



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:01 AM UTC

PDB ID : 1M1L / pdb_00001m1l
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

<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

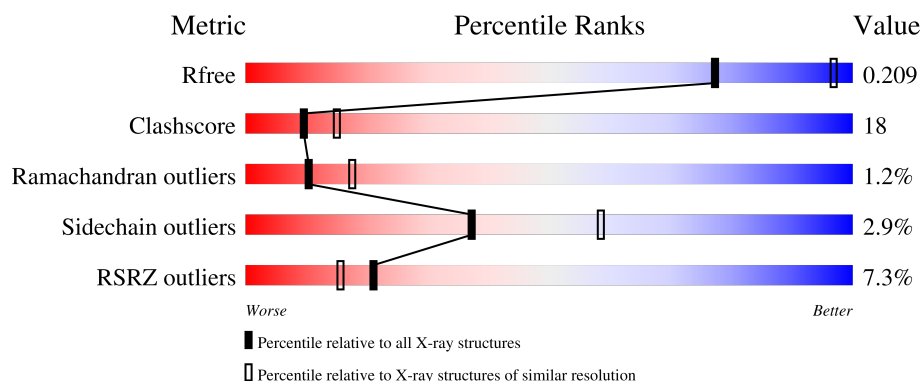
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	236	5% 73% 25% .
1	B	236	8% 72% 26% .
1	C	236	8% 69% 29% ..
1	D	236	8% 67% 28% ..

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			

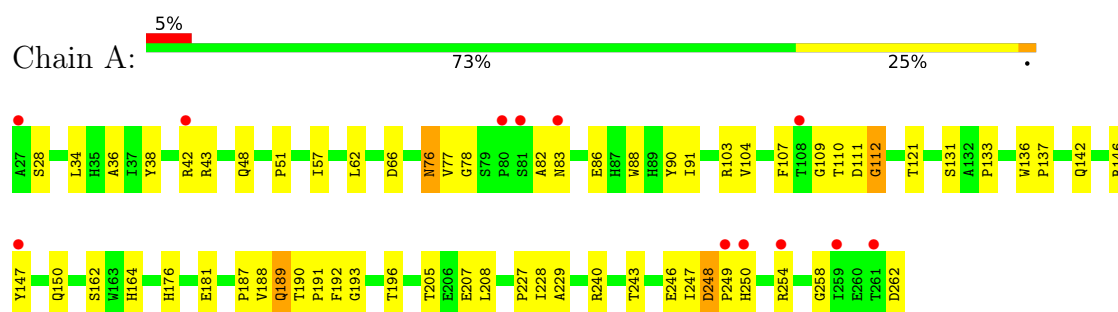
- Molecule 2 is water.

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		

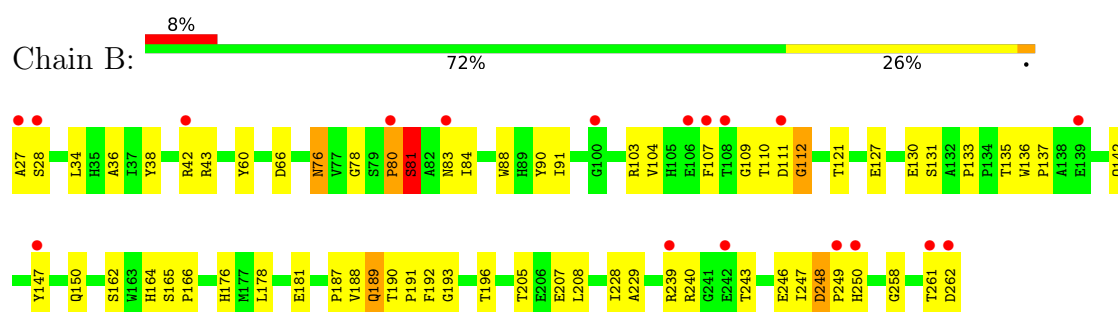
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

