



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:44 AM UTC

PDB ID : 5XJL / pdb_00005xjl
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

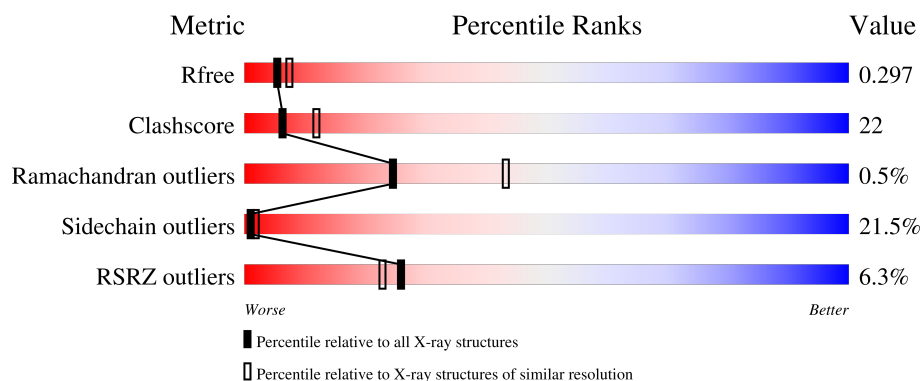
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 $\leq 5\%$. 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	5% 40% 26% 6% 27%
2	A	119	3% 41% 23% • 32%
3	B	118	3% 44% 23% 5% 28%
4	E	92	5% 36% 38% 10% 16%
5	F	86	56% 23% 7% 14%

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Mol	Chain	Length	Quality of chain
6	G	76	16%26%38%18%17%
7	M	37	30%14%.54%

2 Entry composition

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
1	2	204	Total	C	N	O	S	0	0	0
			1644	1042	289	304	9			

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

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

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

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

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

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

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

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

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

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

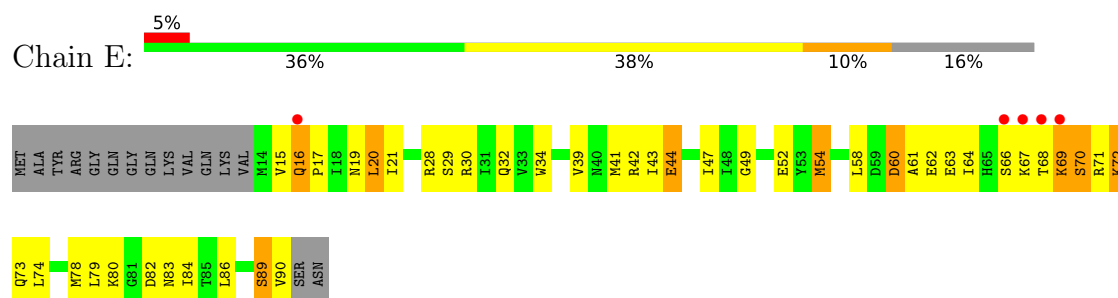
- Molecule 7 is a protein called Survival motor neuron protein.

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

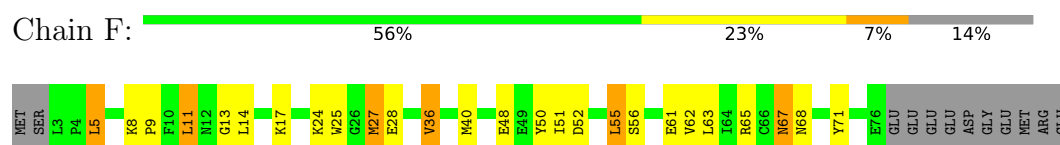
- Molecule 8 is water.

