WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 03:56 am BST

PDB ID	:	3Q6A
Title	:	X-ray crystal structure of the protein SSP2350 from Staphylococcus saprophyticus, Northeast structural genomics consortium target SyR116
Authors	:	Seetharaman, J.; Chen, Y.; Wang, D.; Ciccosanti, C.; Sahdev, S.; Nair, R.; Rost, B.; Acton, T.B.; Xiao, R.; Everett, J.K.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2010-12-31
Resolution	:	1.80 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	:	1.8.5 (274361), CSD as541be (2020)
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 ⓘ

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

The reported resolution of this entry is 1.80 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.
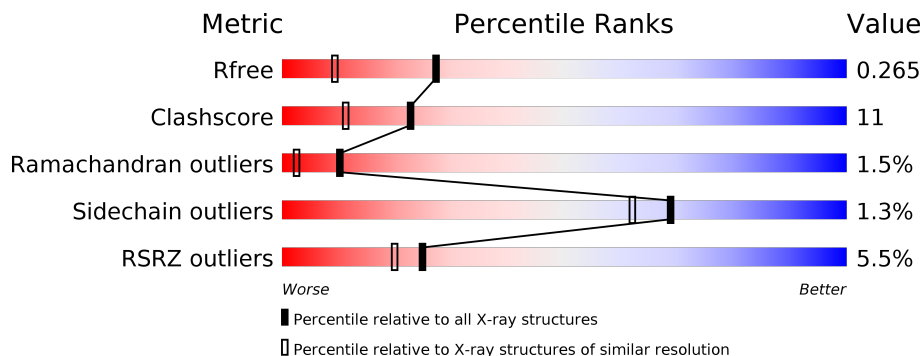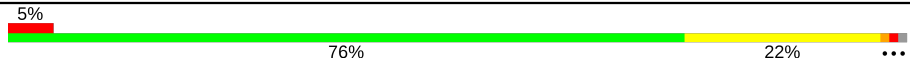

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	135	90% 8% ••
1	B	135	% 87% 13% •
1	C	135	5% 78% 20% •
1	D	135	7% 73% 27%
1	E	135	3% 73% 24% ••
1	F	135	11% 73% 26% •

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Mol	Chain	Length	Quality of chain
1	G	135	5% 76% 22%
1	H	135	11% 75% 24%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8882 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 uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	134	Total	C	N	O	S	Se	0	0	0
			1060	681	168	207	1	3			
1	B	135	Total	C	N	O	S	Se	0	0	0
			1076	691	170	211	1	3			
1	C	135	Total	C	N	O	S	Se	0	0	0
			1027	657	164	202	1	3			
1	D	135	Total	C	N	O	S	Se	0	0	0
			1032	660	170	198	1	3			
1	E	134	Total	C	N	O	S	Se	0	0	0
			1036	662	168	202	1	3			
1	F	135	Total	C	N	O	S	Se	0	0	0
			1011	646	169	192	1	3			
1	G	134	Total	C	N	O	S	Se	0	0	0
			1040	664	169	203	1	3			
1	H	135	Total	C	N	O	S	Se	0	0	0
			1050	673	170	203	1	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	135	LEU	-	EXPRESSION TAG	UNP Q49US3
B	135	LEU	-	EXPRESSION TAG	UNP Q49US3
C	135	LEU	-	EXPRESSION TAG	UNP Q49US3
D	135	LEU	-	EXPRESSION TAG	UNP Q49US3
E	135	LEU	-	EXPRESSION TAG	UNP Q49US3
F	135	LEU	-	EXPRESSION TAG	UNP Q49US3
G	135	LEU	-	EXPRESSION TAG	UNP Q49US3
H	135	LEU	-	EXPRESSION TAG	UNP Q49US3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	127	Total O 127 127	0	0
2	B	133	Total O 133 133	0	0
2	C	46	Total O 46 46	0	0
2	D	50	Total O 50 50	0	0
2	E	82	Total O 82 82	0	0
2	F	15	Total O 15 15	0	0
2	G	79	Total O 79 79	0	0
2	H	18	Total O 18 18	0	0

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 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.

