



Full wwPDB X-ray Structure Validation Report i

Apr 30, 2024 – 06:53 pm BST

PDB ID : 4D18
Title : Crystal structure of the COP9 signalosome
Authors : Bunker, R.D.; Lingaraju, G.M.; Thoma, N.H.
Deposited on : 2014-05-01
Resolution : 4.08 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 i 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](#) ①) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

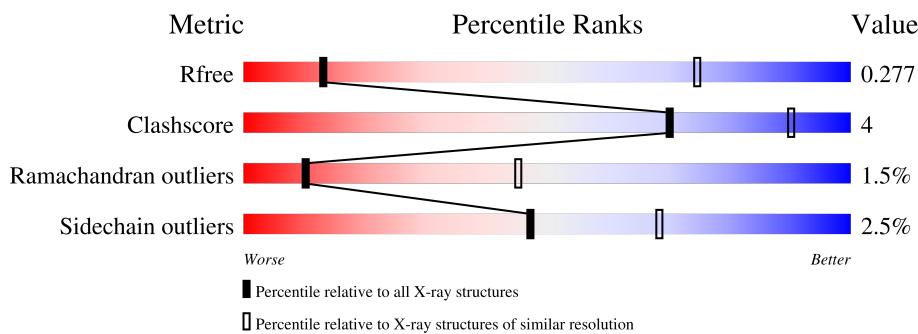
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

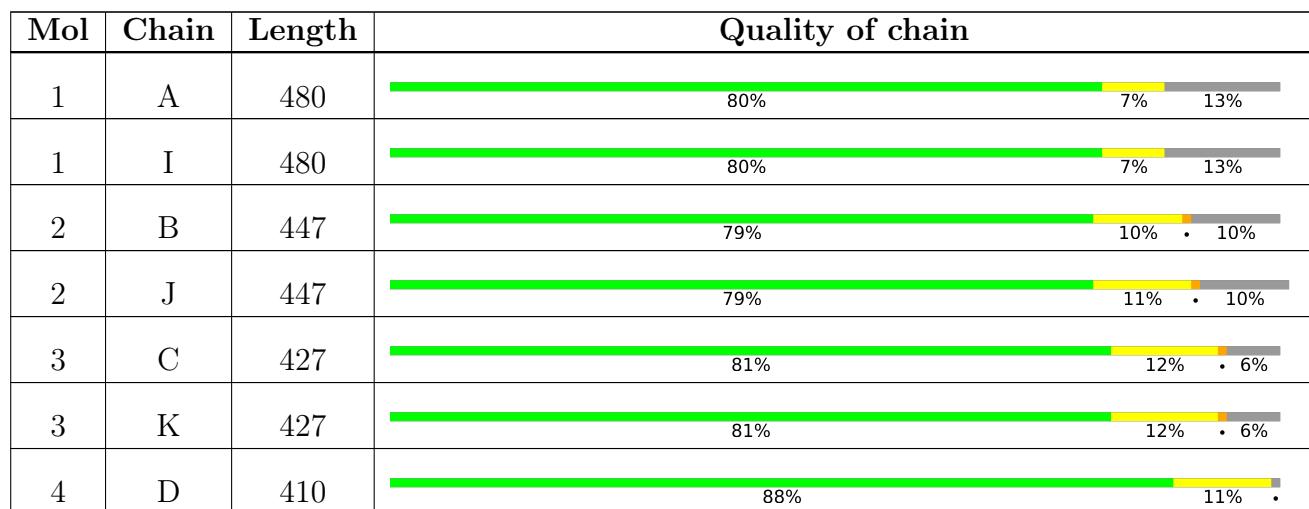
The reported resolution of this entry is 4.08 Å.

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.



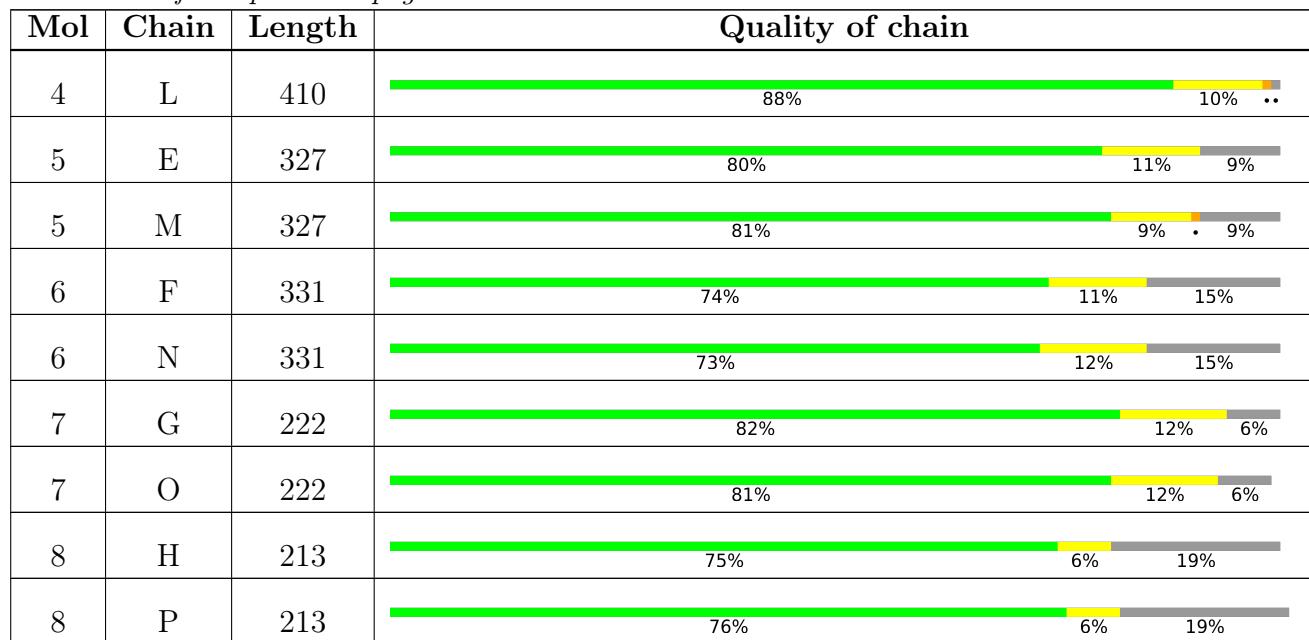
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (4.46-3.70)
Clashscore	141614	1013 (4.42-3.74)
Ramachandran outliers	138981	1151 (4.46-3.70)
Sidechain outliers	138945	1139 (4.46-3.70)

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 <=5%



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2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 41422 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 COP9 SIGNALOSOME COMPLEX SUBUNIT 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	419	3348	2113	588	625	22	0	0	0
1	I	419	3348	2113	588	625	22	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	GLY	-	expression tag	UNP Q13098
A	49	GLY	-	expression tag	UNP Q13098
A	50	GLY	-	expression tag	UNP Q13098
A	51	ARG	-	expression tag	UNP Q13098
I	48	GLY	-	expression tag	UNP Q13098
I	49	GLY	-	expression tag	UNP Q13098
I	50	GLY	-	expression tag	UNP Q13098
I	51	ARG	-	expression tag	UNP Q13098

- Molecule 2 is a protein called COP9 SIGNALOSOME COMPLEX SUBUNIT 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	403	3304	2102	566	621	15	0	0	0
2	J	403	3304	2102	566	621	15	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P61201
B	-2	GLY	-	expression tag	UNP P61201
B	-1	GLY	-	expression tag	UNP P61201
B	0	ARG	-	expression tag	UNP P61201

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-3	GLY	-	expression tag	UNP P61201
J	-2	GLY	-	expression tag	UNP P61201
J	-1	GLY	-	expression tag	UNP P61201
J	0	ARG	-	expression tag	UNP P61201

