Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:16 AM GMT

PDB ID : 3LHF

Title : The Crystal Structure of a Serine Recombinase from Sulfolobus solfataricus to 2.3A

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Deposited on : 2010-01-22

Resolution : 2.30 Å(reported)

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

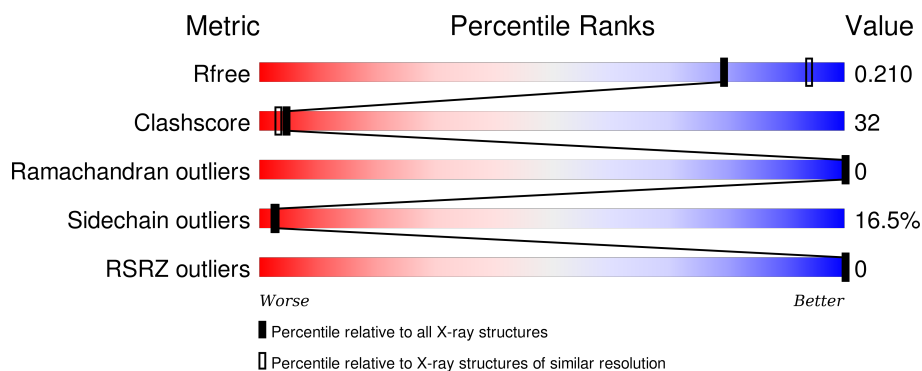|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	Percentile Ranks	Value
Rfree		0.210
Clashscore		32
Ramachandran outliers		0
Sidechain outliers		16.5%
RSRZ outliers		0

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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. 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	140	49% 43% 5% · ·
1	B	140	44% 46% 7% ·
1	C	140	53% 38% 9%
1	D	140	50% 41% 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4427 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 Serine Recombinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	136	Total	C	N	O	S	0	0	0
			1075	685	185	199	6			
1	B	136	Total	C	N	O	S	0	0	0
			1075	685	185	199	6			
1	C	140	Total	C	N	O	S	0	0	0
			1099	698	185	210	6			
1	D	140	Total	C	N	O	S	0	0	0
			1099	700	187	206	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	95	GLY	LYS	engineered	UNP Q97XB5
B	95	GLY	LYS	engineered	UNP Q97XB5
C	95	GLY	LYS	engineered	UNP Q97XB5
D	95	GLY	LYS	engineered	UNP Q97XB5

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	22	Total	O	0	0
			22	22		
2	B	21	Total	O	0	0
			21	21		
2	C	21	Total	O	0	0
			21	21		
2	D	15	Total	O	0	0
			15	15		

3　Residue-property plots ⓘ

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

- Molecule 1: Serine Recombinase
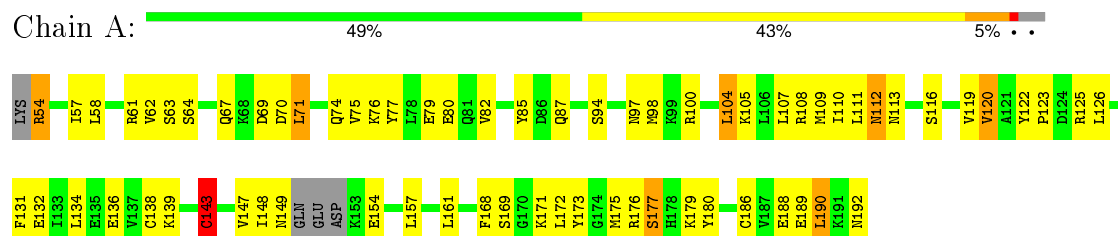
Chain A:

- Molecule 1: Serine Recombinase

Chain B:

- Molecule 1: Serine Recombinase

Chain C:

- Molecule 1: Serine Recombinase

Chain D:
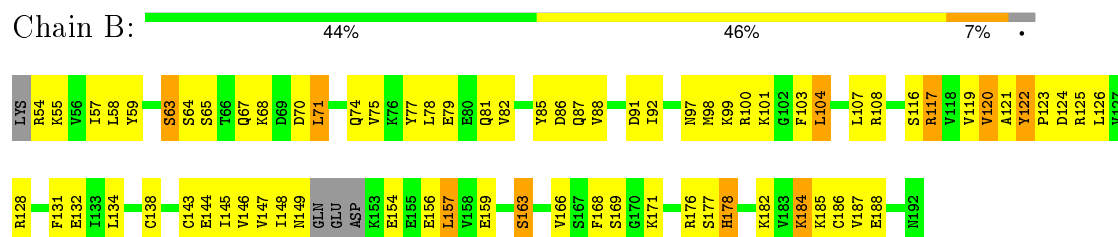
4 Data and refinement statistics (i)

