Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 08:47 PM GMT

PDB ID	:	1M1L
Title	:	Human Suppressor of Fused (N-terminal domain)
Authors	:	Merchant, M.; Vajdos, F.F.; Ultsch, M.; Maun, H.R.; Wendt, U.; Cannon, J.; Lazarus, R.A.; de Vos, A.M.; de Sauvage, F.J.
Deposited on	:	2002-06-19
Resolution	:	2.65 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:

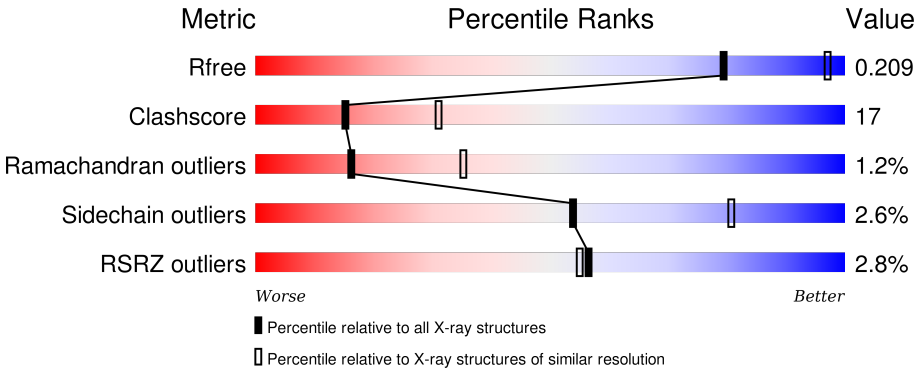
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.65 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	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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	236	2% 72% 26%
1	B	236	4% 74% 24%
1	C	236	3% 71% 27%
1	D	236	2% 68% 29%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7832 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 Suppressor of Fused.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	236	Total	C	N	O	S	0	0	0
			1877	1195	319	355	8			
1	B	236	Total	C	N	O	S	0	0	0
			1877	1195	319	355	8			
1	C	234	Total	C	N	O	S	0	0	0
			1866	1189	317	352	8			
1	D	234	Total	C	N	O	S	0	0	0
			1866	1189	317	352	8			

- Molecule 2 is water.

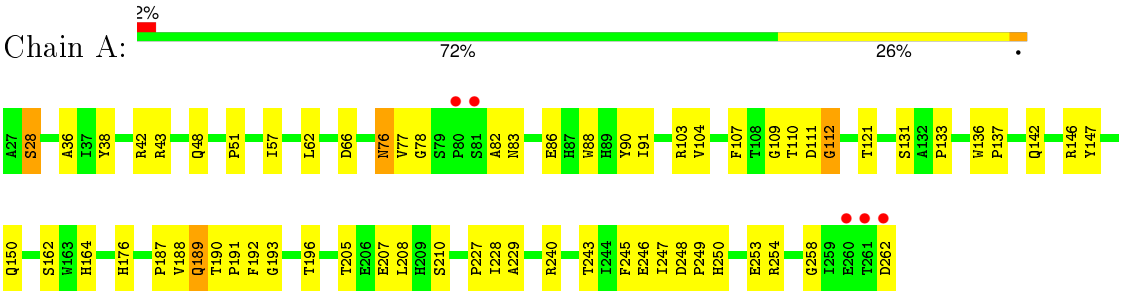
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	96	Total	O	0	0
			96	96		
2	B	73	Total	O	0	0
			73	73		
2	C	77	Total	O	0	0
			77	77		
2	D	100	Total	O	0	0
			100	100		

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.

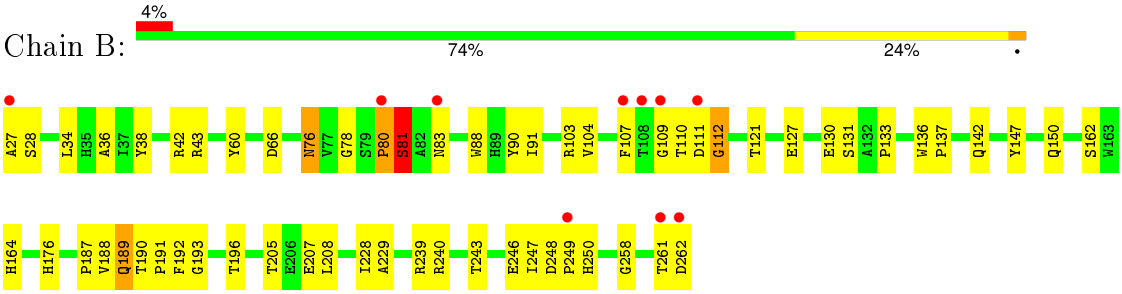
- Molecule 1: Suppressor of Fused

Chain A:



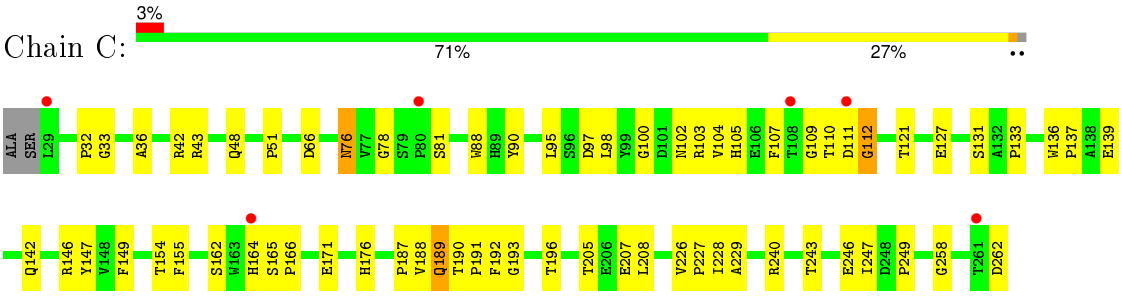
- Molecule 1: Suppressor of Fused

Chain B:



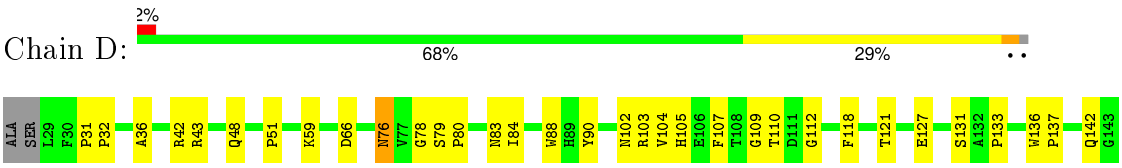
- Molecule 1: Suppressor of Fused

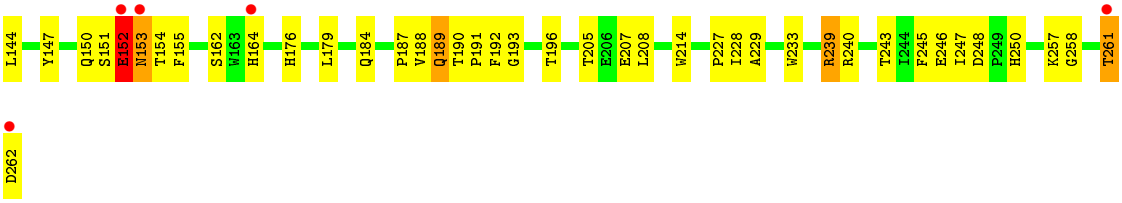
Chain C:



- Molecule 1: Suppressor of Fused

Chain D:




L144
Y147
Q150
S151
E152
N153
T154
F155
S162
W163
H164
H176
L179
Q184
P187
V188
Q189
T190
P191
F192
G193
T196
T205
E206
E207
L208
W214
P227
I228
A229
W233
R239
R240
T243
I244
F245
E246
I247
D248
P249
H250
K257
G258
T261
D262

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	173.03Å 173.03Å 290.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.81 – 2.65 29.81 – 2.65	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.81-2.65) 99.3 (29.81-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.04 (at 2.64Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.256 0.221 , 0.209	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	31.3	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 38.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 48270 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7832	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.53	1/1936 (0.1%)	0.68	1/2642 (0.0%)
1	B	0.53	0/1936	0.71	2/2642 (0.1%)
1	C	0.53	1/1925 (0.1%)	0.71	3/2627 (0.1%)
1	D	0.51	0/1925	0.74	2/2627 (0.1%)
All	All	0.52	2/7722 (0.0%)	0.71	8/10538 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	139	GLU	CB-CG	-6.13	1.40	1.52
1	A	253	GLU	CD-OE2	-5.09	1.20	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	152	GLU	N-CA-C	-9.26	86.01	111.00
1	C	139	GLU	CA-CB-CG	-7.50	96.89	113.40
1	C	139	GLU	OE1-CD-OE2	6.68	131.31	123.30
1	A	253	GLU	OE1-CD-OE2	-6.54	115.45	123.30
1	D	42	ARG	NE-CZ-NH1	-6.47	117.06	120.30
1	B	80	PRO	N-CA-C	-6.35	95.58	112.10
1	B	28	SER	N-CA-C	-5.34	96.59	111.00
1	C	42	ARG	NE-CZ-NH2	-5.07	117.76	120.30

