



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:45 PM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

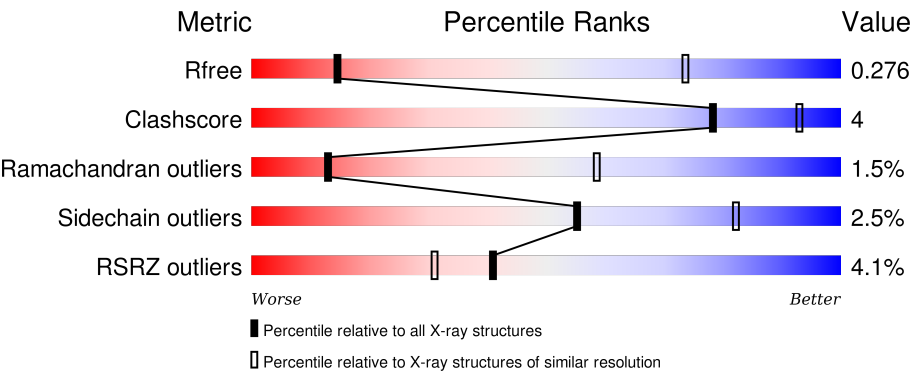
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1009 (4.52-3.60)
Clashscore	102246	1107 (4.52-3.60)
Ramachandran outliers	100387	1053 (4.52-3.60)
Sidechain outliers	100360	1039 (4.52-3.60)
RSRZ outliers	91569	1012 (4.52-3.60)

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. 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	480	
1	I	480	
2	B	447	
2	J	447	
3	C	427	

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Mol	Chain	Length	Quality of chain
3	K	427	
4	D	410	
4	L	410	
5	E	327	
5	M	327	
6	F	331	
6	N	331	
7	G	222	
7	O	222	
8	H	213	
8	P	213	

2 Entry composition

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
1	A	419	Total	C	N	O	S	0	0	0
			3348	2113	588	625	22			
1	I	419	Total	C	N	O	S	0	0	0
			3348	2113	588	625	22			

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
2	B	403	Total	C	N	O	S	0	0	0
			3304	2102	566	621	15			
2	J	403	Total	C	N	O	S	0	0	0
			3304	2102	566	621	15			

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	N	O	S	0	0	0
			2366	1510	393	450	13			
5	M	298	Total	C	N	O	S	0	0	0
			2366	1510	393	450	13			

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	N	O	S	0	0	0
			2236	1429	371	421	15			
6	N	281	Total	C	N	O	S	0	0	0
			2236	1429	371	421	15			

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
7	G	208	Total	C	N	O	S	0	0	0
			1631	1028	287	312	4			
7	O	208	Total	C	N	O	S	0	0	0
			1631	1028	287	312	4			

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
8	H	173	Total	C	N	O	S	0	0	0
			1383	885	240	254	4			
8	P	173	Total	C	N	O	S	0	0	0
			1383	885	240	254	4			

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

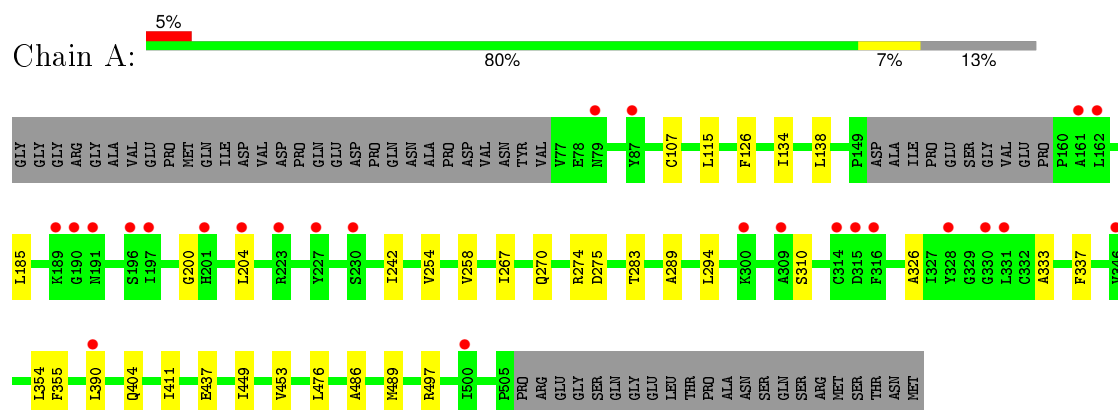
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

