Full wwPDB X-ray Structure Validation Report (i)

Jun 27, 2016 – 04:50 PM EDT

PDB ID	:	5EN7
Title	:	Crystal structure of the Smu1-RED complex (native) of Caenorhabditis elegans.
Authors	:	Ulrich, A.K.C.; Wahl, M.C.
Deposited on	:	2015-11-09
Resolution	:	2.94 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
http://wwpdb.org/validation/2016/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:

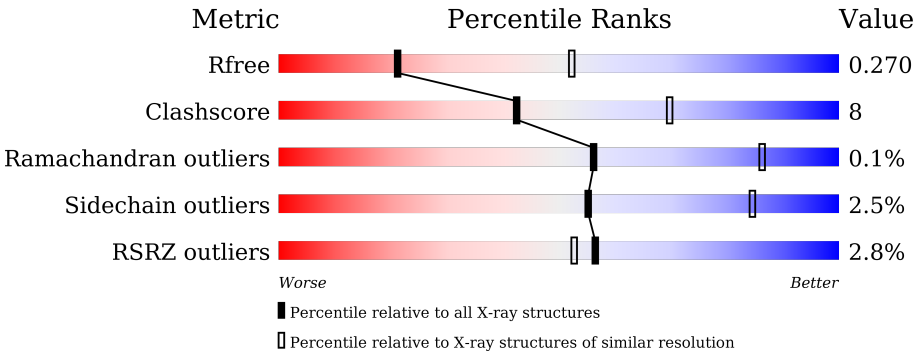
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

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 2.94 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}	91344	2057 (2.98-2.90)
Clashscore	102246	2308 (2.98-2.90)
Ramachandran outliers	100387	2245 (2.98-2.90)
Sidechain outliers	100360	2247 (2.98-2.90)
RSRZ outliers	91569	2065 (2.98-2.90)

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	184	% 72% 24%
1	C	184	68% 28%
1	E	184	77% 18%
1	G	184	80% 16%
2	B	63	8% 21% 75%
2	D	63	5% 11% 13% 76%

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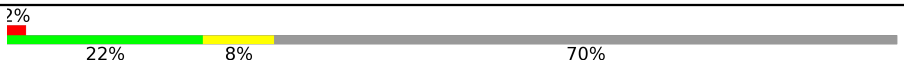
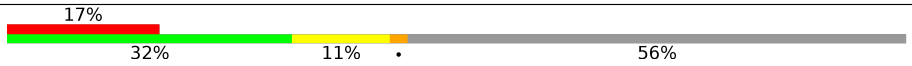
Mol	Chain	Length	Quality of chain
2	F	63	
2	H	63	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6461 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 SMU-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	177	Total	C	N	O	S	0	0	0
			1418	900	246	270	2			
1	C	177	Total	C	N	O	S	0	0	0
			1418	900	246	270	2			
1	E	176	Total	C	N	O	S	0	0	0
			1406	891	245	268	2			
1	G	177	Total	C	N	O	S	0	0	0
			1417	898	246	271	2			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP G5EEG7
A	-1	ALA	-	expression tag	UNP G5EEG7
A	0	MET	-	expression tag	UNP G5EEG7
A	1	GLY	-	expression tag	UNP G5EEG7
C	-2	GLY	-	expression tag	UNP G5EEG7
C	-1	ALA	-	expression tag	UNP G5EEG7
C	0	MET	-	expression tag	UNP G5EEG7
C	1	GLY	-	expression tag	UNP G5EEG7
E	-2	GLY	-	expression tag	UNP G5EEG7
E	-1	ALA	-	expression tag	UNP G5EEG7
E	0	MET	-	expression tag	UNP G5EEG7
E	1	GLY	-	expression tag	UNP G5EEG7
G	-2	GLY	-	expression tag	UNP G5EEG7
G	-1	ALA	-	expression tag	UNP G5EEG7
G	0	MET	-	expression tag	UNP G5EEG7
G	1	GLY	-	expression tag	UNP G5EEG7