- Molecule 3 is a protein called COP9 SIGNALOSOME COMPLEX SUBUNIT 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	401	Total	C	N	O	S	0	0	0
			3191	2032	535	598	26			
3	K	401	Total	C	N	O	S	0	0	0
			3191	2032	535	598	26			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP Q9UNS2
C	-2	GLY	-	expression tag	UNP Q9UNS2
C	-1	GLY	-	expression tag	UNP Q9UNS2
C	0	ARG	-	expression tag	UNP Q9UNS2
K	-3	GLY	-	expression tag	UNP Q9UNS2
K	-2	GLY	-	expression tag	UNP Q9UNS2
K	-1	GLY	-	expression tag	UNP Q9UNS2
K	0	ARG	-	expression tag	UNP Q9UNS2

- Molecule 4 is a protein called COP9 SIGNALOSOME COMPLEX SUBUNIT 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	406	Total	C	N	O	S	0	0	0
			3251	2047	566	622	16			
4	L	406	Total	C	N	O	S	0	0	0
			3251	2047	566	622	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP Q9BT78
D	-2	GLY	-	expression tag	UNP Q9BT78
D	-1	GLY	-	expression tag	UNP Q9BT78
D	0	ARG	-	expression tag	UNP Q9BT78
L	-3	GLY	-	expression tag	UNP Q9BT78
L	-2	GLY	-	expression tag	UNP Q9BT78

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-1	GLY	-	expression tag	UNP Q9BT78
L	0	ARG	-	expression tag	UNP Q9BT78

- Molecule 5 is a protein called COP9 SIGNALOSOME COMPLEX SUBUNIT 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	298	Total	C 2366	N 1510	O 393	S 450	13	0	0
5	M	298	Total	C 2366	N 1510	O 393	S 450	13	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	8	GLY	-	expression tag	UNP Q92905
E	9	GLY	-	expression tag	UNP Q92905
E	10	GLY	-	expression tag	UNP Q92905
E	11	ARG	-	expression tag	UNP Q92905
M	8	GLY	-	expression tag	UNP Q92905
M	9	GLY	-	expression tag	UNP Q92905
M	10	GLY	-	expression tag	UNP Q92905
M	11	ARG	-	expression tag	UNP Q92905

- Molecule 6 is a protein called COP9 SIGNALOSOME COMPLEX SUBUNIT 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	281	Total	C 2236	N 1429	O 371	S 421	15	0	0
6	N	281	Total	C 2236	N 1429	O 371	S 421	15	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-3	GLY	-	expression tag	UNP Q7L5N1
F	-2	GLY	-	expression tag	UNP Q7L5N1
F	-1	GLY	-	expression tag	UNP Q7L5N1
F	0	ARG	-	expression tag	UNP Q7L5N1
N	-3	GLY	-	expression tag	UNP Q7L5N1
N	-2	GLY	-	expression tag	UNP Q7L5N1
N	-1	GLY	-	expression tag	UNP Q7L5N1
N	0	ARG	-	expression tag	UNP Q7L5N1

- Molecule 7 is a protein called COP9 SIGNALOSOME COMPLEX SUBUNIT 7A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	208	1631	1028	287	312	4	0	0	0
7	O	208	1631	1028	287	312	4	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	GLY	-	expression tag	UNP Q9UBW8
G	-2	GLY	-	expression tag	UNP Q9UBW8
G	-1	GLY	-	expression tag	UNP Q9UBW8
G	0	ARG	-	expression tag	UNP Q9UBW8
O	-3	GLY	-	expression tag	UNP Q9UBW8
O	-2	GLY	-	expression tag	UNP Q9UBW8
O	-1	GLY	-	expression tag	UNP Q9UBW8
O	0	ARG	-	expression tag	UNP Q9UBW8

- Molecule 8 is a protein called COP9 SIGNALOSOME COMPLEX SUBUNIT 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	173	1383	885	240	254	4	0	0	0
8	P	173	1383	885	240	254	4	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-3	GLY	-	expression tag	UNP Q99627
H	-2	GLY	-	expression tag	UNP Q99627
H	-1	GLY	-	expression tag	UNP Q99627
H	0	ARG	-	expression tag	UNP Q99627
P	-3	GLY	-	expression tag	UNP Q99627
P	-2	GLY	-	expression tag	UNP Q99627
P	-1	GLY	-	expression tag	UNP Q99627
P	0	ARG	-	expression tag	UNP Q99627

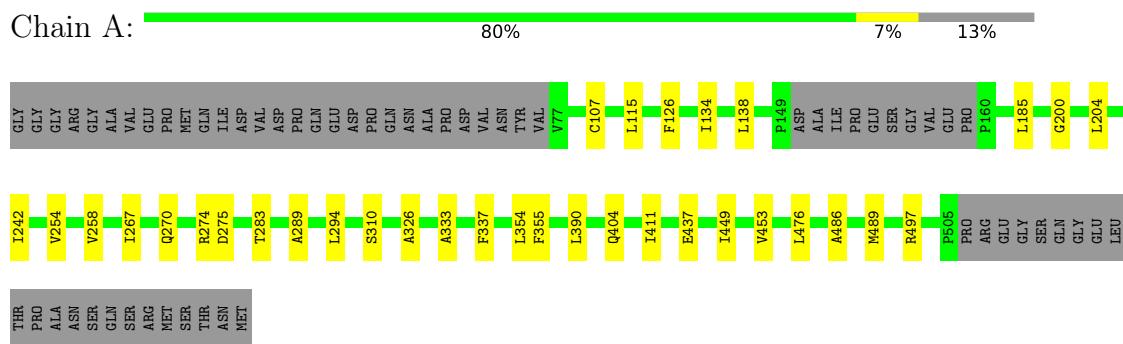
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	E	1	Total Zn 1 1	0	0
9	M	1	Total Zn 1 1	0	0

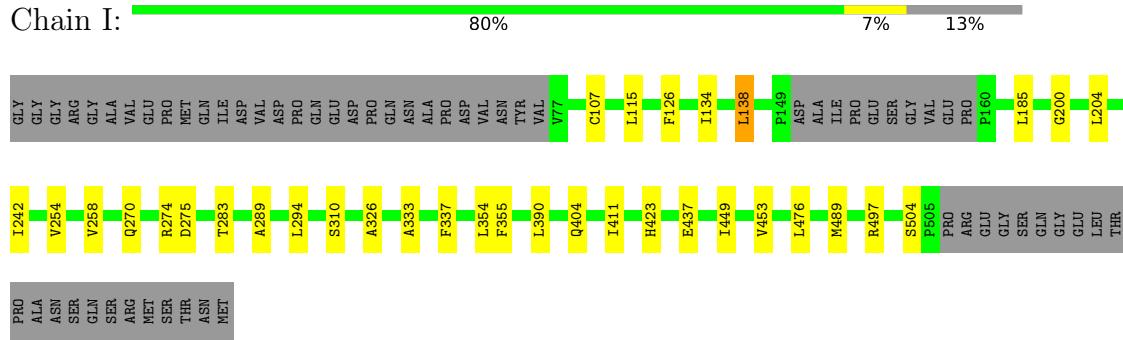
3 Residue-property plots

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. 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. 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.