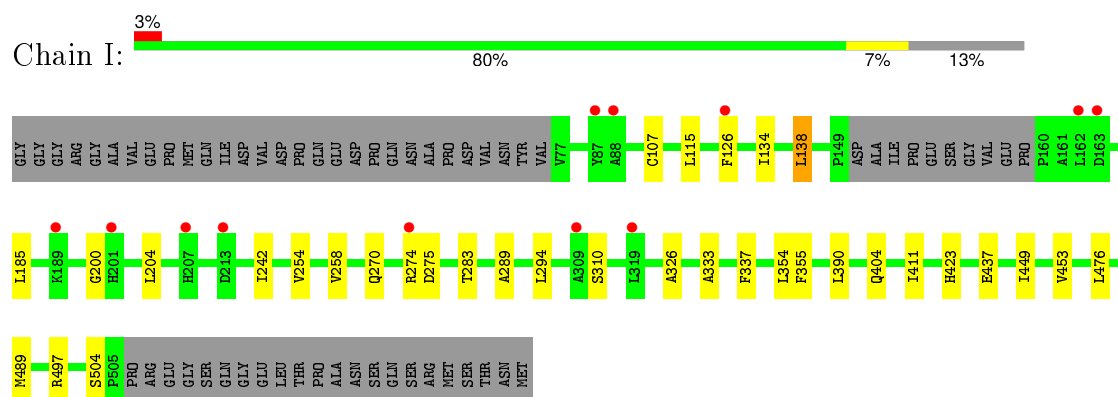
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

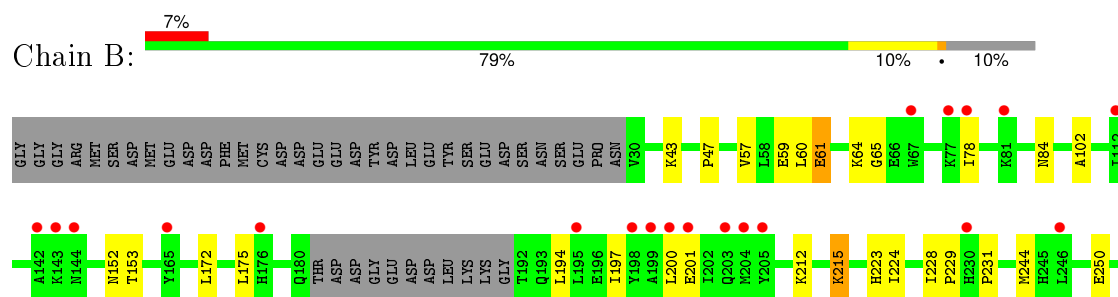
• Molecule 1: COP9 SIGNALOSOME COMPLEX SUBUNIT 1

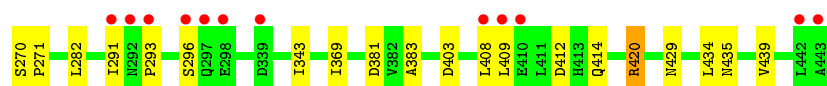


• Molecule 1: COP9 SIGNALOSOME COMPLEX SUBUNIT 1

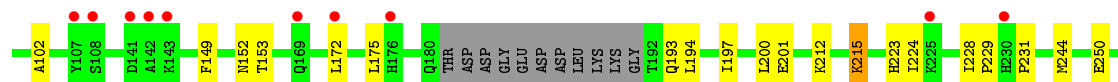
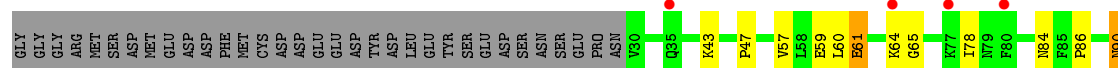
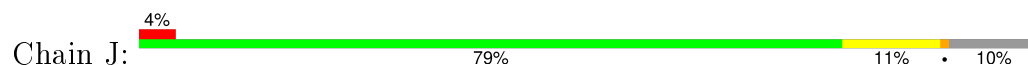


