE:HB	2.17	0.45
1:C:53:LEU:HB3	1:C:57:ARG:NH2	2.32	0.45
1:E:44:HIS:O	1:E:107:LYS:HE3	2.17	0.45
1:F:27:LEU:C	1:F:27:LEU:HD13	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:LEU:HD22	1:E:142:ASN:HD22	1.82	0.44
1:E:28:GLU:O	1:E:28:GLU:HG3	2.17	0.44
1:E:104:HIS:O	1:E:106:ALA:N	2.50	0.44
1:A:13:LEU:HD23	1:A:13:LEU:C	2.37	0.44
1:D:97:LYS:O	1:D:98:GLY:O	2.36	0.44
1:F:49:TRP:NE1	1:F:53:LEU:HD21	2.32	0.44
1:D:44:HIS:O	1:D:107:LYS:HD2	2.18	0.44
1:E:96:LYS:HZ3	1:F:159:ASP:HB3	1.82	0.44
1:C:2:ARG:HD2	1:C:92:PHE:CE1	2.53	0.44
1:D:48:THR:O	1:D:115:PHE:CZ	2.70	0.44
1:D:48:THR:O	1:D:115:PHE:HZ	2.00	0.44
1:F:120:ILE:O	1:F:123:PHE:HB2	2.18	0.44
1:C:144:ASP:HA	1:D:145:VAL:O	2.18	0.44
1:B:58:LYS:O	1:B:62:LEU:HG	2.18	0.44
1:D:43:ILE:HG22	1:D:44:HIS:N	2.33	0.44
1:B:122:GLU:CD	1:B:125:LYS:HD3	2.38	0.43
1:C:137:PHE:O	1:C:139:ASN:N	2.48	0.43
1:D:128:ASN:ND2	1:D:130:ASP:N	2.66	0.43
1:E:9:LYS:HE2	1:E:148:ASP:CG	2.38	0.43
1:F:3:VAL:HG23	1:F:41:LEU:CA	2.48	0.43
1:F:114:ILE:HG23	1:F:115:PHE:H	1.82	0.43
1:F:5:ILE:CG2	1:F:37:LEU:HD13	2.48	0.43
1:A:33:ILE:HG22	1:A:133:LYS:HG3	2.01	0.43
1:B:125:LYS:O	1:B:125:LYS:HG2	2.17	0.43
1:C:27:LEU:N	1:C:27:LEU:CD2	2.79	0.43
1:E:6:GLN:HB2	1:E:38:ILE:CG2	2.47	0.43
1:D:43:ILE:HG22	1:D:107:LYS:HD2	2.01	0.43
1:E:44:HIS:N	1:E:47:ASP:OD2	2.50	0.43
1:A:58:LYS:O	1:A:62:LEU:HG	2.19	0.43
1:B:35:ASN:O	1:B:81:TYR:HB3	2.18	0.43
1:A:19:ASN:C	1:A:21:GLY:H	2.22	0.43
1:A:44:HIS:HE1	1:A:46:ASN:HD22	1.67	0.43
1:C:57:ARG:O	1:C:61:ASN:ND2	2.50	0.43
1:F:113:LEU:O	1:F:116:TYR:N	2.52	0.43
1:A:48:THR:HG22	1:A:49:TRP:H	1.83	0.43
1:D:9:LYS:HE2	1:D:9:LYS:HB3	1.88	0.43
1:D:6:GLN:HB2	1:D:38:ILE:CG2	2.46	0.43
1:D:7:ARG:CB	1:D:151:VAL:HB	2.49	0.43
1:F:108:GLU:OE1	1:F:108:GLU:N	2.42	0.43
