



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:30 PM UTC

PDB ID : 4GFA / pdb_00004gfa
Title : N-terminal coiled-coil dimer of C.elegans SAS-6, crystal form A
Authors : Erat, M.C.; Vakonakis, I.
Deposited on : 2012-08-03
Resolution : 3.55 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
Mogul : 2022.3.0, CSD as543be (2022)
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

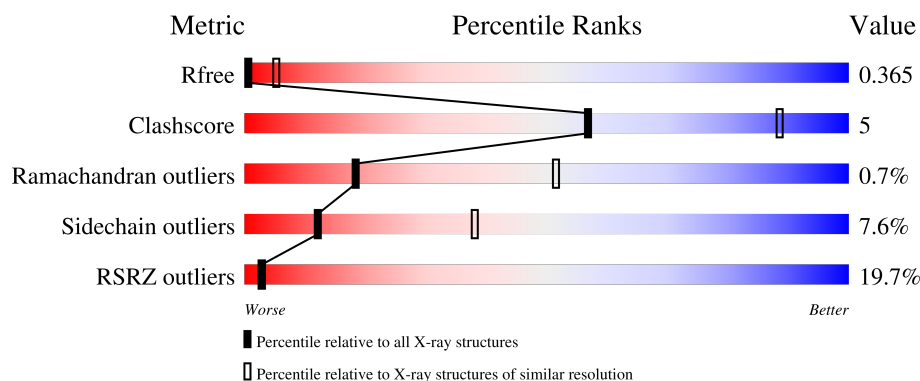
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 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	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)

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	A	183	9% 68% 14% • 15%
1	B	183	23% 65% 18% • 15%
1	C	183	11% 63% 19% • 16%
1	D	183	22% 63% 15% • 20%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4958 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 Spindle assembly abnormal protein 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	155	Total	C	N	O	S	0	0	0
			1260	814	207	236	3			
1	B	155	Total	C	N	O	S	0	0	0
			1260	814	207	236	3			
1	C	153	Total	C	N	O	S	0	0	0
			1242	802	205	232	3			
1	D	146	Total	C	N	O	S	0	0	0
			1188	772	193	220	3			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP O62479
A	0	SER	-	expression tag	UNP O62479
A	?	-	ILE	deletion	UNP O62479
A	?	-	VAL	deletion	UNP O62479
A	?	-	LYS	deletion	UNP O62479
A	?	-	ASN	deletion	UNP O62479
A	?	-	LEU	deletion	UNP O62479
A	?	-	GLU	deletion	UNP O62479
A	?	-	GLU	deletion	UNP O62479
A	?	-	ASP	deletion	UNP O62479
A	?	-	GLY	deletion	UNP O62479
A	?	-	GLU	deletion	UNP O62479
A	?	-	VAL	deletion	UNP O62479
A	?	-	ASP	deletion	UNP O62479
A	?	-	ALA	deletion	UNP O62479
A	?	-	ARG	deletion	UNP O62479
A	?	-	LYS	deletion	UNP O62479
A	?	-	LYS	deletion	UNP O62479
A	?	-	ALA	deletion	UNP O62479
A	?	-	GLY	deletion	UNP O62479
A	?	-	TYR	deletion	UNP O62479

