Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 12:13 am BST

PDB ID	:	3E1E
Title	:	Crystal structure of a Thioesterase family protein from Silicibacter pomeroyi. NorthEast Structural Genomics target SiR180A
Authors	:	Seetharaman, J.; Abashidze, M.; Wang, H.; Janjua, H.; Foote, E.L.; Xiao, R.; Nair, R.; Acton, T.B.; Rost, B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2008-08-04
Resolution	:	2.00 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

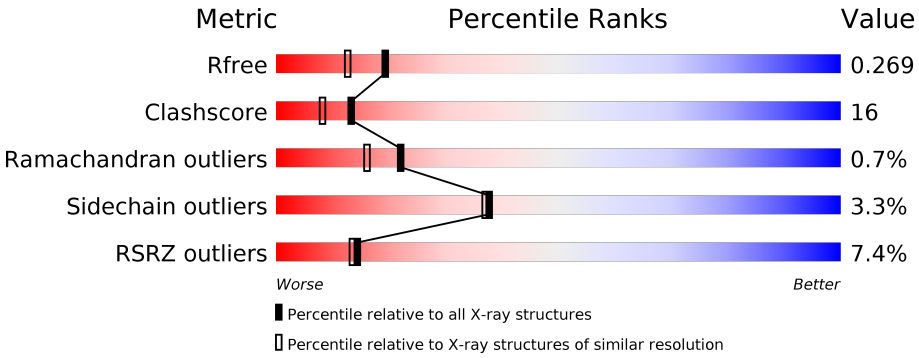
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	141	8% 70% 25%
1	B	141	10% 71% 24%
1	C	141	6% 72% 24%
1	D	141	6% 69% 27%
1	E	141	10% 71% 26%
1	F	141	5% 75% 21%

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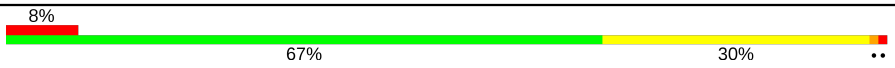
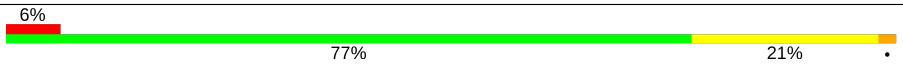
Mol	Chain	Length	Quality of chain
1	G	141	
1	H	141	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8932 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 Thioesterase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	136	Total	C	N	O	S	0	0	0
			1034	655	179	193	7			
1	B	140	Total	C	N	O	S	0	0	0
			1068	678	186	197	7			
1	C	141	Total	C	N	O	S	0	0	0
			1077	683	187	200	7			
1	D	137	Total	C	N	O	S	0	0	0
			1039	658	180	194	7			
1	E	141	Total	C	N	O	S	0	0	0
			1077	683	187	200	7			
1	F	141	Total	C	N	O	S	0	0	0
			1077	683	187	200	7			
1	G	141	Total	C	N	O	S	0	0	0
			1077	683	187	200	7			
1	H	141	Total	C	N	O	S	0	0	0
			1077	683	187	200	7			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	38	Total	O	0	0
			38	38		
2	B	63	Total	O	0	0
			63	63		
2	C	70	Total	O	0	0
			70	70		
2	D	41	Total	O	0	0
			41	41		
2	E	43	Total	O	0	0
			43	43		
2	F	52	Total	O	0	0
			52	52		

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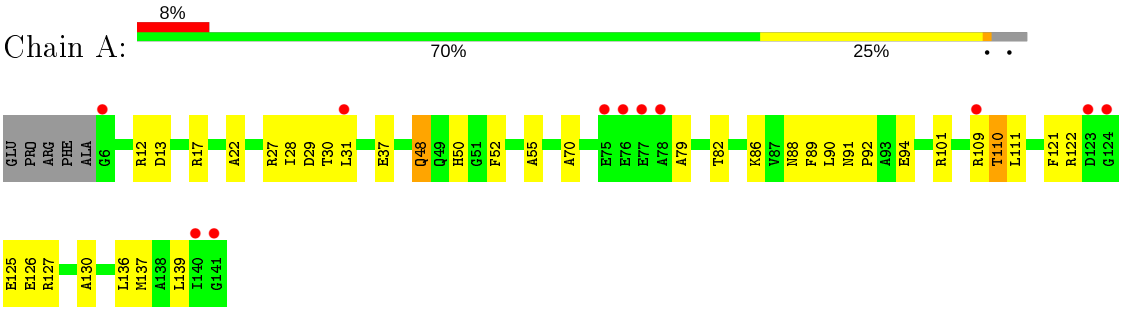
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	28	Total O 28 28	0	0
2	H	71	Total O 71 71	0	0

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.

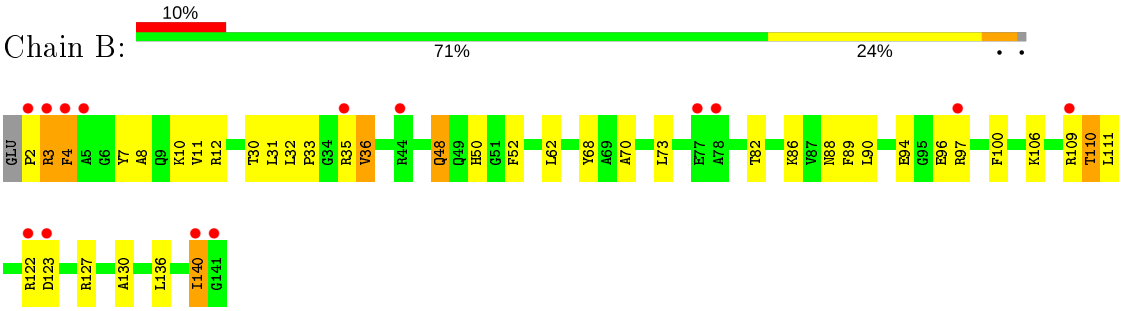
- Molecule 1: Thioesterase family protein

