



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:19 AM UTC

PDB ID : 4FVJ / pdb_00004fvj
Title : SPFH domain of the mouse stomatin (Crystal form 2)
Authors : Brand, J.; Schwefel, D.; Daumke, O.
Deposited on : 2012-06-29
Resolution : 2.69 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

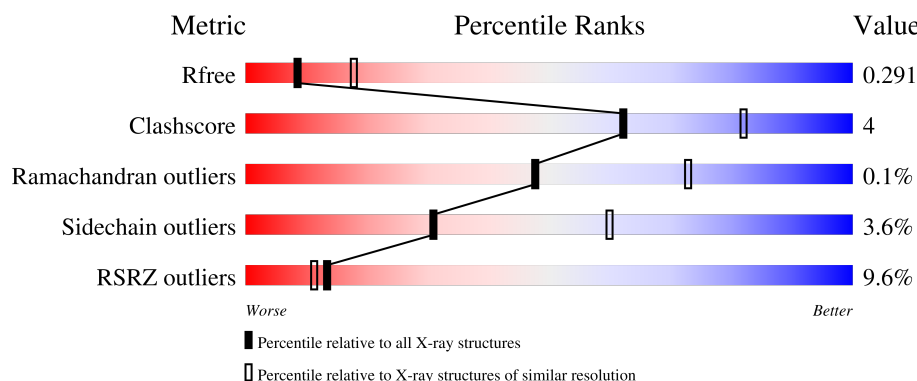
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	A	133	0% 72% 13% 15%
1	B	133	5% 67% 16% 14%
1	C	133	8% 65% 18% 16%
1	D	133	3% 73% 11% 16%
1	E	133	2% 74% 11% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	133	14% 68% 14% • 15%
1	G	133	8% 73% 11% • 15%
1	H	133	23% 68% 13% 5% 14%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 7068 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 Stomatin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	113	Total	C	N	O	S	19	1	0
			889	552	156	179	2			
1	B	114	Total	C	N	O	S	26	0	0
			887	553	154	178	2			
1	C	112	Total	C	N	O	S	32	1	0
			880	548	154	176	2			
1	D	112	Total	C	N	O	S	7	0	0
			871	541	151	177	2			
1	E	113	Total	C	N	O	S	21	0	0
			879	547	153	177	2			
1	F	113	Total	C	N	O	S	73	0	0
			878	546	152	178	2			
1	G	113	Total	C	N	O	S	33	0	0
			878	546	152	178	2			
1	H	114	Total	C	N	O	S	73	0	0
			887	553	154	178	2			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	81	GLY	-	expression tag	UNP P54116
A	82	PRO	-	expression tag	UNP P54116
A	83	LEU	-	expression tag	UNP P54116
A	84	GLY	-	expression tag	UNP P54116
A	85	SER	-	expression tag	UNP P54116
A	87	SER	CYS	engineered mutation	UNP P54116
B	81	GLY	-	expression tag	UNP P54116
B	82	PRO	-	expression tag	UNP P54116
B	83	LEU	-	expression tag	UNP P54116
B	84	GLY	-	expression tag	UNP P54116
B	85	SER	-	expression tag	UNP P54116
B	87	SER	CYS	engineered mutation	UNP P54116
C	81	GLY	-	expression tag	UNP P54116

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	82	PRO	-	expression tag	UNP P54116
C	83	LEU	-	expression tag	UNP P54116
C	84	GLY	-	expression tag	UNP P54116
C	85	SER	-	expression tag	UNP P54116
C	87	SER	CYS	engineered mutation	UNP P54116
D	81	GLY	-	expression tag	UNP P54116
D	82	PRO	-	expression tag	UNP P54116
D	83	LEU	-	expression tag	UNP P54116
D	84	GLY	-	expression tag	UNP P54116
D	85	SER	-	expression tag	UNP P54116
D	87	SER	CYS	engineered mutation	UNP P54116
E	81	GLY	-	expression tag	UNP P54116
E	82	PRO	-	expression tag	UNP P54116
E	83	LEU	-	expression tag	UNP P54116
E	84	GLY	-	expression tag	UNP P54116
E	85	SER	-	expression tag	UNP P54116
E	87	SER	CYS	engineered mutation	UNP P54116
F	81	GLY	-	expression tag	UNP P54116
F	82	PRO	-	expression tag	UNP P54116
F	83	LEU	-	expression tag	UNP P54116
F	84	GLY	-	expression tag	UNP P54116
F	85	SER	-	expression tag	UNP P54116
F	87	SER	CYS	engineered mutation	UNP P54116
G	81	GLY	-	expression tag	UNP P54116
G	82	PRO	-	expression tag	UNP P54116
G	83	LEU	-	expression tag	UNP P54116
G	84	GLY	-	expression tag	UNP P54116
G	85	SER	-	expression tag	UNP P54116
G	87	SER	CYS	engineered mutation	UNP P54116
H	81	GLY	-	expression tag	UNP P54116
H	82	PRO	-	expression tag	UNP P54116
H	83	LEU	-	expression tag	UNP P54116
H	84	GLY	-	expression tag	UNP P54116
H	85	SER	-	expression tag	UNP P54116
H	87	SER	CYS	engineered mutation	UNP P54116