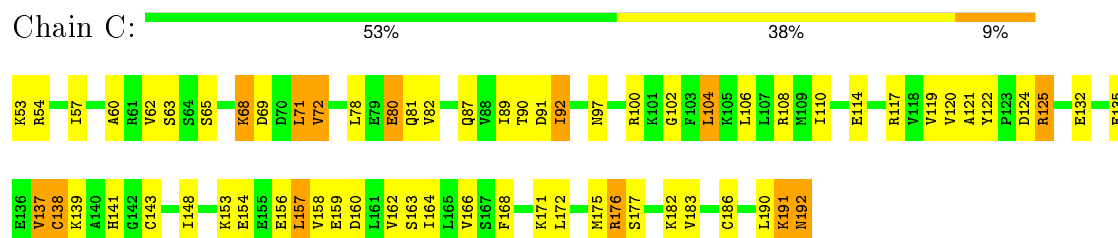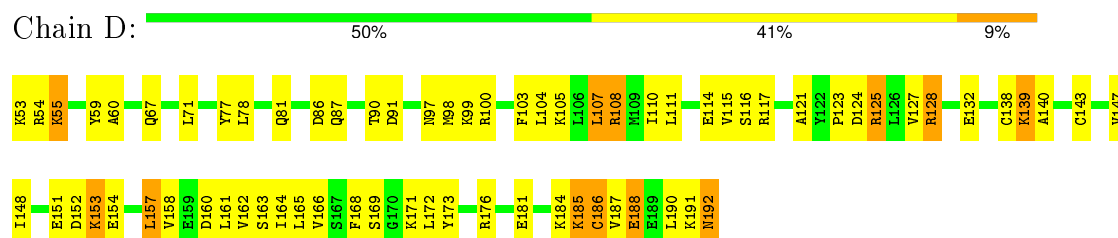| Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	83.36Å 83.36Å 83.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.46 – 2.30 37.46 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.9 (37.46-2.30) 98.7 (37.46-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 2.29Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.178 , 0.226 0.187 , 0.210	Depositor DCC
R_{free} test set	1285 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	46.4	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 35.3	EDS
Estimated twinning fraction	0.019 for -h,-l,-k 0.005 for -h,l,k 0.012 for l,-k,h 0.019 for -l,-k,-h 0.476 for h,-k,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	0 of 25200 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4427	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	1.24	1/1086 (0.1%)	0.71	0/1459
1	B	1.21	0/1086	0.72	0/1459
1	C	1.31	1/1110 (0.1%)	0.74	0/1494
1	D	1.22	0/1110	0.73	0/1492
All	All	1.25	2/4392 (0.0%)	0.73	0/5904

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	CYS	CB-SG	-5.94	1.72	1.81
1	C	138	CYS	CB-SG	-5.89	1.72	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1075	0	1094	79	4
1	B	1075	0	1095	90	4
1	C	1099	0	1103	63	0
1	D	1099	0	1118	90	0
2	A	22	0	0	0	0
2	B	21	0	0	1	0
2	C	21	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	15	0	0	1	0
All	All	4427	0	4410	279	4

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 32.