1:C:100:LYS:HA	1:C:101:PRO:HD2	1.90	0.43
1:D:159:ASP:C	1:D:160:ILE:CG1	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:90:THR:C	1:E:92:PHE:H	2.21	0.43
1:A:156:ASP:C	1:A:158:HIS:H	2.22	0.42
1:C:41:LEU:O	1:C:88:GLN:N	2.50	0.42
1:F:97:LYS:HB3	1:F:97:LYS:HZ3	1.83	0.42
1:A:40:PHE:CD1	1:A:88:GLN:NE2	2.82	0.42
1:F:110:ASN:O	1:F:113:LEU:N	2.51	0.42
1:B:58:LYS:HA	1:B:58:LYS:HD3	1.89	0.42
1:B:119:ILE:C	1:B:121:ASP:N	2.71	0.42
1:D:9:LYS:HA	1:D:35:ASN:HA	2.00	0.42
1:D:114:ILE:O	1:D:118:LYS:HG3	2.19	0.42
1:B:124:LYS:C	1:B:126:GLN:N	2.71	0.42
1:C:62:LEU:HB3	1:C:64:LEU:HD21	2.01	0.42
1:D:91:LEU:HD23	1:D:91:LEU:HA	1.85	0.42
1:A:60:LEU:HD23	1:A:60:LEU:HA	1.83	0.42
1:A:140:TYR:HE1	1:B:149:GLY:H	1.67	0.42
1:C:137:PHE:CD2	1:C:138:GLY:N	2.88	0.42
1:C:124:LYS:O	1:C:125:LYS:C	2.58	0.42
1:E:57:ARG:HH11	1:E:57:ARG:HB2	1.84	0.42
1:A:108:GLU:HA	1:A:109:PRO:HD3	1.92	0.42
1:D:2:ARG:HD3	1:D:92:PHE:CE1	2.55	0.42
1:D:67:ASN:O	1:D:70:LYS:HG2	2.20	0.42
1:A:67:ASN:O	1:A:70:LYS:HB2	2.19	0.42
1:D:128:ASN:ND2	1:D:130:ASP:H	2.18	0.42
1:C:96:LYS:NZ	1:D:159:ASP:HB3	2.35	0.42
1:E:38:ILE:HG23	1:E:38:ILE:O	2.20	0.42
1:F:114:ILE:O	1:F:118:LYS:HG3	2.20	0.42
1:F:122:GLU:OE2	1:F:122:GLU:HA	2.19	0.42
1:A:110:ASN:O	1:A:111:GLU:C	2.58	0.42
1:A:17:LYS:N	1:A:26:GLU:O	2.39	0.41
1:B:113:LEU:HA	1:B:137:PHE:CD1	2.54	0.41
1:C:13:LEU:HD23	1:C:13:LEU:C	2.41	0.41
1:E:45:LYS:HE3	1:E:46:ASN:ND2	2.33	0.41
1:E:59:CYS:O	1:E:76:VAL:HG21	2.19	0.41
1:D:128:ASN:ND2	1:D:129:ASP:N	2.68	0.41
1:E:45:LYS:HA	1:E:107:LYS:HB2	2.02	0.41
1:E:58:LYS:HA	1:E:58:LYS:HD3	1.84	0.41
1:F:54:TYR:HE1	1:F:58:LYS:HG3	1.85	0.41
1:B:49:TRP:CZ3	1:B:118:LYS:HG2	2.55	0.41
1:D:159:ASP:O	1:D:160:ILE:HG23	2.20	0.41
1:A:100:LYS:HA	1:A:101:PRO:HD2	1.84	0.41
