WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 12:01 am BST

PDB ID	:	4GFA
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)

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

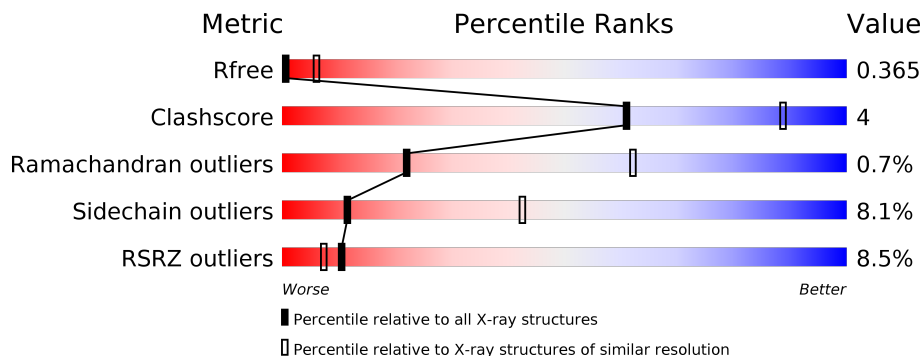|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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	Percentile Ranks	Value
Rfree		0.365
Clashscore		4
Ramachandran outliers		0.7%
Sidechain outliers		8.1%
RSRZ outliers		8.5%

Worse ← → *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1020 (3.62-3.50)
Clashscore	141614	1100 (3.62-3.50)
Ramachandran outliers	138981	1065 (3.62-3.50)
Sidechain outliers	138945	1066 (3.62-3.50)
RSRZ outliers	127900	1009 (3.64-3.48)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	183	69% 14% • 15%
1	B	183	13% / 67% 17% • 15%
1	C	183	2% / 66% 16% • 16%
1	D	183	14% / 63% 16% • 20%

2 Entry composition (i)

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 (three-letter code: MPD) (formula: $C_6H_{14}O_2$).

MPD

O4

OH

C1

C5

C4(S)