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total O 2 2	0	0
2	B	4	Total O 4 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	3	Total 3	O 3	0	0
2	D	3	Total 3	O 3	0	0
2	E	2	Total 2	O 2	0	0
2	F	2	Total 2	O 2	0	0
2	G	1	Total 1	O 1	0	0
2	H	2	Total 2	O 2	0	0

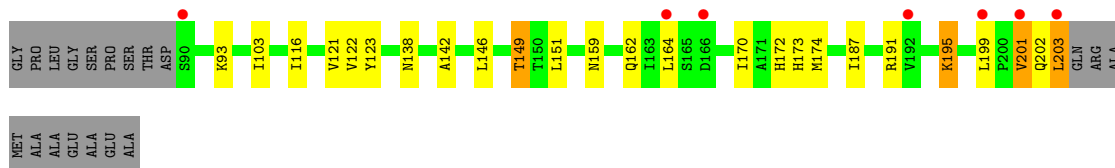
3 Residue-property plots [i](#)

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.

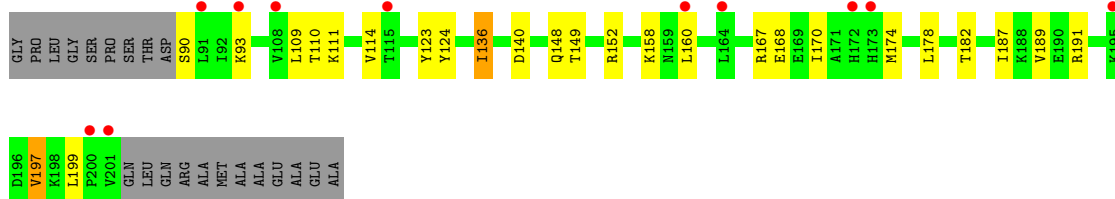
• Molecule 1: Stomatin



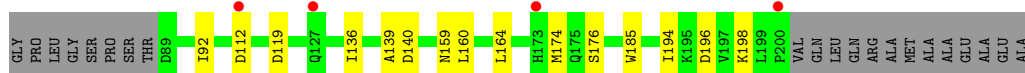
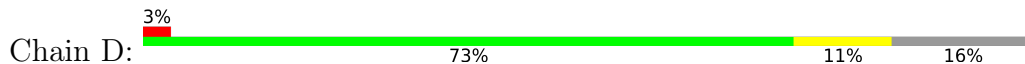
• Molecule 1: Stomatin



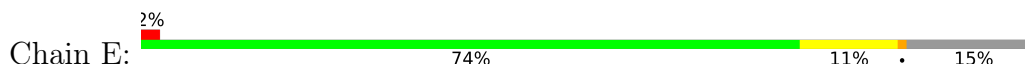
• Molecule 1: Stomatin



• Molecule 1: Stomatin

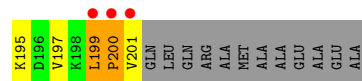
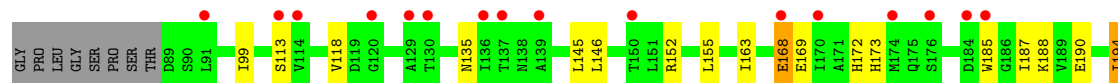