All (279) 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:77:TYR:OH	1:A:148:ILE:CG2	1.67	1.41
1:A:186:CYS:CB	1:D:186:CYS:SG	2.17	1.32
1:B:177:SER:OG	1:C:154:GLU:OE1	1.61	1.15
1:A:186:CYS:SG	1:D:186:CYS:CB	2.37	1.11
1:B:186:CYS:CB	1:C:186:CYS:SG	2.40	1.09
1:B:138:CYS:SG	1:B:145:ILE:HD11	1.93	1.06
1:D:186:CYS:O	1:D:190:LEU:HD13	1.52	1.05
1:B:148:ILE:HG22	1:B:149:ASN:OD1	1.58	1.03
1:B:77:TYR:CZ	1:B:148:ILE:HG21	1.94	1.02
1:B:77:TYR:OH	1:B:148:ILE:CG2	2.06	1.02
1:A:186:CYS:HG	1:D:186:CYS:CB	1.74	1.00
1:D:192:ASN:HD22	1:D:192:ASN:H	1.01	0.99
1:A:77:TYR:OH	1:A:148:ILE:HG21	0.81	0.98
1:A:76:LYS:O	1:A:80:GLU:HG3	1.63	0.98
1:A:136:GLU:OE1	1:D:108:ARG:NH2	1.98	0.96
1:C:62:VAL:HG23	1:C:92:ILE:HG13	1.52	0.90
1:A:77:TYR:CZ	1:A:148:ILE:HG21	2.07	0.90
1:A:147:VAL:O	1:A:147:VAL:HG23	1.69	0.90
1:A:190:LEU:N	1:A:190:LEU:HD23	1.87	0.89
1:C:162:VAL:O	1:C:166:VAL:HG23	1.73	0.88
1:B:186:CYS:SG	1:C:186:CYS:CB	2.62	0.86
1:D:97:ASN:HB3	1:D:100:ARG:HD2	1.57	0.85
1:B:154:GLU:OE1	1:C:177:SER:HB2	1.79	0.82
1:A:147:VAL:HG11	1:C:176:ARG:HG3	1.62	0.81
1:B:154:GLU:OE1	1:C:177:SER:CB	2.29	0.79
1:B:119:VAL:HG22	1:B:146:VAL:HB	1.65	0.79
1:B:122:TYR:HB2	1:B:123:PRO:CD	2.13	0.79
1:B:92:ILE:HD12	1:B:92:ILE:N	1.98	0.79
1:D:192:ASN:HD22	1:D:192:ASN:N	1.78	0.78
1:B:97:ASN:O	1:B:100:ARG:HD3	1.84	0.78
1:B:147:VAL:HG23	1:B:147:VAL:O	1.84	0.78
1:B:77:TYR:CZ	1:B:148:ILE:CG2	2.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LEU:HD22	1:D:140:ALA:CB	2.14	0.77
1:D:53:LYS:CE	1:D:54:ARG:H	1.98	0.77
1:A:100:ARG:NH2	1:A:126:LEU:O	2.17	0.76
1:D:192:ASN:ND2	1:D:192:ASN:H	1.82	0.76
1:A:122:TYR:HB2	1:A:123:PRO:CD	2.16	0.76
1:C:192:ASN:HD22	1:C:192:ASN:N	1.84	0.76
1:D:128:ARG:HD2	1:D:160:ASP:OD2	1.86	0.75
1:C:106:LEU:O	1:C:110:ILE:HG13	1.87	0.75
1:D:124:ASP:HB3	1:D:125:ARG:HH11	1.50	0.74
1:C:82:VAL:HG21	1:C:119:VAL:HG11	1.70	0.74
1:B:138:CYS:HB3	1:B:143:CYS:O	1.87	0.73
1:B:54:ARG:NE	1:B:116:SER:HB3	2.02	0.73
1:B:54:ARG:CD	1:B:116:SER:HB3	2.18	0.73
1:B:122:TYR:CB	1:B:123:PRO:CD	2.66	0.73
1:B:123:PRO:O	1:B:124:ASP:HB2	1.88	0.72
1:A:87:GLN:HE22	1:A:109:MET:CE	2.02	0.72
1:C:57:ILE:HD13	1:C:87:GLN:HB2	1.71	0.72
1:B:157:LEU:CD2	1:C:168:PHE:CE1	2.73	0.71
1:C:68:LYS:HG2	1:C:69:ASP:N	2.05	0.71
1:A:132:GLU:OE1	1:D:98:MET:HG3	1.90	0.71
1:A:97:ASN:O	1:A:100:ARG:HD3	1.92	0.69
1:A:186:CYS:O	1:A:190:LEU:HG	1.91	0.69
1:D:185:LYS:O	1:D:188:GLU:HG2	1.92	0.69
1:D:55:LYS:HB2	1:D:114:GLU:O	1.91	0.69
1:B:122:TYR:CB	1:B:123:PRO:HD3	2.23	0.69
1:B:168:PHE:CE1	1:C:157:LEU:HD22	2.29	0.68
1:A:147:VAL:O	1:A:147:VAL:CG2	2.42	0.68
1:D:55:LYS:HA	1:D:86:ASP:OD2	1.94	0.68
1:B:98:MET:HG3	1:C:132:GLU:OE1	1.93	0.68
1:B:54:ARG:HD3	1:B:116:SER:HB3	1.77	0.67
1:D:110:ILE:HG12	1:D:115:VAL:HG21	1.77	0.67
1:C:137:VAL:O	1:C:141:HIS:HD2	1.77	0.67
1:B:91:ASP:C	1:B:92:ILE:HD12	2.14	0.67
1:A:173:TYR:HB2	1:A:180:TYR:CE1	2.30	0.67
1:A:175:MET:SD	1:D:154:GLU:HG3	2.34	0.67
1:A:190:LEU:H	1:A:190:LEU:HD23	1.61	0.66
1:D:53:LYS:HG3	1:D:54:ARG:N	2.09	0.66
1:A:54:ARG:HD3	1:A:116:SER:HB3	1.77	0.66