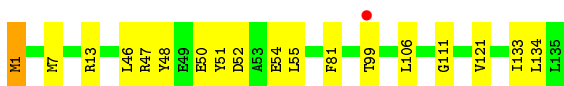- Molecule 1: uncharacterized protein

Chain A:

- Molecule 1: uncharacterized protein

Chain B:

- Molecule 1: uncharacterized protein

Chain C:

- Molecule 1: uncharacterized protein

Chain D:

- Molecule 1: uncharacterized protein

Chain E:

M1 D2 I3 V21 G27 F31 S32 S35 W38 I44 T45 L46 R47 Y48 E49 E50 Y51 D52 A53 E54 L55 N56 I57 N58 I59 E60 R61 G73 A74 T93 E94 K95 D96 F97 V102 L105 L106 V121 I129 I133 L134 LEU

• Molecule 1: uncharacterized protein

Chain F:

11%

73% 26%

M1 D2 K6 M7 Q8 V9 D10 V11 E14 T15 V16 V21 F31 S35 W38 E39 Q40 T43 L46 R47 Y48 D52 A53 E60 R61 D64 N65 Q66 L67 I68 W72 I79 Q80 F81 S84 E85 A86 G87 T88 V89 F97 D98 T99 Q100

L105 L106 G111 S117 C118 L119 K120 V121 E124 V127 T128 I129 I133 L134 L135

• Molecule 1: uncharacterized protein

Chain G:

5%

76% 22%

M1 D2 I3 V21 G27 F31 S32 S35 W38 I44 T45 L46 R47 Y48 E49 E50 Y51 D52 A53 E54 L55 N56 I57 L67 Q80 E94 F97 D98 T99 V102 L106 Y114 V121 I129 R130 A131 A132 I133 L134 LEU

• Molecule 1: uncharacterized protein

Chain H:

11%

75% 24%

M1 D2 I3 Q8 V9 D10 V11 E14 T15 V16 V21 D22 S34 S35 W38 E39 Q40 Y48 D52 I57 N58 I59 E60 R61 V62 E63 D64 N65 Q66 L67 I68 A69 F70 T71 W72 I79 Q80 F81 S84 E85 A86 G87 T88 V89 F97 D98 T99 Q100

L105 L106 G111 S117 K120 V121 V127 I133 L134 L135

4 Data and refinement statistics (i)

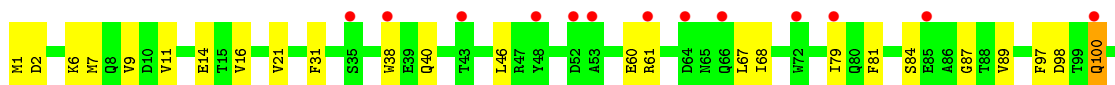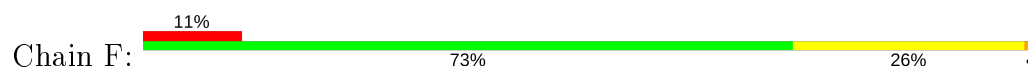| Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.57Å　　66.45Å　　128.66Å 90.00°　　90.12°　　90.00°	Depositor
Resolution (Å)	43.59　－　1.80 43.59　－　1.76	Depositor EDS
% Data completeness (in resolution range)	95.1 (43.59-1.80) 96.3 (43.59-1.76)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	4.54 (at 1.76Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.218　,　0.262 0.229　,　0.265	Depositor DCC
R_{free} test set	5759 reflections (5.43%)	wwPDB-VP
Wilson B-factor (Å^2)	22.4	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 31.3	EDS
L-test for twinning[2]	$<|L|> = 0.47, <L^2> = 0.30$	Xtriage
Estimated twinning fraction	0.025 for -k,-h,-l 0.025 for k,h,-l 0.479 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8882	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% of the height of the origin peak. No significant pseudotranslation is detected.*
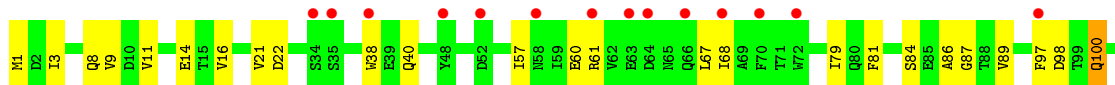
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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 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	0.51	0/1080	0.72	0/1462
1	B	0.53	1/1097 (0.1%)	0.72	0/1486
1	C	0.45	0/1046	0.64	0/1415
1	D	0.45	0/1051	0.62	0/1421
1	E	0.44	0/1055	0.68	0/1428
1	F	0.39	0/1031	0.52	0/1393
1	G	0.44	0/1059	0.79	3/1433 (0.2%)
1	H	0.39	0/1071	0.53	0/1448
All	All	0.46	1/8490 (0.0%)	0.66	3/11486 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	7	MSE	SE-CE	-6.36	1.57	1.95

