Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 11:22 PM EDT

PDB ID	:	5XJL
Title	:	Crystal Structure of the Gemin2-binding domain of SMN, Gemin2 in Complex with SmD1/D2/F/E/G from Human
Authors	:	Zhang, R.
Deposited on	:	2017-05-02
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

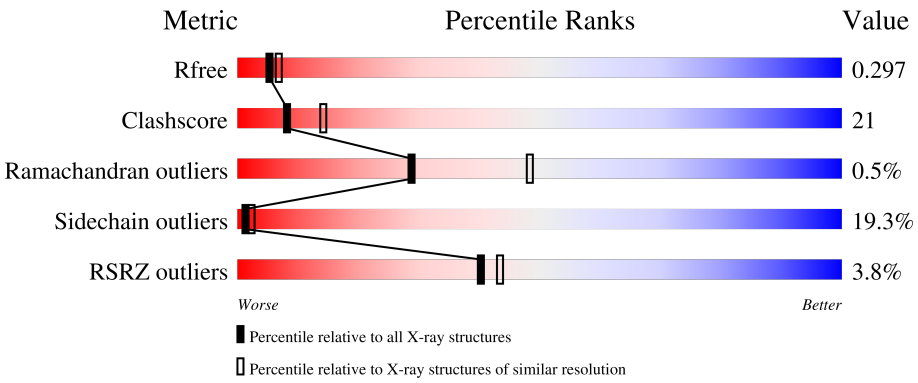
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 of 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	2	280	4%, 41%, 28%, 5%, 27%
2	A	119	%, 46%, 17%, 5%, 32%
3	B	118	47%, 19%, 6%, 28%
4	E	92	4%, 40%, 35%, 9%, 16%
5	F	86	%, 58%, 23%, 5%, 14%

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Mol	Chain	Length	Quality of chain
6	G	76	8% 25% 42% 16% 17%
7	M	37	3% 30% 16% 54%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 4826 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 Gem-associated protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	2	204	1644	1042	289	304	9	0	0	0

- Molecule 2 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	81	641	409	112	116	4	0	0	0

- Molecule 3 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	85	681	429	125	122	5	0	0	0

- Molecule 4 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	77	638	405	113	115	5	0	0	0

- Molecule 5 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	74	576	372	95	104	5	0	0	0

- Molecule 6 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	G	63	485	307	85	87	6	0	0	0

- Molecule 7 is a protein called Survival motor neuron protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	M	17	130	84	20	26	0	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	2	12	12	12	0	0
8	A	5	5	5	0	0
8	B	5	5	5	0	0
8	E	4	4	4	0	0
8	F	4	4	4	0	0
8	G	1	1	1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Gem-associated protein 2

Chain 2: 4% 41% 28% 5% 27%

MET ARG ARG ALA GLU LEU ALA GLY LEU LYS THR MET ALA TRP VAL PRO ALA GLU SER ALA VAL E22 E23 L24 M25 P26 R27 L28 V31 GLU PRO CYS ASP LEU THR GLU GLY PHE ASP PRO SER VAL PRO PRO ARG T48 P49 Y52 L53 R54 R55 V56 Q57 I58 V66 V67 V68

A69 Q70 I71 D72 P73 LYS LYS LEU LYS ARG K79 Q80 S81 V82 S85 L86 G95 Y96 S97 P98 T99 L100 Q101 W102 Q103 Q106 S111 Q115 K119 H120 R121 S122 H123 W124 LYS SER GLN GLN LEU ASP SER ASN VAL THR M135 P136 K137 D140 W144 K145 K146 F147

C148 L149 G150 E151 LYS LEU CYS ALA ASP GLY ALA VAL GLY PRO ALA THR ASN GLU SER PRO GLY ILE ASP TYR VAL GLN I174 G175 F176 P177 P178 L179 L180 S181 I182 V183 S184 R185 M186 S193 V194 L195 G203 E204 R205 T208 L211 G212 R213 W214 L215 L218 L219 A220 C221