1:A:186:CYS:HB2	1:D:186:CYS:SG	2.33	0.66
1:D:121:ALA:HA	1:D:148:ILE:HG12	1.77	0.66
1:B:82:VAL:HG12	1:B:82:VAL:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:TYR:OH	1:B:148:ILE:HG22	1.95	0.65
1:C:68:LYS:HG3	2:C:36:HOH:O	1.96	0.65
1:B:91:ASP:OD2	1:B:100:ARG:HB3	1.96	0.65
1:A:190:LEU:N	1:A:190:LEU:CD2	2.58	0.65
1:D:97:ASN:O	1:D:100:ARG:HD3	1.97	0.65
1:B:131:PHE:CZ	1:D:176:ARG:HD2	2.30	0.65
1:D:191:LYS:O	1:D:192:ASN:C	2.34	0.65
1:B:77:TYR:CE1	1:B:148:ILE:HG21	2.32	0.64
1:B:63:SER:HB3	1:B:156:GLU:OE2	1.98	0.64
1:B:149:ASN:N	1:B:149:ASN:OD1	2.30	0.64
1:B:178:HIS:ND1	1:B:178:HIS:N	2.45	0.64
1:D:151:GLU:CD	1:D:153:LYS:HE3	2.18	0.64
1:B:77:TYR:CE2	1:B:81:GLN:HG3	2.32	0.64
1:D:53:LYS:CG	1:D:54:ARG:H	2.10	0.64
1:C:60:ALA:O	1:C:90:THR:HA	1.98	0.63
1:A:131:PHE:HA	1:A:134:LEU:HD12	1.81	0.63
1:D:97:ASN:O	1:D:100:ARG:CD	2.46	0.63
1:D:162:VAL:O	1:D:166:VAL:HG23	2.00	0.62
1:A:87:GLN:HE22	1:A:109:MET:HE1	1.63	0.62
1:A:87:GLN:NE2	1:A:109:MET:HE1	2.15	0.62
1:B:147:VAL:CG2	1:B:147:VAL:O	2.48	0.62
1:B:71:LEU:O	1:B:75:VAL:HG23	2.00	0.61
1:A:186:CYS:O	1:A:190:LEU:CD2	2.48	0.61
1:B:70:ASP:O	1:B:74:GLN:N	2.30	0.61
1:B:92:ILE:CD1	1:B:92:ILE:N	2.62	0.61
1:D:125:ARG:HD2	1:D:125:ARG:N	2.16	0.61
1:B:64:SER:HB3	1:B:67:GLN:OE1	2.01	0.60
1:C:162:VAL:HG11	1:C:191:LYS:HG2	1.83	0.60
1:D:60:ALA:O	1:D:90:THR:HA	2.02	0.60
1:D:187:VAL:HG12	1:D:191:LYS:CE	2.32	0.60
1:B:126:LEU:HD13	1:B:134:LEU:HD13	1.84	0.59
1:D:151:GLU:OE2	1:D:153:LYS:HE3	2.01	0.59
1:C:104:LEU:O	1:C:108:ARG:HD2	2.01	0.59
1:A:132:GLU:HB2	1:D:98:MET:HB3	1.84	0.59
1:B:132:GLU:HG3	1:D:173:TYR:OH	2.03	0.59
1:B:78:LEU:HD23	1:B:148:ILE:HD12	1.83	0.59
1:A:120:VAL:CG1	1:A:122:TYR:O	2.50	0.59
1:A:122:TYR:HB2	1:A:123:PRO:HD3	1.85	0.59
1:D:55:LYS:NZ	1:D:87:GLN:HE22	2.01	0.58
1:A:132:GLU:CB	1:D:98:MET:HB3	2.33	0.58
1:D:188:GLU:HA	1:D:191:LYS:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:LYS:CG	1:D:54:ARG:N	2.65	0.57
1:A:57:ILE:HD13	1:A:87:GLN:HB3	1.86	0.57
1:D:187:VAL:HG12	1:D:191:LYS:HE2	1.86	0.57
1:D:185:LYS:HA	1:D:188:GLU:OE1	2.05	0.57
1:D:151:GLU:HG2	1:D:152:ASP:N	2.19	0.57
1:B:122:TYR:HB2	1:B:123:PRO:HD2	1.84	0.57
1:B:79:GLU:HG2	1:B:85:TYR:CZ	2.40	0.56
1:A:171:LYS:HD3	1:D:157:LEU:HD11	1.87	0.56
1:A:179:LYS:NZ	1:D:192:ASN:HB2	2.21	0.56
1:C:57:ILE:CD1	1:C:87:GLN:HB2	2.36	0.56
1:C:62:VAL:HG22	1:C:71:LEU:HG	1.87	0.56
1:D:99:LYS:HA	1:D:104:LEU:HD11	1.88	0.56
1:A:171:LYS:NZ	1:D:152:ASP:OD2	2.28	0.55
1:C:97:ASN:O	1:C:100:ARG:HD3	2.06	0.55
1:B:154:GLU:OE1	1:C:177:SER:HB3	2.06	0.55
1:A:94:SER:O	1:A:100:ARG:HD2	2.07	0.55
1:A:186:CYS:O	1:A:190:LEU:CG	2.54	0.55
1:C:62:VAL:CG2	1:C:92:ILE:HG13	2.33	0.54
1:A:64:SER:N	1:A:67:GLN:OE1	2.39	0.54
1:A:147:VAL:HG21	1:C:176:ARG:HB2	1.88	0.54
1:C:175:MET:C	1:C:176:ARG:HG2	2.27	0.54
1:D:104:LEU:O	1:D:108:ARG:HB2	2.07	0.54
1:A:112:ASN:O	1:A:113:ASN:HB2	2.07	0.54
1:C:68:LYS:CG	1:C:69:ASP:N	2.71	0.54
1:B:79:GLU:HG2	1:B:85:TYR:CE1	2.43	0.54
1:C:137:VAL:O	1:C:141:HIS:CD2	2.60	0.53
1:B:156:GLU:HA	1:B:159:GLU:OE2	2.08	0.53
1:B:120:VAL:CG1	1:B:122:TYR:O	2.57	0.53