Chain A:



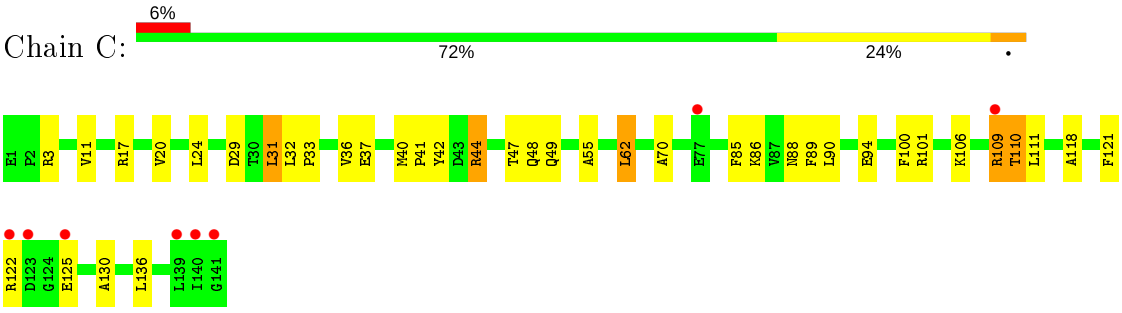
- Molecule 1: Thioesterase family protein

Chain B:



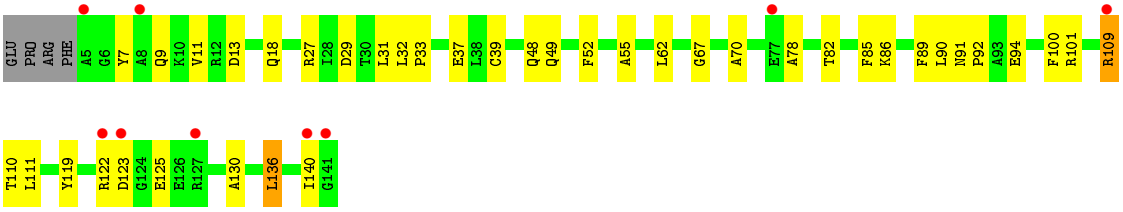
- Molecule 1: Thioesterase family protein

Chain C:

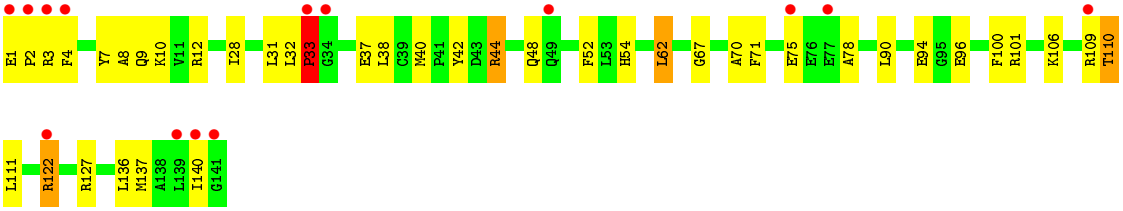


- Molecule 1: Thioesterase family protein

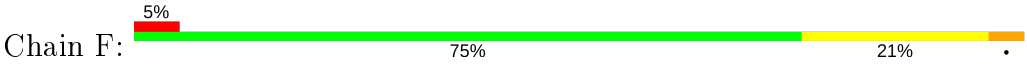
Chain D:



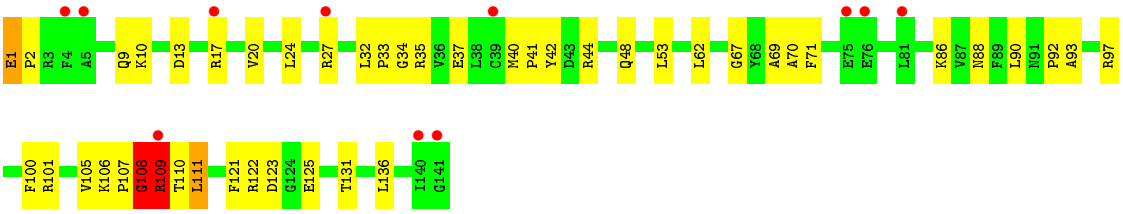
• Molecule 1: Thioesterase family protein



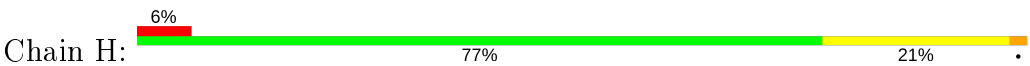
• Molecule 1: Thioesterase family protein