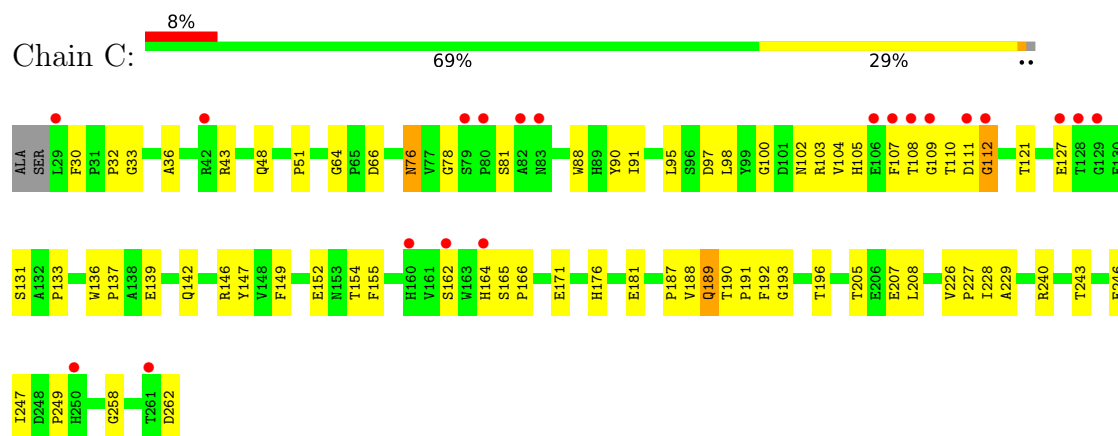
• Molecule 1: Suppressor of Fused



• Molecule 1: Suppressor of Fused



• Molecule 1: Suppressor of Fused



• Molecule 1: Suppressor of Fused



4 Data and refinement statistics

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) 99.2 (29.81-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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	2515 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	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.*

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	0.56	0/1936	0.98	2/2642 (0.1%)
1	B	0.58	0/1936	1.02	7/2642 (0.3%)
1	C	0.56	0/1925	1.01	6/2627 (0.2%)
1	D	0.57	0/1925	1.06	10/2627 (0.4%)
All	All	0.57	0/7722	1.02	25/10538 (0.2%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	152	GLU	N-CA-C	-11.64	86.01	110.80
1	B	80	PRO	N-CA-C	-9.21	95.58	111.32
1	C	139	GLU	CA-CB-CG	-8.60	96.89	114.10
1	D	84	ILE	N-CA-C	-8.03	99.60	107.55
1	B	28	SER	N-CA-C	-6.67	96.59	110.80
1	A	248	ASP	CA-C-N	6.36	127.79	119.84
1	A	248	ASP	C-N-CA	6.36	127.79	119.84
1	C	30	PHE	N-CA-C	-5.90	102.21	109.65
1	D	151	SER	CA-C-N	5.87	132.75	121.54
1	D	151	SER	C-N-CA	5.87	132.75	121.54
1	C	108	THR	N-CA-C	5.77	118.27	110.88
1	B	178	LEU	N-CA-C	-5.64	100.70	109.72
1	D	151	SER	N-CA-C	5.56	122.64	110.80
1	C	64	GLY	CA-C-N	5.46	125.15	119.64
1	C	64	GLY	C-N-CA	5.46	125.15	119.64
1	D	178	LEU	N-CA-C	-5.43	101.03	109.72
1	D	248	ASP	CA-C-N	5.40	126.59	119.84
1	D	248	ASP	C-N-CA	5.40	126.59	119.84
1	B	84	ILE	N-CA-C	5.32	120.38	108.88
1	B	135	THR	N-CA-C	5.32	119.77	113.28
1	B	81	SER	N-CA-C	-5.28	99.55	110.80
1	D	43	ARG	N-CA-C	-5.22	105.59	111.28
1	D	135	THR	N-CA-C	5.06	119.46	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	152	GLU	N-CA-C	-5.06	106.70	112.92
1	B	248	ASP	O-C-N	5.04	125.06	121.12

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	71	0
1	B	1877	0	1779	71	0
1	C	1866	0	1769	58	0
1	D	1866	0	1769	69	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	259	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 18.