1:B:157:LEU:HD22	1:C:168:PHE:CD1	2.44	0.53
1:B:104:LEU:O	1:B:108:ARG:HD2	2.09	0.53
1:D:151:GLU:CG	1:D:152:ASP:N	2.72	0.53
1:C:168:PHE:HA	1:C:171:LYS:HG3	1.90	0.52
1:B:120:VAL:HG13	1:B:121:ALA:N	2.25	0.52
1:D:53:LYS:HE3	1:D:54:ARG:H	1.73	0.52
1:C:192:ASN:HD22	1:C:192:ASN:H	1.55	0.52
1:B:131:PHE:CZ	1:D:176:ARG:CD	2.93	0.52
1:B:159:GLU:O	1:B:163:SER:OG	2.27	0.51
1:D:53:LYS:HE2	1:D:54:ARG:H	1.75	0.51
1:C:80:GLU:HG3	1:C:81:GLN:N	2.20	0.51
1:C:53:LYS:HG2	1:C:54:ARG:N	2.26	0.51
1:A:62:VAL:HG22	1:A:71:LEU:HG	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:LYS:O	1:C:72:VAL:HG13	2.10	0.51
1:C:68:LYS:HG2	1:C:69:ASP:H	1.73	0.51
1:A:179:LYS:HZ1	1:D:192:ASN:HB2	1.76	0.51
1:A:87:GLN:HE22	1:A:109:MET:HE3	1.73	0.51
1:B:119:VAL:HA	1:B:146:VAL:O	2.11	0.51
1:C:139:LYS:HD3	1:C:139:LYS:C	2.31	0.50
1:A:77:TYR:OH	1:A:148:ILE:HG22	1.95	0.50
1:A:122:TYR:HB2	1:A:123:PRO:HD2	1.94	0.50
1:B:85:TYR:O	1:B:85:TYR:CG	2.64	0.50
1:A:161:LEU:HD13	1:D:168:PHE:CD1	2.46	0.50
1:B:117:ARG:HG3	1:B:144:GLU:HB3	1.94	0.50
1:A:120:VAL:HG21	1:A:126:LEU:HG	1.94	0.50
1:D:78:LEU:HD11	2:D:3:HOH:O	2.12	0.50
1:B:120:VAL:HG11	1:B:122:TYR:O	2.12	0.49
1:D:98:MET:CE	1:D:98:MET:HA	2.42	0.49
1:A:189:GLU:HA	1:A:192:ASN:HB2	1.94	0.49
1:A:79:GLU:HG2	1:A:85:TYR:CZ	2.47	0.49
1:D:186:CYS:O	1:D:190:LEU:CD1	2.44	0.49
1:C:192:ASN:N	1:C:192:ASN:ND2	2.55	0.49
1:B:57:ILE:HG22	1:B:58:LEU:N	2.28	0.48
1:D:115:VAL:HG12	1:D:143:CYS:SG	2.53	0.48
1:D:55:LYS:HZ1	1:D:87:GLN:HE22	1.62	0.48
1:B:87:GLN:HG3	1:B:88:VAL:N	2.28	0.48
1:C:160:ASP:O	1:C:164:ILE:N	2.32	0.48
1:B:185:LYS:O	1:B:188:GLU:HG2	2.13	0.48
1:B:58:LEU:HD13	1:B:78:LEU:HB3	1.94	0.48
1:D:77:TYR:O	1:D:81:GLN:HG2	2.14	0.48
1:A:57:ILE:HD11	1:A:109:MET:HE1	1.96	0.48
1:B:75:VAL:HG13	1:B:88:VAL:HG11	1.94	0.48
1:C:138:CYS:HB3	1:C:143:CYS:HB3	1.95	0.48
1:B:120:VAL:CG1	1:B:121:ALA:N	2.73	0.47
1:A:168:PHE:CE1	1:D:157:LEU:HD22	2.48	0.47
1:A:120:VAL:HG13	1:A:122:TYR:O	2.14	0.47
1:A:98:MET:HG3	1:D:132:GLU:OE1	2.14	0.47
1:D:165:LEU:HD13	1:D:190:LEU:HD22	1.97	0.47
1:B:148:ILE:HG22	1:B:149:ASN:CG	2.31	0.46
1:B:78:LEU:HD11	2:B:24:HOH:O	2.15	0.46
1:D:97:ASN:O	1:D:100:ARG:HD2	2.15	0.46
1:A:61:ARG:H	1:A:74:GLN:HE22	1.61	0.46
1:A:138:CYS:HB3	1:A:143:CYS:HB3	1.97	0.46
1:D:107:LEU:HD13	1:D:111:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:PRO:HD3	1:D:147:VAL:HG11	1.97	0.46
1:B:87:GLN:CG	1:B:88:VAL:N	2.79	0.46
1:A:71:LEU:O	1:A:75:VAL:HG23	2.15	0.46
1:D:161:LEU:HG	1:D:165:LEU:HD12	1.98	0.45
1:D:115:VAL:CG1	1:D:143:CYS:SG	3.05	0.45
1:D:158:VAL:O	1:D:162:VAL:HG23	2.16	0.45
1:A:104:LEU:HD12	1:A:104:LEU:HA	1.77	0.45
1:B:91:ASP:OD2	1:B:103:PHE:N	2.48	0.45
1:C:124:ASP:OD2	1:C:125:ARG:HD2	2.17	0.45
1:D:192:ASN:ND2	1:D:192:ASN:N	2.51	0.45
1:D:123:PRO:HD3	1:D:147:VAL:CG1	2.47	0.45
1:A:186:CYS:O	1:A:190:LEU:HD23	2.14	0.45
1:A:147:VAL:HG11	1:C:176:ARG:CG	2.41	0.45
1:B:86:ASP:N	1:B:86:ASP:OD1	2.49	0.45
1:C:132:GLU:HA	1:C:135:GLU:OE1	2.17	0.44
1:A:58:LEU:HD23	1:A:119:VAL:HB	1.99	0.44
1:B:182:LYS:HB3	1:C:190:LEU:HD21	2.00	0.44