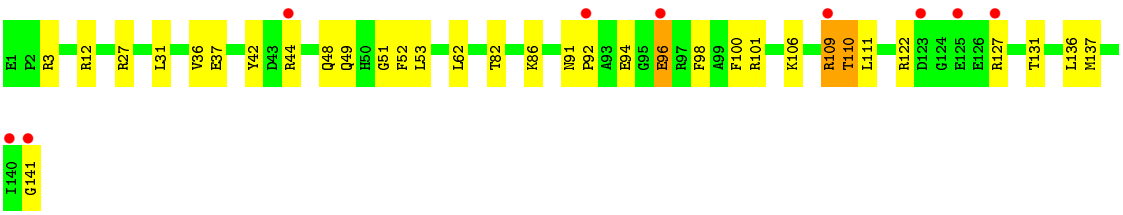


• Molecule 1: Thioesterase family protein



• Molecule 1: Thioesterase family protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.11Å 107.31Å 112.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.39 – 2.00 48.39 – 2.00	Depositor EDS
% Data completeness (in resolution range)	86.4 (48.39-2.00) 88.4 (48.39-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	6.91 (at 2.00Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.223 , 0.252 0.230 , 0.269	Depositor DCC
R_{free} test set	11792 reflections (9.22%)	wwPDB-VP
Wilson B-factor (Å^2)	16.5	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 57.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8932	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 66.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.8262e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.36	0/1052	0.71	2/1424 (0.1%)
1	B	0.38	0/1088	0.71	2/1472 (0.1%)
1	C	0.36	0/1097	0.70	2/1485 (0.1%)
1	D	0.35	0/1057	0.72	2/1431 (0.1%)
1	E	0.36	0/1097	0.70	2/1485 (0.1%)
1	F	0.37	0/1097	0.69	2/1485 (0.1%)
1	G	1.05	7/1097 (0.6%)	0.91	6/1485 (0.4%)
1	H	0.37	0/1097	0.69	2/1485 (0.1%)
All	All	0.51	7/8682 (0.1%)	0.73	20/11752 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	105	VAL	CB-CG1	-16.61	1.18	1.52
1	G	108	GLY	C-O	-14.61	1.00	1.23
1	G	105	VAL	C-O	-10.80	1.02	1.23
1	G	109	ARG	N-CA	-8.14	1.30	1.46
1	G	111	LEU	CG-CD2	-6.54	1.27	1.51
1	G	107	PRO	CB-CG	-6.33	1.18	1.50
1	G	106	LYS	CG-CD	-5.64	1.33	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	109	ARG	NE-CZ-NH1	-16.50	112.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	110	THR	N-CA-CB	-12.81	85.96	110.30
1	F	110	THR	N-CA-CB	-12.28	86.96	110.30
1	A	110	THR	N-CA-CB	-11.76	87.96	110.30
1	E	110	THR	N-CA-CB	-11.61	88.24	110.30
1	B	110	THR	N-CA-CB	-11.17	89.08	110.30
1	C	110	THR	N-CA-CB	-10.76	89.85	110.30
1	H	110	THR	N-CA-CB	-10.54	90.27	110.30
1	G	109	ARG	NE-CZ-NH2	8.79	124.70	120.30
1	D	109	ARG	CB-CA-C	8.71	127.83	110.40
1	G	109	ARG	N-CA-CB	-8.48	95.33	110.60
1	C	109	ARG	N-CA-C	7.73	131.87	111.00
1	H	109	ARG	N-CA-C	7.33	130.78	111.00
1	B	109	ARG	N-CA-C	7.15	130.31	111.00
1	E	109	ARG	N-CA-C	6.66	128.98	111.00
1	G	108	GLY	O-C-N	-6.28	112.66	122.70
1	G	111	LEU	CB-CG-CD1	5.81	120.88	111.00
1	G	105	VAL	CA-CB-CG2	5.46	119.09	110.90
1	F	109	ARG	N-CA-C	5.42	125.63	111.00
1	A	109	ARG	CB-CA-C	5.40	121.20	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	108	GLY	Peptide