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	131	ALA	N-CA-CB	11.24	125.84	110.10
1	G	130	ARG	N-CA-C	-6.68	92.97	111.00
1	G	130	ARG	CB-CA-C	6.15	122.70	110.40

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	1060	0	1008	12	0
1	B	1076	0	1030	21	0
1	C	1027	0	964	24	0
1	D	1032	0	978	28	0
1	E	1036	0	990	26	0
1	F	1011	0	937	35	0
1	G	1040	0	996	36	0
1	H	1050	0	998	33	0
2	A	127	0	0	0	0
2	B	133	0	0	0	0
2	C	46	0	0	1	0
2	D	50	0	0	0	0
2	E	82	0	0	0	0
2	F	15	0	0	0	0
2	G	79	0	0	0	0
2	H	18	0	0	0	0
All	All	8882	0	7901	186	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 11.

All (186) 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:B:1:MSE:HG3	1:B:99:THR:HG22	1.61	0.83
1:G:1:MSE:HE2	1:G:3:ILE:HD13	1.61	0.82
1:B:121:VAL:HG21	1:C:121:VAL:HG21	1.61	0.82
1:D:114:TYR:CD2	1:D:132:ALA:HB2	2.16	0.81
1:E:1:MSE:HE2	1:E:3:ILE:HD13	1.63	0.79
1:A:121:VAL:HG21	1:D:121:VAL:HG21	1.65	0.78
1:H:67:LEU:HD23	1:H:68:ILE:N	2.00	0.75
1:D:114:TYR:HD2	1:D:132:ALA:HB2	1.53	0.73
1:F:67:LEU:HD23	1:F:68:ILE:N	2.02	0.73
1:G:132:ALA:O	1:G:133:ILE:HD13	1.89	0.72
1:F:121:VAL:HG21	1:G:121:VAL:HG21	1.72	0.72
1:H:40:GLN:HG3	1:H:60:GLU:O	1.89	0.72
1:H:21:VAL:HG12	1:H:38:TRP:HB2	1.70	0.72
1:A:121:VAL:HG22	1:D:129:ILE:HG21	1.74	0.70
1:D:21:VAL:HG12	1:D:38:TRP:HB2	1.74	0.69
1:B:1:MSE:HG3	1:B:99:THR:CG2	2.23	0.68
1:H:111:GLY:HA3	1:H:134:LEU:HD13	1.76	0.67
1:H:133:ILE:HG13	1:H:134:LEU:N	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:133:ILE:HG13	1:H:134:LEU:H	1.59	0.67
1:A:46:LEU:HD12	1:A:55:LEU:HD11	1.76	0.66
1:E:102:VAL:O	1:E:106:LEU:HD13	1.95	0.66
1:B:121:VAL:HG22	1:C:129:ILE:HG21	1.78	0.66
1:C:21:VAL:HG12	1:C:38:TRP:HB2	1.78	0.66
1:F:111:GLY:HA3	1:F:134:LEU:HD13	1.79	0.64
1:C:45:THR:HA	1:C:56:ASN:ND2	2.12	0.64
1:F:9:VAL:HG12	1:F:11:VAL:HG22	1.81	0.62