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	HIS	deletion	UNP O62479
A	?	-	SER	deletion	UNP O62479
A	?	-	ILE	deletion	UNP O62479
A	?	-	ALA	deletion	UNP O62479
A	?	-	ASP	deletion	UNP O62479
A	?	-	PRO	deletion	UNP O62479
A	?	-	GLY	deletion	UNP O62479
A	?	-	LYS	deletion	UNP O62479
A	?	-	PRO	deletion	UNP O62479
A	?	-	LYS	deletion	UNP O62479
A	?	-	THR	deletion	UNP O62479
A	?	-	PRO	deletion	UNP O62479
A	?	-	ILE	deletion	UNP O62479
A	?	-	SER	deletion	UNP O62479
A	?	-	LYS	deletion	UNP O62479
B	-1	GLY	-	expression tag	UNP O62479
B	0	SER	-	expression tag	UNP O62479
B	?	-	ILE	deletion	UNP O62479
B	?	-	VAL	deletion	UNP O62479
B	?	-	LYS	deletion	UNP O62479
B	?	-	ASN	deletion	UNP O62479
B	?	-	LEU	deletion	UNP O62479
B	?	-	GLU	deletion	UNP O62479
B	?	-	GLU	deletion	UNP O62479
B	?	-	ASP	deletion	UNP O62479
B	?	-	GLY	deletion	UNP O62479
B	?	-	GLU	deletion	UNP O62479
B	?	-	VAL	deletion	UNP O62479
B	?	-	ASP	deletion	UNP O62479
B	?	-	ALA	deletion	UNP O62479
B	?	-	ARG	deletion	UNP O62479
B	?	-	LYS	deletion	UNP O62479
B	?	-	LYS	deletion	UNP O62479
B	?	-	ALA	deletion	UNP O62479
B	?	-	GLY	deletion	UNP O62479
B	?	-	TYR	deletion	UNP O62479
B	?	-	HIS	deletion	UNP O62479
B	?	-	SER	deletion	UNP O62479
B	?	-	ILE	deletion	UNP O62479
B	?	-	ALA	deletion	UNP O62479
B	?	-	ASP	deletion	UNP O62479
B	?	-	PRO	deletion	UNP O62479

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLY	deletion	UNP O62479
B	?	-	LYS	deletion	UNP O62479
B	?	-	PRO	deletion	UNP O62479
B	?	-	LYS	deletion	UNP O62479
B	?	-	THR	deletion	UNP O62479
B	?	-	PRO	deletion	UNP O62479
B	?	-	ILE	deletion	UNP O62479
B	?	-	SER	deletion	UNP O62479
B	?	-	LYS	deletion	UNP O62479
C	-1	GLY	-	expression tag	UNP O62479
C	0	SER	-	expression tag	UNP O62479
C	?	-	ILE	deletion	UNP O62479
C	?	-	VAL	deletion	UNP O62479
C	?	-	LYS	deletion	UNP O62479
C	?	-	ASN	deletion	UNP O62479
C	?	-	LEU	deletion	UNP O62479
C	?	-	GLU	deletion	UNP O62479
C	?	-	GLU	deletion	UNP O62479
C	?	-	ASP	deletion	UNP O62479
C	?	-	GLY	deletion	UNP O62479
C	?	-	GLU	deletion	UNP O62479
C	?	-	VAL	deletion	UNP O62479
C	?	-	ASP	deletion	UNP O62479
C	?	-	ALA	deletion	UNP O62479
C	?	-	ARG	deletion	UNP O62479
C	?	-	LYS	deletion	UNP O62479
C	?	-	LYS	deletion	UNP O62479
C	?	-	ALA	deletion	UNP O62479
C	?	-	GLY	deletion	UNP O62479
C	?	-	TYR	deletion	UNP O62479
C	?	-	HIS	deletion	UNP O62479
C	?	-	SER	deletion	UNP O62479
C	?	-	ILE	deletion	UNP O62479
C	?	-	ALA	deletion	UNP O62479
C	?	-	ASP	deletion	UNP O62479
C	?	-	PRO	deletion	UNP O62479
C	?	-	GLY	deletion	UNP O62479
C	?	-	LYS	deletion	UNP O62479
C	?	-	PRO	deletion	UNP O62479
C	?	-	LYS	deletion	UNP O62479
C	?	-	THR	deletion	UNP O62479
C	?	-	PRO	deletion	UNP O62479