• Molecule 1: Stomatin

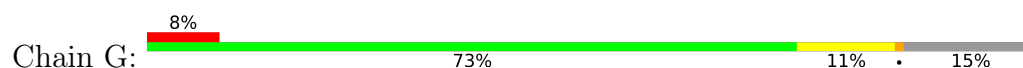




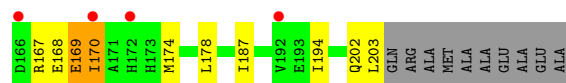
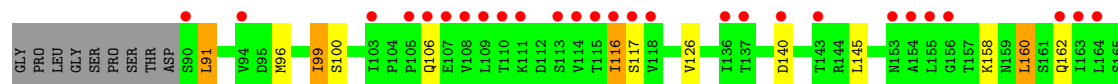
• Molecule 1: Stomatin



• Molecule 1: Stomatin



• Molecule 1: Stomatin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	178.53Å 91.38Å 86.14Å 90.00° 111.88° 90.00°	Depositor
Resolution (Å)	82.76 – 2.69 82.76 – 2.69	Depositor EDS
% Data completeness (in resolution range)	91.1 (82.76-2.69) 91.1 (82.76-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.246 , 0.290 0.245 , 0.291	Depositor DCC
R_{free} test set	1608 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	47.4	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7068	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% 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	A	0.76	3/898 (0.3%)	0.92	3/1221 (0.2%)
1	B	0.99	3/896 (0.3%)	0.95	3/1219 (0.2%)
1	C	1.65	6/890 (0.7%)	1.39	13/1211 (1.1%)
1	D	0.97	2/880 (0.2%)	0.82	1/1197 (0.1%)
1	E	1.50	3/888 (0.3%)	1.08	6/1208 (0.5%)
1	F	2.04	14/887 (1.6%)	1.11	8/1207 (0.7%)
1	G	1.24	6/887 (0.7%)	1.09	7/1207 (0.6%)
1	H	1.99	16/896 (1.8%)	1.60	21/1219 (1.7%)
All	All	1.46	53/7122 (0.7%)	1.14	62/9689 (0.6%)

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	136	ILE	CA-CB	-36.97	1.09	1.54
1	F	173	HIS	CA-CB	-30.89	1.04	1.53
1	C	136	ILE	CA-CB	-29.47	1.18	1.54
1	C	168	GLU	CA-CB	-27.08	1.11	1.53
1	H	169	GLU	CA-CB	-25.85	1.12	1.53
1	B	93	LYS	CA-CB	-23.60	1.16	1.53
1	F	169	GLU	CA-CB	-22.02	1.19	1.53
1	F	195	LYS	CA-CB	-20.40	1.28	1.53
1	E	152	ARG	CA-CB	-20.30	1.21	1.53
1	G	167	ARG	CA-CB	-19.56	1.22	1.53
1	F	145	LEU	CA-CB	-19.51	1.22	1.53
1	H	160	LEU	CA-CB	-19.46	1.23	1.53
1	F	187	ILE	CA-CB	-18.98	1.31	1.54
1	D	198	LYS	CA-CB	-18.87	1.24	1.53
1	G	144	ARG	CA-CB	-18.01	1.25	1.53
1	D	176	SER	CA-CB	-17.51	1.25	1.53
1	H	116	ILE	CA-CB	-17.23	1.25	1.55
1	H	145	LEU	CA-CB	-16.42	1.27	1.53
1	H	162	GLN	CA-CB	-15.94	1.28	1.53
1	C	160	LEU	CA-CB	-15.71	1.28	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	158	LYS	CA-CB	15.62	1.77	1.53
1	H	170	ILE	CA-CB	-15.18	1.34	1.54
1	F	113	SER	CA-CB	-14.91	1.31	1.53
1	H	168	GLU	CA-CB	-14.64	1.30	1.53
1	A	195	LYS	CG-CD	-14.28	1.09	1.52
1	H	178	LEU	CA-CB	-13.87	1.31	1.53
1	H	187	ILE	CA-CB	-13.50	1.38	1.54
1	C	109	LEU	CA-CB	-12.70	1.36	1.53
1	C	93	LYS	CA-CB	-12.11	1.34	1.53
1	G	195	LYS	CG-CD	-11.88	1.16	1.52
1	G	168	GLU	CA-CB	-11.84	1.34	1.53
1	F	185	TRP	CA-CB	-11.81	1.32	1.53
1	F	172	HIS	CA-CB	-11.63	1.34	1.53
1	F	194	ILE	CA-CB	-11.49	1.40	1.54
1	H	202	GLN	CA-CB	-10.74	1.38	1.54
1	H	167	ARG	CA-CB	-10.41	1.37	1.53
1	F	152	ARG	CA-CB	-9.52	1.38	1.53
1	G	138	ASN	CA-CB	9.38	1.68	1.53
1	C	111	LYS	CA-CB	-8.94	1.39	1.53
1	G	141	SER	CA-CB	8.84	1.69	1.53
1	A	169	GLU	CA-CB	-8.73	1.39	1.53
1	F	146	LEU	CA-CB	-8.57	1.40	1.53
1	H	174	MET	CG-SD	-8.40	1.59	1.80
1	B	172	HIS	CA-CB	-8.13	1.40	1.53
1	H	96	MET	CG-SD	7.16	1.98	1.80
1	B	173	HIS	CA-CB	-7.05	1.42	1.53
1	A	172	HIS	CA-CB	-6.95	1.42	1.53
1	F	168	GLU	CB-CG	6.18	1.71	1.52
1	H	194	ILE	CA-CB	-5.87	1.47	1.53
1	E	111	LYS	CA-CB	-5.80	1.44	1.53
1	F	155	LEU	CA-CB	5.64	1.62	1.53
1	F	185	TRP	NE1-CE2	-5.49	1.31	1.37
1	H	174	MET	CA-CB	-5.13	1.45	1.53