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	1034	0	1034	30	0
1	B	1068	0	1069	41	0
1	C	1077	0	1077	31	0
1	D	1039	0	1039	41	0
1	E	1077	0	1077	36	0
1	F	1077	0	1077	40	0
1	G	1077	0	1077	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1077	0	1077	37	0
2	A	38	0	0	1	0
2	B	63	0	0	0	0
2	C	70	0	0	2	0
2	D	41	0	0	3	0
2	E	43	0	0	1	0
2	F	52	0	0	6	0
2	G	28	0	0	3	0
2	H	71	0	0	5	0
All	All	8932	0	8527	276	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (276) 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:G:108:GLY:HA2	1:G:109:ARG:HB2	1.27	1.14
1:G:108:GLY:CA	1:G:109:ARG:HB2	1.77	1.06
1:B:140:ILE:HD13	1:B:140:ILE:H	1.24	0.99
1:G:108:GLY:CA	1:G:109:ARG:CB	2.45	0.94
1:H:27:ARG:HH11	1:H:27:ARG:HB3	1.35	0.91
1:B:32:LEU:HD12	1:B:35:ARG:HE	1.43	0.84
1:G:27:ARG:HH11	1:G:27:ARG:HB3	1.45	0.82
1:H:27:ARG:NH1	1:H:27:ARG:HB3	1.96	0.80
1:E:110:THR:HG22	1:E:111:LEU:HD13	1.63	0.80
1:H:122:ARG:HH21	1:H:127:ARG:HE	1.30	0.79
1:B:94:GLU:HG3	1:B:122:ARG:HD3	1.63	0.78
1:E:78:ALA:HB2	1:E:140:ILE:HG22	1.65	0.78
1:B:110:THR:HG22	1:B:111:LEU:HD13	1.64	0.77
1:E:37:GLU:HG3	1:E:101:ARG:HG2	1.65	0.77
1:F:86:LYS:HB2	1:H:86:LYS:HD3	1.69	0.75
1:B:12:ARG:NH1	1:B:31:LEU:HD23	2.02	0.74
1:A:12:ARG:NH1	1:A:31:LEU:HD12	2.02	0.74
1:H:3:ARG:HH22	1:H:109:ARG:HG2	1.53	0.73
1:C:110:THR:HG22	1:C:111:LEU:HD13	1.70	0.73
1:D:37:GLU:HG2	1:D:101:ARG:HG2	1.70	0.73
1:E:62:LEU:HD13	1:E:100:PHE:HD1	1.53	0.73
1:F:86:LYS:CB	1:H:86:LYS:HD3	2.20	0.71
1:D:82:THR:HG22	2:D:156:HOH:O	1.92	0.70
1:A:90:LEU:HD23	1:A:130:ALA:HA	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:LEU:HB3	1:E:106:LYS:HD2	1.75	0.68
1:F:90:LEU:HD22	1:F:90:LEU:N	2.08	0.68
1:C:86:LYS:HE3	1:C:88:ASN:ND2	2.08	0.67
1:C:86:LYS:HE3	1:C:88:ASN:HD21	1.57	0.67
1:D:90:LEU:HD22	1:D:90:LEU:N	2.10	0.67
1:B:32:LEU:HD12	1:B:35:ARG:NE	2.08	0.67
1:H:110:THR:HG22	1:H:111:LEU:HD13	1.77	0.66
1:E:3:ARG:HB3	1:E:75:GLU:OE1	1.96	0.65
1:B:140:ILE:H	1:B:140:ILE:CD1	2.01	0.65
1:G:27:ARG:NH1	1:G:27:ARG:HB3	2.11	0.64
1:F:110:THR:HG22	1:F:111:LEU:HD13	1.79	0.64
1:H:31:LEU:HD22	1:H:36:VAL:HG22	1.78	0.64
1:D:67:GLY:HA2	1:D:136:LEU:HD22	1.80	0.63
1:H:127:ARG:HH11	1:H:127:ARG:HG2	1.63	0.63
1:C:90:LEU:HD12	1:C:90:LEU:N	2.14	0.63
1:E:127:ARG:HH11	1:E:127:ARG:HG2	1.64	0.62
1:F:10:LYS:HE2	1:F:71:PHE:CZ	2.34	0.61
1:A:110:THR:HG22	1:A:111:LEU:HD13	1.82	0.61
1:C:94:GLU:HG3	1:C:122:ARG:HD3	1.83	0.61
1:E:10:LYS:HE2	1:E:71:PHE:CZ	2.35	0.61
1:B:70:ALA:CB	1:B:136:LEU:HD12	2.31	0.60
1:A:90:LEU:N	1:A:90:LEU:HD22	2.15	0.60
1:D:90:LEU:HD23	1:D:130:ALA:HA	1.82	0.60
1:F:90:LEU:HB3	1:H:106:LYS:HD2	1.84	0.60
1:C:3:ARG:HH22	1:C:109:ARG:HG2	1.67	0.60
1:H:27:ARG:HH11	1:H:27:ARG:CB	2.12	0.60
1:D:140:ILE:O	1:D:140:ILE:HD12	2.02	0.59
1:F:90:LEU:O	1:H:106:LYS:HE3	2.02	0.59
1:G:70:ALA:CB	1:G:136:LEU:HD12	2.32	0.59
1:H:52:PHE:CD1	1:H:94:GLU:HB3	2.36	0.59
1:B:90:LEU:N	1:B:90:LEU:HD22	2.17	0.59
1:H:3:ARG:NH2	1:H:109:ARG:HG2	2.17	0.59
1:F:48:GLN:HE22	1:F:50:HIS:HD2	1.50	0.58
1:D:62:LEU:HD13	1:D:100:PHE:HD1	1.69	0.58
1:A:37:GLU:HG2	1:A:101:ARG:HG2	1.84	0.58
1:G:97:ARG:HH11	1:G:97:ARG:HG2	1.69	0.58
1:C:17:ARG:HB3	1:D:49:GLN:HG3	1.86	0.58
1:G:41:PRO:HA	1:G:97:ARG:HD3	1.86	0.58