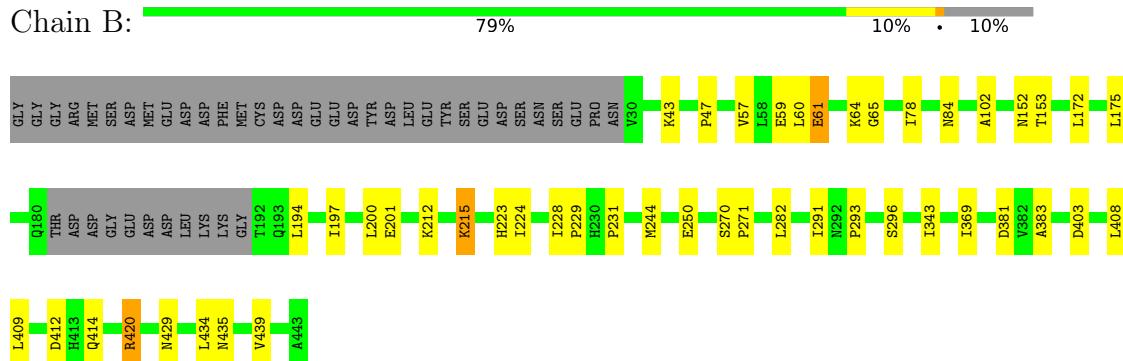
- Molecule 1: COP9 SIGNALOSOME COMPLEX SUBUNIT 1



- Molecule 1: COP9 SIGNALOSOME COMPLEX SUBUNIT 1

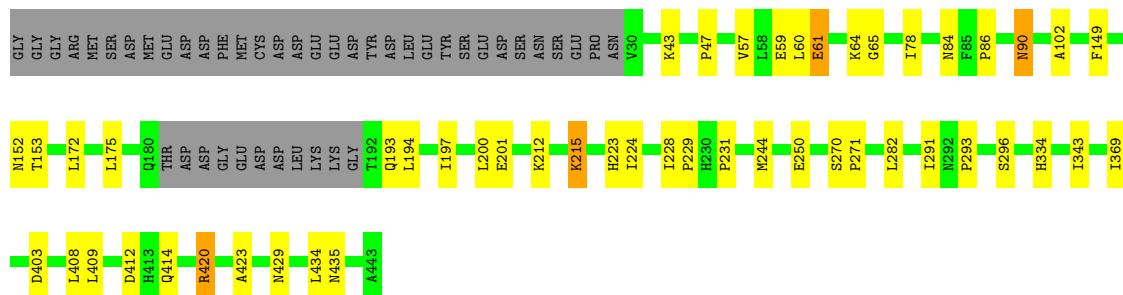


- Molecule 2: COP9 SIGNALOSOME COMPLEX SUBUNIT 2



- Molecule 2: COP9 SIGNALOSOME COMPLEX SUBUNIT 2

Chain J: 



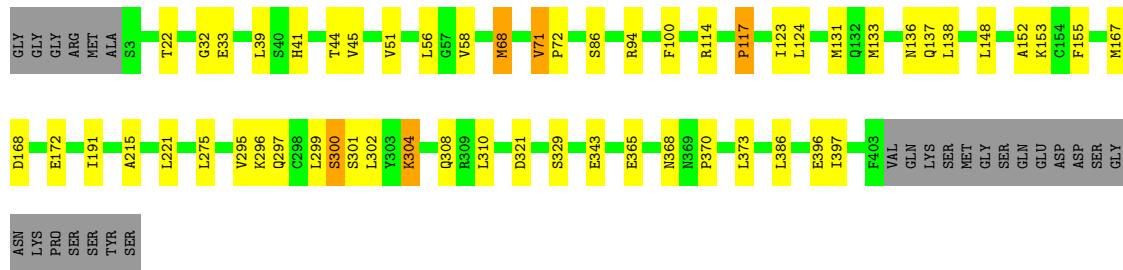
- Molecule 3: COP9 SIGNALOSOME COMPLEX SUBUNIT 3

Chain C: 



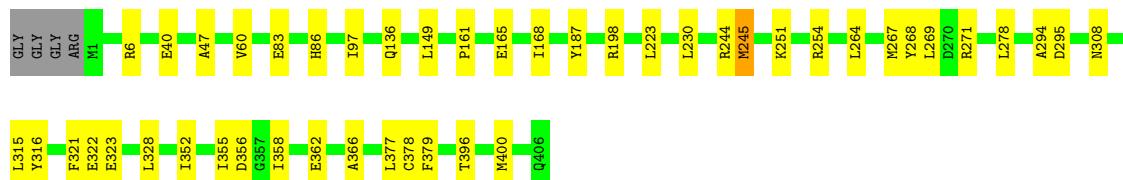
- Molecule 3: COP9 SIGNALOSOME COMPLEX SUBUNIT 3

Chain K: 



- Molecule 4: COP9 SIGNALOSOME COMPLEX SUBUNIT 4

Chain D: 



- Molecule 4: COP9 SIGNALOSOME COMPLEX SUBUNIT 4

Chain L: 

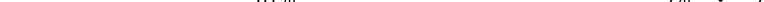


- A diagram showing a sequence of colored bars representing different components or stages. The colors are green, yellow, and red. The labels for each bar are: A294, D295, G296 (green); V304 (yellow); H307, N308 (green); L315, Y316 (yellow); L328 (green); T355 (yellow); E362 (green); A366 (yellow); L377, C378, F379 (green); T396 (yellow); M400 (green); Q406 (red).

- Molecule 5: COP9 SIGNALOSOME COMPLEX SUBUNIT 5

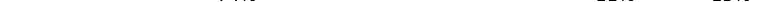


- Molecule 5: COP9 SIGNALOSOME COMPLEX SUBUNIT 5

Chain M:  81% 9% • 9%



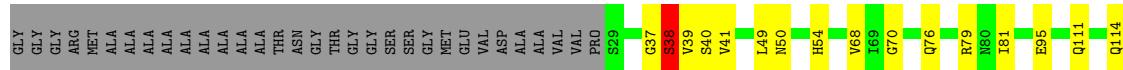
- Molecule 6: COP9 SIGNALOSOME COMPLEX SUBUNIT 6

Chain F:  74% 11% 15%

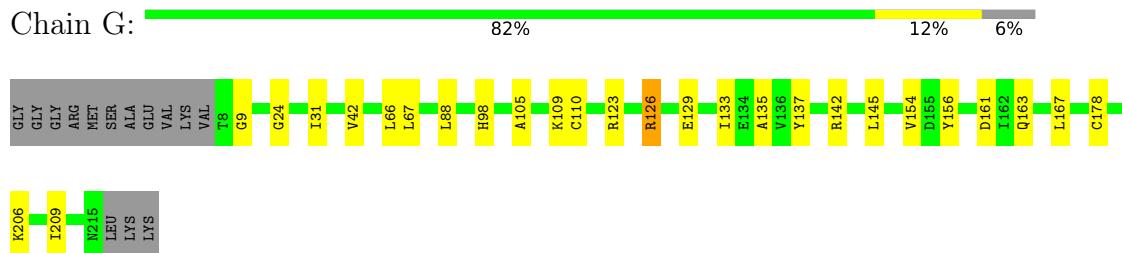


- Molecule 6: COP9 SIGNALOSOME COMPLEX SUBUNIT 6

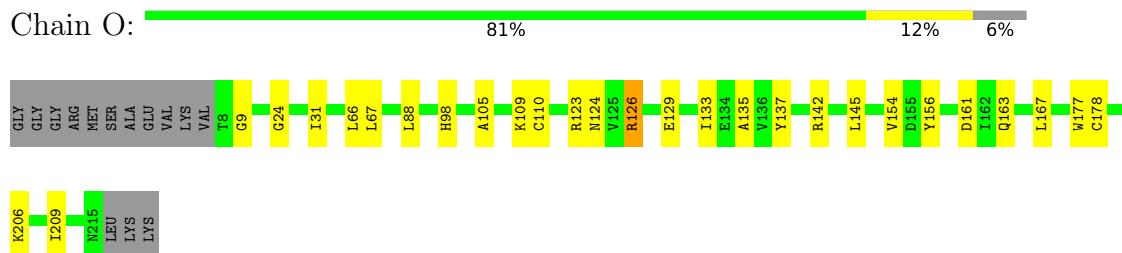
Chain N: 73% 12% 15%



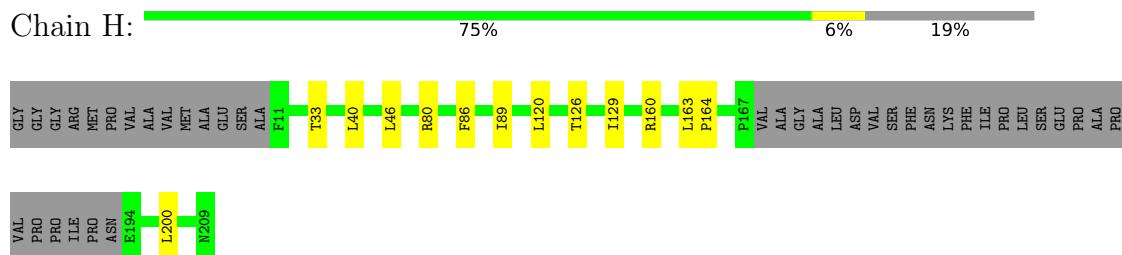
- Molecule 7: COP9 SIGNALOSOME COMPLEX SUBUNIT 7A