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	1877	0	1779	70	0
1	B	1877	0	1779	70	0
1	C	1866	0	1769	57	0
1	D	1866	0	1769	67	0
2	A	96	0	0	3	0
2	B	73	0	0	2	0
2	C	77	0	0	7	0
2	D	100	0	0	8	0
All	All	7832	0	7096	254	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 17.

All (254) 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:190:THR:HG22	1:B:192:PHE:H	1.13	1.14
1:D:176:HIS:HE1	1:D:205:THR:HG22	1.15	1.10
1:B:176:HIS:HE1	1:B:205:THR:HG22	1.14	1.10
1:A:176:HIS:HE1	1:A:205:THR:HG22	1.17	1.09
1:B:176:HIS:CE1	1:B:205:THR:HG22	1.87	1.08
1:A:190:THR:HG22	1:A:192:PHE:H	1.12	1.08
1:D:176:HIS:CE1	1:D:205:THR:HG22	1.89	1.07
1:A:176:HIS:CE1	1:A:205:THR:HG22	1.89	1.06
1:D:190:THR:HG22	1:D:192:PHE:H	1.15	1.06
1:C:190:THR:HG22	1:C:192:PHE:H	1.17	1.05
1:C:176:HIS:CE1	1:C:205:THR:HG22	1.94	1.01
1:C:176:HIS:HE1	1:C:205:THR:HG22	1.21	1.01
1:A:146:ARG:O	1:A:150:GLN:HG2	1.63	0.97
1:B:80:PRO:O	1:B:81:SER:HB3	1.76	0.83
1:D:103:ARG:HG3	1:D:104:VAL:HG23	1.62	0.81
1:C:103:ARG:HG3	1:C:104:VAL:HG23	1.62	0.81
1:B:27:ALA:N	2:B:314:HOH:O	2.14	0.80
1:B:103:ARG:HG3	1:B:104:VAL:HG23	1.62	0.79
1:A:103:ARG:HG3	1:A:104:VAL:HG23	1.63	0.79
1:C:110:THR:HG22	1:C:191:PRO:O	1.84	0.77
1:D:110:THR:HG22	1:D:191:PRO:O	1.85	0.77
1:C:76:ASN:HD22	1:C:78:GLY:H	1.33	0.76
1:A:150:GLN:HG3	1:B:147:TYR:OH	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:LYS:O	1:D:261:THR:HG23	1.87	0.74
1:C:190:THR:HG21	2:C:312:HOH:O	1.86	0.74
1:D:59:LYS:HG2	2:D:343:HOH:O	1.88	0.74
1:D:228:ILE:HG23	2:D:296:HOH:O	1.88	0.74
1:A:76:ASN:HD22	1:A:78:GLY:H	1.35	0.73
1:B:190:THR:HG22	1:B:192:PHE:N	1.97	0.72
1:D:227:PRO:HG2	2:D:296:HOH:O	1.90	0.72
1:C:32:PRO:HB3	1:C:191:PRO:HG3	1.71	0.72
1:B:76:ASN:HD22	1:B:78:GLY:H	1.36	0.71
1:B:110:THR:HG22	1:B:191:PRO:O	1.91	0.71
1:C:258:GLY:O	1:C:262:ASP:HB2	1.90	0.71
1:D:76:ASN:HD22	1:D:78:GLY:H	1.39	0.71
1:A:38:TYR:CE2	1:A:42:ARG:HD2	2.26	0.70
1:A:38:TYR:CZ	1:A:42:ARG:HD2	2.27	0.70
1:C:190:THR:HG22	1:C:192:PHE:N	2.02	0.69
1:B:76:ASN:ND2	1:B:78:GLY:H	1.91	0.69
1:D:184:GLN:HG2	2:D:285:HOH:O	1.92	0.68
1:A:162:SER:HA	1:A:176:HIS:HD2	1.59	0.68
1:A:76:ASN:ND2	1:A:78:GLY:H	1.92	0.68
1:A:258:GLY:O	1:A:262:ASP:HB2	1.94	0.67
1:A:190:THR:HG22	1:A:192:PHE:N	1.97	0.67
1:D:190:THR:HG22	1:D:192:PHE:N	2.00	0.66
1:C:76:ASN:ND2	1:C:78:GLY:H	1.92	0.66