1:C:35:SER:HB3	1:C:45:THR:HB	1.82	0.61
1:F:40:GLN:HG3	1:F:60:GLU:O	1.99	0.61
1:G:32:SER:HB2	1:G:49:GLU:H	1.66	0.60
1:C:46:LEU:HD12	1:C:55:LEU:HD11	1.83	0.60
1:B:121:VAL:HG21	1:C:121:VAL:CG2	2.31	0.60
1:G:102:VAL:O	1:G:106:LEU:HD13	2.01	0.60
1:F:121:VAL:HG21	1:G:121:VAL:CG2	2.32	0.60
1:E:1:MSE:CE	1:E:3:ILE:HD13	2.29	0.59
1:E:27:GLY:HA2	1:E:31:PHE:O	2.03	0.59
1:F:21:VAL:HG12	1:F:38:TRP:HB2	1.85	0.59
1:C:132:ALA:HB1	2:C:304:HOH:O	2.02	0.59
1:F:61:ARG:HB3	1:F:61:ARG:NH1	2.20	0.57
1:F:38:TRP:HE3	1:F:68:ILE:HD11	1.70	0.57
1:G:32:SER:CB	1:G:49:GLU:H	2.17	0.57
1:C:45:THR:HA	1:C:56:ASN:HD22	1.71	0.56
1:F:106:LEU:CD2	1:G:1:MSE:HE1	2.36	0.56
1:E:129:ILE:HG21	1:H:121:VAL:HG22	1.88	0.56
1:A:121:VAL:HG21	1:D:121:VAL:CG2	2.34	0.55
1:F:121:VAL:HG22	1:G:129:ILE:HG21	1.89	0.55
1:D:94:GLU:HG2	1:D:97:PHE:HE2	1.71	0.55
1:B:48:TYR:CE2	1:B:50:GLU:HB3	2.42	0.55
1:B:46:LEU:HD12	1:B:55:LEU:HD11	1.89	0.54
1:D:111:GLY:HA3	1:D:134:LEU:HD13	1.89	0.54
1:E:121:VAL:HG21	1:H:121:VAL:HG21	1.89	0.54
1:D:35:SER:HB3	1:D:45:THR:HB	1.90	0.54
1:E:21:VAL:HG12	1:E:38:TRP:HB2	1.91	0.53
1:E:46:LEU:HD12	1:E:55:LEU:HD11	1.89	0.53
1:E:48:TYR:O	1:E:50:GLU:N	2.41	0.53
1:B:121:VAL:CG2	1:C:121:VAL:HG21	2.36	0.53
1:F:61:ARG:HH11	1:F:61:ARG:CB	2.22	0.53
1:E:49:GLU:C	1:E:51:TYR:H	2.12	0.53
1:E:32:SER:HB2	1:E:49:GLU:H	1.73	0.53
1:G:132:ALA:O	1:G:133:ILE:O	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:9:VAL:HG12	1:H:11:VAL:HG22	1.91	0.52
1:D:43:THR:HG23	1:D:43:THR:O	2.10	0.52
1:D:94:GLU:HG2	1:D:97:PHE:CE2	2.44	0.52
1:C:2:ASP:OD2	1:C:95:LYS:HG2	2.10	0.52
1:A:111:GLY:HA3	1:A:134:LEU:HD13	1.91	0.52
1:G:67:LEU:HD12	1:G:80:GLN:HG2	1.91	0.52
1:C:30:TRP:CZ2	1:C:134:LEU:HD23	2.45	0.52
1:G:46:LEU:HD12	1:G:55:LEU:HD11	1.92	0.52
1:C:57:ILE:HD12	1:C:70:PHE:CD1	2.46	0.51
1:B:55:LEU:HD12	1:B:55:LEU:O	2.10	0.51