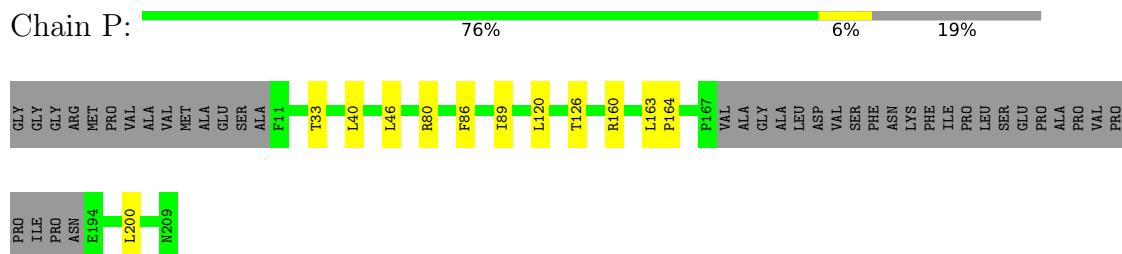
- Molecule 7: COP9 SIGNALOSOME COMPLEX SUBUNIT 7A



- Molecule 8: COP9 SIGNALOSOME COMPLEX SUBUNIT 8



- Molecule 8: COP9 SIGNALOSOME COMPLEX SUBUNIT 8



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	147.68Å 147.68Å 317.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	52.98 – 4.08 52.98 – 4.08	Depositor EDS
% Data completeness (in resolution range)	100.0 (52.98-4.08) 100.0 (52.98-4.08)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	1.30 (at 4.14Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R , R_{free}	0.236 , 0.253 0.263 , 0.277	Depositor DCC
R_{free} test set	3085 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	175.9	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 196.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.059 for -h,-k,l 0.115 for h,-h-k,-l 0.067 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	41422	wwPDB-VP
Average B, all atoms (Å ²)	213.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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 i

5.1 Standard geometry i

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

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	0.38	0/3404	0.48	0/4588
1	I	0.37	0/3404	0.48	0/4588
2	B	0.42	0/3361	0.51	0/4522
2	J	0.42	0/3361	0.51	0/4522
3	C	0.55	2/3250 (0.1%)	0.64	3/4390 (0.1%)
3	K	0.56	2/3250 (0.1%)	0.64	3/4390 (0.1%)
4	D	0.41	0/3303	0.52	0/4460
4	L	0.39	0/3303	0.53	0/4460
5	E	0.40	0/2417	0.54	0/3266
5	M	0.42	0/2417	0.54	0/3266
6	F	0.66	1/2282 (0.0%)	0.57	1/3092 (0.0%)
6	N	0.38	0/2281	0.57	2/3089 (0.1%)
7	G	0.37	0/1652	0.48	0/2239
7	O	0.38	0/1652	0.48	0/2239
8	H	0.39	0/1416	0.49	0/1924
8	P	0.39	0/1416	0.48	0/1924
All	All	0.44	5/42169 (0.0%)	0.54	9/56959 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	6
3	K	0	6
All	All	0	12

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	40	SER	C-N	26.22	1.94	1.34
3	K	301	SER	C-O	-5.74	1.12	1.23
3	C	301	SER	C-O	-5.72	1.12	1.23
3	C	297	GLN	C-O	-5.40	1.13	1.23
3	K	297	GLN	C-O	-5.38	1.13	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	40	SER	O-C-N	-7.22	111.15	122.70
3	K	304	LYS	CA-C-O	-5.30	108.97	120.10
3	C	304	LYS	CA-C-O	-5.30	108.98	120.10
3	K	301	SER	CA-C-O	-5.29	109.00	120.10
3	C	301	SER	CA-C-O	-5.26	109.05	120.10
6	N	37	GLY	C-N-CA	5.23	134.78	121.70
3	C	300	SER	CA-C-O	-5.07	109.47	120.10
3	K	300	SER	CA-C-O	-5.06	109.48	120.10
6	N	132	ASP	CB-CA-C	-5.04	100.33	110.40

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	295	VAL	Mainchain
3	C	296	LYS	Mainchain
3	C	300	SER	Mainchain
3	C	304	LYS	Mainchain
3	C	308	GLN	Mainchain
3	C	310	LEU	Mainchain
3	K	295	VAL	Mainchain
3	K	296	LYS	Mainchain
3	K	300	SER	Mainchain
3	K	304	LYS	Mainchain
3	K	308	GLN	Mainchain
3	K	310	LEU	Mainchain