1:A:176:HIS:HE1	1:A:205:THR:CG2	2.04	0.65
1:B:162:SER:HA	1:B:176:HIS:HD2	1.61	0.65
1:C:107:PHE:CZ	1:C:109:GLY:HA2	2.33	0.64
1:D:118:PHE:CE2	1:D:154:THR:HG23	2.32	0.64
1:A:62:LEU:HD12	2:A:284:HOH:O	1.96	0.64
1:D:190:THR:HG21	2:D:275:HOH:O	1.96	0.64
1:D:32:PRO:HB3	1:D:191:PRO:HG3	1.79	0.64
1:C:162:SER:HA	1:C:176:HIS:HD2	1.63	0.63
1:D:228:ILE:HD11	1:D:247:ILE:CD1	2.29	0.63
1:D:76:ASN:ND2	1:D:78:GLY:H	1.96	0.63
1:B:190:THR:HB	1:B:193:GLY:O	1.99	0.62
1:C:32:PRO:HB3	1:C:191:PRO:CG	2.29	0.62
1:A:83:ASN:HD21	1:A:227:PRO:HB3	1.63	0.62
1:A:82:ALA:O	1:A:83:ASN:HB3	1.99	0.62
1:A:110:THR:HG22	1:A:191:PRO:O	2.00	0.61
1:B:258:GLY:O	1:B:262:ASP:HB2	2.01	0.61
1:B:243:THR:OG1	1:B:246:GLU:HG3	2.01	0.61
1:A:147:TYR:OH	1:B:150:GLN:OE1	2.11	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:TRP:CG	1:A:137:PRO:HD3	2.36	0.61
1:C:243:THR:OG1	1:C:246:GLU:HG3	2.00	0.61
1:B:80:PRO:O	1:B:81:SER:CB	2.49	0.60
1:D:162:SER:HA	1:D:176:HIS:HD2	1.66	0.60
1:A:190:THR:HG23	1:A:191:PRO:HD2	1.84	0.60
1:D:228:ILE:HD11	1:D:247:ILE:HD13	1.84	0.59
1:A:243:THR:OG1	1:A:246:GLU:HG3	2.02	0.59
1:C:228:ILE:HD11	1:C:247:ILE:CD1	2.32	0.59
1:B:66:ASP:HB3	1:B:142:GLN:CD	2.22	0.59
1:D:190:THR:HB	1:D:193:GLY:O	2.02	0.59
1:C:76:ASN:HD22	1:C:78:GLY:N	2.00	0.59
1:A:228:ILE:HD11	1:A:247:ILE:CD1	2.32	0.59
1:B:228:ILE:HD11	1:B:247:ILE:CD1	2.31	0.59
1:C:190:THR:HB	1:C:193:GLY:O	2.03	0.58
1:B:76:ASN:HD22	1:B:78:GLY:N	2.00	0.58
1:D:154:THR:HG22	1:D:155:PHE:O	2.03	0.58
1:B:228:ILE:HD11	1:B:247:ILE:HD13	1.86	0.58
1:D:118:PHE:HE2	1:D:154:THR:HG23	1.67	0.58
1:A:43:ARG:HH11	1:A:43:ARG:HG2	1.69	0.57
1:C:229:ALA:HB1	1:C:240:ARG:NH1	2.19	0.57
1:A:36:ALA:HB1	1:A:188:VAL:HG11	1.86	0.57
1:D:136:TRP:CG	1:D:137:PRO:HD3	2.40	0.57
1:A:66:ASP:HB3	1:A:142:GLN:CD	2.24	0.57
1:C:171:GLU:HB2	2:C:268:HOH:O	2.04	0.57
1:C:240:ARG:HD3	2:C:280:HOH:O	2.05	0.56
1:A:190:THR:HB	1:A:193:GLY:O	2.05	0.56
1:C:190:THR:HG23	1:C:191:PRO:HD2	1.86	0.56
1:B:43:ARG:HH11	1:B:43:ARG:HG2	1.71	0.56
1:D:190:THR:HG23	1:D:191:PRO:HD2	1.88	0.56
1:A:228:ILE:HD11	1:A:247:ILE:HD13	1.87	0.56
1:B:136:TRP:CG	1:B:137:PRO:HD3	2.41	0.55
1:B:176:HIS:CD2	1:B:208:LEU:HD22	2.42	0.55
1:C:66:ASP:HB3	1:C:142:GLN:CD	2.26	0.55
1:B:189:GLN:HE21	1:B:190:THR:N	2.05	0.55
1:D:90:TYR:O	1:D:121:THR:HA	2.07	0.55
1:D:43:ARG:HH11	1:D:43:ARG:HG2	1.72	0.55