K224 P225 Q236 R239 R240 R245 K251 D252 D253 E254 R255 V256 P257 N260 R268 R273 D274 L275 E278 PRO SER

• Molecule 2: Small nuclear ribonucleoprotein Sm D1

Chain A: % 46% 17% 5% 32%

M1 K2 L3 V4 R5 F6 S11 T14 E18 Q24 T30 D33 M36 H39 L40 K41 K44 Q54 S59 R66 P71 D72 S73 L74 P75 L76 L80 V81 ASP VAL GLU PRO LYS VAL LYS SER LYS LYS ARG GLU ALA VAL ALA GLY ARG GLY

ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY GLY GLY PRO ARG ARG

• Molecule 3: Small nuclear ribonucleoprotein Sm D2

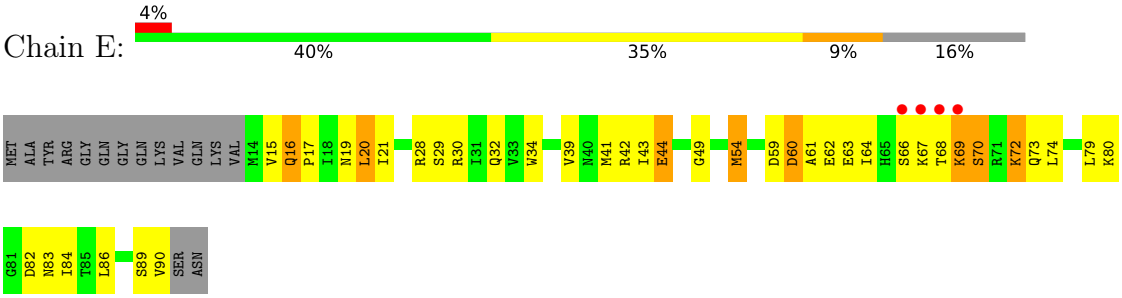
Chain B: 47% 19% 6% 28%

MET SER LEU LEU ASN LYS PRO LYS SER GLU MET THR PRO GLU GLU LEU GLN LYS ARG GLU GLU E22 E23 F24 N25 T26 S30 V31 L32 T33 R47 K51 L52 R55 V56 K57 D60 R61 H62 V70 K71 E72 M73 V77 PRO LYS SER GLY LYS GLY LYS LYS LYS

SER LYS P89 R94 K98 M99 F100 L101 R102 G103 D104 S105 V106 I107 V108 V109 L110 R111 N112 G117 LYS

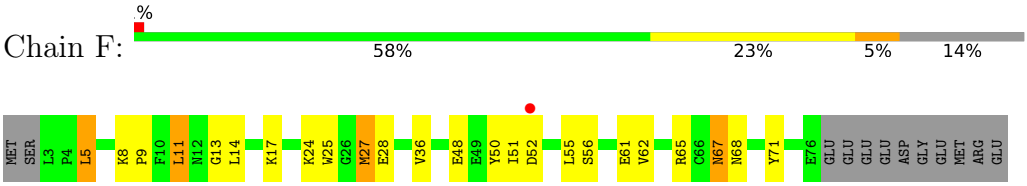
• Molecule 4: Small nuclear ribonucleoprotein E

Chain E:



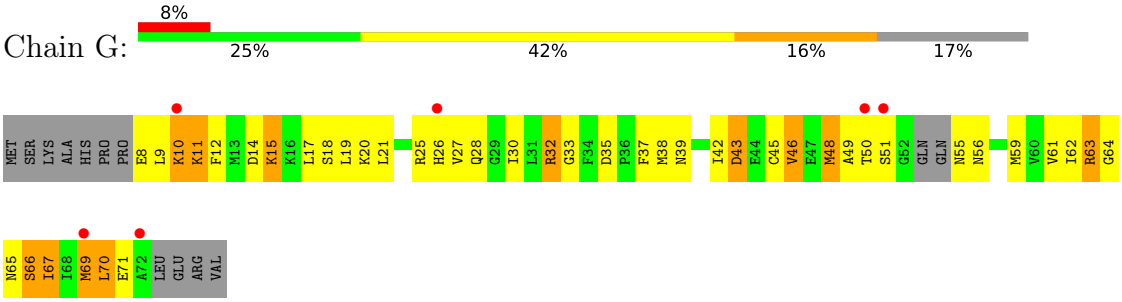
- Molecule 5: Small nuclear ribonucleoprotein F

Chain F:



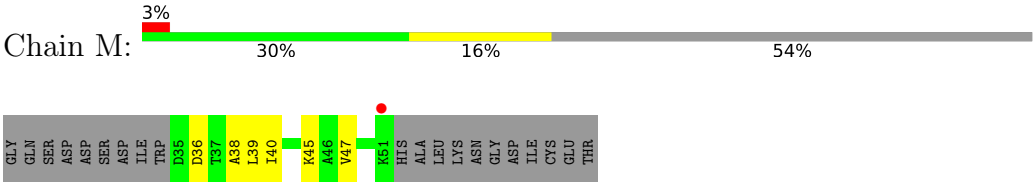
- Molecule 6: Small nuclear ribonucleoprotein G

Chain G:



- Molecule 7: Survival motor neuron protein

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.83Å 84.60Å 104.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.19 – 2.50 39.22 – 2.50	Depositor EDS
% Data completeness (in resolution range)	76.2 (59.19-2.50) 76.2 (39.22-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.95 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.220 , 0.296 0.224 , 0.297	Depositor DCC
R_{free} test set	1015 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	38.1	Xtriage
Anisotropy	0.726	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 58.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4826	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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 (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	2	0.66	0/1678	0.76	0/2276
2	A	0.87	0/649	0.86	0/877
3	B	0.72	0/689	0.83	0/926
4	E	0.68	0/646	0.72	0/867
5	F	0.66	0/588	0.75	0/795
6	G	0.66	0/488	0.81	0/648
7	M	0.60	0/131	0.65	0/175
All	All	0.70	0/4869	0.78	0/6564

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 (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	2	1644	0	1631	67	0
2	A	641	0	689	16	0
3	B	681	0	709	27	0
4	E	638	0	657	44	0
5	F	576	0	581	24	0
6	G	485	0	508	54	0
7	M	130	0	131	7	0
8	2	12	0	0	1	0
8	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	5	0	0	0	0
8	E	4	0	0	0	0
8	F	4	0	0	0	0
8	G	1	0	0	0	0
All	All	4826	0	4906	206	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 21.