- Molecule 2 is a protein called Suppressor of Mec and Unc defects.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	16	Total	C	N	O	S	0	0	0
			140	87	31	21	1			
2	D	15	Total	C	N	O	S	0	0	0
			131	81	29	20	1			
2	F	19	Total	C	N	O	S	0	0	0
			163	99	36	27	1			
2	H	28	Total	C	N	O	S	0	0	0
			227	140	45	41	1			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	161	GLY	-	expression tag	UNP Q9N4U5
B	162	ALA	-	expression tag	UNP Q9N4U5
D	161	GLY	-	expression tag	UNP Q9N4U5
D	162	ALA	-	expression tag	UNP Q9N4U5
F	161	GLY	-	expression tag	UNP Q9N4U5
F	162	ALA	-	expression tag	UNP Q9N4U5
H	161	GLY	-	expression tag	UNP Q9N4U5
H	162	ALA	-	expression tag	UNP Q9N4U5

- Molecule 3 is water.

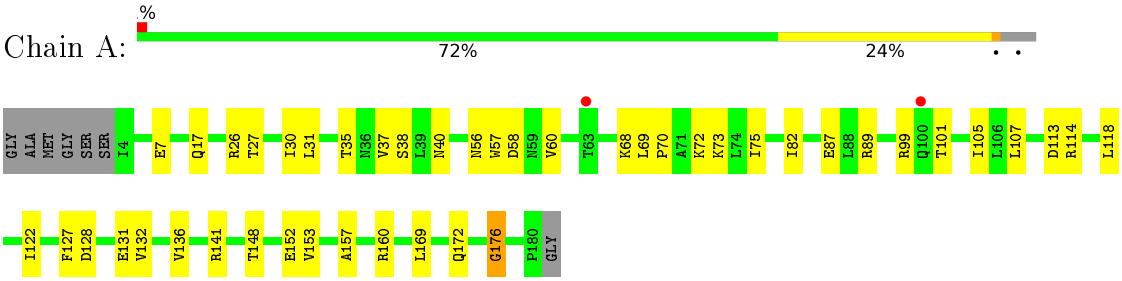
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	B	4	Total	O	0	0
			4	4		
3	C	25	Total	O	0	0
			25	25		
3	D	3	Total	O	0	0
			3	3		
3	E	46	Total	O	0	0
			46	46		
3	F	5	Total	O	0	0
			5	5		
3	G	36	Total	O	0	0
			36	36		
3	H	2	Total	O	0	0
			2	2		

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 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.

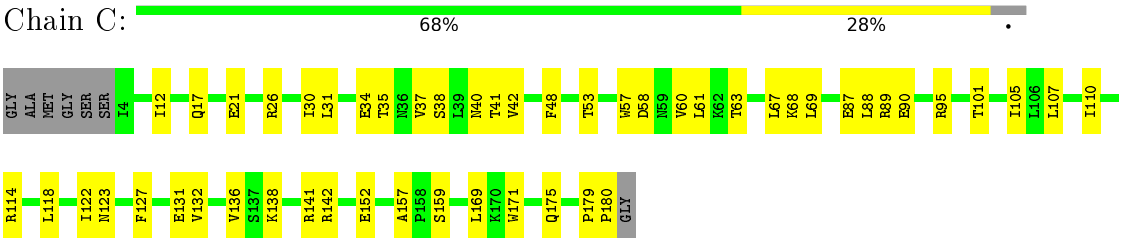
- Molecule 1: SMU-1

Chain A:



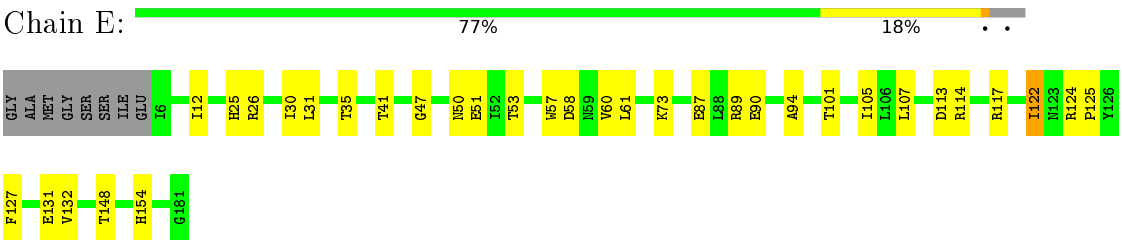
- Molecule 1: SMU-1

Chain C:



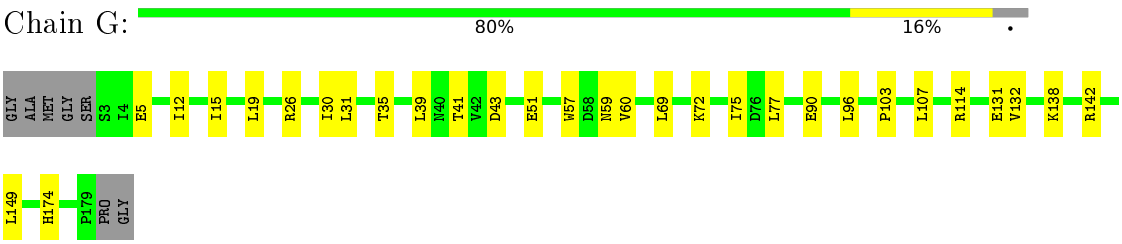
- Molecule 1: SMU-1

Chain E:



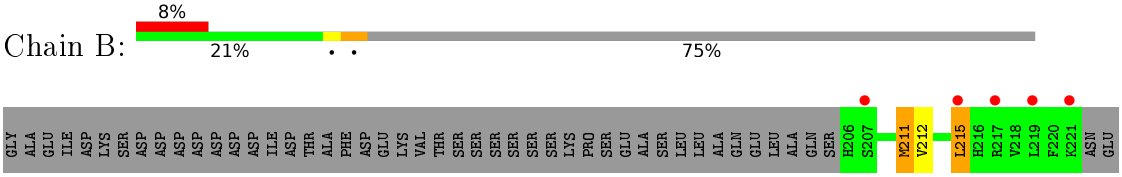
- Molecule 1: SMU-1

Chain G:



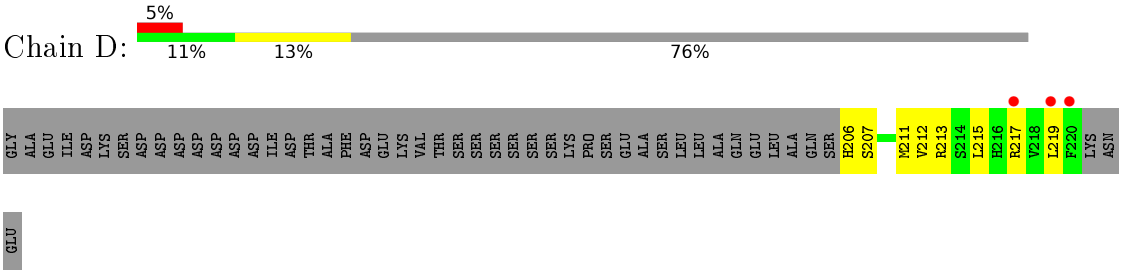
• Molecule 2: Suppressor of Mec and Unc defects

Chain B:



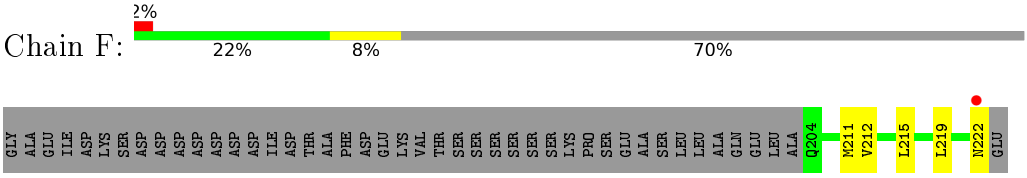
• Molecule 2: Suppressor of Mec and Unc defects

Chain D:



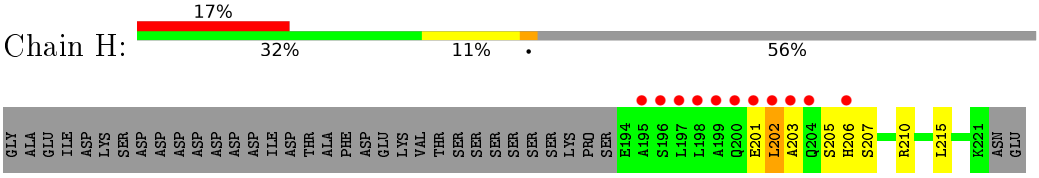
• Molecule 2: Suppressor of Mec and Unc defects

Chain F:



• Molecule 2: Suppressor of Mec and Unc defects

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	122.32Å 41.04Å 126.38Å 90.00° 95.92° 90.00°	Depositor
Resolution (Å)	46.16 – 2.94 46.16 – 2.94	Depositor EDS
% Data completeness (in resolution range)	98.3 (46.16-2.94) 98.3 (46.16-2.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.96Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.222 , 0.269 0.224 , 0.270	Depositor DCC
R_{free} test set	1349 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	61.2	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 39.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.098 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6461	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% 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	0.26	0/1439	0.49	0/1951
1	C	0.28	0/1439	0.48	0/1951
1	E	0.27	0/1427	0.47	0/1933
1	G	0.28	0/1437	0.48	0/1947
2	B	0.23	0/142	0.46	0/187
2	D	0.23	0/133	0.43	0/176
2	F	0.26	0/165	0.44	0/218
2	H	0.24	0/229	0.39	0/305
All	All	0.27	0/6411	0.47	0/8668

There are no bond length outliers.

There are no bond angle outliers.

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	1418	0	1462	31	0
1	C	1418	0	1462	34	0
1	E	1406	0	1448	23	0
1	G	1417	0	1460	18	0
2	B	140	0	145	2	0
2	D	131	0	132	5	0
2	F	163	0	164	3	0
2	H	227	0	231	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	20	0	0	1	0
3	B	4	0	0	0	0
3	C	25	0	0	1	0
3	D	3	0	0	0	0
3	E	46	0	0	1	0
3	F	5	0	0	0	0
3	G	36	0	0	0	0
3	H	2	0	0	0	0
All	All	6461	0	6504	107	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 8.