1:B:12:ARG:HH12	1:B:31:LEU:HD23	1.67	0.58
1:A:90:LEU:HD23	1:A:130:ALA:CA	2.34	0.57
1:A:90:LEU:CD2	1:A:130:ALA:HA	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:THR:O	1:E:137:MET:HA	2.05	0.57
1:E:37:GLU:CG	1:E:101:ARG:HG2	2.35	0.57
1:F:70:ALA:HB2	1:F:136:LEU:HD12	1.86	0.57
1:B:82:THR:HA	1:B:136:LEU:HD23	1.87	0.56
1:D:90:LEU:O	1:E:106:LYS:HE3	2.05	0.56
1:D:70:ALA:HB2	1:D:136:LEU:HD13	1.87	0.56
1:B:35:ARG:O	1:B:36:VAL:HB	2.04	0.56
1:G:32:LEU:HB2	1:G:35:ARG:HB2	1.88	0.56
1:D:31:LEU:C	1:D:32:LEU:HD22	2.26	0.55
1:C:37:GLU:HG2	1:C:101:ARG:HG2	1.87	0.55
1:C:90:LEU:HD13	1:C:130:ALA:HA	1.89	0.55
1:C:106:LYS:HE3	1:G:90:LEU:O	2.06	0.55
1:A:52:PHE:CD1	1:A:94:GLU:HB3	2.42	0.54
1:D:78:ALA:HB2	1:D:140:ILE:HG22	1.89	0.54
1:F:11:VAL:HG11	1:F:31:LEU:HD21	1.90	0.54
1:H:127:ARG:HG3	2:H:159:HOH:O	2.07	0.54
1:F:90:LEU:HD23	1:F:130:ALA:HA	1.90	0.54
1:D:37:GLU:CG	1:D:101:ARG:HG2	2.38	0.53
1:F:48:GLN:HE22	1:F:50:HIS:CD2	2.26	0.53
1:F:90:LEU:H	1:F:90:LEU:HD22	1.73	0.53
1:F:27:ARG:HG3	2:F:156:HOH:O	2.08	0.53
1:D:125:GLU:HB2	2:D:168:HOH:O	2.07	0.53
1:G:86:LYS:HE3	1:G:88:ASN:HD21	1.74	0.53
1:A:126:GLU:OE1	1:E:12:ARG:NH2	2.42	0.53
1:H:37:GLU:HG2	1:H:101:ARG:HG2	1.90	0.53
1:G:9:GLN:HE21	1:G:13:ASP:CG	2.12	0.53
1:H:131:THR:HG23	2:H:148:HOH:O	2.08	0.53
1:H:52:PHE:CE1	1:H:94:GLU:HB3	2.44	0.53
1:B:48:GLN:HE22	1:B:50:HIS:HD2	1.57	0.52
1:F:86:LYS:HB2	1:H:86:LYS:CD	2.39	0.52
1:F:52:PHE:CD1	1:F:94:GLU:HB3	2.44	0.52
1:A:86:LYS:NZ	1:A:88:ASN:HD21	2.07	0.52
1:E:140:ILE:O	1:E:140:ILE:HD12	2.09	0.52
1:E:96:GLU:OE1	1:E:122:ARG:O	2.28	0.52
1:F:31:LEU:HD22	1:F:36:VAL:HG22	1.91	0.52
1:G:109:ARG:NH1	1:G:110:THR:OG1	2.43	0.52
1:E:70:ALA:HB2	1:E:136:LEU:HD13	1.91	0.52
1:B:96:GLU:OE2	1:B:122:ARG:O	2.28	0.52
1:D:122:ARG:HB3	2:D:168:HOH:O	2.09	0.52
1:E:44:ARG:HG2	1:E:44:ARG:HH11	1.75	0.52
1:G:92:PRO:HG2	2:G:151:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:TYR:CZ	1:D:33:PRO:HD3	2.45	0.52
1:E:4:PHE:CD1	1:E:10:LYS:HD2	2.45	0.51
1:B:3:ARG:HB2	1:B:73:LEU:O	2.10	0.51
1:G:90:LEU:HD22	1:G:90:LEU:N	2.24	0.51
1:C:90:LEU:N	1:C:90:LEU:CD1	2.74	0.51
1:E:42:TYR:OH	1:E:44:ARG:HD3	2.10	0.51
1:A:125:GLU:HG2	1:E:9:GLN:NE2	2.26	0.51
1:D:29:ASP:OD1	1:D:39:CYS:HB3	2.11	0.51
1:E:52:PHE:CD1	1:E:94:GLU:HB3	2.45	0.51
1:B:110:THR:HG22	1:B:111:LEU:CD1	2.37	0.51
1:H:82:THR:HA	1:H:136:LEU:HD23	1.91	0.51
1:A:27:ARG:NH1	1:A:27:ARG:HB3	2.26	0.51
1:C:11:VAL:HG11	1:C:31:LEU:HD21	1.93	0.51
1:C:40:MET:HE2	1:C:100:PHE:CZ	2.46	0.51
1:D:52:PHE:CD1	1:D:94:GLU:HB3	2.46	0.51
1:A:91:ASN:HB3	1:A:92:PRO:HD2	1.93	0.50
1:F:86:LYS:HE3	1:F:88:ASN:HD21	1.77	0.50
1:G:20:VAL:O	1:G:24:LEU:HG	2.11	0.50
1:A:30:THR:O	1:A:31:LEU:HD23	2.11	0.50
1:D:27:ARG:HB3	1:D:27:ARG:NH1	2.25	0.50
1:F:62:LEU:HD13	1:F:100:PHE:HD1	1.75	0.50
1:G:67:GLY:HA2	1:G:136:LEU:HD13	1.94	0.50
1:A:82:THR:HA	1:A:136:LEU:HD23	1.94	0.50
1:C:44:ARG:HH11	1:C:44:ARG:CG	2.25	0.50
1:A:91:ASN:OD1	1:B:106:LYS:HE3	2.13	0.49
1:H:94:GLU:HG3	1:H:122:ARG:HD3	1.92	0.49
1:B:90:LEU:HD23	1:B:130:ALA:HA	1.92	0.49
1:E:28:ILE:HA	1:E:38:LEU:HD23	1.95	0.49
1:C:62:LEU:HD21	1:C:118:ALA:HB2	1.94	0.49
1:B:70:ALA:HB2	1:B:136:LEU:HD12	1.94	0.49
1:B:2:PRO:HG3	1:B:33:PRO:HB2	1.95	0.49