All (206) 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)
4:E:44:GLU:HB2	4:E:64:ILE:HD11	1.42	0.98
1:2:224:LYS:HB2	1:2:225:PRO:HA	1.49	0.94
4:E:83:ASN:HD21	5:F:24:LYS:HG2	1.39	0.87
2:A:18:GLU:HG3	2:A:24:GLN:NE2	1.90	0.87
6:G:28:GLN:HB2	6:G:48:MET:CE	2.05	0.86
4:E:68:THR:O	4:E:69:LYS:HG3	1.78	0.84
2:A:18:GLU:HG3	2:A:24:GLN:HE22	1.42	0.82
1:2:204:GLU:N	1:2:204:GLU:OE1	2.13	0.82
4:E:83:ASN:HD21	5:F:24:LYS:CG	1.92	0.82
4:E:41:MET:SD	4:E:63:GLU:OE1	2.40	0.80
1:2:119:LYS:O	1:2:122:SER:HB2	1.81	0.80
6:G:64:GLY:O	6:G:67:ILE:HG23	1.83	0.79
4:E:83:ASN:ND2	5:F:24:LYS:HD3	1.98	0.78
6:G:70:LEU:HD12	6:G:70:LEU:H	1.49	0.76
5:F:25:TRP:HB2	5:F:27:MET:SD	2.26	0.76
4:E:44:GLU:HB2	4:E:64:ILE:CD1	2.15	0.75
1:2:135:MET:CG	1:2:182:ILE:HD11	2.17	0.75
6:G:67:ILE:HD11	6:G:70:LEU:HG	1.68	0.75
4:E:64:ILE:HD12	4:E:64:ILE:N	2.02	0.75
6:G:37:PHE:O	6:G:38:MET:HB2	1.86	0.75
6:G:28:GLN:HB2	6:G:48:MET:HE1	1.67	0.75
3:B:47:ARG:HG2	3:B:105:SER:O	1.86	0.74
1:2:135:MET:SD	1:2:182:ILE:HD11	2.27	0.74
4:E:44:GLU:OE1	4:E:90:VAL:HG11	1.88	0.74
4:E:83:ASN:HD21	5:F:24:LYS:CD	2.00	0.73
1:2:177:PRO:HB2	7:M:40:ILE:HD11	1.70	0.73
1:2:203:GLY:C	1:2:204:GLU:OE1	2.27	0.73
4:E:15:VAL:O	6:G:33:GLY:HA3	1.88	0.72
6:G:70:LEU:HD12	6:G:70:LEU:N	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:27:VAL:HG13	6:G:45:CYS:SG	2.29	0.72
1:2:182:ILE:HD12	1:2:182:ILE:O	1.91	0.71
6:G:19:LEU:N	6:G:27:VAL:O	2.21	0.71
4:E:30:ARG:NH2	4:E:60:ASP:O	2.24	0.71
3:B:22:GLU:C	3:B:23:GLU:OE2	2.29	0.70
1:2:120:HIS:CD2	1:2:180:LEU:HD13	2.27	0.69
1:2:203:GLY:CA	1:2:204:GLU:OE1	2.40	0.69
2:A:3:LEU:O	2:A:6:PHE:HB3	1.93	0.69
6:G:19:LEU:O	6:G:26:HIS:HA	1.93	0.69
4:E:17:PRO:O	4:E:21:ILE:HG13	1.93	0.69
1:2:70:GLN:HG2	1:2:71:ILE:H	1.59	0.68
3:B:30:SER:HA	3:B:33:THR:HG23	1.74	0.68
4:E:68:THR:C	4:E:69:LYS:HG3	2.12	0.67
6:G:67:ILE:C	6:G:67:ILE:HD12	2.14	0.67
6:G:19:LEU:HD23	6:G:70:LEU:HB3	1.77	0.66
6:G:70:LEU:O	6:G:70:LEU:HD13	1.95	0.66
1:2:66:VAL:HG21	3:B:23:GLU:HB3	1.78	0.66
4:E:39:VAL:HG23	6:G:25:ARG:HD3	1.78	0.65
6:G:42:ILE:HG22	6:G:45:CYS:HB2	1.79	0.64
6:G:43:ASP:OD1	6:G:59:MET:CE	2.46	0.64
4:E:83:ASN:ND2	5:F:24:LYS:CD	2.60	0.63
2:A:72:ASP:O	3:B:98:LYS:NZ	2.30	0.63
5:F:51:ILE:HD12	5:F:56:SER:CB	2.30	0.62
6:G:19:LEU:CD2	6:G:70:LEU:HB3	2.29	0.62
1:2:268:ARG:NH2	1:2:278:GLU:OE2	2.27	0.62
2:A:2:LYS:O	2:A:5:ARG:HB2	1.99	0.61
1:2:203:GLY:HA3	1:2:204:GLU:OE1	2.00	0.61
1:2:177:PRO:HB2	7:M:40:ILE:CD1	2.29	0.61
6:G:43:ASP:OD1	6:G:59:MET:HE2	1.99	0.61
6:G:10:LYS:HD3	6:G:11:LYS:N	2.15	0.61
1:2:135:MET:HG3	1:2:182:ILE:CD1	2.31	0.60
1:2:180:LEU:O	1:2:184:SER:HB2	2.01	0.60
3:B:111:ARG:HG3	3:B:112:ASN:OD1	2.02	0.59
5:F:65:ARG:HB3	5:F:68:ASN:ND2	2.17	0.59
2:A:66:ARG:NH1	2:A:66:ARG:HG3	2.18	0.59
6:G:63:ARG:O	6:G:65:ASN:O	2.21	0.59
2:A:66:ARG:CG	2:A:66:ARG:HH11	2.16	0.58
6:G:21:LEU:N	6:G:25:ARG:O	2.27	0.58
1:2:135:MET:HG3	1:2:182:ILE:HD11	1.85	0.58
1:2:214:TRP:O	1:2:218:LEU:HG	2.03	0.58
3:B:23:GLU:OE2	3:B:23:GLU:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:11:LEU:HD13	5:F:36:VAL:HG11	1.87	0.57
1:2:121:ARG:HG2	1:2:121:ARG:O	2.05	0.56
6:G:10:LYS:HD2	6:G:11:LYS:HB2	1.88	0.56
6:G:63:ARG:O	6:G:67:ILE:HG22	2.06	0.56