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	3348	0	3385	22	0
1	I	3348	0	3385	26	0
2	B	3304	0	3351	25	0
2	J	3304	0	3351	35	0
3	C	3191	0	3208	26	0
3	K	3191	0	3208	21	0
4	D	3251	0	3253	31	0
4	L	3251	0	3253	39	0
5	E	2366	0	2340	29	0
5	M	2366	0	2340	31	0
6	F	2236	0	2226	29	0
6	N	2236	0	2226	33	0
7	G	1631	0	1654	18	0
7	O	1631	0	1654	24	0
8	H	1383	0	1366	7	0
8	P	1383	0	1366	5	0
9	E	1	0	0	0	0
9	M	1	0	0	0	0
All	All	41422	0	41566	297	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 (297) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:40:SER:C	6:F:41:VAL:N	1.94	1.21
1:A:200:GLY:O	1:A:204:LEU:HD13	1.63	0.98
1:I:200:GLY:O	1:I:204:LEU:HD13	1.64	0.98
5:M:70:ARG:NH2	5:M:257:THR:HG22	1.78	0.97
3:K:41:HIS:O	3:K:44:THR:HG22	1.63	0.96
3:C:41:HIS:O	3:C:44:THR:HG22	1.63	0.95
5:E:70:ARG:NH2	5:E:257:THR:HG22	1.83	0.94
5:M:173:THR:CG2	5:M:261:TYR:HB2	1.98	0.93
4:D:83:GLU:HG3	2:J:90:ASN:HB2	1.53	0.91
1:I:354:LEU:CD2	2:J:212:LYS:HB3	2.01	0.89
2:J:420:ARG:HD3	5:M:263:THR:HG22	1.58	0.86
5:E:173:THR:CG2	5:E:261:TYR:HB2	2.05	0.85
4:L:161:PRO:HB3	4:L:197:TYR:HB3	1.59	0.84
4:L:165:GLU:HA	4:L:194:VAL:HG11	1.61	0.83
4:D:254:ARG:HG2	6:F:174:ILE:HD11	1.61	0.81
5:M:173:THR:HG21	5:M:261:TYR:HB2	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:96:PHE:CD1	5:M:120:TYR:CE2	2.68	0.80
5:E:70:ARG:HH21	5:E:257:THR:HG22	1.44	0.80
5:E:96:PHE:CD1	5:E:120:TYR:CE2	2.70	0.79
6:N:40:SER:HA	6:N:41:VAL:N	1.99	0.78
1:I:275:ASP:HB3	2:J:223:HIS:CE1	2.19	0.76
2:B:420:ARG:HD3	5:E:263:THR:HG22	1.68	0.76
1:I:354:LEU:HD21	2:J:212:LYS:HB3	1.67	0.75
5:M:70:ARG:HH21	5:M:257:THR:HG22	1.49	0.74
1:A:275:ASP:HB3	2:B:223:HIS:CE1	2.22	0.74
4:L:178:SER:HB3	4:L:184:GLN:HE21	1.51	0.74
7:G:126:ARG:NH2	7:G:129:GLU:HB3	2.02	0.73
7:O:126:ARG:NH2	7:O:129:GLU:HB3	2.03	0.72
8:H:129:ILE:HD11	7:O:123:ARG:CZ	2.20	0.71
1:I:200:GLY:O	1:I:204:LEU:CD1	2.38	0.71
1:A:200:GLY:O	1:A:204:LEU:CD1	2.38	0.71
5:E:173:THR:HG21	5:E:261:TYR:HB2	1.74	0.69
4:L:180:ASN:O	4:L:184:GLN:HG3	1.92	0.69
1:A:354:LEU:HD21	2:B:212:LYS:HB3	1.74	0.69
3:C:353:GLN:HB3	7:O:123:ARG:HH12	1.58	0.69
1:A:185:LEU:HD22	1:A:204:LEU:HD21	1.74	0.68
1:I:185:LEU:HD22	1:I:204:LEU:HD21	1.74	0.68
4:D:315:LEU:HD13	7:G:133:ILE:HG12	1.76	0.68
3:C:353:GLN:HB3	7:O:123:ARG:HH22	1.59	0.67
4:L:268:TYR:OH	6:N:38:SER:HA	1.95	0.67
6:N:40:SER:CA	6:N:41:VAL:N	2.58	0.66
2:B:153:THR:HG23	2:B:200:LEU:HD11	1.79	0.65
6:F:116:PHE:HB3	6:F:119:LEU:HD13	1.79	0.65
4:D:268:TYR:OH	6:F:38:SER:HA	1.97	0.64
1:I:354:LEU:HD23	2:J:212:LYS:HB3	1.79	0.64
4:D:321:PHE:HZ	4:D:352:ILE:HG23	1.63	0.64
4:L:254:ARG:HG2	6:N:174:ILE:HD11	1.80	0.63
6:N:116:PHE:HB3	6:N:119:LEU:HD13	1.79	0.63
7:G:126:ARG:NH2	7:G:129:GLU:CB	2.61	0.63
2:J:153:THR:HG23	2:J:200:LEU:HD11	1.79	0.62
2:B:383:ALA:HB2	4:L:296:GLY:HA3	1.81	0.62
7:O:126:ARG:NH2	7:O:129:GLU:CB	2.62	0.62
8:H:126:THR:O	8:H:164:PRO:HD2	2.00	0.62
2:B:420:ARG:CD	5:E:263:THR:HG22	2.30	0.62
8:P:126:THR:O	8:P:164:PRO:HD2	2.00	0.62
3:C:117:PRO:HD2	3:C:152:ALA:HB2	1.81	0.61
3:K:117:PRO:HD2	3:K:152:ALA:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:HB3	1:A:138:LEU:HG	1.82	0.61
3:K:44:THR:HG23	3:K:45:VAL:HG23	1.83	0.61
1:A:275:ASP:HB3	2:B:223:HIS:HE1	1.65	0.60
6:F:39:VAL:HG11	6:F:81:ILE:HD11	1.82	0.60
3:C:397:ILE:CG2	6:F:312:LEU:HD23	2.30	0.60
6:F:39:VAL:HG11	6:F:81:ILE:CD1	2.31	0.60
5:M:173:THR:HG22	5:M:261:TYR:HB2	1.82	0.59
4:D:83:GLU:HG3	2:J:90:ASN:CB	2.29	0.59
3:C:44:THR:HG23	3:C:45:VAL:HG23	1.84	0.59
4:L:269:LEU:HD13	4:L:271:ARG:HH21	1.67	0.59
4:D:251:LYS:O	6:F:171:VAL:HG13	2.03	0.59
5:M:63:LEU:HD22	6:N:49:LEU:HD12	1.83	0.59
2:J:270:SER:HB2	2:J:271:PRO:HA	1.85	0.58
2:J:420:ARG:CD	5:M:263:THR:HG22	2.33	0.58
2:B:270:SER:HB2	2:B:271:PRO:HA	1.84	0.57
4:L:244:ARG:HG2	6:N:76:GLN:HE22	1.69	0.57
4:L:251:LYS:O	6:N:171:VAL:HG13	2.05	0.56
4:L:245:MET:HG2	6:N:147:GLU:HG2	1.88	0.56
3:C:343:GLU:HG3	8:H:120:LEU:HD13	1.88	0.56
4:L:70:CYS:HA	4:L:73:LEU:HD12	1.88	0.56
4:D:245:MET:HG2	6:F:147:GLU:HG2	1.86	0.56
1:I:115:LEU:HB3	1:I:138:LEU:HG	1.87	0.56
1:I:275:ASP:HB3	2:J:223:HIS:HE1	1.67	0.56
4:L:271:ARG:HD2	7:O:137:TYR:CD2	2.40	0.56
4:L:308:ASN:HB3	4:L:328:LEU:HD22	1.87	0.56
6:N:40:SER:C	6:N:41:VAL:N	2.59	0.56
4:L:165:GLU:CA	4:L:194:VAL:HG11	2.35	0.55
4:L:168:ILE:HG12	4:L:191:TYR:HA	1.89	0.55
3:C:275:LEU:HD23	3:C:299:LEU:HD12	1.87	0.55
3:K:275:LEU:HD23	3:K:299:LEU:HD12	1.87	0.55
5:M:96:PHE:CE1	5:M:120:TYR:CE2	2.95	0.55
4:D:295:ASP:HB3	2:J:334:HIS:CE1	2.42	0.55
2:J:215:LYS:HE3	2:J:244:MET:SD	2.48	0.55
4:L:315:LEU:HD13	7:O:133:ILE:HG12	1.87	0.54
3:K:71:VAL:HB	3:K:72:PRO:CD	2.37	0.54
3:C:71:VAL:HB	3:C:72:PRO:CD	2.37	0.54
6:F:39:VAL:HG21	6:F:81:ILE:HD12	1.89	0.54
4:D:379:PHE:CZ	6:F:189:THR:HB	2.43	0.54
1:A:486:ALA:HB1	3:C:386:LEU:HD21	1.88	0.54
4:L:180:ASN:O	4:L:184:GLN:CG	2.56	0.54