1:D:164:ILE:HG23	1:D:168:PHE:CE2	2.53	0.44
1:B:128:ARG:HD2	1:C:168:PHE:HZ	1.82	0.44
1:C:89:ILE:CG2	1:C:102:GLY:HA3	2.48	0.44
1:B:157:LEU:CD2	1:C:168:PHE:CD1	2.99	0.44
1:B:117:ARG:HA	1:B:144:GLU:O	2.17	0.44
1:D:139:LYS:HG3	1:D:140:ALA:N	2.31	0.44
1:B:166:VAL:O	1:B:169:SER:HB3	2.17	0.44
1:D:164:ILE:O	1:D:168:PHE:HD2	2.01	0.44
1:C:78:LEU:HD21	1:C:121:ALA:HB2	1.99	0.44
1:D:78:LEU:HD23	1:D:148:ILE:CD1	2.48	0.43
1:A:82:VAL:O	1:A:85:TYR:CE1	2.72	0.43
1:C:138:CYS:HB3	1:C:143:CYS:O	2.17	0.43
1:B:121:ALA:O	1:B:149:ASN:OD1	2.36	0.43
1:B:68:LYS:HE2	1:B:92:ILE:HG12	2.00	0.43
1:D:168:PHE:O	1:D:172:LEU:HG	2.19	0.43
1:A:148:ILE:HG22	1:A:149:ASN:ND2	2.32	0.43
1:C:183:VAL:HA	1:C:186:CYS:HB2	1.99	0.43
1:B:157:LEU:HD22	1:C:168:PHE:CE1	2.51	0.43
1:B:187:VAL:HG12	1:B:188:GLU:N	2.32	0.43
1:D:97:ASN:HB3	1:D:100:ARG:CD	2.39	0.43
1:A:161:LEU:HD13	1:D:168:PHE:CG	2.54	0.43
1:C:138:CYS:HA	1:C:143:CYS:HB3	2.01	0.43
1:A:104:LEU:O	1:A:108:ARG:HD2	2.18	0.43
1:A:108:ARG:O	1:A:112:ASN:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:GLU:HA	1:C:159:GLU:HB2	2.00	0.43
1:C:162:VAL:O	1:C:166:VAL:N	2.35	0.43
1:A:111:LEU:HD22	1:D:140:ALA:HB3	1.94	0.43
1:D:78:LEU:HD23	1:D:148:ILE:HD11	1.99	0.43
1:A:57:ILE:CD1	1:A:109:MET:HE1	2.49	0.43
1:B:57:ILE:CG2	1:B:58:LEU:N	2.81	0.42
1:D:184:LYS:O	1:D:188:GLU:CD	2.58	0.42
1:C:158:VAL:O	1:C:162:VAL:HG23	2.19	0.42
1:C:91:ASP:OD2	1:C:100:ARG:HB3	2.18	0.42
1:B:59:TYR:O	1:B:120:VAL:HG22	2.19	0.42
1:B:156:GLU:O	1:B:159:GLU:HB2	2.20	0.42
1:C:138:CYS:CB	1:C:143:CYS:HB3	2.50	0.42
1:D:91:ASP:CG	1:D:100:ARG:HB3	2.40	0.42
1:D:139:LYS:HE2	1:D:139:LYS:HB2	1.67	0.42
1:C:104:LEU:HA	1:C:104:LEU:HD12	1.82	0.42
1:B:138:CYS:SG	1:B:145:ILE:CD1	2.86	0.42
1:B:185:LYS:HA	1:B:188:GLU:HG2	2.02	0.42
1:A:179:LYS:HD3	1:A:179:LYS:HA	1.91	0.41
1:B:157:LEU:HD23	1:C:168:PHE:CE1	2.55	0.41
1:D:173:TYR:O	1:D:173:TYR:CD1	2.73	0.41
1:B:131:PHE:CE2	1:D:176:ARG:CD	3.03	0.41
1:A:67:GLN:O	1:A:70:ASP:HB2	2.19	0.41
1:A:79:GLU:O	1:A:82:VAL:O	2.39	0.41
1:B:77:TYR:CE1	1:B:148:ILE:CG2	3.02	0.41
1:B:77:TYR:OH	1:B:148:ILE:HG23	2.11	0.41
1:D:53:LYS:HB2	1:D:53:LYS:HE3	1.63	0.41
1:A:189:GLU:O	1:A:192:ASN:CB	2.69	0.41
1:C:122:TYR:O	1:C:125:ARG:HB2	2.20	0.41
1:A:139:LYS:HG2	1:A:139:LYS:O	2.21	0.41
1:A:132:GLU:OE1	1:A:132:GLU:N	2.40	0.41
1:A:172:LEU:HA	1:A:172:LEU:HD23	1.89	0.41
1:D:161:LEU:HG	1:D:165:LEU:CD1	2.51	0.41
1:B:123:PRO:O	1:B:124:ASP:CB	2.56	0.41
1:B:120:VAL:O	1:B:147:VAL:HA	2.21	0.41
1:D:100:ARG:HB2	1:D:103:PHE:HB3	2.03	0.41
1:C:54:ARG:HA	1:C:114:GLU:O	2.20	0.41
1:A:69:ASP:N	1:A:69:ASP:OD1	2.54	0.41
1:B:104:LEU:HD12	1:B:104:LEU:HA	1.84	0.41
1:D:59:TYR:C	1:D:59:TYR:CD1	2.95	0.40
1:A:111:LEU:HD22	1:D:140:ALA:HB2	1.99	0.40
1:A:177:SER:HB2	1:D:154:GLU:OE1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:LEU:HB3	1:C:177:SER:OG	2.22	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ASP:OD2	1:B:184:LYS:NZ[2_544]	0.72	1.48
1:A:69:ASP:CG	1:B:184:LYS:NZ[2_544]	1.34	0.86
1:A:69:ASP:OD1	1:B:184:LYS:NZ[2_544]	1.82	0.38
1:A:69:ASP:OD2	1:B:184:LYS:CE[2_544]	2.09	0.11