6:G:65:ASN:C	6:G:67:ILE:H	2.08	0.56
1:2:27:ARG:HG2	1:2:27:ARG:HH21	1.71	0.55
5:F:24:LYS:NZ	5:F:67:ASN:O	2.31	0.55
3:B:47:ARG:HG3	3:B:105:SER:HA	1.87	0.55
4:E:32:GLN:HB2	4:E:90:VAL:HG21	1.88	0.55
1:2:70:GLN:HG2	1:2:71:ILE:N	2.21	0.55
1:2:135:MET:SD	1:2:182:ILE:CD1	2.95	0.54
1:2:137:LYS:HG3	1:2:140:ASP:HB2	1.90	0.54
6:G:10:LYS:CD	6:G:11:LYS:HB2	2.38	0.54
1:2:224:LYS:HB2	1:2:225:PRO:CA	2.32	0.54
6:G:20:LYS:HB3	6:G:69:MET:HG3	1.90	0.53
4:E:41:MET:HE3	4:E:43:ILE:HD11	1.91	0.53
5:F:51:ILE:HD12	5:F:56:SER:HB2	1.90	0.53
1:2:257:PRO:HB2	7:M:47:VAL:HG13	1.91	0.53
2:A:71:PRO:O	2:A:74:LEU:HB2	2.08	0.53
2:A:30:THR:OG1	2:A:39:HIS:HB2	2.09	0.53
4:E:64:ILE:HD12	4:E:64:ILE:H	1.73	0.52
6:G:70:LEU:N	6:G:70:LEU:CD1	2.73	0.52
3:B:22:GLU:O	3:B:25:ASN:HB2	2.09	0.52
1:2:52:TYR:O	1:2:56:VAL:HG23	2.09	0.52
1:2:253:ASP:OD1	1:2:255:ARG:HD3	2.10	0.52
1:2:71:ILE:H	1:2:71:ILE:HD12	1.75	0.52
1:2:136:PRO:HD3	1:2:147:PHE:CD2	2.45	0.51
1:2:213:ARG:NH1	7:M:40:ILE:HG23	2.26	0.51
1:2:122:SER:C	1:2:124:TRP:H	2.13	0.51
6:G:21:LEU:HA	6:G:66:SER:O	2.09	0.51
1:2:236:GLN:OE1	1:2:239:ARG:NH1	2.44	0.50
4:E:83:ASN:ND2	5:F:24:LYS:HG2	2.16	0.50
1:2:186:MET:HE1	1:2:194:VAL:HG21	1.94	0.50
1:2:182:ILE:HD12	1:2:182:ILE:C	2.33	0.49
6:G:20:LYS:CB	6:G:69:MET:HG3	2.43	0.49
6:G:28:GLN:HB2	6:G:48:MET:SD	2.52	0.49
4:E:34:TRP:CE2	4:E:86:LEU:HD22	2.48	0.49
6:G:14:ASP:OD1	6:G:32:ARG:NH1	2.45	0.49
1:2:23:GLU:OE2	1:2:23:GLU:N	2.43	0.49
3:B:99:MET:CE	3:B:101:LEU:HD13	2.42	0.49
1:2:54:ARG:O	1:2:58:ILE:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:224:LYS:CB	1:2:225:PRO:HA	2.28	0.49
1:2:183:VAL:O	1:2:186:MET:HG3	2.13	0.48
2:A:66:ARG:NH1	2:A:66:ARG:CG	2.74	0.48
3:B:52:LEU:HD22	3:B:70:VAL:HG11	1.96	0.48
2:A:66:ARG:HG3	2:A:66:ARG:HH11	1.75	0.47
4:E:82:ASP:O	6:G:63:ARG:NH2	2.47	0.47
4:E:66:SER:O	4:E:67:LYS:HB2	2.14	0.47
1:2:181:SER:OG	7:M:36:ASP:OD2	2.31	0.47
3:B:22:GLU:N	3:B:25:ASN:OD1	2.47	0.47
5:F:50:TYR:CZ	5:F:55:LEU:HD23	2.49	0.47
2:A:76:LEU:HD11	3:B:98:LYS:HD3	1.96	0.47
6:G:10:LYS:HD3	6:G:11:LYS:CB	2.45	0.47
6:G:12:PHE:O	6:G:15:LYS:HB2	2.14	0.47
4:E:15:VAL:HG21	6:G:59:MET:HE1	1.97	0.47
6:G:9:LEU:HD23	6:G:12:PHE:CD1	2.50	0.47
6:G:39:ASN:OD1	6:G:63:ARG:HA	2.15	0.47
6:G:42:ILE:CG2	6:G:45:CYS:HB2	2.43	0.47
1:2:103:GLN:OE1	1:2:268:ARG:NH1	2.47	0.46
1:2:174:ILE:HG23	1:2:175:GLY:N	2.30	0.46
3:B:107:ILE:HG22	3:B:108:VAL:HG13	1.97	0.46
4:E:49:GLY:HA3	5:F:5:LEU:O	2.15	0.46
4:E:89:SER:O	4:E:90:VAL:HG23	2.15	0.46
1:2:71:ILE:N	1:2:71:ILE:HD12	2.31	0.46
4:E:16:GLN:O	4:E:19:ASN:HB2	2.15	0.45
1:2:80:GLN:NE2	3:B:112:ASN:O	2.46	0.45
6:G:43:ASP:OD1	6:G:59:MET:HE3	2.16	0.45
6:G:46:VAL:HA	6:G:55:ASN:O	2.15	0.45
1:2:24:LEU:O	5:F:67:ASN:ND2	2.45	0.45
4:E:62:GLU:HA	4:E:72:LYS:O	2.16	0.45
5:F:65:ARG:HB3	5:F:68:ASN:HD22	1.81	0.45
4:E:20:LEU:HD11	6:G:59:MET:HG2	1.99	0.45
4:E:79:LEU:HD12	5:F:71:TYR:HB3	1.99	0.45
1:2:174:ILE:HG13	1:2:175:GLY:H	1.82	0.45
1:2:205:ARG:HE	1:2:205:ARG:HB2	1.72	0.45
1:2:95:GLY:O	1:2:251:LYS:HE2	2.17	0.44
3:B:111:ARG:CG	3:B:112:ASN:OD1	2.65	0.44
1:2:183:VAL:HB	1:2:221:CYS:SG	2.57	0.44
3:B:47:ARG:HG2	3:B:47:ARG:H	1.62	0.44
4:E:68:THR:C	4:E:69:LYS:CG	2.86	0.44
4:E:72:LYS:N	4:E:72:LYS:CD	2.79	0.44