4:D:308:ASN:HB3	4:D:328:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:70:ARG:HH21	5:M:257:THR:CG2	2.17	0.53
3:K:343:GLU:HG3	8:P:120:LEU:HD13	1.90	0.53
3:K:397:ILE:CG2	6:N:312:LEU:HD23	2.38	0.53
2:B:215:LYS:HE3	2:B:244:MET:SD	2.49	0.53
5:E:96:PHE:CE1	5:E:120:TYR:CE2	2.97	0.53
4:L:178:SER:CB	4:L:184:GLN:HE21	2.19	0.53
2:B:194:LEU:HA	2:B:197:ILE:HD12	1.91	0.53
7:G:123:ARG:HD3	1:I:423:HIS:CG	2.44	0.52
3:C:397:ILE:HG23	6:F:312:LEU:HD23	1.90	0.52
7:G:123:ARG:HH11	1:I:423:HIS:HB2	1.74	0.52
4:D:230:LEU:HD11	4:D:264:LEU:HB2	1.92	0.52
1:A:486:ALA:CB	3:C:386:LEU:HD21	2.40	0.51
2:B:47:PRO:HB3	2:B:78:ILE:HG21	1.92	0.51
1:I:107:CYS:HB2	1:I:390:LEU:HD22	1.92	0.51
5:M:315:ILE:HG23	8:P:200:LEU:HD22	1.93	0.51
5:E:173:THR:HG22	5:E:261:TYR:HB2	1.89	0.51
4:L:278:LEU:CD2	4:L:304:VAL:HG21	2.41	0.51
4:L:378:CYS:HB3	5:M:247:VAL:HG22	1.92	0.51
2:B:282:LEU:HD13	2:B:343:ILE:HG23	1.91	0.51
2:J:47:PRO:HB3	2:J:78:ILE:HG21	1.92	0.51
4:L:187:TYR:CD1	4:L:188:LYS:N	2.78	0.51
3:C:353:GLN:HB3	7:O:123:ARG:NH1	2.26	0.51
1:A:107:CYS:HB2	1:A:390:LEU:HD22	1.93	0.51
4:D:378:CYS:HB3	5:E:247:VAL:HG22	1.92	0.51
1:I:200:GLY:C	1:I:204:LEU:HD13	2.31	0.51
4:L:379:PHE:CZ	6:N:189:THR:HB	2.46	0.51
2:J:282:LEU:HD13	2:J:343:ILE:HG23	1.92	0.51
1:A:326:ALA:HB2	1:A:355:PHE:HB3	1.93	0.50
4:D:295:ASP:HA	2:J:334:HIS:CE1	2.46	0.50
5:E:249:THR:HG23	6:F:197:ARG:NH1	2.25	0.50
1:A:200:GLY:C	1:A:204:LEU:HD13	2.31	0.50
1:A:489:MET:HB3	2:B:439:VAL:HG13	1.94	0.50
2:J:194:LEU:HA	2:J:197:ILE:HD12	1.93	0.50
6:N:39:VAL:HG11	6:N:81:ILE:CD1	2.40	0.50
2:B:434:LEU:HD21	5:E:300:LEU:HD11	1.93	0.50
3:C:353:GLN:HB3	7:O:123:ARG:NH2	2.27	0.50
3:K:397:ILE:HG23	6:N:312:LEU:HD23	1.93	0.50
3:C:354:LYS:O	7:O:124:ASN:HB3	2.10	0.50
4:L:222:ARG:NH2	6:N:179:ALA:HB3	2.26	0.50
5:M:60:LEU:HD11	6:N:50:ASN:OD1	2.11	0.50
5:M:120:TYR:N	6:N:111:GLN:HE22	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:161:PRO:CB	4:L:197:TYR:HB3	2.38	0.50
1:I:326:ALA:HB2	1:I:355:PHE:HB3	1.93	0.49
2:B:420:ARG:HD3	5:E:263:THR:CG2	2.41	0.49
4:D:316:TYR:CD1	7:G:145:LEU:HB2	2.47	0.49
5:M:173:THR:HG22	5:M:261:TYR:CB	2.41	0.49
1:I:504:SER:HA	3:K:215:ALA:HB2	1.95	0.49
5:E:60:LEU:HD11	6:F:50:ASN:OD1	2.13	0.49
1:I:497:ARG:HG3	6:N:313:TYR:CE1	2.48	0.49
5:M:318:LEU:HD23	8:P:200:LEU:HD21	1.94	0.49
7:O:105:ALA:HB1	7:O:154:VAL:HG11	1.94	0.49
3:C:117:PRO:HB2	3:C:148:LEU:HD22	1.95	0.49
7:G:105:ALA:HB1	7:G:154:VAL:HG11	1.93	0.49
5:E:245:TYR:HD1	6:F:190:LEU:HD13	1.77	0.49
2:B:64:LYS:HB3	2:B:65:GLY:HA2	1.95	0.48
3:K:117:PRO:HB2	3:K:148:LEU:HD22	1.95	0.48
4:L:230:LEU:HD11	4:L:264:LEU:HB2	1.95	0.48
4:L:278:LEU:HD21	4:L:304:VAL:HG21	1.94	0.48
2:J:64:LYS:HB3	2:J:65:GLY:HA2	1.96	0.48
3:K:368:ASN:O	6:N:280:TYR:HB3	2.13	0.48
8:H:86:PHE:HA	8:H:89:ILE:HD12	1.95	0.48
7:O:66:LEU:HD21	7:O:88:LEU:HD21	1.96	0.48
5:M:207:PRO:HA	5:M:268:ASP:OD2	2.13	0.47
2:B:172:LEU:HD22	2:B:201:GLU:HG3	1.96	0.47
4:L:267:MET:HA	4:L:307:HIS:CE1	2.48	0.47
4:D:244:ARG:HB3	6:F:147:GLU:HB2	1.97	0.47
6:N:267:LEU:HD11	7:O:177:TRP:CE3	2.49	0.47
4:D:271:ARG:HD2	7:G:137:TYR:CD2	2.50	0.47
5:E:327:LEU:HD11	6:F:228:ILE:HG12	1.95	0.47
2:J:172:LEU:HD22	2:J:201:GLU:HG3	1.96	0.47
2:J:420:ARG:HD3	5:M:263:THR:CG2	2.39	0.47
2:B:408:LEU:HD22	4:D:355:ILE:HG12	1.96	0.47
2:B:403:ASP:HB3	2:B:408:LEU:HG	1.96	0.47
3:C:353:GLN:CB	7:O:123:ARG:HH12	2.27	0.47
4:D:295:ASP:HA	2:J:334:HIS:HE1	1.80	0.47
1:I:437:GLU:HG3	1:I:453:VAL:HG11	1.96	0.47
5:M:245:TYR:HD1	6:N:190:LEU:HD13	1.79	0.47
2:B:59:GLU:C	2:B:61:GLU:H	2.19	0.47
4:D:6:ARG:HG2	4:D:47:ALA:HB1	1.97	0.46
4:D:295:ASP:CB	2:J:334:HIS:CE1	2.98	0.46
1:I:411:ILE:HA	1:I:449:ILE:HD11	1.97	0.46
8:H:129:ILE:CG1	7:O:123:ARG:NH2	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:86:PHE:HA	8:P:89:ILE:HD12	1.96	0.46
4:D:161:PRO:HB2	4:D:198:ARG:HG2	1.97	0.46
7:G:66:LEU:HD21	7:G:88:LEU:HD21	1.96	0.46
1:A:437:GLU:HG3	1:A:453:VAL:HG11	1.96	0.46
1:I:283:THR:HG22	1:I:310:SER:H	1.80	0.46
2:J:403:ASP:HB3	2:J:408:LEU:HG	1.97	0.46
1:A:185:LEU:HD22	1:A:204:LEU:CD2	2.44	0.46
1:A:411:ILE:HA	1:A:449:ILE:HD11	1.98	0.46
5:E:70:ARG:HH21	5:E:257:THR:CG2	2.23	0.46
2:B:175:LEU:HB3	2:B:197:ILE:HG12	1.98	0.45
4:D:271:ARG:HD2	7:G:137:TYR:CG	2.51	0.45
7:G:126:ARG:HH22	7:G:129:GLU:HB3	1.76	0.45
3:C:39:LEU:HD22	3:C:58:VAL:HG22	1.98	0.45
5:M:253:SER:HA	5:M:321:GLN:HE22	1.81	0.45
4:D:86:HIS:NE2	2:J:86:PRO:HG2	2.32	0.45
3:K:370:PRO:O	3:K:373:LEU:HB3	2.17	0.45
1:A:283:THR:HG22	1:A:310:SER:H	1.81	0.45
4:D:295:ASP:CB	2:J:334:HIS:HE1	2.30	0.45
1:I:185:LEU:HD22	1:I:204:LEU:CD2	2.45	0.45
3:K:39:LEU:HD22	3:K:58:VAL:HG22	1.98	0.45
3:C:370:PRO:O	3:C:373:LEU:HB3	2.16	0.45
2:J:175:LEU:HB3	2:J:197:ILE:HG12	1.99	0.45
7:O:126:ARG:HH22	7:O:129:GLU:HB3	1.77	0.45
1:A:134:ILE:HG22	1:A:138:LEU:HD12	1.98	0.45
1:A:497:ARG:HG3	6:F:313:TYR:CE1	2.52	0.44
5:E:253:SER:HA	5:E:321:GLN:HE22	1.82	0.44
2:J:59:GLU:C	2:J:61:GLU:H	2.21	0.44