1:G:108:GLY:HA3	1:G:109:ARG:HB3	1.95	0.49
1:G:10:LYS:HE3	1:G:71:PHE:CZ	2.48	0.49
1:E:54:HIS:CD2	1:G:20:VAL:HG11	2.48	0.49
1:D:31:LEU:O	1:D:32:LEU:HD22	2.13	0.48
1:F:44:ARG:HG2	1:F:44:ARG:HH11	1.78	0.48
1:B:62:LEU:HD13	1:B:100:PHE:HD1	1.78	0.48
1:G:109:ARG:CD	1:G:110:THR:H	2.26	0.48
1:D:27:ARG:HB2	1:D:39:CYS:SG	2.54	0.48
1:E:12:ARG:NH1	1:E:31:LEU:HD23	2.28	0.48
1:F:90:LEU:CD2	1:F:130:ALA:HA	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:90:LEU:CD2	1:F:90:LEU:N	2.76	0.48
2:E:142:HOH:O	1:G:17:ARG:HG3	2.12	0.48
1:B:4:PHE:CD1	1:B:10:LYS:HD2	2.49	0.48
1:F:33:PRO:HG2	2:F:144:HOH:O	2.14	0.48
1:B:4:PHE:HD1	1:B:10:LYS:HD2	1.79	0.48
1:A:27:ARG:HB3	1:A:27:ARG:HH11	1.79	0.48
1:A:22:ALA:HA	2:A:148:HOH:O	2.12	0.48
1:C:42:TYR:OH	1:C:47:THR:HG21	2.14	0.48
1:G:70:ALA:HB3	1:G:136:LEU:HD12	1.95	0.48
1:E:4:PHE:HD1	1:E:10:LYS:HD2	1.78	0.47
1:H:49:GLN:O	1:H:49:GLN:HG2	2.14	0.47
1:G:70:ALA:HB2	1:G:136:LEU:HD12	1.95	0.47
1:H:31:LEU:CD2	1:H:36:VAL:HG22	2.44	0.47
1:D:90:LEU:HD23	1:D:130:ALA:CA	2.44	0.47
1:D:90:LEU:CD2	1:D:90:LEU:N	2.77	0.47
1:B:31:LEU:O	1:B:32:LEU:HD23	2.15	0.47
1:B:48:GLN:HE22	1:B:50:HIS:CD2	2.33	0.47
1:E:32:LEU:HB3	1:E:33:PRO:HD2	1.96	0.47
1:F:1:GLU:HA	2:F:143:HOH:O	2.13	0.47
1:A:79:ALA:HB3	1:A:139:LEU:HB2	1.97	0.47
1:E:140:ILE:C	1:E:140:ILE:HD12	2.35	0.47
1:E:7:TYR:OH	1:E:33:PRO:HD3	2.15	0.47
1:F:4:PHE:CE1	1:F:76:GLU:HG3	2.50	0.46
1:F:70:ALA:CB	1:F:136:LEU:HD12	2.45	0.46
1:G:121:PHE:HA	1:G:125:GLU:O	2.16	0.46
1:G:53:LEU:HB2	1:G:93:ALA:HB1	1.97	0.46
1:A:121:PHE:CE2	1:A:126:GLU:HG3	2.50	0.46
1:G:62:LEU:HD13	1:G:100:PHE:HD1	1.81	0.46
1:C:70:ALA:CB	1:C:136:LEU:HD13	2.45	0.46
1:F:27:ARG:HH11	1:F:27:ARG:HB3	1.81	0.46
1:A:70:ALA:CB	1:A:136:LEU:HD13	2.46	0.46
1:A:70:ALA:HB2	1:A:136:LEU:HD13	1.98	0.46
1:C:55:ALA:HB1	1:C:89:PHE:CZ	2.51	0.46
1:H:110:THR:HG22	1:H:111:LEU:CD1	2.44	0.46
1:E:127:ARG:HG2	1:E:127:ARG:NH1	2.29	0.46
1:B:127:ARG:HG2	1:B:127:ARG:HH11	1.82	0.45
1:H:122:ARG:NH2	1:H:127:ARG:HE	2.07	0.45
1:B:52:PHE:CD1	1:B:94:GLU:HB3	2.51	0.45
1:B:70:ALA:HB3	1:B:136:LEU:HD12	1.99	0.45
1:C:41:PRO:HG2	2:C:155:HOH:O	2.16	0.45
1:G:34:GLY:HA2	1:G:69:ALA:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:122:ARG:HB3	1:G:123:ASP:H	1.67	0.45
1:B:90:LEU:CD2	1:B:130:ALA:HA	2.46	0.45
1:A:127:ARG:HH11	1:A:127:ARG:HG2	1.82	0.45
1:B:32:LEU:HB2	1:B:35:ARG:HD3	1.98	0.45
1:C:85:PHE:HE1	1:D:85:PHE:HE1	1.65	0.45
1:E:8:ALA:HA	1:E:31:LEU:HD21	1.98	0.45
1:C:20:VAL:O	1:C:24:LEU:HG	2.17	0.45
1:F:131:THR:HG23	2:F:172:HOH:O	2.16	0.45
1:D:90:LEU:CD2	1:D:130:ALA:HA	2.46	0.44
1:B:86:LYS:NZ	1:B:88:ASN:HD21	2.15	0.44
1:D:101:ARG:HD2	1:D:119:TYR:CE1	2.52	0.44
1:H:127:ARG:NH1	1:H:127:ARG:HG2	2.31	0.44
1:H:3:ARG:HH22	1:H:109:ARG:CG	2.26	0.44
1:A:48:GLN:HE22	1:A:50:HIS:CD2	2.35	0.44
1:G:42:TYR:OH	1:G:44:ARG:HD2	2.17	0.44
1:D:91:ASN:HB3	1:D:92:PRO:HD2	1.99	0.44
1:G:32:LEU:HB3	1:G:33:PRO:HD2	1.99	0.44
1:B:35:ARG:O	1:B:36:VAL:CB	2.65	0.44
1:D:55:ALA:HB1	1:D:89:PHE:CE1	2.52	0.44
1:E:40:MET:HE2	1:E:40:MET:HB3	1.82	0.44
1:F:127:ARG:HD3	2:F:147:HOH:O	2.18	0.44
1:F:9:GLN:HG3	1:F:13:ASP:OD2	2.18	0.44
1:D:55:ALA:HB1	1:D:89:PHE:CZ	2.53	0.43
1:H:51:GLY:HA2	2:H:174:HOH:O	2.17	0.43