All (107) 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:C:90:GLU:HG2	2:D:212:VAL:HG11	1.58	0.86
1:A:40:ASN:HD21	1:A:68:LYS:HG2	1.51	0.76
1:E:30:ILE:HG13	1:G:30:ILE:HG13	1.67	0.76
1:G:107:LEU:HD11	1:G:114:ARG:HD3	1.71	0.73
1:C:107:LEU:HD11	1:C:114:ARG:HD3	1.71	0.72
1:A:107:LEU:HD11	1:A:114:ARG:HD3	1.72	0.69
1:E:107:LEU:HD11	1:E:114:ARG:HD3	1.76	0.68
1:A:157:ALA:HB3	1:A:160:ARG:HG2	1.78	0.65
1:C:89:ARG:HH12	1:C:127:PHE:H	1.43	0.64
1:A:30:ILE:HG13	1:C:30:ILE:HG13	1.80	0.64
1:C:42:VAL:HG11	1:C:48:PHE:HB2	1.79	0.63
1:G:96:LEU:HD21	2:H:203:ALA:HA	1.82	0.62
1:A:7:GLU:N	1:A:7:GLU:OE1	2.32	0.62
1:C:12:ILE:HG21	1:C:35:THR:HG21	1.83	0.59
1:A:38:SER:HB2	1:A:68:LYS:HD2	1.85	0.59
1:C:136:VAL:O	1:C:141:ARG:NH1	2.36	0.59
1:G:31:LEU:O	1:G:35:THR:HG22	2.04	0.56
1:E:113:ASP:OD1	1:E:117:ARG:NH2	2.36	0.56
1:G:138:LYS:HG2	1:G:142:ARG:HD2	1.86	0.56
1:C:38:SER:OG	1:C:68:LYS:HD2	2.06	0.56
1:E:124:ARG:HG3	1:E:125:PRO:HD2	1.87	0.56
1:E:61:LEU:HD13	2:F:219:LEU:HD21	1.89	0.55
1:C:61:LEU:HD12	2:D:215:LEU:HD11	1.90	0.54
2:H:202:LEU:HA	2:H:205:SER:HB3	1.90	0.54
1:A:70:PRO:HB2	1:A:73:LYS:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ASN:ND2	3:A:201:HOH:O	2.41	0.53
2:B:212:VAL:HA	2:B:215:LEU:HD23	1.90	0.53
1:A:136:VAL:O	1:A:141:ARG:NH1	2.42	0.52
1:A:72:LYS:HA	1:A:75:ILE:HG12	1.92	0.52
1:E:31:LEU:O	1:E:35:THR:HG22	2.09	0.52
1:E:12:ILE:HG21	1:E:35:THR:HG21	1.91	0.52
1:C:40:ASN:ND2	1:C:152:GLU:O	2.43	0.51
1:C:57:TRP:HA	1:C:60:VAL:HG22	1.93	0.51
1:A:113:ASP:OD1	1:A:114:ARG:N	2.44	0.50
1:A:57:TRP:HA	1:A:60:VAL:HG22	1.94	0.49
1:A:87:GLU:HG3	1:A:127:PHE:CD2	2.47	0.49
1:A:31:LEU:O	1:A:35:THR:HG22	2.12	0.49
1:C:89:ARG:NH1	1:C:127:PHE:H	2.11	0.49
1:C:35:THR:HG23	1:C:37:VAL:H	1.78	0.49
1:C:61:LEU:HD13	2:D:219:LEU:HD21	1.95	0.48
1:E:73:LYS:HD3	1:E:148:THR:HG22	1.95	0.48
1:G:51:GLU:OE1	1:G:59:ASN:ND2	2.34	0.48
1:G:77:LEU:HD22	1:G:149:LEU:HD11	1.94	0.48
1:C:26:ARG:O	1:C:30:ILE:HG12	2.12	0.48
1:G:96:LEU:HD11	2:H:203:ALA:HB2	1.96	0.47
1:C:31:LEU:O	1:C:35:THR:HG22	2.13	0.47
1:C:53:THR:O	1:C:142:ARG:NH2	2.46	0.47
1:G:57:TRP:HA	1:G:60:VAL:HG22	1.97	0.47
1:G:72:LYS:O	1:G:75:ILE:HG12	2.15	0.47
1:E:90:GLU:HG2	2:F:212:VAL:HG11	1.96	0.47
1:G:90:GLU:OE1	2:H:207:SER:OG	2.32	0.47
1:C:138:LYS:NZ	3:C:203:HOH:O	2.48	0.47
1:E:57:TRP:HA	1:E:60:VAL:HG22	1.97	0.46
1:G:26:ARG:O	1:G:30:ILE:HG12	2.15	0.46
1:A:118:LEU:O	1:A:122:ILE:HG13	2.15	0.46
1:E:131:GLU:HG3	1:E:132:VAL:N	2.31	0.46
1:A:131:GLU:HG3	1:A:132:VAL:N	2.31	0.46
1:A:17:GLN:NE2	1:A:157:ALA:O	2.30	0.46