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

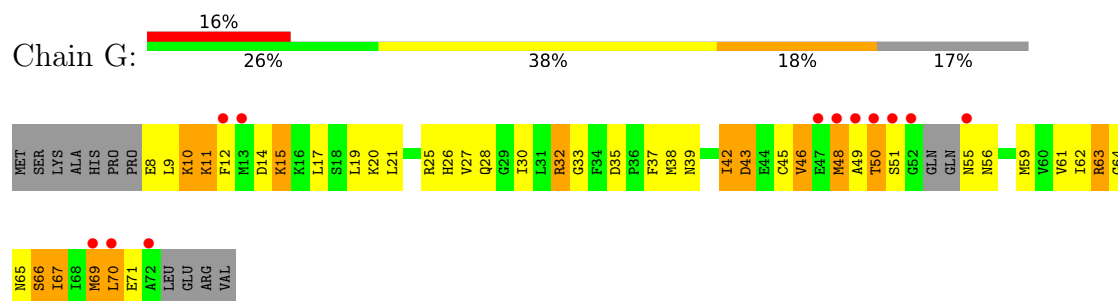
- Molecule 4: Small nuclear ribonucleoprotein E



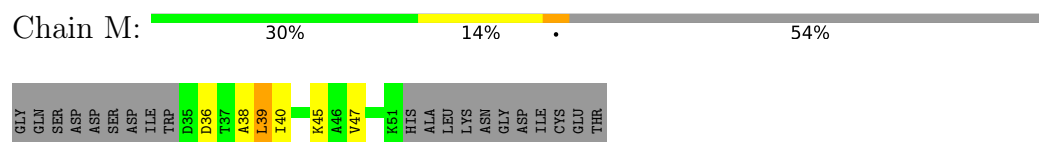
- Molecule 5: Small nuclear ribonucleoprotein F



- Molecule 6: Small nuclear ribonucleoprotein G



- Molecule 7: Survival motor neuron protein



4 Data and refinement statistics

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 59.19 – 2.50	Depositor EDS
% Data completeness (in resolution range)	76.2 (59.19-2.50) 76.2 (59.19-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.33 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	2	0.92	0/1678	1.03	3/2276 (0.1%)
2	A	1.25	1/649 (0.2%)	1.06	0/877
3	B	1.02	0/689	1.06	1/926 (0.1%)
4	E	0.91	0/646	0.98	0/867
5	F	0.92	0/588	0.96	0/795
6	G	0.96	0/488	1.03	1/648 (0.2%)
7	M	0.87	0/131	1.04	2/175 (1.1%)
All	All	0.99	1/4869 (0.0%)	1.02	7/6564 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	26	HIS	C-O	-5.62	1.17	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	50	THR	N-CA-C	-8.47	101.42	112.68
1	2	224	LYS	C-N-CD	8.21	138.67	120.60
1	2	256	VAL	CB-CA-C	-5.81	108.18	113.70
1	2	56	VAL	CB-CA-C	-5.26	105.13	112.02
3	B	97	SER	N-CA-C	5.23	116.67	111.07
7	M	39	LEU	CA-C-N	5.15	127.25	120.60
7	M	39	LEU	C-N-CA	5.15	127.25	120.60

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	2	1644	0	1631	69	0
2	A	641	0	689	18	0
3	B	681	0	709	31	0
4	E	638	0	657	47	0
5	F	576	0	581	26	0
6	G	485	0	508	51	0
7	M	130	0	131	7	0
8	2	12	0	0	1	0
8	A	5	0	0	0	0
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	215	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 22.