1:H:1:MSE:HA	1:H:1:MSE:HE2	1.91	0.51
1:B:47:ARG:HH11	1:B:54:GLU:HB2	1.75	0.51
1:F:6:LYS:O	1:G:133:ILE:HA	2.11	0.51
1:C:67:LEU:HD23	1:C:67:LEU:C	2.31	0.51
1:F:106:LEU:HD12	1:G:106:LEU:HD12	1.93	0.51
1:E:121:VAL:CG2	1:H:121:VAL:HG21	2.40	0.51
1:E:106:LEU:HD12	1:H:106:LEU:HD12	1.93	0.51
1:H:14:GLU:H	1:H:14:GLU:CD	2.15	0.50
1:A:46:LEU:HD12	1:A:55:LEU:CD1	2.42	0.50
1:B:47:ARG:HD2	1:B:54:GLU:HG3	1.94	0.50
1:B:46:LEU:HD12	1:B:55:LEU:CD1	2.42	0.50
1:G:27:GLY:HA2	1:G:31:PHE:O	2.12	0.50
1:B:46:LEU:HB2	1:B:55:LEU:CD1	2.42	0.50
1:H:61:ARG:HB3	1:H:61:ARG:NH1	2.27	0.50
1:F:31:PHE:CD2	1:F:46:LEU:HD13	2.47	0.49
1:F:106:LEU:HD22	1:G:1:MSE:HE1	1.95	0.49
1:H:38:TRP:HE3	1:H:68:ILE:HD11	1.76	0.49
1:H:57:ILE:O	1:H:57:ILE:HG13	2.12	0.49
1:B:111:GLY:HA3	1:B:134:LEU:HD13	1.94	0.49
1:F:7:MSE:SE	1:G:132:ALA:HB1	2.63	0.49
1:D:67:LEU:C	1:D:67:LEU:HD23	2.32	0.49
1:H:98:ASP:C	1:H:100:GLN:H	2.17	0.49
1:A:121:VAL:CG2	1:D:121:VAL:HG21	2.40	0.48
1:D:114:TYR:CE2	1:D:132:ALA:HB2	2.47	0.48
1:G:130:ARG:HG3	1:G:130:ARG:HH21	1.77	0.48
1:F:120:LYS:HG3	1:F:124:GLU:OE2	2.13	0.48
1:F:97:PHE:HB3	1:F:105:LEU:HD21	1.96	0.48
1:G:27:GLY:O	1:G:130:ARG:HD3	2.14	0.48
1:E:3:ILE:HD11	1:E:105:LEU:HD22	1.97	0.47
1:H:68:ILE:CG2	1:H:79:ILE:HB	2.45	0.47
1:F:61:ARG:NH1	1:F:67:LEU:HD22	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:21:VAL:HG12	1:G:38:TRP:HB2	1.97	0.47
1:B:106:LEU:HD12	1:C:106:LEU:HD12	1.96	0.47
1:B:48:TYR:CG	1:B:133:ILE:HG22	2.50	0.46
1:F:1:MSE:HE2	1:F:1:MSE:HA	1.97	0.46
1:E:1:MSE:HE1	1:H:106:LEU:CD2	2.44	0.46
1:H:117:SER:O	1:H:121:VAL:HG23	2.16	0.46
1:H:133:ILE:O	1:H:134:LEU:HB3	2.16	0.46
1:B:13:ARG:HG3	1:B:81:PHE:HB3	1.98	0.46
1:E:106:LEU:HD12	1:H:106:LEU:CD1	2.46	0.46
1:A:3:ILE:HD11	1:A:105:LEU:HD23	1.97	0.46
1:H:121:VAL:HG12	1:H:127:VAL:HG23	1.98	0.46