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	162	GLN	N-CA-CB	21.02	140.55	110.07
1	C	136	ILE	N-CA-CB	17.88	132.82	110.47
1	H	116	ILE	CB-CA-C	-16.07	84.98	110.69
1	C	111	LYS	N-CA-CB	15.93	133.96	110.06
1	E	202	GLN	CB-CA-C	13.90	136.51	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	158	LYS	N-CA-CB	-13.21	91.01	110.70
1	C	160	LEU	N-CA-CB	12.84	129.07	109.94
1	C	136	ILE	CB-CA-C	-12.72	95.38	112.04
1	H	168	GLU	CA-CB-CG	-12.69	88.73	114.10
1	F	135	ASN	CB-CA-C	-12.59	95.21	111.70
1	G	167	ARG	N-CA-CB	12.55	128.56	110.12
1	H	187	ILE	CB-CA-C	11.43	126.39	110.84
1	C	109	LEU	CB-CA-C	-11.18	92.36	110.81
1	C	168	GLU	CA-CB-CG	-11.18	91.74	114.10
1	G	144	ARG	N-CA-CB	10.68	125.49	110.01
1	G	188	LYS	CB-CA-C	-10.48	93.19	111.22
1	B	173	HIS	CA-CB-CG	10.43	124.23	113.80
1	H	160	LEU	N-CA-CB	10.35	125.34	110.12
1	H	178	LEU	N-CA-CB	10.10	124.65	110.01
1	E	136	ILE	N-CA-CB	9.98	122.95	110.47
1	H	203	LEU	CB-CA-C	-9.88	91.33	110.10
1	G	188	LYS	N-CA-CB	9.74	126.92	110.46
1	E	152	ARG	N-CA-CB	9.64	124.29	110.12
1	E	152	ARG	CB-CA-C	-9.49	95.03	110.79
1	A	168	GLU	CA-CB-CG	-9.25	95.59	114.10
1	E	202	GLN	N-CA-CB	-9.25	94.78	110.50
1	C	136	ILE	CA-CB-CG1	-9.08	94.96	110.40
1	H	116	ILE	CA-CB-CG1	-8.97	95.16	110.40
1	F	169	GLU	CB-CA-C	8.63	125.11	110.79
1	A	195	LYS	CG-CD-CE	8.35	130.50	111.30
1	F	146	LEU	N-CA-CB	8.17	122.13	110.12
1	G	138	ASN	N-CA-CB	-8.13	97.68	110.28
1	B	173	HIS	N-CA-CB	8.03	122.04	110.16
1	E	136	ILE	CA-CB-CG2	-7.61	97.56	110.50
1	C	111	LYS	CA-CB-CG	7.53	129.16	114.10
1	H	96	MET	N-CA-CB	7.36	122.02	110.46
1	H	194	ILE	CB-CA-C	-7.30	101.98	111.25
1	G	141	SER	CB-CA-C	-7.21	95.47	110.17
1	C	93	LYS	N-CA-CB	7.07	122.19	110.52
1	H	145	LEU	N-CA-CB	6.98	120.38	110.12
1	H	160	LEU	CA-CB-CG	6.96	140.65	116.30
1	H	116	ILE	N-CA-CB	-6.90	99.16	111.93
1	G	141	SER	N-CA-CB	-6.87	98.37	110.39
1	H	162	GLN	CB-CA-C	-6.80	100.15	110.90
1	F	152	ARG	N-CA-CB	6.64	119.64	110.01
1	F	169	GLU	N-CA-CB	-6.43	100.67	110.12
1	H	168	GLU	CB-CA-C	6.32	121.28	110.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	169	GLU	N-CA-CB	6.24	119.30	110.12
1	D	198	LYS	N-CA-CB	6.24	120.82	110.52
1	C	109	LEU	CA-CB-CG	-6.20	94.61	116.30
1	A	169	GLU	N-CA-CB	6.18	119.30	110.16
1	F	194	ILE	CB-CA-C	6.17	118.30	111.08
1	H	145	LEU	CB-CA-C	-5.88	101.03	110.79
1	F	172	HIS	CB-CA-C	5.82	120.74	110.85
1	C	168	GLU	CB-CA-C	5.72	120.29	110.79
1	H	202	GLN	N-CA-CB	-5.69	100.68	110.86
1	H	174	MET	CB-CA-C	-5.67	101.37	110.79
1	C	136	ILE	N-CA-C	5.65	117.06	110.62
1	H	116	ILE	CA-CB-CG2	5.59	120.00	110.50
1	B	172	HIS	CA-CB-CG	5.51	119.31	113.80
1	C	158	LYS	CB-CA-C	-5.48	100.24	109.83
1	F	173	HIS	N-CA-CB	5.42	118.17	110.16