1:2:254:GLU:OE2	1:2:255:ARG:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:46:VAL:HG12	6:G:55:ASN:O	2.18	0.44
1:2:245:ARG:NH1	1:2:260:ASN:OD1	2.50	0.43
4:E:34:TRP:N	4:E:34:TRP:CD1	2.84	0.43
5:F:61:GLU:C	5:F:62:VAL:HG23	2.39	0.43
4:E:68:THR:HG23	4:E:70:SER:OG	2.18	0.43
1:2:135:MET:HG3	1:2:182:ILE:HD13	2.00	0.43
1:2:147:PHE:C	1:2:147:PHE:CD1	2.92	0.43
1:2:49:PRO:HG3	4:E:19:ASN:OD1	2.19	0.43
1:2:174:ILE:HD12	1:2:174:ILE:HA	1.84	0.43
4:E:44:GLU:O	4:E:61:ALA:HA	2.18	0.43
6:G:15:LYS:HD2	6:G:15:LYS:HA	1.86	0.43
6:G:35:ASP:OD1	6:G:39:ASN:N	2.50	0.43
1:2:53:LEU:HD23	1:2:53:LEU:HA	1.85	0.43
6:G:10:LYS:HD3	6:G:11:LYS:HG3	2.01	0.43
2:A:36:MET:SD	3:B:102:ARG:HG2	2.59	0.43
5:F:13:GLY:O	5:F:17:LYS:HE2	2.19	0.43
5:F:48:GLU:HB3	5:F:55:LEU:HD21	2.01	0.43
1:2:151:GLU:HA	1:2:151:GLU:OE1	2.17	0.43
6:G:27:VAL:CG1	6:G:45:CYS:SG	3.03	0.43
4:E:62:GLU:HG2	4:E:73:GLN:OE1	2.20	0.42
1:2:97:SER:HA	1:2:98:PRO:HD2	1.91	0.42
6:G:46:VAL:HG12	6:G:55:ASN:C	2.40	0.42
1:2:148:CYS:HB3	1:2:214:TRP:NE1	2.34	0.42
3:B:55:ARG:NE	3:B:56:VAL:O	2.53	0.42
5:F:14:LEU:O	5:F:17:LYS:HG3	2.20	0.42
6:G:65:ASN:C	6:G:67:ILE:N	2.73	0.42
3:B:62:HIS:O	3:B:103:GLY:HA3	2.20	0.42
1:2:180:LEU:HD11	7:M:38:ALA:HB3	2.02	0.42
2:A:1:MET:HB2	3:B:60:ASP:OD2	2.19	0.41
2:A:6:PHE:CD1	2:A:80:LEU:HD13	2.55	0.41
1:2:49:PRO:HG3	4:E:19:ASN:HA	2.02	0.41
6:G:19:LEU:O	6:G:27:VAL:N	2.51	0.41
4:E:86:LEU:HD12	6:G:62:ILE:HG12	2.01	0.41
6:G:70:LEU:H	6:G:70:LEU:CD1	2.27	0.41
1:2:28:LEU:HB2	4:E:54:MET:HB2	2.03	0.41
2:A:3:LEU:HD23	3:B:60:ASP:HB3	2.02	0.41
3:B:57:LYS:HD2	3:B:57:LYS:HA	1.90	0.41
6:G:28:GLN:CB	6:G:48:MET:CE	2.88	0.41
1:2:96:TYR:O	1:2:98:PRO:HD3	2.21	0.41
1:2:137:LYS:O	1:2:144:TRP:NE1	2.51	0.41
4:E:80:LYS:O	4:E:83:ASN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:28:GLU:HG3	5:F:50:TYR:HB2	2.01	0.41
8:2:308:HOH:O	3:B:73:MET:HG2	2.21	0.41
5:F:8:LYS:N	5:F:9:PRO:HD2	2.36	0.41
4:E:64:ILE:CD1	4:E:64:ILE:N	2.73	0.40
3:B:22:GLU:HB2	3:B:23:GLU:H	1.59	0.40
3:B:32:LEU:HA	3:B:32:LEU:HD23	1.80	0.40
4:E:20:LEU:HD13	6:G:61:VAL:HG23	2.03	0.40
3:B:110:LEU:HG	5:F:62:VAL:HG22	2.02	0.40
4:E:54:MET:CE	4:E:84:ILE:HG21	2.52	0.40
7:M:39:LEU:HA	7:M:39:LEU:HD23	1.75	0.40
1:2:148:CYS:HB3	1:2:214:TRP:CD1	2.55	0.40
1:2:256:VAL:N	1:2:257:PRO:CD	2.84	0.40
1:2:120:HIS:C	1:2:122:SER:H	2.24	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	2	194/280 (69%)	188 (97%)	5 (3%)	1 (0%)	29	48
2	A	79/119 (66%)	75 (95%)	3 (4%)	1 (1%)	12	21
3	B	81/118 (69%)	77 (95%)	4 (5%)	0	100	100
4	E	75/92 (82%)	74 (99%)	1 (1%)	0	100	100
5	F	72/86 (84%)	71 (99%)	1 (1%)	0	100	100
6	G	59/76 (78%)	53 (90%)	5 (8%)	1 (2%)	9	16
7	M	15/37 (40%)	15 (100%)	0	0	100	100
All	All	575/808 (71%)	553 (96%)	19 (3%)	3 (0%)	29	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	G	49	ALA
1	2	123	HIS
2	A	75	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	2	184/248 (74%)	145 (79%)	39 (21%)	1	2
2	A	76/101 (75%)	61 (80%)	15 (20%)	1	2
3	B	79/110 (72%)	68 (86%)	11 (14%)	3	6
4	E	72/84 (86%)	59 (82%)	13 (18%)	1	3
5	F	62/74 (84%)	57 (92%)	5 (8%)	11	23
6	G	54/66 (82%)	34 (63%)	20 (37%)	0	0
7	M	13/30 (43%)	12 (92%)	1 (8%)	13	25
All	All	540/713 (76%)	436 (81%)	104 (19%)	1	2