1:C:77:ILE:HG12	1:C:94:GLU:HG3	1.97	0.46
1:B:46:LEU:HB2	1:B:55:LEU:HD12	1.98	0.45
1:G:46:LEU:HD12	1:G:55:LEU:CD1	2.46	0.45
1:A:1:MSE:HE1	1:D:106:LEU:CD1	2.47	0.45
1:H:8:GLN:OE1	1:H:86:ALA:HB3	2.16	0.45
1:E:44:ILE:HD12	1:E:44:ILE:N	2.32	0.45
1:G:1:MSE:CE	1:G:3:ILE:HD13	2.38	0.45
1:G:35:SER:HB3	1:G:45:THR:HB	1.97	0.45
1:C:45:THR:HG23	1:C:56:ASN:HD21	1.81	0.45
1:F:7:MSE:SE	1:G:132:ALA:CB	3.15	0.45
1:D:45:THR:HA	1:D:56:ASN:HD22	1.82	0.45
1:F:106:LEU:CD1	1:G:106:LEU:HD12	2.47	0.45
1:F:21:VAL:HA	1:F:38:TRP:HB2	1.99	0.45
1:C:44:ILE:HD12	1:C:44:ILE:N	2.32	0.45
1:C:17:PHE:CG	1:C:65:ASN:HA	2.51	0.45
1:D:43:THR:HA	1:D:58:ASN:HA	1.98	0.45
1:H:97:PHE:HB3	1:H:105:LEU:HD21	1.99	0.44
1:B:48:TYR:CE2	1:B:133:ILE:HG23	2.52	0.44
1:F:121:VAL:HG12	1:F:127:VAL:HG23	2.00	0.44
1:F:84:SER:HB3	1:F:89:VAL:HG23	1.98	0.44
1:E:94:GLU:HG2	1:E:97:PHE:CE2	2.53	0.44
1:A:55:LEU:HD12	1:A:55:LEU:C	2.38	0.44
1:C:39:GLU:N	1:C:59:ILE:HD12	2.33	0.44
1:F:16:VAL:HG12	1:F:81:PHE:CE2	2.53	0.44
1:D:27:GLY:HA2	1:D:31:PHE:O	2.18	0.44
1:D:33:SER:OG	1:D:47:ARG:HB2	2.18	0.44
1:G:114:TYR:CE2	1:G:133:ILE:HD12	2.53	0.44
1:H:8:GLN:HE21	1:H:8:GLN:HA	1.83	0.44
1:F:14:GLU:H	1:F:14:GLU:CD	2.21	0.43
1:B:55:LEU:C	1:B:55:LEU:HD12	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:GLU:H	1:C:59:ILE:HD12	1.83	0.43
1:G:114:TYR:CD2	1:G:133:ILE:HD12	2.52	0.43
1:G:44:ILE:HD12	1:G:44:ILE:N	2.34	0.43
1:C:1:MSE:HA	1:C:1:MSE:HE2	2.00	0.43
1:H:61:ARG:NH1	1:H:67:LEU:HD22	2.33	0.43
1:D:17:PHE:CG	1:D:65:ASN:HA	2.53	0.43
1:A:21:VAL:HG12	1:A:38:TRP:HB2	2.01	0.43
1:D:38:TRP:HA	1:D:59:ILE:CD1	2.49	0.43
1:F:98:ASP:C	1:F:100:GLN:H	2.22	0.43
1:H:3:ILE:HD11	1:H:105:LEU:HD22	1.99	0.43
1:H:21:VAL:HG23	1:H:22:ASP:N	2.33	0.43
1:F:117:SER:O	1:F:121:VAL:HG23	2.18	0.43
1:G:130:ARG:HG3	1:G:130:ARG:NH2	2.33	0.43
1:E:35:SER:HB3	1:E:45:THR:HB	2.00	0.43