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	A	889	0	904	5	0
1	B	887	0	907	13	0
1	C	880	0	894	15	0
1	D	871	0	883	10	0
1	E	879	0	896	8	0
1	F	878	0	892	3	0
1	G	878	0	892	6	0
1	H	887	0	907	7	0
2	A	2	0	0	0	0
2	B	4	0	0	1	0
2	C	3	0	0	1	0
2	D	3	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	1	0	0	1	0
2	H	2	0	0	0	0
All	All	7068	0	7175	55	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 4.

All (55) 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:140:ASP:HB3	1:H:91:LEU:HB2	1.47	0.95
1:C:140:ASP:CB	1:H:91:LEU:HB2	2.08	0.82
1:E:99:ILE:HG13	1:E:100:SER:H	1.55	0.72
1:E:99:ILE:HG13	1:E:100:SER:N	2.04	0.71
1:B:199:LEU:HB2	1:C:197:VAL:HG13	1.73	0.69
1:D:174:MET:HE1	1:D:194:ILE:HD11	1.75	0.66
1:D:136:ILE:O	1:D:140:ASP:HB2	2.00	0.60
1:D:119:ASP:OD1	1:D:196:ASP:HB2	2.03	0.58
1:B:170:ILE:HG22	1:B:174:MET:HE2	1.86	0.57
1:F:188:LYS:HE3	1:F:190:GLU:HG3	1.88	0.56
1:C:123:TYR:HB2	1:C:191:ARG:HB3	1.88	0.56
1:B:187:ILE:O	2:B:304:HOH:O	2.18	0.55
1:B:121:VAL:HG22	1:B:195:LYS:HE3	1.89	0.54
1:A:171:ALA:HB1	1:A:192:VAL:O	2.10	0.52
1:F:118:VAL:HG22	1:F:197:VAL:HG12	1.91	0.51
1:B:123:TYR:HB2	1:B:191:ARG:HB3	1.93	0.51
1:D:140:ASP:OD1	1:G:90:SER:HA	2.11	0.51
1:B:164:LEU:HD11	1:C:199:LEU:HD13	1.92	0.50
1:H:106:GLN:O	1:H:117:SER:HA	2.11	0.49
1:D:139:ALA:HA	1:D:185:TRP:CD1	2.48	0.48
1:B:201:VAL:HG13	1:C:167:ARG:HD2	1.95	0.48
1:C:148:GLN:O	1:C:152:ARG:HG3	2.15	0.47
1:E:170:ILE:HG22	1:E:174:MET:HE2	1.97	0.46
1:A:117:SER:HB3	1:A:198:LYS:HB2	1.97	0.46
1:D:160:LEU:O	1:D:164:LEU:HG	2.17	0.45
1:C:170:ILE:HG22	1:C:174:MET:HE2	1.98	0.45
1:G:182:THR:HB	1:G:187:ILE:HB	1.98	0.45
1:C:187:ILE:O	2:C:303:HOH:O	2.21	0.44
1:C:110:THR:HG22	1:C:114:VAL:H	1.83	0.44
1:E:117:SER:HB3	1:E:198:LYS:HB2	1.99	0.44
1:E:185:TRP:HD1	1:E:187:ILE:HD12	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:SER:HA	1:H:140:ASP:OD1	2.18	0.44
1:D:92:ILE:HD13	1:G:136:ILE:HG22	2.00	0.44
1:A:108:VAL:HG22	1:A:152[B]:ARG:HG2	1.99	0.44