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ILE	deletion	UNP O62479
C	?	-	SER	deletion	UNP O62479
C	?	-	LYS	deletion	UNP O62479
D	-1	GLY	-	expression tag	UNP O62479
D	0	SER	-	expression tag	UNP O62479
D	?	-	ILE	deletion	UNP O62479
D	?	-	VAL	deletion	UNP O62479
D	?	-	LYS	deletion	UNP O62479
D	?	-	ASN	deletion	UNP O62479
D	?	-	LEU	deletion	UNP O62479
D	?	-	GLU	deletion	UNP O62479
D	?	-	GLU	deletion	UNP O62479
D	?	-	ASP	deletion	UNP O62479
D	?	-	GLY	deletion	UNP O62479
D	?	-	GLU	deletion	UNP O62479
D	?	-	VAL	deletion	UNP O62479
D	?	-	ASP	deletion	UNP O62479
D	?	-	ALA	deletion	UNP O62479
D	?	-	ARG	deletion	UNP O62479
D	?	-	LYS	deletion	UNP O62479
D	?	-	LYS	deletion	UNP O62479
D	?	-	ALA	deletion	UNP O62479
D	?	-	GLY	deletion	UNP O62479
D	?	-	TYR	deletion	UNP O62479
D	?	-	HIS	deletion	UNP O62479
D	?	-	SER	deletion	UNP O62479
D	?	-	ILE	deletion	UNP O62479
D	?	-	ALA	deletion	UNP O62479
D	?	-	ASP	deletion	UNP O62479
D	?	-	PRO	deletion	UNP O62479
D	?	-	GLY	deletion	UNP O62479
D	?	-	LYS	deletion	UNP O62479
D	?	-	PRO	deletion	UNP O62479
D	?	-	LYS	deletion	UNP O62479
D	?	-	THR	deletion	UNP O62479
D	?	-	PRO	deletion	UNP O62479
D	?	-	ILE	deletion	UNP O62479
D	?	-	SER	deletion	UNP O62479
D	?	-	LYS	deletion	UNP O62479

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).

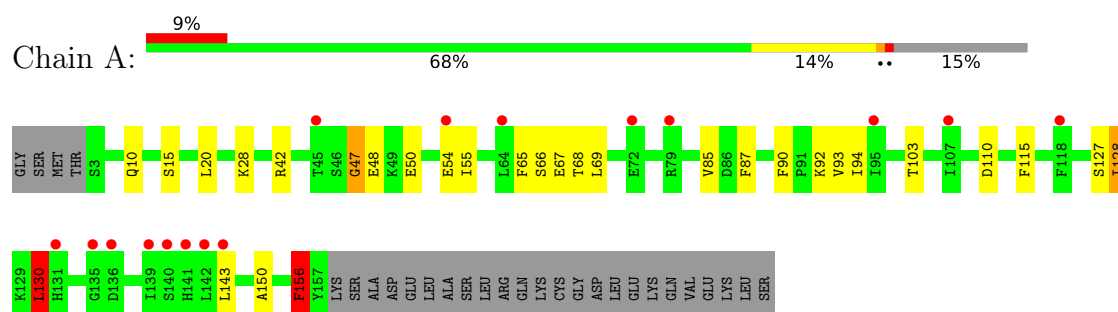


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			8	6	2		

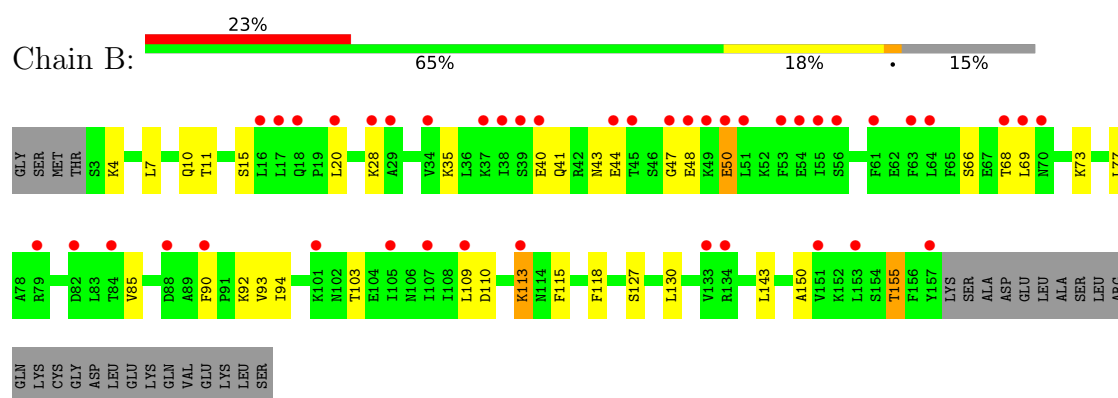
3 Residue-property plots [i](#)

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.