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	132/140 (94%)	129 (98%)	3 (2%)	0	100	100
1	B	132/140 (94%)	132 (100%)	0	0	100	100
1	C	138/140 (99%)	138 (100%)	0	0	100	100
1	D	138/140 (99%)	138 (100%)	0	0	100	100
All	All	540/560 (96%)	537 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	119/130 (92%)	101 (85%)	18 (15%)		3	3
1	B	119/130 (92%)	101 (85%)	18 (15%)		3	3
1	C	121/130 (93%)	101 (84%)	20 (16%)		3	2
1	D	121/130 (93%)	98 (81%)	23 (19%)		2	1
All	All	480/520 (92%)	401 (84%)	79 (16%)		3	2

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ARG
1	A	63	SER
1	A	71	LEU
1	A	104	LEU
1	A	105	LYS
1	A	107	LEU
1	A	110	ILE
1	A	112	ASN
1	A	120	VAL
1	A	125	ARG
1	A	143	CYS
1	A	154	GLU
1	A	157	LEU
1	A	169	SER
1	A	176	ARG
1	A	177	SER
1	A	188	GLU
1	A	190	LEU
1	B	55	LYS
1	B	63	SER
1	B	65	SER
1	B	71	LEU
1	B	99	LYS
1	B	101	LYS
1	B	104	LEU
1	B	107	LEU
1	B	117	ARG
1	B	120	VAL
1	B	122	TYR
1	B	125	ARG
1	B	157	LEU
1	B	163	SER
1	B	171	LYS