1:A:89:ARG:NH2	1:A:127:PHE:H	2.14	0.46
1:C:63:THR:O	1:C:67:LEU:HG	2.16	0.46
1:E:26:ARG:O	1:E:30:ILE:HG12	2.16	0.45
1:A:82:ILE:HD12	1:A:118:LEU:HD21	1.98	0.45
1:C:95:ARG:NH2	1:C:123:ASN:OD1	2.43	0.45
1:A:40:ASN:ND2	1:A:152:GLU:O	2.48	0.45
1:E:101:THR:O	1:E:105:ILE:HG12	2.17	0.45
1:E:61:LEU:HD12	2:F:215:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:69:LEU:HA	1:G:69:LEU:HD23	1.86	0.45
1:C:88:LEU:HD23	1:E:89:ARG:HG3	1.99	0.45
2:D:206:HIS:CD2	2:D:207:SER:H	2.36	0.44
1:E:87:GLU:HG3	1:E:127:PHE:CE2	2.52	0.44
2:H:201:GLU:O	2:H:205:SER:N	2.50	0.44
1:E:41:THR:HA	1:E:154:HIS:O	2.16	0.44
1:C:171:TRP:CZ3	1:C:175:GLN:HG3	2.53	0.44
2:B:211:MET:O	2:B:215:LEU:HB3	2.18	0.44
1:C:131:GLU:HG3	1:C:132:VAL:N	2.33	0.44
1:E:58:ASP:N	1:E:58:ASP:OD1	2.51	0.44
1:C:17:GLN:NE2	1:C:157:ALA:O	2.27	0.43
1:C:101:THR:O	1:C:105:ILE:HG13	2.17	0.43
1:E:50:ASN:HA	1:E:53:THR:HG22	1.99	0.43
1:G:131:GLU:HG3	1:G:132:VAL:N	2.33	0.43
1:A:73:LYS:HD3	1:A:148:THR:HG22	1.99	0.43
1:C:21:GLU:OE1	1:C:159:SER:OG	2.35	0.43
1:C:58:ASP:N	1:C:58:ASP:OD1	2.52	0.43
1:A:58:ASP:N	1:A:58:ASP:OD1	2.52	0.43
1:G:39:LEU:HD22	1:G:41:THR:HG23	2.02	0.42
1:A:101:THR:O	1:A:105:ILE:HG12	2.20	0.42
1:C:118:LEU:O	1:C:122:ILE:HG13	2.20	0.42
1:E:61:LEU:HA	1:E:61:LEU:HD23	1.81	0.42
1:A:128:ASP:O	1:A:131:GLU:HG2	2.19	0.42
1:E:25:HIS:HB3	3:E:232:HOH:O	2.19	0.42
1:E:47:GLY:O	1:E:51:GLU:HG2	2.20	0.42
1:G:15:ILE:O	1:G:19:LEU:HD13	2.20	0.41
1:C:169:LEU:HA	1:C:169:LEU:HD12	1.88	0.41
1:E:94:ALA:HB1	1:E:122:ILE:HD11	2.02	0.41
1:A:30:ILE:HG23	1:C:26:ARG:HD2	2.03	0.41
1:C:87:GLU:HG3	1:C:127:PHE:CD2	2.56	0.41
1:A:27:THR:OG1	1:C:34:GLU:OE1	2.28	0.41
1:G:75:ILE:HG22	1:G:103:PRO:O	2.20	0.41
1:C:179:PRO:HA	1:C:180:PRO:HD3	1.93	0.41
1:A:169:LEU:HA	1:A:169:LEU:HD12	1.87	0.41
1:A:172:GLN:O	1:A:176:GLY:HA2	2.20	0.41
1:A:26:ARG:O	1:A:30:ILE:HG12	2.21	0.41
1:A:99:ARG:O	1:A:105:ILE:HD11	2.21	0.41
2:D:213:ARG:HG2	2:D:217:ARG:NH1	2.36	0.41
1:G:12:ILE:HG21	1:G:35:THR:HG21	2.02	0.41
1:A:35:THR:HG23	1:A:37:VAL:H	1.86	0.40
1:C:61:LEU:HD23	1:C:61:LEU:HA	1.85	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	175/184 (95%)	171 (98%)	3 (2%)	1 (1%)	30 66
1	C	175/184 (95%)	172 (98%)	3 (2%)	0	100 100
1	E	174/184 (95%)	173 (99%)	1 (1%)	0	100 100
1	G	175/184 (95%)	172 (98%)	3 (2%)	0	100 100
2	B	14/63 (22%)	14 (100%)	0	0	100 100
2	D	13/63 (21%)	13 (100%)	0	0	100 100
2	F	17/63 (27%)	17 (100%)	0	0	100 100
2	H	26/63 (41%)	26 (100%)	0	0	100 100
All	All	769/988 (78%)	758 (99%)	10 (1%)	1 (0%)	56 86