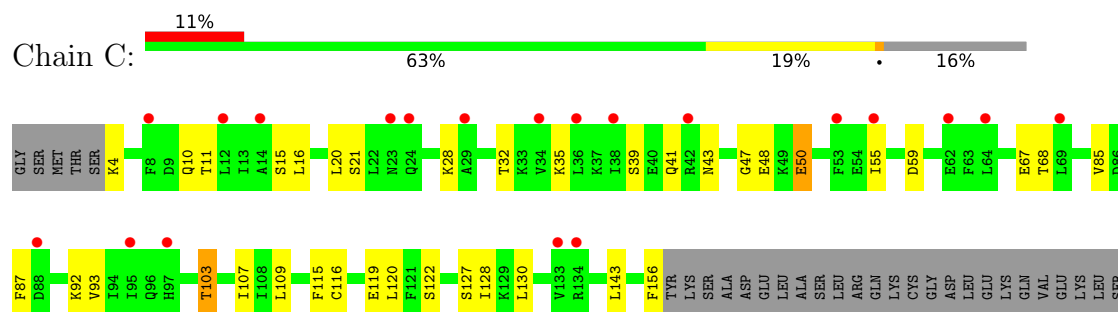
• Molecule 1: Spindle assembly abnormal protein 6



• Molecule 1: Spindle assembly abnormal protein 6

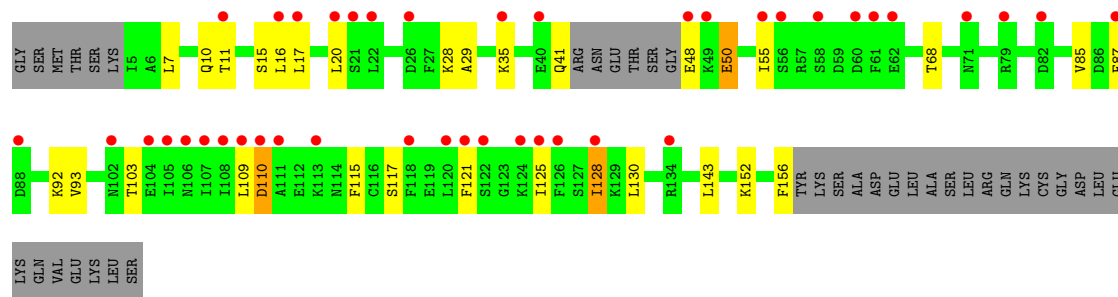


• Molecule 1: Spindle assembly abnormal protein 6



• Molecule 1: Spindle assembly abnormal protein 6





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	73.15Å 118.94Å 121.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.31 – 3.55 62.31 – 3.55	Depositor EDS
% Data completeness (in resolution range)	99.1 (62.31-3.55) 98.8 (62.31-3.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 3.57Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.310 , 0.357 0.318 , 0.365	Depositor DCC
R_{free} test set	660 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	87.4	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 105.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	4958	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.44 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7641e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MPD

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	0.89	1/1283 (0.1%)	1.35	7/1725 (0.4%)
1	B	0.88	0/1283	1.36	7/1725 (0.4%)
1	C	0.83	0/1264	1.34	6/1699 (0.4%)
1	D	0.82	0/1209	1.37	4/1625 (0.2%)
All	All	0.86	1/5039 (0.0%)	1.35	24/6774 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	130	LEU	CA-C	7.21	1.61	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	92	LYS	CA-C-N	6.35	128.56	120.56
1	D	92	LYS	C-N-CA	6.35	128.56	120.56
1	C	92	LYS	CA-C-N	6.32	128.65	120.56
1	C	92	LYS	C-N-CA	6.32	128.65	120.56
1	C	43	ASN	CA-CB-CG	6.20	118.80	112.60
1	A	156	PHE	CA-CB-CG	6.14	119.94	113.80
1	B	43	ASN	CA-CB-CG	6.14	118.74	112.60
1	B	92	LYS	CA-C-N	6.06	128.32	120.56
1	B	92	LYS	C-N-CA	6.06	128.32	120.56
1	A	65	PHE	CA-CB-CG	5.91	119.71	113.80
1	A	92	LYS	CA-C-N	5.83	128.02	120.56
1	A	92	LYS	C-N-CA	5.83	128.02	120.56
1	A	87	PHE	CA-CB-CG	5.81	119.61	113.80
1	C	115	PHE	CA-CB-CG	5.80	119.60	113.80
1	C	87	PHE	CA-CB-CG	5.62	119.42	113.80
1	A	150	ALA	CA-C-N	5.25	127.28	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	ALA	C-N-CA	5.25	127.28	120.56
1	D	87	PHE	CA-CB-CG	5.25	119.05	113.80
1	D	110	ASP	CA-CB-CG	5.18	117.78	112.60
1	B	155	THR	CA-C-N	5.16	128.67	121.24
1	B	155	THR	C-N-CA	5.16	128.67	121.24
1	C	59	ASP	CA-CB-CG	5.08	117.68	112.60
1	B	150	ALA	CA-C-N	5.03	127.00	120.56
1	B	150	ALA	C-N-CA	5.03	127.00	120.56