1:B:38:TYR:CE2	1:B:42:ARG:HD2	2.42	0.55
1:A:76:ASN:HD22	1:A:78:GLY:N	2.01	0.55
1:D:243:THR:OG1	1:D:246:GLU:HG3	2.07	0.54
1:D:164:HIS:O	1:D:164:HIS:CD2	2.60	0.54
1:C:147:TYR:CE2	1:C:155:PHE:HZ	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:GLN:HE21	1:B:189:GLN:CA	2.20	0.54
1:D:240:ARG:HD3	2:D:322:HOH:O	2.08	0.54
1:C:228:ILE:HD11	1:C:247:ILE:HD13	1.88	0.54
1:D:66:ASP:HB3	1:D:142:GLN:CD	2.28	0.54
1:D:76:ASN:HD22	1:D:78:GLY:N	2.04	0.54
1:C:136:TRP:CG	1:C:137:PRO:HD3	2.43	0.53
1:B:36:ALA:HB1	1:B:188:VAL:HG11	1.90	0.53
1:B:261:THR:O	1:B:261:THR:HG22	2.08	0.53
1:C:176:HIS:CD2	1:C:208:LEU:HD22	2.44	0.53
1:D:147:TYR:OH	1:D:152:GLU:OE2	2.26	0.53
1:D:176:HIS:CD2	1:D:208:LEU:HD22	2.43	0.53
1:B:90:TYR:O	1:B:121:THR:HA	2.09	0.52
1:C:205:THR:HG23	2:C:265:HOH:O	2.09	0.52
1:D:144:LEU:HD22	1:D:155:PHE:HE1	1.74	0.52
1:B:190:THR:HG23	1:B:191:PRO:HD2	1.92	0.52
1:A:150:GLN:HG3	1:B:147:TYR:CE1	2.44	0.52
1:C:95:LEU:HD23	1:C:149:PHE:HE1	1.75	0.52
1:D:127:GLU:HG3	1:D:239:ARG:NH1	2.24	0.52
1:A:147:TYR:CE1	1:B:150:GLN:OE1	2.63	0.51
1:A:164:HIS:CD2	1:A:164:HIS:O	2.63	0.51
1:A:147:TYR:CE2	1:B:147:TYR:CE2	2.98	0.51
1:A:88:TRP:CE3	1:A:133:PRO:HB3	2.45	0.51
1:C:111:ASP:O	1:C:112:GLY:O	2.29	0.51
1:A:38:TYR:CE2	1:A:42:ARG:NH1	2.79	0.51
1:A:90:TYR:O	1:A:121:THR:HA	2.11	0.51
1:C:189:GLN:HE21	1:C:190:THR:N	2.09	0.51
1:B:107:PHE:CZ	1:B:109:GLY:HA2	2.46	0.51
1:B:189:GLN:HE21	1:B:190:THR:H	1.58	0.50
1:D:189:GLN:HE21	1:D:190:THR:N	2.09	0.50
1:A:38:TYR:HE2	1:A:42:ARG:NH1	2.09	0.50
1:A:240:ARG:HD3	2:A:338:HOH:O	2.10	0.50
1:B:187:PRO:HB3	1:B:196:THR:HG22	1.92	0.50
1:C:43:ARG:HG2	1:C:43:ARG:HH11	1.77	0.50
1:A:229:ALA:HA	1:A:240:ARG:HD2	1.93	0.50
1:D:164:HIS:HD2	1:D:164:HIS:O	1.94	0.50
1:C:36:ALA:HB1	1:C:188:VAL:HG11	1.94	0.50
1:B:38:TYR:CZ	1:B:42:ARG:HD2	2.47	0.50
1:A:207:GLU:OE1	1:A:240:ARG:NH2	2.44	0.50
1:A:176:HIS:CD2	1:A:208:LEU:HD22	2.46	0.50
1:A:150:GLN:HG3	1:B:147:TYR:CZ	2.46	0.49
1:C:228:ILE:HB	2:C:273:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ASP:OD1	1:A:250:HIS:HB2	2.11	0.49
1:D:32:PRO:HB3	1:D:191:PRO:CG	2.41	0.48
1:A:147:TYR:CZ	1:B:150:GLN:OE1	2.65	0.48
1:A:210:SER:HG	1:A:245:PHE:HZ	1.60	0.48
1:B:88:TRP:CE3	1:B:133:PRO:HB3	2.49	0.48
1:D:36:ALA:HB1	1:D:188:VAL:HG11	1.95	0.48
1:D:151:SER:OG	1:D:152:GLU:N	2.47	0.48