All (259) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:HIS:HE1	1:C:205:THR:HG22	1.21	1.01
1:C:176:HIS:CE1	1:C:205:THR:HG22	1.94	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
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:B:66:ASP:HB3	1:B:142:GLN:CD	2.22	0.64
1:A:62:LEU:HD12	2:A:284:HOH:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:PHE:CE2	1:D:154:THR:HG23	2.32	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:66:ASP:HB3	1:A:142:GLN:CD	2.24	0.62
1:A:82:ALA:O	1:A:83:ASN:HB3	1.99	0.62
1:A:83:ASN:HD21	1:A:227:PRO:HB3	1.63	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
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:C:66:ASP:HB3	1:C:142:GLN:CD	2.26	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: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:76:ASN:HD22	1:C:78:GLY:N	2.00	0.59
1:D:190:THR:HB	1:D:193:GLY:O	2.02	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:B:228:ILE:HD11	1:B:247:ILE:HD13	1.86	0.58
1:D:154:THR:HG22	1:D:155:PHE:O	2.03	0.58
1:D:66:ASP:HB3	1:D:142:GLN:CD	2.28	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:THR:HG23	1:C:191:PRO:HD2	1.86	0.56
1:B:43:ARG:HG2	1:B:43:ARG:HH11	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: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:B:38:TYR:CE2	1:B:42:ARG:HD2	2.42	0.55
1:D:43:ARG:HG2	1:D:43:ARG:HH11	1.72	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:C:147:TYR:CE2	1:C:155:PHE:HZ	2.25	0.54
1:D:164:HIS:O	1:D:164:HIS:CD2	2.60	0.54
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:76:ASN:HD22	1:D:78:GLY:N	2.04	0.54
1:B:36:ALA:HB1	1:B:188:VAL:HG11	1.90	0.53
1:C:136:TRP:CG	1:C:137:PRO:HD3	2.43	0.53
1:B:261:THR:HG22	1:B:261:THR:O	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:O	1:A:164:HIS:CD2	2.63	0.51
1:A:147:TYR:CE2	1:B:147:TYR:CE2	2.98	0.51
1:A:207:GLU:CD	1:A:240:ARG:HH22	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:36:ALA:HB1	1:C:188:VAL:HG11	1.94	0.50
1:D:164:HIS:O	1:D:164:HIS:HD2	1.94	0.50
1:A:207:GLU:OE1	1:A:240:ARG:NH2	2.44	0.50
1:B:38:TYR:CZ	1:B:42:ARG:HD2	2.47	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
1:A:248:ASP:OD1	1:A:250:HIS:HB2	2.11	0.49
1:B:90:TYR:C	1:B:91:ILE:HD12	2.37	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:B:207:GLU:CD	1:B:240:ARG:HH22	2.21	0.48
1:C:207:GLU:CD	1:C:240:ARG:HH22	2.22	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:B:164:HIS:CD2	1:B:164:HIS:O	2.66	0.48
1:D:151:SER:OG	1:D:152:GLU:N	2.47	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:B:127:GLU:O	1:B:130:GLU:HG3	2.15	0.47
1:C:102:ASN:HA	1:C:105:HIS:O	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:C:90:TYR:O	1:C:121:THR:HA	2.15	0.47
1:D:107:PHE:CZ	1:D:109:GLY:HA2	2.50	0.47
1:D:187:PRO:HB3	1:D:196:THR:HG22	1.95	0.47
1:A:187:PRO:HB3	1:A:196:THR:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:ASP:HB3	1:C:142:GLN:NE2	2.30	0.46
1:D:207:GLU:CD	1:D:240:ARG:HH22	2.23	0.46