1:D:139:ALA:HB1	1:G:92:ILE:HD11	2.00	0.44
1:A:91:LEU:HD22	1:E:140:ASP:HA	1.99	0.43
1:B:146:LEU:HA	1:B:149:THR:HB	2.00	0.43
1:B:159:ASN:HB2	1:B:162:GLN:HG2	1.99	0.43
1:B:202:GLN:HA	1:B:203:LEU:HB3	2.01	0.43
1:C:182:THR:HB	1:C:187:ILE:HB	2.01	0.43
1:G:187:ILE:O	2:G:301:HOH:O	2.21	0.43
1:D:174:MET:CE	1:D:194:ILE:HD11	2.47	0.43
1:E:159:ASN:HB2	1:E:162:GLN:HB2	1.99	0.42
1:C:178:LEU:HG	1:C:189:VAL:HG21	2.00	0.42
1:H:99:ILE:HG22	1:H:100:SER:H	1.83	0.42
1:A:175:GLN:O	1:A:179:ASP:HB2	2.19	0.42
1:F:199:LEU:HA	1:F:200:PRO:HD3	1.82	0.42
1:E:185:TRP:CD1	1:E:187:ILE:HD12	2.54	0.42
1:C:140:ASP:HB2	1:H:91:LEU:HB2	1.96	0.41
1:D:112:ASP:HB2	1:D:159:ASN:HA	2.03	0.41
1:B:103:ILE:HD11	1:B:122:VAL:HG23	2.02	0.41
1:G:116:ILE:HG22	1:G:199:LEU:HD23	2.03	0.41
1:B:116:ILE:HG22	1:B:199:LEU:HD23	2.03	0.40
1:C:124:TYR:CE1	1:H:91:LEU:HD13	2.57	0.40
1:B:138:ASN:O	1:B:142:ALA:HB3	2.21	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	112/133 (84%)	107 (96%)	5 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	112/133 (84%)	108 (96%)	4 (4%)	0	100	100
1	C	111/133 (84%)	108 (97%)	3 (3%)	0	100	100
1	D	110/133 (83%)	108 (98%)	2 (2%)	0	100	100
1	E	111/133 (84%)	109 (98%)	2 (2%)	0	100	100
1	F	111/133 (84%)	104 (94%)	6 (5%)	1 (1%)	14	35
1	G	111/133 (84%)	107 (96%)	4 (4%)	0	100	100
1	H	112/133 (84%)	106 (95%)	6 (5%)	0	100	100
All	All	890/1064 (84%)	857 (96%)	32 (4%)	1 (0%)	48	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	200	PRO

5.3.2 Protein sidechains ⓘ

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	102/114 (90%)	98 (96%)	4 (4%)	28	57
1	B	102/114 (90%)	97 (95%)	5 (5%)	22	49
1	C	101/114 (89%)	98 (97%)	3 (3%)	36	66
1	D	100/114 (88%)	100 (100%)	0	100	100
1	E	101/114 (89%)	100 (99%)	1 (1%)	68	86
1	F	101/114 (89%)	95 (94%)	6 (6%)	18	42
1	G	101/114 (89%)	98 (97%)	3 (3%)	36	66
1	H	102/114 (90%)	95 (93%)	7 (7%)	14	34
All	All	810/912 (89%)	781 (96%)	29 (4%)	31	60