1:G:44:ARG:HG2	2:G:150:HOH:O	2.18	0.43
1:D:37:GLU:HG2	1:D:101:ARG:CG	2.45	0.43
1:A:28:ILE:CG2	1:A:31:LEU:HG	2.48	0.43
1:B:30:THR:O	1:B:36:VAL:HA	2.19	0.43
1:F:31:LEU:C	1:F:31:LEU:HD13	2.38	0.43
1:B:70:ALA:HB3	1:B:136:LEU:CD1	2.49	0.43
1:F:3:ARG:HB3	1:F:75:GLU:OE1	2.19	0.43
1:H:82:THR:O	1:H:82:THR:HG23	2.19	0.43
1:B:35:ARG:HG2	1:B:35:ARG:HH21	1.84	0.43
1:F:90:LEU:CD2	1:F:90:LEU:H	2.30	0.43
1:C:121:PHE:HA	1:C:125:GLU:O	2.19	0.42
1:C:31:LEU:HD22	1:C:36:VAL:HG22	2.00	0.42
1:F:90:LEU:HD23	1:F:130:ALA:CA	2.48	0.42
1:C:86:LYS:HD2	1:C:86:LYS:C	2.40	0.42
1:F:131:THR:HG21	2:F:187:HOH:O	2.18	0.42
1:A:110:THR:O	1:A:137:MET:HA	2.19	0.42
1:G:109:ARG:HD2	1:G:110:THR:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:LYS:HG2	1:D:86:LYS:HB2	2.01	0.42
1:H:12:ARG:NH1	2:H:198:HOH:O	2.53	0.42
1:F:53:LEU:HA	1:F:53:LEU:HD12	1.92	0.42
1:G:111:LEU:N	1:G:111:LEU:HD23	2.34	0.42
1:D:52:PHE:CE1	1:D:94:GLU:HB3	2.54	0.42
1:E:70:ALA:CB	1:E:136:LEU:HD13	2.50	0.42
1:E:67:GLY:HA2	1:E:136:LEU:HD22	2.00	0.42
1:E:3:ARG:HD3	1:E:75:GLU:OE1	2.19	0.42
1:B:89:PHE:CD2	1:F:82:THR:HG23	2.54	0.42
1:H:31:LEU:C	1:H:31:LEU:HD13	2.40	0.42
1:A:13:ASP:O	1:A:17:ARG:HG2	2.19	0.42
1:A:55:ALA:HB1	1:A:89:PHE:CZ	2.55	0.42
1:B:97:ARG:HD3	1:D:32:LEU:CB	2.50	0.42
1:C:94:GLU:HA	2:C:167:HOH:O	2.20	0.42
1:F:110:THR:O	1:F:137:MET:HA	2.20	0.42
1:A:90:LEU:CD2	1:A:90:LEU:N	2.82	0.42
1:D:27:ARG:CB	1:D:27:ARG:NH1	2.83	0.41
1:E:52:PHE:CE1	1:E:94:GLU:HB3	2.55	0.41
1:F:52:PHE:CE1	1:F:94:GLU:HB3	2.55	0.41
1:C:94:GLU:CD	1:C:122:ARG:HH11	2.24	0.41
1:F:82:THR:O	1:F:82:THR:HG23	2.19	0.41
1:G:37:GLU:HG2	1:G:101:ARG:HG2	2.01	0.41
1:H:141:GLY:HA3	2:H:187:HOH:O	2.21	0.41
1:D:122:ARG:HB3	1:D:123:ASP:H	1.58	0.41
1:D:27:ARG:CB	1:D:27:ARG:HH11	2.33	0.41
1:B:7:TYR:CG	1:B:8:ALA:N	2.88	0.41
1:C:44:ARG:NH1	1:C:44:ARG:CG	2.81	0.41
1:H:110:THR:O	1:H:137:MET:HA	2.20	0.41
1:E:1:GLU:HA	1:E:2:PRO:HD3	1.90	0.41
1:D:9:GLN:HE21	1:D:13:ASP:CG	2.24	0.41
1:D:11:VAL:HB	1:D:31:LEU:HD11	2.03	0.41
1:C:32:LEU:HB3	1:C:33:PRO:HD2	2.01	0.41
1:H:62:LEU:HD13	1:H:100:PHE:HD1	1.86	0.41
1:B:90:LEU:N	1:B:90:LEU:CD2	2.84	0.41
1:G:40:MET:HE2	1:G:100:PHE:CE2	2.55	0.41
1:E:37:GLU:HG3	1:E:101:ARG:CG	2.44	0.40
1:H:42:TYR:HB2	1:H:96:GLU:HA	2.03	0.40
1:C:49:GLN:HB2	1:D:18:GLN:HE22	1.86	0.40
1:D:140:ILE:C	1:D:140:ILE:HD12	2.41	0.40
1:G:131:THR:HG23	2:G:168:HOH:O	2.21	0.40
1:G:1:GLU:OE1	1:G:2:PRO:HD2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:91:ASN:HB3	1:H:92:PRO:HD2	2.03	0.40
1:B:11:VAL:HG13	1:B:68:TYR:CD1	2.56	0.40
1:A:90:LEU:O	1:B:106:LYS:HE3	2.21	0.40
1:C:62:LEU:CD2	1:C:118:ALA:HB2	2.51	0.40
1:H:53:LEU:HD23	1:H:98:PHE:CZ	2.56	0.40
1:G:108:GLY:HA3	1:G:109:ARG:CB	2.38	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	134/141 (95%)	129 (96%)	4 (3%)	1 (1%)	22 16
1	B	138/141 (98%)	128 (93%)	7 (5%)	3 (2%)	6 2
1	C	139/141 (99%)	135 (97%)	4 (3%)	0	100 100
1	D	135/141 (96%)	131 (97%)	3 (2%)	1 (1%)	22 16
1	E	139/141 (99%)	133 (96%)	4 (3%)	2 (1%)	11 5
1	F	139/141 (99%)	135 (97%)	4 (3%)	0	100 100
1	G	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	22 16
1	H	139/141 (99%)	136 (98%)	3 (2%)	0	100 100
All	All	1102/1128 (98%)	1061 (96%)	33 (3%)	8 (1%)	22 16