C2

CM

C3

OH

O2
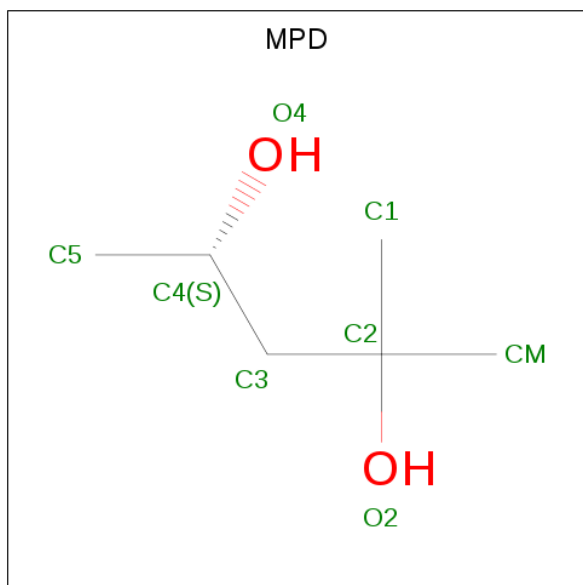
| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total 8	C 6	O 2	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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.
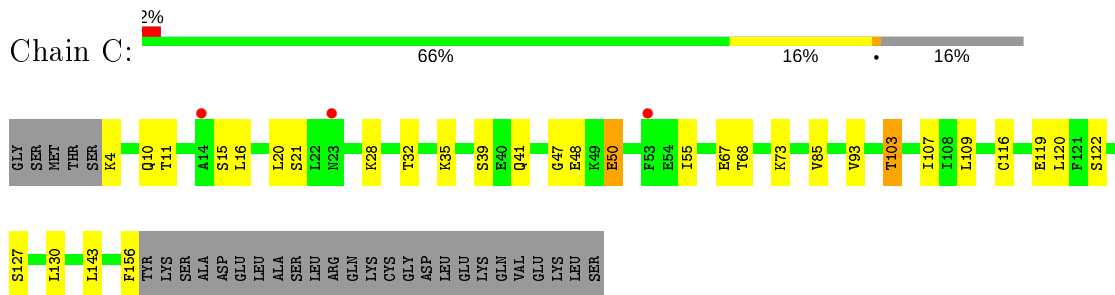
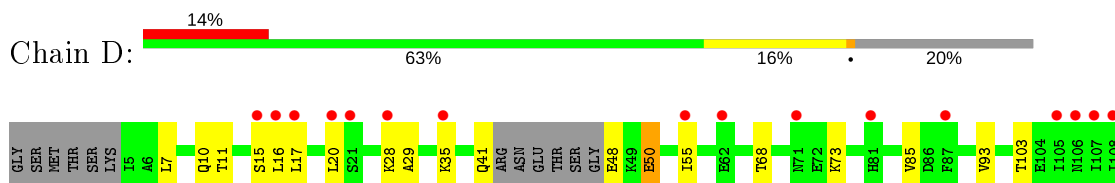• Molecule 1: Spindle assembly abnormal protein 6
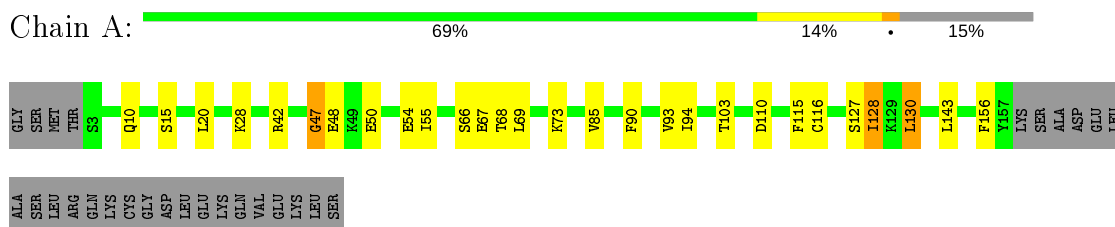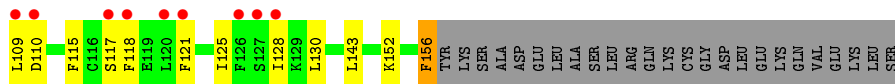
Chain A:

• Molecule 1: Spindle assembly abnormal protein 6

Chain B:

• Molecule 1: Spindle assembly abnormal protein 6

Chain C:

• Molecule 1: Spindle assembly abnormal protein 6

Chain D:
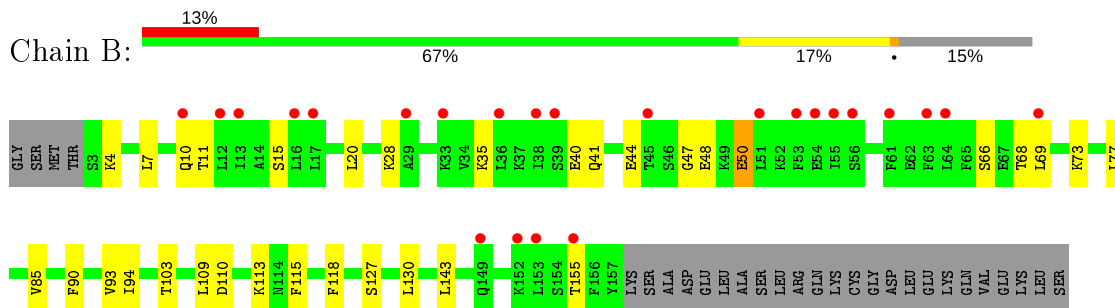
4 Data and refinement statistics (i)

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
$<I/\sigma(I)>$ [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 (4.97%)	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)	0.29 , 102.0	EDS
L-test for twinning [2]	$<|L|> = 0.43, <L^2> = 0.26$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.84	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.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.52	0/1283	0.69	0/1725
1	B	0.50	0/1283	0.69	0/1725
1	C	0.50	0/1264	0.70	0/1699
1	D	0.46	0/1209	0.67	0/1625
All	All	0.50	0/5039	0.69	0/6774