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	22	GLU
1	2	23	GLU
1	2	24	LEU
1	2	25	MET
1	2	27	ARG
1	2	31	VAL
1	2	67	VAL
1	2	68	VAL
1	2	71	ILE
1	2	79	LYS
1	2	82	VAL
1	2	85	SER
1	2	86	LEU
1	2	97	SER
1	2	100	LEU

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Mol	Chain	Res	Type
1	2	101	GLN
1	2	106	GLN
1	2	111	SER
1	2	115	GLN
1	2	122	SER
1	2	124	TRP
1	2	145	LYS
1	2	149	LEU
1	2	179	LEU
1	2	181	SER
1	2	182	ILE
1	2	186	MET
1	2	193	SER
1	2	195	LEU
1	2	205	ARG
1	2	208	THR
1	2	211	LEU
1	2	215	LEU
1	2	219	LEU
1	2	240	ARG
1	2	254	GLU
1	2	268	ARG
1	2	273	ARG
1	2	275	LEU
2	A	1	MET
2	A	3	LEU
2	A	4	VAL
2	A	5	ARG
2	A	11	SER
2	A	14	THR
2	A	33	ASP
2	A	41	LYS
2	A	44	LYS
2	A	54	GLN
2	A	59	SER
2	A	66	ARG
2	A	73	SER
2	A	74	LEU
2	A	80	LEU
3	B	22	GLU
3	B	23	GLU
3	B	26	THR