1:B:164:HIS:CD2	1:B:164:HIS:O	2.66	0.48
1:D:214:TRP:CE2	1:D:258:GLY:HA3	2.48	0.48
1:B:189:GLN:HA	1:B:189:GLN:NE2	2.28	0.48
1:D:228:ILE:HD11	1:D:247:ILE:HD11	1.95	0.48
1:B:205:THR:HG23	2:B:270:HOH:O	2.13	0.48
1:C:33:GLY:HA3	1:C:98:LEU:HA	1.96	0.48
1:D:88:TRP:CE3	1:D:133:PRO:HB3	2.48	0.47
1:C:102:ASN:HA	1:C:105:HIS:O	2.15	0.47
1:B:127:GLU:O	1:B:130:GLU:HG3	2.15	0.47
1:A:190:THR:HG21	2:A:266:HOH:O	2.14	0.47
1:A:36:ALA:HB1	1:A:188:VAL:CG1	2.45	0.47
1:A:164:HIS:O	1:A:164:HIS:HD2	1.98	0.47
1:C:187:PRO:HB3	1:C:196:THR:HG22	1.97	0.47
1:B:66:ASP:HB3	1:B:142:GLN:NE2	2.30	0.47
1:D:187:PRO:HB3	1:D:196:THR:HG22	1.95	0.47
1:D:107:PHE:CZ	1:D:109:GLY:HA2	2.50	0.47
1:C:90:TYR:O	1:C:121:THR:HA	2.15	0.47
1:A:207:GLU:CD	1:A:240:ARG:HH22	2.18	0.47
1:A:187:PRO:HB3	1:A:196:THR:HG22	1.97	0.47
1:C:66:ASP:HB3	1:C:142:GLN:NE2	2.30	0.46
1:A:147:TYR:CE2	1:B:147:TYR:CD2	3.03	0.46
1:D:248:ASP:OD1	1:D:250:HIS:HB2	2.14	0.46
1:C:48:GLN:O	1:C:51:PRO:HD3	2.16	0.46
1:A:189:GLN:HE21	1:A:190:THR:N	2.14	0.45
1:B:38:TYR:CE2	1:B:42:ARG:NH1	2.85	0.45
1:D:102:ASN:HA	1:D:105:HIS:O	2.16	0.45
1:B:127:GLU:HG3	1:B:239:ARG:CZ	2.46	0.45
1:B:189:GLN:NE2	1:B:189:GLN:CA	2.79	0.45
1:B:127:GLU:HG3	1:B:239:ARG:NH2	2.32	0.45
1:C:88:TRP:CE3	1:C:133:PRO:HB3	2.52	0.45
1:C:189:GLN:HE21	1:C:190:THR:H	1.65	0.45
1:B:111:ASP:O	1:B:112:GLY:O	2.33	0.45
1:B:43:ARG:HG2	1:B:43:ARG:NH1	2.32	0.45
1:C:142:GLN:O	1:C:146:ARG:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:ALA:HB1	1:D:240:ARG:NH1	2.32	0.45
1:D:189:GLN:CA	1:D:189:GLN:HE21	2.28	0.44
1:D:152:GLU:O	1:D:153:ASN:HB2	2.17	0.44
1:A:43:ARG:NH1	1:A:43:ARG:HG2	2.31	0.44
1:B:38:TYR:HE2	1:B:42:ARG:NH1	2.15	0.44
1:C:228:ILE:HD11	1:C:247:ILE:HD11	1.98	0.44
1:B:90:TYR:C	1:B:91:ILE:HD12	2.37	0.44
1:C:107:PHE:CZ	1:C:109:GLY:CA	3.00	0.44
1:D:43:ARG:HG2	1:D:43:ARG:NH1	2.32	0.44
1:D:48:GLN:O	1:D:51:PRO:HD3	2.17	0.44
1:B:207:GLU:OE1	1:B:240:ARG:NH2	2.50	0.44
1:A:136:TRP:CD2	1:A:137:PRO:HD3	2.53	0.44
1:A:228:ILE:HD11	1:A:247:ILE:HD11	1.99	0.44
1:C:164:HIS:CD2	1:C:164:HIS:O	2.70	0.44
1:D:245:PHE:HB2	2:D:274:HOH:O	2.17	0.44
1:B:136:TRP:CD2	1:B:137:PRO:HD3	2.53	0.44
1:D:127:GLU:HG3	1:D:239:ARG:NH2	2.32	0.44
1:D:150:GLN:HG3	2:D:339:HOH:O	2.17	0.43
1:D:127:GLU:HG3	1:D:239:ARG:CZ	2.49	0.43
1:C:154:THR:HA	2:C:313:HOH:O	2.19	0.43