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	1260	0	1281	10	0
1	B	1260	0	1281	12	0
1	C	1242	0	1267	13	0
1	D	1188	0	1213	11	0
2	C	8	0	14	0	0
All	All	4958	0	5056	46	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 5.

All (46) 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:69:LEU:HD23	1:B:73:LYS:HB3	1.72	0.71
1:C:119:GLU:HG2	1:C:127:SER:HB2	1.82	0.62
1:D:16:LEU:HD11	1:D:109:LEU:HD13	1.82	0.61
1:B:4:LYS:HD2	1:B:41:GLN:HB3	1.85	0.58
1:C:16:LEU:HD22	1:C:32:THR:HG21	1.85	0.57
1:A:85:VAL:HG11	1:A:93:VAL:HG21	1.88	0.55
1:A:54:GLU:HG3	1:A:66:SER:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:PHE:O	1:B:127:SER:HA	2.08	0.54
1:C:67:GLU:HB3	1:C:130:LEU:HD23	1.89	0.54
1:B:11:THR:HA	1:B:35:LYS:HA	1.88	0.53
1:D:55:ILE:HG12	1:D:130:LEU:HD13	1.88	0.53
1:A:110:ASP:HB2	1:A:115:PHE:O	2.10	0.51
1:B:85:VAL:HG11	1:B:93:VAL:HG21	1.91	0.51
1:C:67:GLU:CB	1:C:130:LEU:HD23	2.41	0.51
1:B:41:GLN:HG3	1:B:50:GLU:HB3	1.95	0.48
1:D:85:VAL:HG11	1:D:93:VAL:HG21	1.95	0.48
1:B:110:ASP:HB2	1:B:115:PHE:O	2.13	0.47
1:D:110:ASP:HB2	1:D:115:PHE:O	2.15	0.47
1:D:41:GLN:HG3	1:D:50:GLU:HB3	1.96	0.47
1:C:85:VAL:HG11	1:C:93:VAL:HG21	1.95	0.47
1:C:41:GLN:HG3	1:C:50:GLU:HB3	1.97	0.47
1:A:69:LEU:HD11	1:A:128:ILE:HD11	1.96	0.46
1:A:42:ARG:HD3	1:A:47:GLY:O	2.15	0.46
1:B:66:SER:HA	1:B:130:LEU:HD23	1.98	0.45
1:C:4:LYS:HE2	1:C:39:SER:OG	2.16	0.45
1:D:117:SER:HA	1:D:128:ILE:O	2.15	0.45
1:D:121:PHE:HB2	1:D:125:ILE:HD12	1.97	0.44
1:A:156:PHE:CD1	1:A:156:PHE:C	2.95	0.44
1:A:55:ILE:HG12	1:A:130:LEU:HD13	2.00	0.44
1:D:20:LEU:HD21	1:D:28:LYS:HB2	1.99	0.43
1:B:90:PHE:CE1	1:B:94:ILE:HG13	2.54	0.43
1:A:90:PHE:CE1	1:A:94:ILE:HG13	2.54	0.43
1:C:20:LEU:HD21	1:C:28:LYS:HB2	2.00	0.42
1:C:16:LEU:HD12	1:C:107:ILE:HB	2.01	0.42
1:D:11:THR:HA	1:D:35:LYS:HA	2.01	0.42
1:D:152:LYS:O	1:D:156:PHE:HB2	2.19	0.42
1:C:11:THR:HA	1:C:35:LYS:HA	2.02	0.42
1:D:17:LEU:CD2	1:D:29:ALA:HB2	2.49	0.42
1:A:20:LEU:HD21	1:A:28:LYS:HB2	2.01	0.42
1:B:20:LEU:HD21	1:B:28:LYS:HB2	2.01	0.41
1:C:103:THR:CG2	1:C:120:LEU:HD22	2.50	0.41
1:C:55:ILE:HG12	1:C:130:LEU:HD13	2.03	0.41
1:A:67:GLU:HB3	1:A:130:LEU:HD23	2.03	0.40
1:B:7:LEU:HD11	1:B:40:GLU:HB2	2.02	0.40
1:C:119:GLU:HG2	1:C:127:SER:CB	2.50	0.40
1:B:109:LEU:HD21	1:B:113:LYS:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	153/183 (84%)	145 (95%)	7 (5%)	1 (1%)	18	51
1	B	153/183 (84%)	144 (94%)	8 (5%)	1 (1%)	18	51
1	C	151/183 (82%)	140 (93%)	9 (6%)	2 (1%)	9	40
1	D	142/183 (78%)	136 (96%)	6 (4%)	0	100	100
All	All	599/732 (82%)	565 (94%)	30 (5%)	4 (1%)	18	51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	47	GLY
1	C	47	GLY
1	A	47	GLY
1	C	116	CYS