3:K:68:MET:HB3	3:K:71:VAL:H	1.81	0.44
4:D:165:GLU:HA	4:D:168:ILE:HG22	1.99	0.44
5:E:233:LEU:HD22	6:F:55:TRP:CE3	2.52	0.44
1:I:258:VAL:HG11	1:I:289:ALA:HB2	1.99	0.44
4:L:187:TYR:HE1	4:L:188:LYS:HD3	1.82	0.44
6:F:38:SER:OG	6:F:39:VAL:HG13	2.17	0.44
5:M:116:TYR:HE2	6:N:114:GLN:HG3	1.83	0.44
3:K:94:ARG:HH22	3:K:137:GLN:HE22	1.64	0.44
3:C:68:MET:HB3	3:C:71:VAL:H	1.81	0.44
3:C:94:ARG:HH22	3:C:137:GLN:HE22	1.64	0.44
4:D:378:CYS:HB2	5:E:247:VAL:HG13	1.98	0.44
5:M:173:THR:HG22	5:M:261:TYR:CG	2.52	0.44
5:M:269:LEU:HD21	5:M:307:SER:HB3	2.00	0.44
4:L:316:TYR:CD1	7:O:145:LEU:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:155:PHE:HB3	3:K:191:ILE:HG23	2.00	0.44
3:C:155:PHE:HB3	3:C:191:ILE:HG23	2.00	0.44
4:D:269:LEU:HD13	4:D:271:ARG:HH21	1.81	0.43
5:E:248:ASN:OD1	6:F:192:THR:HG22	2.18	0.43
6:F:54:HIS:CE1	6:F:68:VAL:HB	2.53	0.43
5:M:248:ASN:OD1	6:N:192:THR:HG22	2.18	0.43
6:N:54:HIS:CE1	6:N:68:VAL:HB	2.53	0.43
2:J:434:LEU:HD23	6:N:299:CYS:SG	2.58	0.43
2:J:57:VAL:HA	2:J:60:LEU:HD12	1.99	0.43
5:E:318:LEU:HD11	6:F:283:CYS:SG	2.58	0.43
5:M:62:LEU:HD11	5:M:181:VAL:HG11	2.01	0.43
2:B:57:VAL:HA	2:B:60:LEU:HD12	2.00	0.43
1:A:258:VAL:HG11	1:A:289:ALA:HB2	2.00	0.43
2:J:149:PHE:CZ	2:J:193:GLN:HB2	2.53	0.43
2:B:152:ASN:HB3	2:B:175:LEU:HD21	2.00	0.43
5:E:318:LEU:HD23	8:H:200:LEU:HD21	2.01	0.43
7:G:142:ARG:HB2	7:G:156:TYR:HB3	2.00	0.43
4:L:244:ARG:HB3	6:N:147:GLU:HB2	2.01	0.43
7:O:126:ARG:NH2	7:O:129:GLU:HB2	2.34	0.43
7:O:142:ARG:HB2	7:O:156:TYR:HB3	2.00	0.43
2:J:152:ASN:HB3	2:J:175:LEU:HD21	2.01	0.43
4:D:356:ASP:HB3	4:D:358:ILE:HD12	2.00	0.42
5:E:173:THR:HG22	5:E:261:TYR:CG	2.53	0.42
7:O:31:ILE:HG23	7:O:67:LEU:HD13	2.01	0.42
5:E:173:THR:HG22	5:E:261:TYR:CB	2.49	0.42
3:K:386:LEU:HD23	6:N:298:THR:HG21	2.00	0.42
7:O:206:LYS:HA	7:O:209:ILE:HD12	2.01	0.42
7:G:126:ARG:NH2	7:G:129:GLU:HB2	2.35	0.42
5:E:62:LEU:HD11	5:E:181:VAL:HG11	2.02	0.42
1:I:134:ILE:HG22	1:I:138:LEU:HD12	2.01	0.42
5:M:96:PHE:CE1	5:M:120:TYR:CD2	3.08	0.42
3:K:56:LEU:HD11	3:K:100:PHE:HA	2.02	0.42
5:M:176:ILE:HG23	6:N:194:GLU:HG2	2.01	0.42
7:G:123:ARG:HD3	1:I:423:HIS:CD2	2.55	0.42
1:I:333:ALA:O	1:I:337:PHE:HB2	2.20	0.42
2:J:408:LEU:HD22	4:L:355:ILE:HG12	2.01	0.42
1:A:333:ALA:O	1:A:337:PHE:HB2	2.20	0.42
6:F:70:GLY:HA3	6:F:125:TYR:CE2	2.54	0.42
3:C:370:PRO:O	3:C:373:LEU:N	2.53	0.42
7:G:206:LYS:HA	7:G:209:ILE:HD12	2.01	0.42
4:L:33:ALA:HA	4:L:36:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:369:ILE:HG23	2:B:409:LEU:HB3	2.02	0.41
3:C:56:LEU:HD11	3:C:100:PHE:HA	2.02	0.41
4:D:396:THR:O	4:D:400:MET:HB2	2.20	0.41
6:F:258:ARG:HD2	7:G:42:VAL:HG21	2.02	0.41
6:N:70:GLY:HA3	6:N:125:TYR:CE2	2.54	0.41
7:G:31:ILE:HG23	7:G:67:LEU:HD13	2.00	0.41
2:J:369:ILE:HG23	2:J:409:LEU:HB3	2.02	0.41
5:M:173:THR:CG2	5:M:261:TYR:CB	2.83	0.41
3:K:370:PRO:O	3:K:373:LEU:N	2.53	0.41
4:L:378:CYS:HB2	5:M:247:VAL:HG13	2.01	0.41
2:B:381:ASP:OD2	4:L:294:ALA:O	2.39	0.41
8:H:129:ILE:HG13	7:O:123:ARG:NH2	2.35	0.41
3:K:275:LEU:HD22	3:K:302:LEU:HD22	2.02	0.41
3:C:39:LEU:HB3	3:C:58:VAL:HG13	2.02	0.41
3:C:275:LEU:HD22	3:C:302:LEU:HD22	2.02	0.41
4:D:321:PHE:CZ	4:D:352:ILE:HG23	2.51	0.41
7:G:98:HIS:HD2	7:G:135:ALA:HB2	1.86	0.41
3:K:39:LEU:HB3	3:K:58:VAL:HG13	2.02	0.41
7:O:98:HIS:HD2	7:O:135:ALA:HB2	1.86	0.41
5:E:240:LEU:HD13	6:F:164:PRO:HD3	2.03	0.41
1:I:242:ILE:HG23	1:I:254:VAL:HG13	2.02	0.41
4:L:222:ARG:HH22	6:N:179:ALA:HB3	1.86	0.41
4:L:396:THR:O	4:L:400:MET:HB2	2.21	0.41
6:N:254:HIS:O	6:N:258:ARG:HB2	2.21	0.41
4:L:153:ARG:NH2	4:L:186:HIS:HB3	2.36	0.40
6:N:38:SER:HB2	6:N:169:GLU:OE1	2.21	0.40
1:A:242:ILE:HG23	1:A:254:VAL:HG13	2.02	0.40
6:F:132:ASP:HB2	6:F:133:PRO:CD	2.51	0.40
6:F:254:HIS:O	6:F:258:ARG:HB2	2.22	0.40
2:J:423:ALA:HB2	5:M:267:PHE:CE2	2.56	0.40
6:N:39:VAL:HA	6:N:79:ARG:O	2.21	0.40
5:E:140:HIS:CG	5:E:143:TYR:CE1	3.10	0.40
5:E:318:LEU:HD11	6:F:283:CYS:HA	2.03	0.40
1:I:275:ASP:HB3	2:J:223:HIS:ND1	2.35	0.40
4:L:377:LEU:HD21	7:O:177:TRP:CH2	2.56	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	415/480 (86%)	395 (95%)	16 (4%)	4 (1%)	15 52
1	I	415/480 (86%)	395 (95%)	17 (4%)	3 (1%)	22 61
2	B	399/447 (89%)	365 (92%)	24 (6%)	10 (2%)	5 35
2	J	399/447 (89%)	365 (92%)	24 (6%)	10 (2%)	5 35
3	C	399/427 (93%)	360 (90%)	26 (6%)	13 (3%)	4 30
3	K	399/427 (93%)	360 (90%)	25 (6%)	14 (4%)	3 29
4	D	404/410 (98%)	399 (99%)	2 (0%)	3 (1%)	22 61
4	L	404/410 (98%)	400 (99%)	1 (0%)	3 (1%)	22 61
5	E	294/327 (90%)	283 (96%)	8 (3%)	3 (1%)	15 52
5	M	294/327 (90%)	283 (96%)	9 (3%)	2 (1%)	22 61
6	F	277/331 (84%)	267 (96%)	8 (3%)	2 (1%)	22 61
6	N	275/331 (83%)	264 (96%)	8 (3%)	3 (1%)	14 51
7	G	206/222 (93%)	195 (95%)	8 (4%)	3 (2%)	10 45
7	O	206/222 (93%)	195 (95%)	8 (4%)	3 (2%)	10 45
8	H	169/213 (79%)	162 (96%)	7 (4%)	0	100 100
8	P	169/213 (79%)	162 (96%)	7 (4%)	0	100 100
All	All	5124/5714 (90%)	4850 (95%)	198 (4%)	76 (2%)	10 45