1:E:57:ILE:O	1:E:57:ILE:HG13	2.17	0.43
1:D:133:ILE:O	1:D:135:LEU:N	2.52	0.43
1:D:2:ASP:OD2	1:D:95:LYS:HG2	2.19	0.43
1:F:61:ARG:CB	1:F:61:ARG:NH1	2.79	0.42
1:E:60:GLU:O	1:E:61:ARG:HG3	2.19	0.42
1:C:11:VAL:HG23	1:C:16:VAL:HG23	2.01	0.42
1:G:48:TYR:C	1:G:50:GLU:N	2.72	0.42
1:D:45:THR:HA	1:D:56:ASN:ND2	2.34	0.42
1:E:44:ILE:HD13	1:E:59:ILE:HG12	2.02	0.42
1:D:73:GLY:O	1:D:74:ALA:HB3	2.19	0.42
1:G:94:GLU:HG2	1:G:97:PHE:CE2	2.55	0.42
1:E:73:GLY:O	1:E:74:ALA:HB3	2.19	0.42
1:E:93:THR:HG22	1:E:95:LYS:HG2	2.01	0.42
1:H:61:ARG:CB	1:H:61:ARG:HH11	2.33	0.42
1:H:84:SER:HB3	1:H:89:VAL:HG23	2.01	0.41
1:G:46:LEU:HB2	1:G:55:LEU:CD1	2.50	0.41
1:G:57:ILE:O	1:G:57:ILE:HG13	2.20	0.41
1:B:51:TYR:O	1:B:52:ASP:C	2.57	0.41
1:C:21:VAL:CG1	1:C:38:TRP:HB2	2.49	0.41
1:F:7:MSE:SE	1:G:133:ILE:HG22	2.71	0.41
1:A:61:ARG:HB3	1:A:61:ARG:CZ	2.50	0.41
1:F:121:VAL:CG2	1:G:121:VAL:HG21	2.46	0.41
1:D:59:ILE:CG2	1:D:62:VAL:HG23	2.51	0.41
1:E:129:ILE:HB	1:H:120:LYS:HD3	2.01	0.41
1:E:31:PHE:CE2	1:E:46:LEU:HD13	2.55	0.41
1:F:68:ILE:CG2	1:F:79:ILE:HB	2.51	0.41
1:D:55:LEU:HD12	1:D:57:ILE:HG13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:16:VAL:HG12	1:H:81:PHE:CE2	2.56	0.40
1:G:31:PHE:CE2	1:G:46:LEU:HD13	2.56	0.40
1:D:81:PHE:CD1	1:D:81:PHE:N	2.89	0.40
1:F:118:CYS:SG	1:F:129:ILE:HG13	2.62	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	130/135 (96%)	119 (92%)	11 (8%)	0	100	100
1	B	133/135 (98%)	123 (92%)	10 (8%)	0	100	100
1	C	133/135 (98%)	114 (86%)	16 (12%)	3 (2%)	6	1
1	D	133/135 (98%)	115 (86%)	16 (12%)	2 (2%)	10	2
1	E	132/135 (98%)	116 (88%)	13 (10%)	3 (2%)	6	1
1	F	133/135 (98%)	118 (89%)	13 (10%)	2 (2%)	10	2
1	G	132/135 (98%)	117 (89%)	11 (8%)	4 (3%)	4	0
1	H	133/135 (98%)	117 (88%)	14 (10%)	2 (2%)	10	2
All	All	1059/1080 (98%)	939 (89%)	104 (10%)	16 (2%)	10	2