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	144/168 (86%)	133 (92%)	11 (8%)	12	38
1	B	144/168 (86%)	133 (92%)	11 (8%)	12	38
1	C	142/168 (84%)	130 (92%)	12 (8%)	10	35
1	D	136/168 (81%)	127 (93%)	9 (7%)	15	42
All	All	566/672 (84%)	523 (92%)	43 (8%)	12	38

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	15	SER
1	A	48	GLU
1	A	50	GLU
1	A	68	THR
1	A	103	THR
1	A	127	SER
1	A	128	ILE
1	A	130	LEU
1	A	143	LEU
1	A	156	PHE
1	B	10	GLN
1	B	15	SER
1	B	44	GLU
1	B	48	GLU
1	B	50	GLU
1	B	68	THR
1	B	77	LEU
1	B	103	THR
1	B	113	LYS
1	B	143	LEU
1	B	155	THR
1	C	10	GLN
1	C	15	SER
1	C	21	SER
1	C	48	GLU
1	C	50	GLU
1	C	68	THR
1	C	103	THR
1	C	109	LEU
1	C	122	SER
1	C	128	ILE
1	C	143	LEU
1	C	156	PHE
1	D	7	LEU
1	D	10	GLN
1	D	15	SER
1	D	48	GLU
1	D	50	GLU
1	D	68	THR
1	D	103	THR
1	D	128	ILE