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	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	163/166 (98%)	161 (99%)	2 (1%)	78 93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	163/166 (98%)	160 (98%)	3 (2%)	66 89
1	E	161/166 (97%)	160 (99%)	1 (1%)	90 97
1	G	163/166 (98%)	160 (98%)	3 (2%)	66 89
2	B	16/57 (28%)	14 (88%)	2 (12%)	6 16
2	D	15/57 (26%)	14 (93%)	1 (7%)	20 50
2	F	19/57 (33%)	17 (90%)	2 (10%)	8 25
2	H	25/57 (44%)	21 (84%)	4 (16%)	3 8
All	All	725/892 (81%)	707 (98%)	18 (2%)	55 84

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LEU
1	A	153	VAL
2	B	211	MET
2	B	215	LEU
1	C	41	THR
1	C	69	LEU
1	C	110	ILE
2	D	211	MET
1	E	122	ILE
2	F	211	MET
2	F	222	ASN
1	G	5	GLU
1	G	43	ASP
1	G	174	HIS
2	H	202	LEU
2	H	206	HIS
2	H	210	ARG
2	H	215	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	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	177/184 (96%)	0.12	2 (1%) 82 81	30, 73, 103, 122	0
1	C	177/184 (96%)	0.02	0 100 100	28, 68, 102, 115	0
1	E	176/184 (95%)	-0.03	0 100 100	27, 53, 81, 101	0
1	G	177/184 (96%)	-0.03	0 100 100	23, 54, 79, 112	0
2	B	16/63 (25%)	1.52	5 (31%) 1 0	119, 134, 144, 152	0
2	D	15/63 (23%)	1.31	3 (20%) 1 1	107, 116, 130, 137	0
2	F	19/63 (30%)	0.77	1 (5%) 30 26	63, 86, 114, 114	0
2	H	28/63 (44%)	2.14	11 (39%) 0 0	67, 103, 143, 156	0
All	All	785/988 (79%)	0.17	22 (2%) 56 53	23, 63, 115, 156	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	219	LEU	7.6
2	H	202	LEU	7.0
2	H	200	GLN	6.1
2	H	201	GLU	6.1
2	H	196	SER	6.1
2	H	199	ALA	5.7
2	D	220	PHE	5.1
2	H	197	LEU	4.8
2	D	219	LEU	4.1
2	H	203	ALA	4.0
2	H	204	GLN	3.7
2	H	195	ALA	3.7
2	H	198	LEU	3.7
2	B	215	LEU	3.4
2	B	217	ARG	3.3
2	D	217	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
2	F	222	ASN	3.2
1	A	100	GLN	2.6
2	B	221	LYS	2.4
1	A	63	THR	2.3
2	H	206	HIS	2.3
2	B	207	SER	2.1

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.