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Mol	Chain	Res	Type
3	B	33	THR
3	B	47	ARG
3	B	51	LYS
3	B	55	ARG
3	B	57	LYS
3	B	71	LYS
3	B	94	ARG
3	B	111	ARG
4	E	16	GLN
4	E	20	LEU
4	E	28	ARG
4	E	29	SER
4	E	42	ARG
4	E	44	GLU
4	E	54	MET
4	E	59	ASP
4	E	60	ASP
4	E	69	LYS
4	E	70	SER
4	E	72	LYS
4	E	74	LEU
5	F	5	LEU
5	F	11	LEU
5	F	27	MET
5	F	52	ASP
5	F	67	ASN
6	G	8	GLU
6	G	10	LYS
6	G	11	LYS
6	G	15	LYS
6	G	17	LEU
6	G	18	SER
6	G	30	ILE
6	G	32	ARG
6	G	43	ASP
6	G	46	VAL
6	G	48	MET
6	G	50	THR
6	G	51	SER
6	G	56	ASN
6	G	63	ARG
6	G	66	SER

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Mol	Chain	Res	Type
6	G	67	ILE
6	G	69	MET
6	G	70	LEU
6	G	71	GLU
7	M	45	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	105	GLN
1	2	106	GLN
1	2	109	GLN
1	2	120	HIS
2	A	24	GLN
3	B	25	ASN
4	E	83	ASN
6	G	65	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 monosaccharides 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	2	204/280 (72%)	0.17	10 (4%)	29	31	21, 51, 92, 109	0
2	A	81/119 (68%)	-0.08	1 (1%)	79	80	21, 37, 65, 78	0
3	B	85/118 (72%)	-0.10	0	100	100	18, 40, 77, 94	0
4	E	77/92 (83%)	0.21	4 (5%)	27	29	31, 50, 89, 109	0
5	F	74/86 (86%)	-0.11	1 (1%)	75	77	28, 42, 72, 91	0
6	G	63/76 (82%)	0.51	6 (9%)	8	8	43, 72, 102, 112	0
7	M	17/37 (45%)	0.35	1 (5%)	22	23	41, 57, 82, 99	0
All	All	601/808 (74%)	0.11	23 (3%)	40	43	18, 49, 92, 112	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	E	67	LYS	6.7
4	E	68	THR	4.8
1	2	72	ASP	4.6
1	2	68	VAL	4.4
6	G	51	SER	4.3
1	2	71	ILE	3.8
4	E	66	SER	3.5
1	2	101	GLN	3.4
6	G	69	MET	3.3
1	2	99	THR	3.1
6	G	10	LYS	3.0
1	2	123	HIS	2.9
4	E	69	LYS	2.7
6	G	50	THR	2.5
1	2	82	VAL	2.5
5	F	52	ASP	2.5
1	2	95	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
6	G	26	HIS	2.3
1	2	100	LEU	2.3
1	2	69	ALA	2.2
6	G	72	ALA	2.1
7	M	51	LYS	2.1
2	A	2	LYS	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 monosaccharides 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.