All (215) 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)
6:G:43:ASP:OD1	6:G:59:MET:HE3	1.50	1.10
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
1:2:203:GLY:C	1:2:204:GLU:OE1	2.27	0.78
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:B:22:GLU:C	3:B:23:GLU:OE2	2.29	0.75
4:E:64:ILE:N	4:E:64:ILE:HD12	2.02	0.75
6:G:37:PHE:O	6:G:38:MET:HB2	1.86	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
6:G:28:GLN:HB2	6:G:48:MET:HE1	1.68	0.73
1:2:177:PRO:HB2	7:M:40:ILE:HD11	1.70	0.73
4:E:68:THR:C	4:E:69:LYS:HG3	2.12	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
6:G:27:VAL:HG13	6:G:45:CYS:SG	2.29	0.72
6:G:67:ILE:C	6:G:67:ILE:HD12	2.14	0.71
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
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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:180:LEU:O	1:2:184:SER:HB2	2.01	0.60
6:G:65:ASN:C	6:G:67:ILE:H	2.08	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:HH11	2:A:66:ARG:CG	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
5:F:11:LEU:HD13	5:F:36:VAL:HG11	1.87	0.57
3:B:23:GLU:OE2	3:B:23:GLU:N	2.38	0.56
1:2:121:ARG:O	1:2:121:ARG:HG2	2.05	0.56
1:2:122:SER:C	1:2:124:TRP:H	2.13	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
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
1:2:182:ILE:HD12	1:2:182:ILE:C	2.33	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
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
6:G:21:LEU:HA	6:G:66:SER:O	2.09	0.51
4:E:41:MET:HE3	4:E:43:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	0.49
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
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
5:F:61:GLU:C	5:F:62:VAL:HG23	2.39	0.48
1:2:147:PHE:CD1	1:2:147:PHE:C	2.92	0.48
3:B:52:LEU:HD22	3:B:70:VAL:HG11	1.96	0.48
4:E:68:THR:C	4:E:69:LYS:CG	2.86	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:46:VAL:HG12	6:G:55:ASN:C	2.40	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
6:G:65:ASN:C	6:G:67:ILE:N	2.73	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:78:MET:HE1	5:F:40:MET:SD	2.56	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:46:VAL:HA	6:G:55:ASN:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:24:LEU:O	5:F:67:ASN:ND2	2.45	0.45
1:2:120:HIS:C	1:2:122:SER:H	2.24	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:72:LYS:CD	4:E:72:LYS:N	2.79	0.44
1:2:254:GLU:OE2	1:2:255:ARG:HG3	2.18	0.44
4:E:71:ARG:C	4:E:72:LYS:CD	2.91	0.44
5:F:71:TYR:C	5:F:71:TYR:CD1	2.96	0.44
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
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
1:2:49: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
1:2:148:CYS:HB3	1:2:214:TRP:NE1	2.34	0.42
3:B:111:ARG:HG3	3:B:112:ASN:CG	2.44	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
3:B:99:MET:HE2	3:B:101:LEU:HB2	2.01	0.42
3:B:73:MET:HE3	3:B:73:MET:HB2	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:62:HIS:O	3:B:103:GLY:HA3	2.20	0.42
4:E:71:ARG:C	4:E:72:LYS:HD2	2.45	0.42
1:2:180:LEU:HD11	7:M:38:ALA:HB3	2.02	0.42
2:A:67:TYR:CG	3:B:99:MET:HE3	2.55	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
4:E:89:SER:C	4:E:90:VAL:HG23	2.45	0.41
6:G:19:LEU:O	6:G:27:VAL:N	2.51	0.41
2:A:49:ASN:C	2:A:50:ARG:HG3	2.45	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
1:2:122:SER:C	1:2:124:TRP:N	2.79	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
5:F:28:GLU:HG3	5:F:50:TYR:HB2	2.01	0.41
1:2:224:LYS:HA	1:2:225:PRO:C	2.46	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

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%)	24	43
2	A	79/119 (66%)	75 (95%)	3 (4%)	1 (1%)	9	18
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%)	7	13
7	M	15/37 (40%)	15 (100%)	0	0	100	100
All	All	575/808 (71%)	553 (96%)	19 (3%)	3 (0%)	24	43

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%)	141 (77%)	43 (23%)	1	1
2	A	76/101 (75%)	60 (79%)	16 (21%)	1	2
3	B	79/110 (72%)	67 (85%)	12 (15%)	3	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	72/84 (86%)	56 (78%)	16 (22%)	1	2
5	F	62/74 (84%)	54 (87%)	8 (13%)	4	9
6	G	54/66 (82%)	34 (63%)	20 (37%)	0	0
7	M	13/30 (43%)	12 (92%)	1 (8%)	12	25
All	All	540/713 (76%)	424 (78%)	116 (22%)	1	2

All (116) 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	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
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	135	MET
1	2	137	LYS
1	2	145	LYS
1	2	146	LYS
1	2	149	LEU
1	2	174	ILE
1	2	179	LEU
1	2	181	SER
1	2	182	ILE
1	2	186	MET
1	2	193	SER
1	2	195	LEU