• Molecule 2: COP9 SIGNALOSOME COMPLEX SUBUNIT 2

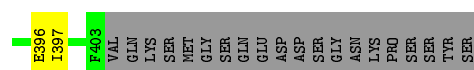
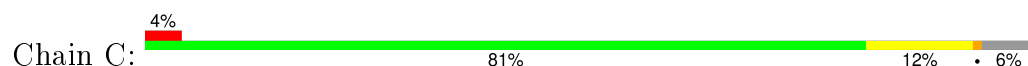




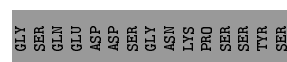
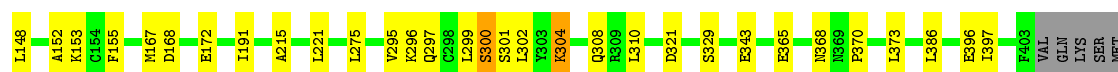
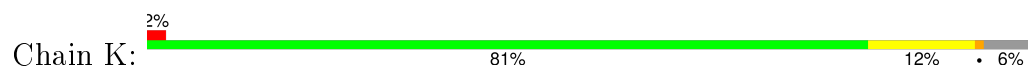
• Molecule 2: COP9 SIGNALOSOME COMPLEX SUBUNIT 2



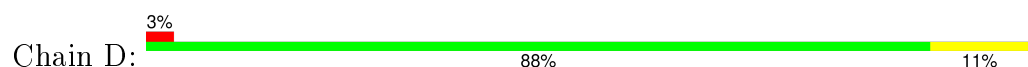
• Molecule 3: COP9 SIGNALOSOME COMPLEX SUBUNIT 3



• Molecule 3: COP9 SIGNALOSOME COMPLEX SUBUNIT 3

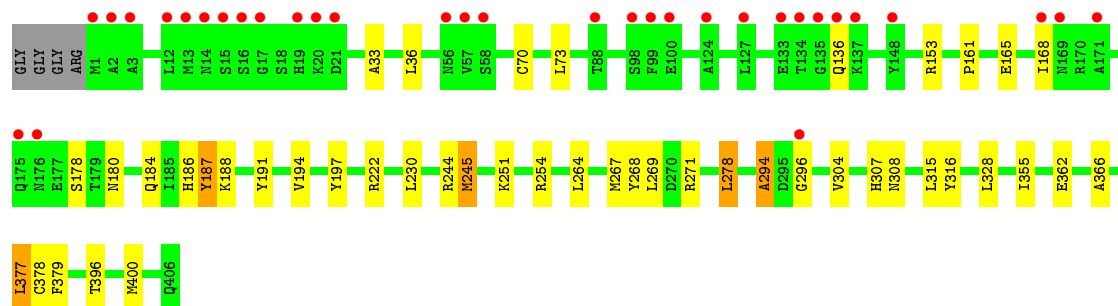
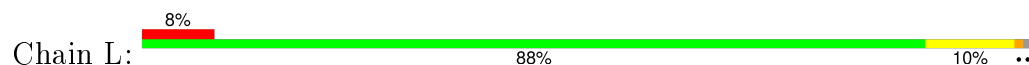