1:A:147:TYR:CE2	1:B:147:TYR:CD2	3.03	0.46
1:C:110:THR:HG22	1:C:191:PRO:C	2.41	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:34:LEU:C	1:B:34:LEU:HD23	2.41	0.45
1:B:38:TYR:CE2	1:B:42:ARG:NH1	2.85	0.45
1:A:90:TYR:C	1:A:91:ILE:HD12	2.41	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:C:165:SER:O	1:C:166:PRO:C	2.58	0.45
1:B:127:GLU:HG3	1:B:239:ARG:NH2	2.32	0.45
1:B:189:GLN:CA	1:B:189:GLN:NE2	2.79	0.45
1:C:88:TRP:CE3	1:C:133:PRO:HB3	2.52	0.45
1:B:111:ASP:O	1:B:112:GLY:O	2.33	0.45
1:C:189:GLN:HE21	1:C:190:THR:H	1.65	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
1:D:229:ALA:HB1	1:D:240:ARG:NH1	2.32	0.45
1:D:189:GLN:HE21	1:D:189:GLN:CA	2.28	0.44
1:D:152:GLU:O	1:D:153:ASN:HB2	2.17	0.44
1:A:43:ARG:HG2	1:A:43:ARG:NH1	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:A:83:ASN:CG	1:A:83:ASN:O	2.59	0.44
1:B:207:GLU:OE1	1:B:240:ARG:NH2	2.50	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: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:O	1:C:164:HIS:CD2	2.70	0.44
1:D:245:PHE:HB2	2:D:274:HOH:O	2.17	0.44
1:C:90:TYR:C	1:C:91:ILE:HD12	2.43	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:C:154:THR:HA	2:C:313:HOH:O	2.19	0.43
1:D:127:GLU:HG3	1:D:239:ARG:CZ	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:91:ILE:HD12	1:B:91:ILE:N	2.33	0.43
1:A:248:ASP:HA	1:A:249:PRO:HD2	1.78	0.43
1:C:189:GLN:HE21	1:C:189:GLN:CA	2.31	0.43
1:B:164:HIS:O	1:B:164:HIS:HD2	2.02	0.42
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:A:189:GLN:HE21	1:A:189:GLN:CA	2.32	0.42
1:B:36:ALA:HB1	1:B:188:VAL:CG1	2.49	0.42
1:D:136:TRP:CD2	1:D:137:PRO:HD3	2.54	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:260:GLU:C	1:D:262:ASP:H	2.28	0.42
1:A:88:TRP:CZ3	1:A:133:PRO:HD3	2.55	0.42
1:D:127:GLU:HG3	1:D:239:ARG:HH12	1.84	0.42
1:B:176:HIS:HE1	1:B:205:THR:CG2	2.05	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:A:164:HIS:CE1	1:B:60:TYR:CE2	3.08	0.41
1:D:155:PHE:HB3	1:D:179:LEU:CD1	2.50	0.41
1:A:77:VAL:HA	1:A:86:GLU:HG3	2.03	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:D:79:SER:HA	1:D:80:PRO:HD2	1.94	0.41
1:D:110:THR:HG22	1:D:191:PRO:C	2.43	0.41
1:A:34:LEU:C	1:A:34:LEU:HD23	2.45	0.41
1:C:226:VAL:HA	1:C:227:PRO:HD2	1.89	0.41
1:B:88:TRP:CZ3	1:B:133:PRO:HD3	2.57	0.40
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:C:164:HIS:O	1:C:164:HIS:HD2	2.03	0.40
1:A:48:GLN:O	1:A:51:PRO:HD3	2.21	0.40
1:A:146:ARG:O	1:A:150:GLN:CG	2.52	0.40
1:B:165:SER:O	1:B:166:PRO:C	2.63	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:A:66:ASP:HB3	1:A:142:GLN:NE2	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ASP:O	1:A:112:GLY:O	2.39	0.40
1:B:248:ASP:OD1	1:B:250:HIS:HB2	2.21	0.40
1:D:189:GLN:HE21	1:D:190:THR:H	1.69	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%)	14	24
1	B	234/236 (99%)	220 (94%)	11 (5%)	3 (1%)	9	16
1	C	232/236 (98%)	218 (94%)	12 (5%)	2 (1%)	14	24
1	D	232/236 (98%)	215 (93%)	13 (6%)	4 (2%)	7	12
All	All	932/944 (99%)	873 (94%)	48 (5%)	11 (1%)	10	17