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	49	GLU
1	E	51	TYR
1	G	52	ASP
1	G	133	ILE
1	C	50	GLU
1	C	134	LEU

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Mol	Chain	Res	Type
1	E	52	ASP
1	F	100	GLN
1	C	130	ARG
1	G	51	TYR
1	H	100	GLN
1	D	50	GLU
1	D	130	ARG
1	G	99	THR
1	H	87	GLY
1	F	87	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	111/117 (95%)	109 (98%)	2 (2%)	59	48
1	B	114/117 (97%)	113 (99%)	1 (1%)	78	75
1	C	106/117 (91%)	104 (98%)	2 (2%)	57	46
1	D	105/117 (90%)	104 (99%)	1 (1%)	76	71
1	E	109/117 (93%)	106 (97%)	3 (3%)	43	30
1	F	99/117 (85%)	98 (99%)	1 (1%)	76	71
1	G	110/117 (94%)	109 (99%)	1 (1%)	78	75
1	H	109/117 (93%)	109 (100%)	0	100	100
All	All	863/936 (92%)	852 (99%)	11 (1%)	69	62

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	106	LEU
1	B	1	MSE
1	C	1	MSE
1	C	106	LEU

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Mol	Chain	Res	Type
1	D	1	MSE
1	E	56	ASN
1	E	133	ILE
1	E	134	LEU
1	F	2	ASP
1	G	133	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	56	ASN
1	B	8	GLN
1	B	56	ASN
1	B	104	GLN
1	B	108	GLN
1	C	8	GLN
1	C	56	ASN
1	C	108	GLN
1	D	8	GLN
1	D	56	ASN
1	D	108	GLN
1	E	8	GLN
1	E	56	ASN
1	F	8	GLN
1	F	56	ASN
1	F	80	GLN
1	G	8	GLN
1	G	56	ASN
1	H	8	GLN
1	H	56	ASN
1	H	80	GLN

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	131/135 (97%)	-0.30	0	100	100	10, 19, 40, 51	0
1	B	132/135 (97%)	-0.30	1 (0%)	86	84	11, 19, 40, 52	0
1	C	132/135 (97%)	0.28	7 (5%)	26	21	14, 30, 54, 62	0
1	D	132/135 (97%)	0.26	9 (6%)	17	13	14, 30, 56, 63	0
1	E	131/135 (97%)	-0.11	4 (3%)	49	43	16, 27, 50, 69	0
1	F	132/135 (97%)	0.93	15 (11%)	5	3	24, 50, 60, 64	0
1	G	131/135 (97%)	0.09	7 (5%)	26	21	15, 27, 49, 68	0
1	H	132/135 (97%)	0.82	15 (11%)	5	3	24, 50, 61, 64	0
All	All	1053/1080 (97%)	0.21	58 (5%)	25	20	10, 29, 59, 69	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	51	TYR	8.0
1	E	51	TYR	6.0
1	D	133	ILE	5.7
1	F	53	ALA	4.7
1	E	52	ASP	4.6
1	G	48	TYR	4.4
1	D	50	GLU	4.4
1	D	134	LEU	4.2
1	D	51	TYR	4.2
1	C	50	GLU	4.1
1	H	35	SER	4.0
1	F	43	THR	3.8
1	E	134	LEU	3.7
1	C	134	LEU	3.5
1	D	53	ALA	3.5
1	F	52	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	64	ASP	3.4
1	E	53	ALA	3.4
1	G	53	ALA	3.4
1	C	53	ALA	3.4
1	D	132	ALA	3.4
1	F	35	SER	3.3
1	C	51	TYR	3.3
1	D	99	THR	3.3
1	H	72	TRP	3.2
1	D	131	ALA	3.1
1	H	48	TYR	3.0
1	H	34	SER	3.0
1	H	133	ILE	3.0
1	G	50	GLU	2.9
1	H	97	PHE	2.9
1	C	131	ALA	2.8
1	F	133	ILE	2.8
1	F	61	ARG	2.8
1	H	64	ASP	2.7
1	F	48	TYR	2.7
1	F	85	GLU	2.7
1	F	134	LEU	2.6
1	H	68	ILE	2.6
1	D	48	TYR	2.6
1	H	66	GLN	2.6
1	C	39	GLU	2.6
1	H	52	ASP	2.5
1	C	133	ILE	2.5
1	F	72	TRP	2.4
1	F	79	ILE	2.4
1	G	134	LEU	2.3
1	B	99	THR	2.3
1	H	63	GLU	2.3
1	G	133	ILE	2.2
1	F	38	TRP	2.2
1	H	70	PHE	2.2
1	H	61	ARG	2.1
1	G	131	ALA	2.1
1	F	66	GLN	2.1
1	H	38	TRP	2.1
1	H	58	ASN	2.1
1	F	100	GLN	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.