1:A:38:TYR:CE2	1:A:42:ARG:CD	3.01	0.43
1:B:228:ILE:HD11	1:B:247:ILE:HD11	1.99	0.43
1:B:207:GLU:CD	1:B:240:ARG:HH22	2.21	0.43
1:B:91:ILE:HD12	1:B:91:ILE:N	2.33	0.43
1:A:57:ILE:HG21	1:D:51:PRO:HD2	1.99	0.43
1:A:107:PHE:CZ	1:A:109:GLY:HA2	2.54	0.43
1:C:189:GLN:CA	1:C:189:GLN:HE21	2.31	0.43
1:A:248:ASP:HA	1:A:249:PRO:HD2	1.78	0.43
1:C:32:PRO:CB	1:C:191:PRO:CG	2.97	0.42
1:D:229:ALA:HA	1:D:240:ARG:HD2	2.01	0.42
1:B:164:HIS:HD2	1:B:164:HIS:O	2.02	0.42
1:A:189:GLN:CA	1:A:189:GLN:HE21	2.32	0.42
1:C:207:GLU:CD	1:C:240:ARG:HH22	2.22	0.42
1:D:136:TRP:CD2	1:D:137:PRO:HD3	2.54	0.42
1:B:36:ALA:HB1	1:B:188:VAL:CG1	2.49	0.42
1:D:176:HIS:HE1	1:D:205:THR:CG2	2.06	0.42
1:C:127:GLU:HG3	2:C:318:HOH:O	2.19	0.42
1:A:190:THR:CG2	1:A:191:PRO:N	2.83	0.42
1:D:207:GLU:CD	1:D:240:ARG:HH22	2.23	0.42
1:D:127:GLU:HG3	1:D:239:ARG:HH12	1.84	0.42
1:A:88:TRP:CZ3	1:A:133:PRO:HD3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:THR:HG22	1:C:191:PRO:C	2.41	0.41
1:B:176:HIS:HE1	1:B:205:THR:CG2	2.05	0.41
1:A:90:TYR:C	1:A:91:ILE:HD12	2.41	0.41
1:C:97:ASP:OD1	1:C:100:GLY:HA2	2.21	0.41
1:B:229:ALA:HA	1:B:240:ARG:HD2	2.01	0.41
1:D:155:PHE:HB3	1:D:179:LEU:CD1	2.50	0.41
1:A:164:HIS:CE1	1:B:60:TYR:CE2	3.08	0.41
1:A:162:SER:HA	1:A:176:HIS:CD2	2.47	0.41
1:B:229:ALA:HB1	1:B:240:ARG:NH1	2.36	0.41
1:A:77:VAL:HA	1:A:86:GLU:HG3	2.03	0.41
1:D:79:SER:HA	1:D:80:PRO:HD2	1.94	0.41
1:A:66:ASP:HB3	1:A:142:GLN:NE2	2.35	0.41
1:B:34:LEU:HD23	1:B:34:LEU:C	2.41	0.41
1:C:226:VAL:HA	1:C:227:PRO:HD2	1.89	0.41
1:B:107:PHE:CZ	1:B:109:GLY:CA	3.04	0.40
1:C:36:ALA:HB1	1:C:188:VAL:CG1	2.51	0.40
1:B:88:TRP:CZ3	1:B:133:PRO:HD3	2.57	0.40
1:C:164:HIS:HD2	1:C:164:HIS:O	2.03	0.40
1:A:146:ARG:O	1:A:150:GLN:CG	2.52	0.40
1:D:66:ASP:HB3	1:D:142:GLN:NE2	2.36	0.40
1:D:84:ILE:HG21	1:D:233:TRP:CE3	2.56	0.40
1:C:165:SER:O	1:C:166:PRO:C	2.58	0.40
1:A:48:GLN:O	1:A:51:PRO:HD3	2.21	0.40
1:D:189:GLN:HE21	1:D:190:THR:H	1.69	0.40
1:B:248:ASP:OD1	1:B:250:HIS:HB2	2.21	0.40
1:A:111:ASP:O	1:A:112:GLY:O	2.39	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	234/236 (99%)	220 (94%)	12 (5%)	2 (1%)	21	44
1	B	234/236 (99%)	220 (94%)	11 (5%)	3 (1%)	15	33
1	C	232/236 (98%)	218 (94%)	12 (5%)	2 (1%)	21	44
1	D	232/236 (98%)	215 (93%)	13 (6%)	4 (2%)	11	25
All	All	932/944 (99%)	873 (94%)	48 (5%)	11 (1%)	16	35