• Molecule 4: COP9 SIGNALOSOME COMPLEX SUBUNIT 4

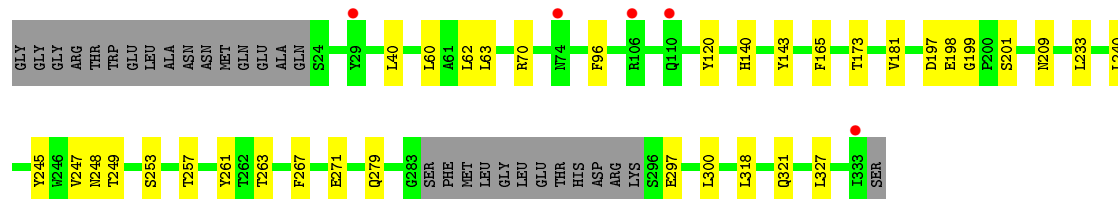




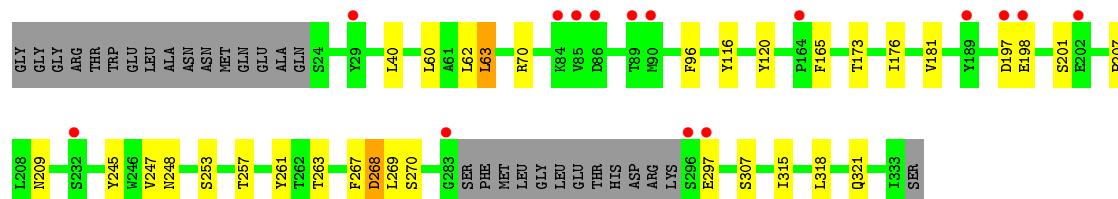
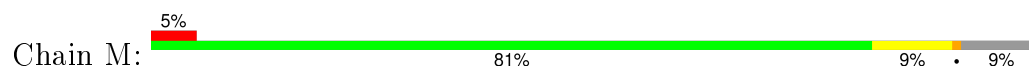
• Molecule 4: COP9 SIGNALOSOME COMPLEX SUBUNIT 4



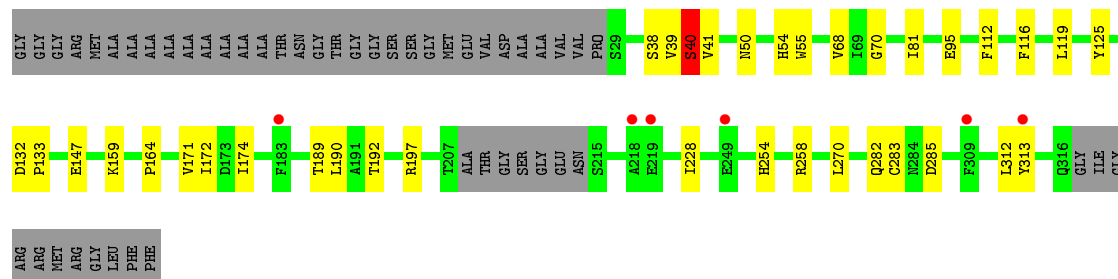
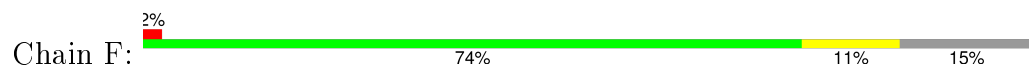
• Molecule 5: COP9 SIGNALOSOME COMPLEX SUBUNIT 5



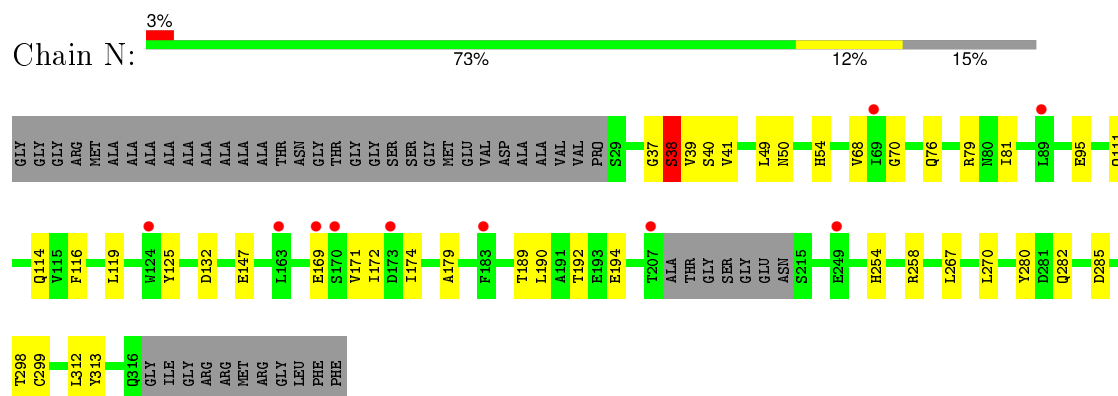
• Molecule 5: COP9 SIGNALOSOME COMPLEX SUBUNIT 5