1:C:112:ALA:O	1:C:115:PHE:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ASN:HB3	1:B:102:ASP:HB3	2.01	0.41
1:B:137:PHE:HD2	1:B:137:PHE:C	2.24	0.41
1:D:7:ARG:NE	1:D:148:ASP:OD2	2.54	0.41
1:E:104:HIS:C	1:E:106:ALA:N	2.74	0.41
1:E:115:PHE:O	1:E:119:ILE:N	2.43	0.41
1:A:139:ASN:N	1:A:139:ASN:HD22	2.18	0.41
1:C:6:GLN:HB2	1:C:38:ILE:CG2	2.50	0.41
1:C:103:PHE:O	1:C:105:LEU:N	2.54	0.41
1:D:108:GLU:HA	1:D:109:PRO:HD3	1.92	0.41
1:E:127:TYR:CE2	1:E:131:LYS:HB2	2.55	0.41
1:F:51:ASP:O	1:F:54:TYR:N	2.50	0.41
1:F:122:GLU:O	1:F:126:GLN:HG3	2.21	0.41
1:A:105:LEU:HG	1:A:105:LEU:O	2.20	0.41
1:B:73:ASP:O	1:B:74:LYS:HD3	2.21	0.41
1:F:112:ALA:O	1:F:115:PHE:HB3	2.21	0.41
1:A:7:ARG:HD2	1:A:65:TRP:NE1	2.35	0.40
1:A:7:ARG:CZ	1:A:151:VAL:HG21	2.52	0.40
1:B:124:LYS:O	1:B:126:GLN:N	2.54	0.40
1:B:137:PHE:C	1:B:137:PHE:CD2	2.94	0.40
1:C:15:VAL:CG1	1:C:16:ARG:N	2.84	0.40
1:C:75:ASN:O	1:C:76:VAL:C	2.60	0.40
1:E:44:HIS:CE1	1:E:105:LEU:HG	2.56	0.40
1:A:153:ILE:HG22	1:A:154:TYR:N	2.35	0.40
1:B:154:TYR:O	1:B:155:ILE:CG1	2.69	0.40
1:E:81:TYR:HB3	1:E:82:GLU:H	1.78	0.40
1:E:116:TYR:HA	1:E:119:ILE:CG2	2.51	0.40
1:F:8:VAL:HG22	1:F:36:GLY:O	2.22	0.40
1:A:12:ILE:O	1:A:12:ILE:HG22	2.20	0.40
1:C:110:ASN:O	1:C:111:GLU:C	2.59	0.40
1:B:119:ILE:O	1:B:120:ILE:C	2.59	0.40
1:B:119:ILE:O	1:B:121:ASP:N	2.55	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	157/164 (96%)	130 (83%)	17 (11%)	10 (6%)	1 9
1	B	158/164 (96%)	123 (78%)	27 (17%)	8 (5%)	2 13
1	C	157/164 (96%)	116 (74%)	32 (20%)	9 (6%)	1 11
1	D	148/164 (90%)	117 (79%)	24 (16%)	7 (5%)	2 14
1	E	144/164 (88%)	121 (84%)	18 (12%)	5 (4%)	3 21
1	F	145/164 (88%)	109 (75%)	28 (19%)	8 (6%)	2 11
All	All	909/984 (92%)	716 (79%)	146 (16%)	47 (5%)	2 13