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 ⓘ

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%)	43	65
1	B	205/205 (100%)	199 (97%)	6 (3%)	37	58
1	C	204/205 (100%)	199 (98%)	5 (2%)	42	64
1	D	204/205 (100%)	196 (96%)	8 (4%)	28	48
All	All	818/820 (100%)	794 (97%)	24 (3%)	37	58

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	131	SER
1	A	181	GLU
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	181	GLU
1	B	189	GLN
1	C	76	ASN
1	C	81	SER
1	C	131	SER
1	C	181	GLU
1	C	189	GLN
1	D	76	ASN
1	D	83	ASN
1	D	131	SER
1	D	181	GLU
1	D	189	GLN
1	D	239	ARG
1	D	261	THR
1	D	262	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) 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	53	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	176	HIS
1	C	189	GLN
1	C	252	GLN
1	D	76	ASN
1	D	164	HIS
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 oligosaccharides 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, 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	236/236 (100%)	0.11	12 (5%) 33 26	14, 28, 63, 92	0
1	B	236/236 (100%)	0.18	18 (7%) 20 15	15, 29, 62, 81	0
1	C	234/236 (99%)	0.30	20 (8%) 16 12	18, 33, 61, 81	0
1	D	234/236 (99%)	0.21	19 (8%) 18 13	14, 30, 57, 89	0
All	All	940/944 (99%)	0.20	69 (7%) 21 15	14, 30, 61, 92	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	249	PRO	5.4
1	D	153	ASN	5.2
1	B	83	ASN	4.7
1	D	155	PHE	4.6
1	B	108	THR	4.5
1	B	111	ASP	4.2
1	C	164	HIS	4.1
1	A	27	ALA	4.0
1	D	154	THR	3.9
1	B	147	TYR	3.7
1	C	42	ARG	3.7
1	B	250	HIS	3.6
1	B	27	ALA	3.6
1	D	42	ARG	3.6
1	B	242	GLU	3.5
1	A	261	THR	3.5
1	B	261	THR	3.5
1	D	152	GLU	3.5
1	B	80	PRO	3.4
1	D	129	GLY	3.4
1	A	250	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	107	PHE	3.3
1	A	147	TYR	3.3
1	D	107	PHE	3.2
1	B	107	PHE	3.2
1	A	81	SER	3.1
1	C	111	ASP	3.1
1	D	250	HIS	3.0
1	C	80	PRO	3.0
1	C	106	GLU	2.9
1	A	108	THR	2.9
1	A	83	ASN	2.9
1	C	29	LEU	2.9
1	D	151	SER	2.9
1	A	80	PRO	2.8
1	C	162	SER	2.8
1	C	250	HIS	2.8
1	D	111	ASP	2.8
1	A	249	PRO	2.7
1	A	42	ARG	2.7
1	D	106	GLU	2.7
1	D	150	GLN	2.6
1	B	106	GLU	2.6
1	C	128	THR	2.6
1	D	109	GLY	2.6
1	C	83	ASN	2.6
1	D	262	ASP	2.5
1	C	112	GLY	2.5
1	B	139	GLU	2.5
1	C	108	THR	2.4
1	A	259	ILE	2.4
1	D	164	HIS	2.3
1	B	28	SER	2.3
1	B	239	ARG	2.3
1	C	109	GLY	2.2
1	C	261	THR	2.2
1	D	254	ARG	2.2
1	C	160	HIS	2.2
1	C	79	SER	2.2
1	B	100	GLY	2.1
1	B	262	ASP	2.1
1	A	254	ARG	2.1
1	D	29	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	129	GLY	2.1
1	C	82	ALA	2.0
1	D	156	CYS	2.0
1	B	42	ARG	2.0
1	C	127	GLU	2.0
1	D	221	GLU	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.