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	THR
1	A	140	ASP
1	A	149	THR
1	A	164	LEU
1	B	149	THR
1	B	151	LEU
1	B	195	LYS
1	B	201	VAL
1	B	203	LEU
1	C	136	ILE
1	C	149	THR
1	C	197	VAL
1	E	99	ILE
1	F	99	ILE
1	F	163	ILE
1	F	168	GLU
1	F	194	ILE
1	F	199	LEU
1	F	201	VAL
1	G	109	LEU
1	G	195	LYS
1	G	197	VAL
1	H	91	LEU
1	H	99	ILE
1	H	116	ILE
1	H	126	VAL
1	H	160	LEU
1	H	169	GLU
1	H	170	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	159	ASN
1	B	153	ASN
1	B	159	ASN
1	E	148	GLN
1	H	153	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	A	113/133 (84%)	0.51	1 (0%) 81 80	19, 45, 58, 68	5 (4%)
1	B	114/133 (85%)	0.51	7 (6%) 27 24	20, 42, 63, 69	5 (4%)
1	C	112/133 (84%)	0.72	11 (9%) 13 11	22, 45, 69, 73	8 (7%)
1	D	112/133 (84%)	0.32	4 (3%) 46 42	19, 39, 49, 63	2 (1%)
1	E	113/133 (84%)	0.41	3 (2%) 56 53	15, 43, 60, 64	4 (3%)
1	F	113/133 (84%)	1.18	19 (16%) 4 3	21, 62, 79, 88	15 (13%)
1	G	113/133 (84%)	0.89	11 (9%) 13 11	21, 56, 75, 80	7 (6%)
1	H	114/133 (85%)	1.45	31 (27%) 1 1	21, 61, 110, 125	17 (14%)
All	All	904/1064 (84%)	0.75	87 (9%) 13 11	15, 48, 76, 125	63 (6%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	113	SER	4.8
1	H	114	VAL	4.7
1	H	117	SER	4.4
1	H	115	THR	4.3
1	C	91	LEU	4.2
1	F	201	VAL	4.1
1	F	130	THR	4.1
1	C	201	VAL	4.0
1	H	108	VAL	3.9
1	H	116	ILE	3.7
1	B	203	LEU	3.6
1	H	154	ALA	3.5
1	H	111	LYS	3.4
1	F	139	ALA	3.4
1	F	200	PRO	3.3
1	H	155	LEU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	173[A]	HIS	3.3
1	H	172	HIS	3.2
1	G	201	VAL	3.2
1	H	110	THR	3.1
1	H	192	VAL	3.1
1	H	143	THR	3.0
1	H	136	ILE	3.0
1	F	113	SER	3.0
1	H	109	LEU	3.0
1	F	137	THR	2.9
1	F	168	GLU	2.9
1	E	141	SER	2.8
1	H	137	THR	2.8
1	F	136	ILE	2.7
1	D	200	PRO	2.7
1	G	166	ASP	2.7
1	H	166	ASP	2.7
1	H	107	GLU	2.6
1	F	129	ALA	2.6
1	F	199	LEU	2.6
1	H	105	PRO	2.6
1	H	162	GLN	2.6
1	F	176	SER	2.5
1	B	192	VAL	2.5
1	B	201	VAL	2.5
1	G	142	ALA	2.5
1	C	115	THR	2.4
1	B	199	LEU	2.4
1	F	184	ASP	2.4
1	F	150	THR	2.4
1	H	153	ASN	2.4
1	B	166	ASP	2.4
1	F	170	ILE	2.3
1	H	90	SER	2.3
1	G	133	VAL	2.3
1	H	118	VAL	2.3
1	F	91	LEU	2.3
1	E	143	THR	2.3
1	H	94	VAL	2.3
1	C	93	LYS	2.2
1	C	164	LEU	2.2
1	G	197	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	163	ILE	2.2
1	F	174	MET	2.2
1	G	136	ILE	2.2
1	H	103	ILE	2.2
1	B	90	SER	2.2
1	B	164	LEU	2.2
1	C	200	PRO	2.2
1	D	127	GLN	2.2
1	F	120	GLY	2.2
1	G	89	ASP	2.2
1	F	185	TRP	2.1
1	G	171	ALA	2.1
1	H	106	GLN	2.1
1	F	114	VAL	2.1
1	H	140	ASP	2.1
1	G	177	THR	2.1
1	C	160	LEU	2.1
1	D	112	ASP	2.1
1	C	195	LYS	2.1
1	A	164	LEU	2.1
1	H	156	GLY	2.1
1	G	190	GLU	2.1
1	C	172	HIS	2.1
1	C	108	VAL	2.1
1	E	201	VAL	2.1
1	G	157	THR	2.0
1	H	170	ILE	2.0
1	H	164	LEU	2.0
1	D	173	HIS	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.