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1260	0	1281	9	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	45	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 (45) 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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 (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	153/183 (84%)	145 (95%)	7 (5%)	1 (1%)	22	62
1	B	153/183 (84%)	144 (94%)	8 (5%)	1 (1%)	22	62
1	C	151/183 (82%)	140 (93%)	9 (6%)	2 (1%)	12	50
1	D	142/183 (78%)	136 (96%)	6 (4%)	0	100	100
All	All	599/732 (82%)	565 (94%)	30 (5%)	4 (1%)	22	62

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 (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	A	144/168 (86%)	131 (91%)	13 (9%)	9	39
1	B	144/168 (86%)	134 (93%)	10 (7%)	15	48
1	C	142/168 (84%)	130 (92%)	12 (8%)	10	41
1	D	136/168 (81%)	125 (92%)	11 (8%)	11	42
All	All	566/672 (84%)	520 (92%)	46 (8%)	11	42

All (46) 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	73	LYS
1	A	103	THR
1	A	116	CYS
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	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	73	LYS

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Mol	Chain	Res	Type
1	C	103	THR
1	C	109	LEU
1	C	122	SER
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	73	LYS
1	D	103	THR
1	D	118	PHE
1	D	143	LEU
1	D	156	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	41	GLN
1	D	41	GLN

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 carbohydrates in this entry.

5.6　Ligand geometry (i)

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	0.46	0	9,10,10	0.34	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	155/183 (84%)	-0.02	0	100	100	17, 73, 116, 170	0
1	B	155/183 (84%)	0.74	24 (15%)	2	1	77, 109, 184, 284	0
1	C	153/183 (83%)	0.17	3 (1%)	65	49	47, 79, 142, 198	0
1	D	146/183 (79%)	0.90	25 (17%)	1	1	87, 119, 162, 210	0
All	All	609/732 (83%)	0.44	52 (8%)	10	7	17, 97, 161, 284	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	106	ASN	5.9
1	D	105	ILE	5.7
1	B	64	LEU	5.0
1	D	81	HIS	4.4
1	D	62	GLU	4.4
1	D	17	LEU	4.3
1	B	17	LEU	4.2
1	D	120	LEU	3.9
1	B	56	SER	3.8
1	D	110	ASP	3.6
1	D	118	PHE	3.6
1	B	29	ALA	3.6
1	B	51	LEU	3.6
1	B	38	ILE	3.6
1	B	55	ILE	3.5
1	D	108	ILE	3.5
1	B	39	SER	3.5
1	B	54	GLU	3.4
1	D	109	LEU	3.4
1	D	121	PHE	3.2
1	C	53	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	53	PHE	3.2
1	D	20	LEU	3.1
1	D	126	PHE	3.1
1	B	149	GLN	3.0
1	D	16	LEU	3.0
1	B	16	LEU	2.9
1	B	63	PHE	2.9
1	D	71	ASN	2.8
1	D	117	SER	2.8
1	D	87	PHE	2.7
1	B	12	LEU	2.7
1	B	153	LEU	2.6
1	B	69	LEU	2.6
1	D	128	ILE	2.6
1	B	10	GLN	2.6
1	C	14	ALA	2.6
1	B	33	LYS	2.6
1	D	21	SER	2.5
1	D	107	ILE	2.5
1	B	61	PHE	2.5
1	C	23	ASN	2.4
1	B	152	LYS	2.2
1	D	28	LYS	2.2
1	D	35	LYS	2.2
1	B	155	THR	2.2
1	D	15	SER	2.1
1	B	13	ILE	2.1
1	B	45	THR	2.1
1	D	55	ILE	2.1
1	D	127	SER	2.0
1	B	36	LEU	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 carbohydrates 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(Å^2)	Q<0.9
2	MPD	C	201	8/8	0.87	0.31	96,97,102,103	0

6.5 Other polymers (i)

There are no such residues in this entry.