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	97	LYS
1	B	18	GLU
1	B	19	ASN
1	B	23	ASN
1	B	24	GLU
1	B	106	ALA
1	B	109	PRO
1	C	25	LYS
1	C	76	VAL
1	C	97	LYS
1	D	48	THR
1	D	98	GLY
1	D	107	LYS
1	A	25	LYS
1	A	68	ASP
1	B	26	GLU
1	C	26	GLU
1	C	66	ASN
1	C	104	HIS
1	E	73	ASP
1	F	110	ASN
1	F	113	LEU
1	F	129	ASP
1	F	136	LYS
1	F	137	PHE
1	A	157	THR

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Mol	Chain	Res	Type
1	E	68	ASP
1	E	129	ASP
1	D	68	ASP
1	A	127	TYR
1	B	68	ASP
1	E	105	LEU
1	E	127	TYR
1	F	55	ILE
1	F	59	CYS
1	A	18	GLU
1	A	53	LEU
1	D	96	LYS
1	D	130	ASP
1	C	20	ILE
1	D	134	ILE
1	F	101	PRO
1	A	30	ILE
1	C	21	GLY
1	A	109	PRO
1	C	138	GLY

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	117/151 (78%)	107 (92%)	10 (8%)	10 35
1	B	118/151 (78%)	107 (91%)	11 (9%)	9 30
1	C	118/151 (78%)	107 (91%)	11 (9%)	9 30
1	D	118/151 (78%)	108 (92%)	10 (8%)	10 35
1	E	117/151 (78%)	104 (89%)	13 (11%)	6 23
1	F	118/151 (78%)	108 (92%)	10 (8%)	10 35
All	All	706/906 (78%)	641 (91%)	65 (9%)	9 31

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	28	GLU
1	A	48	THR
1	A	57	ARG
1	A	76	VAL
1	A	95	THR
1	A	109	PRO
1	A	111	GLU
1	A	121	ASP
1	A	133	LYS
1	B	27	LEU
1	B	32	GLU
1	B	35	ASN
1	B	70	LYS
1	B	88	GLN
1	B	108	GLU
1	B	123	PHE
1	B	130	ASP
1	B	137	PHE
1	B	158	HIS
1	B	159	ASP
1	C	27	LEU
1	C	34	LYS
1	C	63	ARG
1	C	80	ASN
1	C	94	ASN
1	C	102	ASP
1	C	108	GLU
1	C	123	PHE
1	C	130	ASP
1	C	152	THR
1	C	158	HIS
1	D	2	ARG
1	D	46	ASN
1	D	51	ASP
1	D	71	THR
1	D	108	GLU
1	D	123	PHE
1	D	127	TYR
1	D	128	ASN
1	D	133	LYS
1	D	158	HIS
1	E	27	LEU

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Mol	Chain	Res	Type
1	E	28	GLU
1	E	54	TYR
1	E	57	ARG
1	E	66	ASN
1	E	76	VAL
1	E	78	ASP
1	E	97	LYS
1	E	99	ASN
1	E	108	GLU
1	E	109	PRO
1	E	139	ASN
1	E	152	THR
1	F	14	SER
1	F	47	ASP
1	F	54	TYR
1	F	63	ARG
1	F	82	GLU
1	F	97	LYS
1	F	102	ASP
1	F	123	PHE
1	F	128	ASN
1	F	130	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	46	ASN
1	A	61	ASN
1	A	67	ASN
1	A	99	ASN
1	A	117	ASN
1	A	139	ASN
1	B	6	GLN
1	B	139	ASN
1	C	46	ASN
1	C	94	ASN
1	C	117	ASN
1	C	126	GLN
1	C	147	ASN
1	D	6	GLN
1	D	35	ASN

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Mol	Chain	Res	Type
1	D	67	ASN
1	D	126	GLN
1	D	128	ASN
1	D	139	ASN
1	D	147	ASN
1	E	6	GLN
1	E	44	HIS
1	E	80	ASN
1	E	99	ASN
1	E	117	ASN
1	E	139	ASN
1	F	6	GLN
1	F	66	ASN
1	F	67	ASN
1	F	80	ASN
1	F	99	ASN
1	F	117	ASN

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 monosaccharides 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 (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, 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	159/164 (96%)	-0.60	0 100 100	42, 62, 95, 98	2 (1%)
1	B	160/164 (97%)	-0.49	1 (0%) 89 90	44, 58, 88, 96	2 (1%)
1	C	159/164 (96%)	-0.48	0 100 100	49, 70, 90, 101	1 (0%)
1	D	152/164 (92%)	-0.49	0 100 100	42, 69, 91, 106	3 (1%)
1	E	148/164 (90%)	-0.46	0 100 100	52, 71, 90, 99	1 (0%)
1	F	149/164 (90%)	-0.37	0 100 100	52, 81, 105, 109	2 (1%)
All	All	927/984 (94%)	-0.48	1 (0%) 95 97	42, 68, 95, 109	11 (1%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	22	GLU	2.4

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.