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Mol	Chain	Res	Type
1	2	205	ARG
1	2	208	THR
1	2	211	LEU
1	2	215	LEU
1	2	219	LEU
1	2	226	LEU
1	2	240	ARG
1	2	254	GLU
1	2	255	ARG
1	2	273	ARG
1	2	275	LEU
2	A	1	MET
2	A	3	LEU
2	A	4	VAL
2	A	11	SER
2	A	14	THR
2	A	33	ASP
2	A	41	LYS
2	A	44	LYS
2	A	48	LYS
2	A	54	GLN
2	A	56	GLU
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
3	B	33	THR
3	B	47	ARG
3	B	51	LYS
3	B	57	LYS
3	B	71	LYS
3	B	94	ARG
3	B	111	ARG
3	B	114	LEU
3	B	115	ILE
4	E	16	GLN
4	E	20	LEU
4	E	28	ARG

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Mol	Chain	Res	Type
4	E	29	SER
4	E	42	ARG
4	E	44	GLU
4	E	47	ILE
4	E	52	GLU
4	E	54	MET
4	E	58	LEU
4	E	60	ASP
4	E	69	LYS
4	E	70	SER
4	E	72	LYS
4	E	74	LEU
4	E	89	SER
5	F	5	LEU
5	F	11	LEU
5	F	27	MET
5	F	36	VAL
5	F	52	ASP
5	F	55	LEU
5	F	63	LEU
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	30	ILE
6	G	32	ARG
6	G	42	ILE
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
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 (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	105	GLN
1	2	109	GLN
1	2	120	HIS
2	A	24	GLN
2	A	63	ASN
3	B	25	ASN
4	E	65	HIS
4	E	83	ASN
4	E	88	GLN
5	F	43	GLN
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 oligosaccharides 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 ⓘ

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, 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%)	0.47	14 (6%) 23 20	21, 51, 92, 109	0
2	A	81/119 (68%)	0.05	4 (4%) 35 31	21, 37, 65, 78	0
3	B	85/118 (72%)	0.18	3 (3%) 47 42	18, 40, 77, 94	0
4	E	77/92 (83%)	0.46	5 (6%) 25 22	31, 50, 89, 109	0
5	F	74/86 (86%)	0.18	0 100 100	28, 42, 72, 91	0
6	G	63/76 (82%)	1.03	12 (19%) 3 2	43, 72, 102, 112	0
7	M	17/37 (45%)	0.57	0 100 100	41, 57, 82, 99	0
All	All	601/808 (74%)	0.40	38 (6%) 26 23	18, 49, 92, 112	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	77	VAL	4.6
1	2	124	TRP	4.3
1	2	73	PRO	4.1
1	2	82	VAL	3.7
1	2	84	ILE	3.7
1	2	174	ILE	3.6
2	A	81	VAL	3.5
1	2	31	VAL	3.4
1	2	123	HIS	3.4
4	E	67	LYS	3.3
6	G	12	PHE	3.3
6	G	47	GLU	3.2
2	A	72	ASP	3.1
6	G	55	ASN	3.0
6	G	72	ALA	3.0
4	E	69	LYS	2.8
1	2	122	SER	2.8

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Mol	Chain	Res	Type	RSRZ
3	B	89	PRO	2.8
6	G	50	THR	2.8
6	G	49	ALA	2.6
1	2	176	PHE	2.6
4	E	16	GLN	2.5
4	E	66	SER	2.5
2	A	2	LYS	2.4
1	2	48	THR	2.4
1	2	79	LYS	2.3
1	2	81	SER	2.3
6	G	69	MET	2.2
6	G	70	LEU	2.2
3	B	48	ASN	2.2
2	A	33	ASP	2.2
6	G	51	SER	2.1
1	2	83	ASN	2.1
4	E	68	THR	2.1
6	G	52	GLY	2.1
1	2	30	PRO	2.1
6	G	48	MET	2.1
6	G	13	MET	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 oligosaccharides 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.