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Mol	Chain	Res	Type
1	B	176	ARG
1	B	178	HIS
1	B	184	LYS
1	C	63	SER
1	C	65	SER
1	C	68	LYS
1	C	71	LEU
1	C	72	VAL
1	C	80	GLU
1	C	92	ILE
1	C	104	LEU
1	C	117	ARG
1	C	120	VAL
1	C	125	ARG
1	C	137	VAL
1	C	148	ILE
1	C	153	LYS
1	C	157	LEU
1	C	163	SER
1	C	176	ARG
1	C	182	LYS
1	C	191	LYS
1	C	192	ASN
1	D	55	LYS
1	D	67	GLN
1	D	71	LEU
1	D	105	LYS
1	D	107	LEU
1	D	108	ARG
1	D	116	SER
1	D	117	ARG
1	D	125	ARG
1	D	127	VAL
1	D	128	ARG
1	D	138	CYS
1	D	139	LYS
1	D	153	LYS
1	D	157	LEU
1	D	163	SER
1	D	169	SER
1	D	171	LYS
1	D	181	GLU

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Mol	Chain	Res	Type
1	D	185	LYS
1	D	186	CYS
1	D	188	GLU
1	D	192	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	87	GLN
1	B	74	GLN
1	B	87	GLN
1	C	141	HIS
1	C	149	ASN
1	C	192	ASN
1	D	74	GLN
1	D	87	GLN
1	D	192	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	136/140 (97%)	-0.53	0	100	100	37, 55, 70, 75	0
1	B	136/140 (97%)	-0.52	0	100	100	39, 56, 69, 77	0
1	C	140/140 (100%)	-0.69	0	100	100	37, 48, 65, 71	0
1	D	140/140 (100%)	-0.66	0	100	100	40, 52, 71, 76	0
All	All	552/560 (98%)	-0.60	0	100	100	37, 52, 69, 77	0

There are no RSRZ outliers to report.

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.