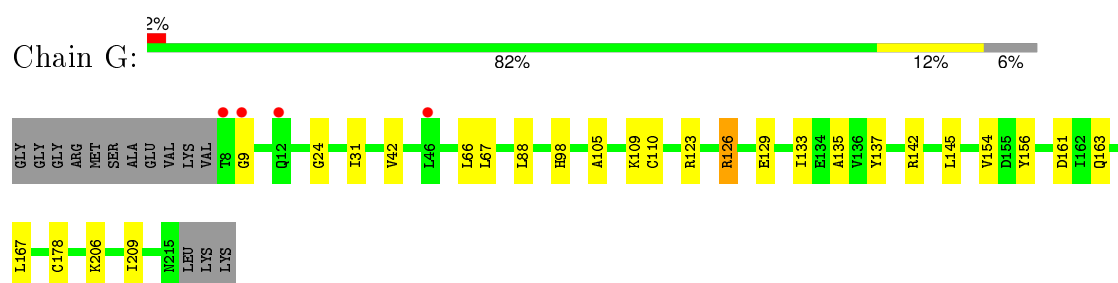
• Molecule 6: COP9 SIGNALOSOME COMPLEX SUBUNIT 6



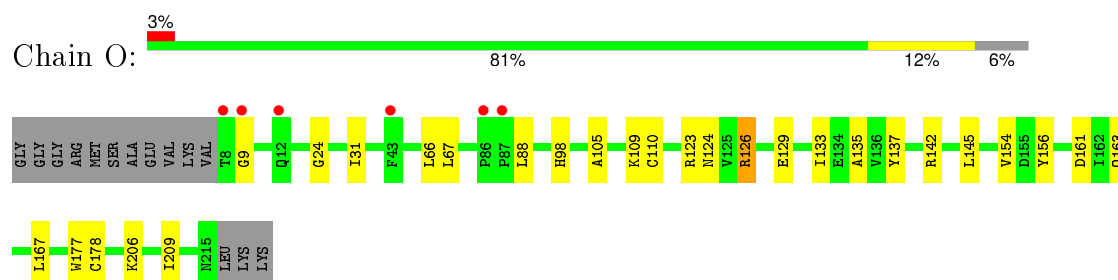
- Molecule 6: COP9 SIGNALOSOME COMPLEX SUBUNIT 6



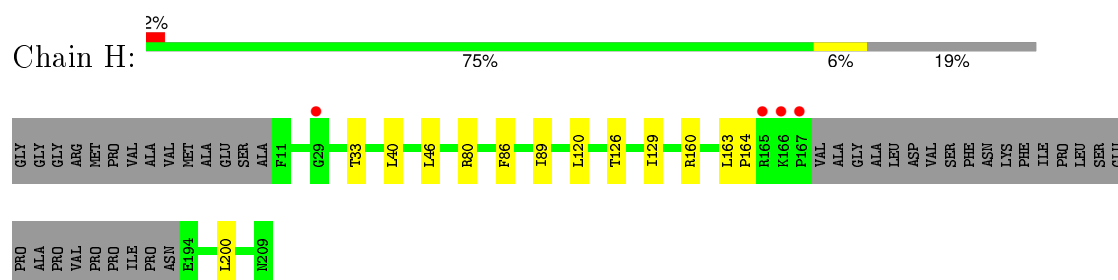
- Molecule 7: COP9 SIGNALOSOME COMPLEX SUBUNIT 7A



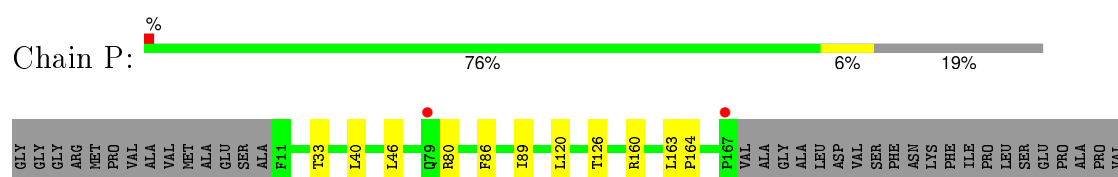
- Molecule 7: COP9 SIGNALOSOME COMPLEX SUBUNIT 7A