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	ARG
1	D	109	ARG
1	A	122	ARG
1	B	36	VAL

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Mol	Chain	Res	Type
1	E	33	PRO
1	G	109	ARG
1	E	122	ARG
1	B	4	PHE

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	104/108 (96%)	102 (98%)	2 (2%)	57	61
1	B	107/108 (99%)	104 (97%)	3 (3%)	43	44
1	C	108/108 (100%)	103 (95%)	5 (5%)	27	23
1	D	104/108 (96%)	101 (97%)	3 (3%)	42	43
1	E	108/108 (100%)	103 (95%)	5 (5%)	27	23
1	F	108/108 (100%)	103 (95%)	5 (5%)	27	23
1	G	108/108 (100%)	106 (98%)	2 (2%)	57	61
1	H	108/108 (100%)	105 (97%)	3 (3%)	43	44
All	All	855/864 (99%)	827 (97%)	28 (3%)	38	37

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ASP
1	A	48	GLN
1	B	48	GLN
1	B	123	ASP
1	B	140	ILE
1	C	29	ASP
1	C	31	LEU
1	C	44	ARG
1	C	48	GLN
1	C	62	LEU
1	D	48	GLN

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Mol	Chain	Res	Type
1	D	111	LEU
1	D	136	LEU
1	E	33	PRO
1	E	44	ARG
1	E	48	GLN
1	E	62	LEU
1	E	90	LEU
1	F	27	ARG
1	F	44	ARG
1	F	48	GLN
1	F	62	LEU
1	F	75	GLU
1	G	1	GLU
1	G	48	GLN
1	H	44	ARG
1	H	48	GLN
1	H	96	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	50	HIS
1	A	88	ASN
1	B	50	HIS
1	B	88	ASN
1	C	18	GLN
1	C	50	HIS
1	C	88	ASN
1	D	9	GLN
1	E	88	ASN
1	F	9	GLN
1	F	49	GLN
1	F	50	HIS
1	F	88	ASN
1	G	9	GLN
1	G	18	GLN
1	G	50	HIS
1	G	88	ASN
1	H	18	GLN
1	H	88	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 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	136/141 (96%)	0.47	11 (8%) 12 11	7, 18, 39, 46	0
1	B	140/141 (99%)	0.65	14 (10%) 7 6	8, 17, 39, 49	1 (0%)
1	C	141/141 (100%)	0.36	8 (5%) 23 23	8, 17, 34, 44	0
1	D	137/141 (97%)	0.43	9 (6%) 18 17	10, 19, 40, 46	0
1	E	141/141 (100%)	0.57	14 (9%) 7 6	10, 18, 40, 47	0
1	F	141/141 (100%)	0.46	7 (4%) 28 28	9, 18, 34, 43	0
1	G	141/141 (100%)	0.64	11 (7%) 13 12	10, 21, 40, 51	0
1	H	141/141 (100%)	0.31	9 (6%) 19 18	7, 17, 36, 43	0
All	All	1118/1128 (99%)	0.49	83 (7%) 14 13	7, 18, 39, 51	1 (0%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	141	GLY	9.3
1	F	141	GLY	7.4
1	B	140	ILE	6.7
1	B	4	PHE	6.5
1	B	141	GLY	6.4
1	A	140	ILE	6.1
1	B	2	PRO	5.7
1	G	140	ILE	5.5
1	B	3	ARG	5.1
1	D	140	ILE	5.1
1	E	141	GLY	5.1
1	E	3	ARG	4.8
1	A	141	GLY	4.7
1	H	141	GLY	4.6
1	D	141	GLY	4.6
1	C	140	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	140	ILE	4.4
1	C	139	LEU	4.3
1	B	123	ASP	4.2
1	B	77	GLU	4.1
1	B	35	ARG	4.0
1	E	1	GLU	3.9
1	H	140	ILE	3.9
1	C	122	ARG	3.9
1	F	77	GLU	3.8
1	F	140	ILE	3.8
1	E	77	GLU	3.7
1	C	141	GLY	3.7
1	E	4	PHE	3.7
1	B	109	ARG	3.6
1	D	77	GLU	3.5
1	H	109	ARG	3.5
1	D	109	ARG	3.5
1	D	5	ALA	3.3
1	A	75	GLU	3.3
1	H	44	ARG	3.2
1	E	2	PRO	3.1
1	G	17	ARG	3.1
1	A	31	LEU	3.1
1	A	124	GLY	3.1
1	G	4	PHE	3.1
1	A	78	ALA	3.0
1	C	123	ASP	3.0
1	C	109	ARG	2.9
1	E	75	GLU	2.9
1	E	109	ARG	2.9
1	G	27	ARG	2.8
1	A	77	GLU	2.8
1	D	127	ARG	2.7
1	D	8	ALA	2.7
1	B	122	ARG	2.7
1	C	125	GLU	2.6
1	B	97	ARG	2.5
1	G	76	GLU	2.5
1	A	6	GLY	2.5
1	E	139	LEU	2.5
1	F	4	PHE	2.5
1	A	109	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	76	GLU	2.4
1	G	5	ALA	2.4
1	H	123	ASP	2.4
1	F	109	ARG	2.4
1	D	123	ASP	2.3
1	H	127	ARG	2.3
1	G	75	GLU	2.3
1	H	125	GLU	2.3
1	B	44	ARG	2.2
1	G	39	CYS	2.2
1	E	33	PRO	2.2
1	F	49	GLN	2.2
1	G	81	LEU	2.2
1	H	96	GLU	2.2
1	H	92	PRO	2.2
1	A	76	GLU	2.2
1	C	77	GLU	2.2
1	A	123	ASP	2.2
1	E	122	ARG	2.2
1	G	109	ARG	2.2
1	E	49	GLN	2.1
1	E	34	GLY	2.1
1	B	5	ALA	2.0
1	B	78	ALA	2.0
1	D	122	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no 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.