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Mol	Chain	Res	Type
1	D	143	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	41	GLN
1	B	10	GLN
1	B	43	ASN
1	B	106	ASN
1	B	149	GLN
1	C	41	GLN
1	C	43	ASN
1	C	106	ASN
1	C	149	GLN
1	D	41	GLN
1	D	106	ASN
1	D	149	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 ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MPD	C	201	-	7,7,7	0.40	0	9,10,10	0.38	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	C	201	-	-	0/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	155/183 (84%)	0.92	16 (10%) 12 8	17, 73, 116, 170	0
1	B	155/183 (84%)	1.52	43 (27%) 1 1	77, 109, 184, 284	0
1	C	153/183 (83%)	0.95	20 (13%) 7 6	47, 79, 142, 198	0
1	D	146/183 (79%)	1.50	41 (28%) 1 1	87, 119, 162, 210	0
All	All	609/732 (83%)	1.22	120 (19%) 3 3	17, 97, 161, 284	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	62	GLU	9.3
1	C	53	PHE	6.8
1	B	51	LEU	5.5
1	B	45	THR	5.4
1	B	17	LEU	5.1
1	D	105	ILE	5.1
1	D	111	ALA	5.0
1	A	139	ILE	4.9
1	B	82	ASP	4.7
1	D	108	ILE	4.7
1	A	143	LEU	4.6
1	B	53	PHE	4.5
1	B	69	LEU	4.3
1	B	54	GLU	4.2
1	B	55	ILE	4.1
1	D	110	ASP	4.0
1	B	64	LEU	4.0
1	D	58	SER	4.0
1	A	131	HIS	4.0
1	D	118	PHE	4.0
1	A	72	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	38	ILE	3.8
1	D	109	LEU	3.8
1	D	26	ASP	3.5
1	C	23	ASN	3.4
1	D	113	LYS	3.4
1	A	64	LEU	3.4
1	D	107	ILE	3.3
1	A	141	HIS	3.2
1	D	120	LEU	3.1
1	D	21	SER	3.1
1	C	36	LEU	3.1
1	D	106	ASN	3.1
1	C	88	ASP	3.0
1	B	47	GLY	3.0
1	B	29	ALA	3.0
1	D	121	PHE	3.0
1	B	18	GLN	3.0
1	B	153	LEU	3.0
1	B	28	LYS	3.0
1	D	22	LEU	3.0
1	B	39	SER	3.0
1	A	79	ARG	2.9
1	A	45	THR	2.9
1	D	55	ILE	2.9
1	D	71	ASN	2.9
1	C	34	VAL	2.9
1	D	17	LEU	2.8
1	B	63	PHE	2.8
1	C	38	ILE	2.8
1	B	107	ILE	2.8
1	A	140	SER	2.8
1	D	11	THR	2.7
1	B	90	PHE	2.7
1	D	61	PHE	2.7
1	B	20	LEU	2.7
1	D	126	PHE	2.7
1	C	24	GLN	2.7
1	C	55	ILE	2.6
1	C	95	ILE	2.6
1	D	125	ILE	2.6
1	B	56	SER	2.6
1	D	60	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	20	LEU	2.6
1	B	50	GLU	2.5
1	D	48	GLU	2.5
1	B	16	LEU	2.5
1	C	97	HIS	2.5
1	A	54	GLU	2.5
1	A	142	LEU	2.5
1	D	87	PHE	2.4
1	D	104	GLU	2.4
1	C	134	ARG	2.4
1	A	135	GLY	2.4
1	B	109	LEU	2.4
1	A	95	ILE	2.4
1	D	134	ARG	2.4
1	D	40	GLU	2.4
1	B	84	THR	2.4
1	D	82	ASP	2.4
1	B	44	GLU	2.4
1	B	34	VAL	2.3
1	B	101	LYS	2.3
1	B	134	ARG	2.3
1	C	29	ALA	2.3
1	B	68	THR	2.3
1	D	102	ASN	2.3
1	B	79	ARG	2.3
1	A	107	ILE	2.3
1	C	42	ARG	2.3
1	B	70	ASN	2.2
1	B	151	VAL	2.2
1	B	40	GLU	2.2
1	C	14	ALA	2.2
1	B	157	TYR	2.2
1	D	79	ARG	2.2
1	C	62	GLU	2.2
1	B	61	PHE	2.2
1	D	128	ILE	2.2
1	D	16	LEU	2.2
1	C	8	PHE	2.2
1	D	88	ASP	2.1
1	A	118	PHE	2.1
1	C	133	VAL	2.1
1	B	113	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	48	GLU	2.1
1	C	64	LEU	2.1
1	B	49	LYS	2.1
1	D	49	LYS	2.1
1	C	12	LEU	2.1
1	B	37	LYS	2.0
1	D	122	SER	2.0
1	C	69	LEU	2.0
1	D	124	LYS	2.0
1	B	88	ASP	2.0
1	D	35	LYS	2.0
1	B	105	ILE	2.0
1	A	136	ASP	2.0
1	D	56	SER	2.0
1	B	133	VAL	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MPD	C	201	8/8	0.67	0.27	96,97,102,103	0

6.5 Other polymers [i](#)

There are no such residues in this entry.