All (76) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	51	VAL
3	C	68	MET
3	C	153	LYS
4	D	294	ALA
5	E	297	GLU
3	K	51	VAL

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Mol	Chain	Res	Type
3	K	68	MET
3	K	153	LYS
4	L	294	ALA
5	M	297	GLU
6	N	38	SER
1	A	274	ARG
2	B	61	GLU
2	B	414	GLN
3	C	86	SER
3	C	172	GLU
7	G	24	GLY
2	J	61	GLU
2	J	414	GLN
3	K	86	SER
3	K	172	GLU
7	O	24	GLY
2	B	43	LYS
2	B	84	ASN
3	C	33	GLU
3	C	71	VAL
3	C	114	ARG
4	D	362	GLU
4	D	366	ALA
6	F	95	GLU
1	I	274	ARG
2	J	43	LYS
2	J	84	ASN
3	K	33	GLU
3	K	71	VAL
3	K	114	ARG
4	L	362	GLU
4	L	366	ALA
6	N	95	GLU
1	A	126	PHE
1	A	270	GLN
3	C	168	ASP
6	F	270	LEU
7	G	9	GLY
1	I	126	PHE
1	I	270	GLN
3	K	117	PRO
3	K	168	ASP

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Mol	Chain	Res	Type
6	N	270	LEU
7	O	9	GLY
2	B	229	PRO
2	B	291	ILE
2	B	296	SER
3	C	117	PRO
3	C	133	MET
3	C	329	SER
5	E	199	GLY
5	E	201	SER
2	J	229	PRO
2	J	291	ILE
2	J	296	SER
3	K	133	MET
3	K	329	SER
5	M	201	SER
7	O	163	GLN
2	B	102	ALA
3	C	32	GLY
7	G	163	GLN
2	J	102	ALA
3	K	32	GLY
3	K	136	ASN
2	B	231	PRO
2	B	293	PRO
2	J	231	PRO
1	A	267	ILE
2	J	293	PRO

5.3.2 Protein sidechains [\(i\)](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	365/415 (88%)	362 (99%)	3 (1%)	81 89
1	I	365/415 (88%)	360 (99%)	5 (1%)	67 80
2	B	367/406 (90%)	359 (98%)	8 (2%)	52 71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	367/406 (90%)	358 (98%)	9 (2%)	47	68
3	C	358/378 (95%)	347 (97%)	11 (3%)	40	63
3	K	358/378 (95%)	348 (97%)	10 (3%)	43	65
4	D	347/348 (100%)	334 (96%)	13 (4%)	34	60
4	L	347/348 (100%)	342 (99%)	5 (1%)	67	80
5	E	255/278 (92%)	246 (96%)	9 (4%)	36	61
5	M	255/278 (92%)	247 (97%)	8 (3%)	40	63
6	F	251/277 (91%)	245 (98%)	6 (2%)	49	69
6	N	251/277 (91%)	247 (98%)	4 (2%)	62	79
7	G	174/184 (95%)	168 (97%)	6 (3%)	37	61
7	O	174/184 (95%)	168 (97%)	6 (3%)	37	61
8	H	144/174 (83%)	138 (96%)	6 (4%)	30	56
8	P	144/174 (83%)	138 (96%)	6 (4%)	30	56
All	All	4522/4920 (92%)	4407 (98%)	115 (2%)	47	68

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	294	LEU
1	A	404	GLN
1	A	476	LEU
2	B	215	LYS
2	B	224	ILE
2	B	228	ILE
2	B	250	GLU
2	B	412	ASP
2	B	420	ARG
2	B	429	ASN
2	B	435	ASN
3	C	22	THR
3	C	123	ILE
3	C	124	LEU
3	C	131	MET
3	C	138	LEU
3	C	167	MET
3	C	221	LEU
3	C	246	SER

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Mol	Chain	Res	Type
3	C	321	ASP
3	C	365	GLU
3	C	396	GLU
4	D	40	GLU
4	D	60	VAL
4	D	97	ILE
4	D	136	GLN
4	D	149	LEU
4	D	187	TYR
4	D	223	LEU
4	D	245	MET
4	D	267	MET
4	D	278	LEU
4	D	322	GLU
4	D	323	GLU
4	D	377	LEU
5	E	40	LEU
5	E	63	LEU
5	E	165	PHE
5	E	197	ASP
5	E	198	GLU
5	E	209	ASN
5	E	267	PHE
5	E	271	GLU
5	E	279	GLN
6	F	40	SER
6	F	112	PHE
6	F	159	LYS
6	F	172	ILE
6	F	282	GLN
6	F	285	ASP
7	G	109	LYS
7	G	110	CYS
7	G	126	ARG
7	G	161	ASP
7	G	167	LEU
7	G	178	CYS
8	H	33	THR
8	H	40	LEU
8	H	46	LEU
8	H	80	ARG
8	H	160	ARG

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Mol	Chain	Res	Type
8	H	163	LEU
1	I	138	LEU
1	I	294	LEU
1	I	404	GLN
1	I	476	LEU
1	I	489	MET
2	J	90	ASN
2	J	215	LYS
2	J	224	ILE
2	J	228	ILE
2	J	250	GLU
2	J	412	ASP
2	J	420	ARG
2	J	429	ASN
2	J	435	ASN
3	K	22	THR
3	K	123	ILE
3	K	124	LEU
3	K	131	MET
3	K	138	LEU
3	K	167	MET
3	K	221	LEU
3	K	321	ASP
3	K	365	GLU
3	K	396	GLU
4	L	136	GLN
4	L	187	TYR
4	L	245	MET
4	L	278	LEU
4	L	377	LEU
5	M	40	LEU
5	M	63	LEU
5	M	165	PHE
5	M	197	ASP
5	M	198	GLU
5	M	209	ASN
5	M	268	ASP
5	M	270	SER
6	N	38	SER
6	N	172	ILE
6	N	282	GLN
6	N	285	ASP

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Mol	Chain	Res	Type
7	O	109	LYS
7	O	110	CYS
7	O	126	ARG
7	O	161	ASP
7	O	167	LEU
7	O	178	CYS
8	P	33	THR
8	P	40	LEU
8	P	46	LEU
8	P	80	ARG
8	P	160	ARG
8	P	163	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	313	HIS
1	A	324	ASN
1	A	412	GLN
1	A	483	GLN
2	B	90	ASN
2	B	223	HIS
2	B	319	GLN
3	C	41	HIS
3	C	89	ASN
4	D	276	ASN
4	D	277	GLN
5	E	321	GLN
6	F	61	GLN
6	F	76	GLN
6	F	111	GLN
7	G	202	GLN
1	I	313	HIS
1	I	324	ASN
1	I	412	GLN
2	J	223	HIS
2	J	319	GLN
2	J	334	HIS
3	K	41	HIS
3	K	89	ASN
4	L	184	GLN
4	L	276	ASN

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Mol	Chain	Res	Type
5	M	321	GLN
6	N	76	GLN
6	N	111	GLN
7	O	202	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 monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	N	1
6	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	40:SER	C	41:VAL	N	2.59
1	F	40:SER	C	41:VAL	N	1.94

6 Fit of model and data [\(i\)](#)

6.1 Protein, DNA and RNA chains [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.