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	B	81	SER
1	D	152	GLU
1	A	112	GLY
1	B	112	GLY
1	C	112	GLY
1	B	249	PRO
1	D	153	ASN
1	D	31	PRO
1	D	112	GLY
1	C	249	PRO

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	205/205 (100%)	200 (98%)	5 (2%)	57	82
1	B	205/205 (100%)	200 (98%)	5 (2%)	57	82
1	C	204/205 (100%)	200 (98%)	4 (2%)	63	86
1	D	204/205 (100%)	197 (97%)	7 (3%)	44	72
All	All	818/820 (100%)	797 (97%)	21 (3%)	54	81

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	76	ASN
1	A	131	SER
1	A	189	GLN
1	A	254	ARG
1	B	76	ASN
1	B	81	SER
1	B	83	ASN
1	B	131	SER
1	B	189	GLN
1	C	76	ASN
1	C	81	SER
1	C	131	SER
1	C	189	GLN
1	D	76	ASN
1	D	83	ASN
1	D	131	SER
1	D	189	GLN
1	D	239	ARG
1	D	261	THR
1	D	262	ASP

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	76	ASN
1	A	83	ASN
1	A	164	HIS
1	A	176	HIS
1	A	189	GLN
1	B	76	ASN
1	B	164	HIS
1	B	176	HIS
1	B	189	GLN
1	C	76	ASN
1	C	164	HIS
1	C	169	ASN
1	C	176	HIS
1	C	189	GLN
1	C	252	GLN
1	D	76	ASN
1	D	164	HIS
1	D	169	ASN

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Mol	Chain	Res	Type
1	D	176	HIS
1	D	189	GLN

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	236/236 (100%)	-0.28	5 (2%)	67	66	14, 28, 63, 92	0
1	B	236/236 (100%)	-0.26	10 (4%)	40	38	15, 29, 62, 81	0
1	C	234/236 (99%)	-0.24	6 (2%)	59	58	18, 33, 61, 81	0
1	D	234/236 (99%)	-0.21	5 (2%)	67	66	14, 30, 57, 89	0
All	All	940/944 (99%)	-0.25	26 (2%)	56	55	14, 30, 61, 92	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	262	ASP	4.0
1	D	153	ASN	3.9
1	B	80	PRO	3.6
1	C	80	PRO	3.6
1	D	152	GLU	3.5
1	A	261	THR	3.5
1	C	164	HIS	3.3
1	B	27	ALA	3.2
1	B	261	THR	3.1
1	B	83	ASN	3.0
1	B	262	ASP	2.9
1	D	262	ASP	2.8
1	B	111	ASP	2.7
1	A	81	SER	2.5
1	B	249	PRO	2.5
1	C	108	THR	2.2
1	A	80	PRO	2.2
1	B	109	GLY	2.2
1	D	164	HIS	2.2
1	B	108	THR	2.2
1	C	111	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	260	GLU	2.1
1	C	29	LEU	2.1
1	C	261	THR	2.1
1	D	261	THR	2.1
1	B	107	PHE	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.