- Molecule 8: COP9 SIGNALOSOME COMPLEX SUBUNIT 8



- Molecule 8: COP9 SIGNALOSOME COMPLEX SUBUNIT 8





4 Data and refinement statistics

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 0.260 , 0.276	Depositor DCC
R_{free} test set	3087 reflections (5.01%)	DCC
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
Estimated twinning fraction	0.059 for -h,-k,l 0.115 for h,-h-k,-l 0.067 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 61643 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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

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
3:C:353:GLN:HB3	7:O:123:ARG:HH12	1.58	0.69
1:A:354:LEU:HD21	2:B:212:LYS:HB3	1.74	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
7:O:126:ARG:NH2	7:O:129:GLU:CB	2.62	0.62
2:B:383:ALA:HB2	4:L:296:GLY:HA3	1.81	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
5:M:63:LEU:HD22	6:N:49:LEU:HD12	1.83	0.59
4:D:251:LYS:O	6:F:171:VAL:HG13	2.03	0.59
2:J:420:ARG:CD	5:M:263:THR:HG22	2.33	0.58
2:J:270:SER:HB2	2:J:271:PRO:HA	1.85	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
4:L:70:CYS:HA	4:L:73:LEU:HD12	1.88	0.56
3:C:343:GLU:HG3	8:H:120:LEU:HD13	1.88	0.56
4:D:245:MET:HG2	6:F:147:GLU:HG2	1.86	0.56
1:I:275:ASP:HB3	2:J:223:HIS:HE1	1.67	0.56
1:I:115:LEU:HB3	1:I:138:LEU:HG	1.87	0.56
6:N:40:SER:C	6:N:41:VAL:N	2.59	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
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
4:L:180:ASN:O	4:L:184:GLN:CG	2.56	0.54
1:A:486:ALA:HB1	3:C:386:LEU:HD21	1.88	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:397:ILE:CG2	6:N:312:LEU:HD23	2.38	0.53
3:K:343:GLU:HG3	8:P:120:LEU:HD13	1.90	0.53
5:E:96:PHE:CE1	5:E:120:TYR:CE2	2.97	0.53
2:B:215:LYS:HE3	2:B:244:MET:SD	2.49	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
4:L:187:TYR:CD1	4:L:188:LYS:N	2.78	0.51
2:J:47:PRO:HB3	2:J:78:ILE:HG21	1.92	0.51
3:C:353:GLN:HB3	7:O:123:ARG:NH1	2.26	0.51
1:I:200:GLY:C	1:I:204:LEU:HD13	2.31	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
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
4:D:295:ASP:HA	2:J:334:HIS:CE1	2.46	0.50
1:A:326:ALA:HB2	1:A:355:PHE:HB3	1.93	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
5:M:120:TYR:N	6:N:111:GLN:HE22	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
3:C:354:LYS:O	7:O:124:ASN:HB3	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
5:M:173:THR:HG22	5:M:261:TYR:CB	2.41	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
1:I:504:SER:HA	3:K:215:ALA:HB2	1.95	0.49
5:M:318:LEU:HD23	8:P:200:LEU:HD21	1.94	0.49
5:E:60:LEU:HD11	6:F:50:ASN:OD1	2.13	0.49
7:O:105:ALA:HB1	7:O:154:VAL:HG11	1.94	0.49
1:I:497:ARG:HG3	6:N:313:TYR:CE1	2.48	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
3:K:117:PRO:HB2	3:K:148:LEU:HD22	1.95	0.48
2:B:64:LYS:HB3	2:B:65:GLY:HA2	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
3:K:368:ASN:O	6:N:280:TYR:HB3	2.13	0.48
2:J:64:LYS:HB3	2:J:65:GLY:HA2	1.96	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
2:J:420:ARG:HD3	5:M:263:THR:CG2	2.39	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
4:D:271:ARG:HD2	7:G:137:TYR:CD2	2.50	0.47
2:B:408:LEU:HD22	4:D:355:ILE:HG12	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
2:B:403:ASP:HB3	2:B:408:LEU:HG	1.96	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:295:ASP:CB	2:J:334:HIS:CE1	2.98	0.46
4:D:6:ARG:HG2	4:D:47:ALA:HB1	1.97	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
7:G:66:LEU:HD21	7:G:88:LEU:HD21	1.96	0.46
4:D:161:PRO:HB2	4:D:198:ARG:HG2	1.97	0.46
2:J:403:ASP:HB3	2:J:408:LEU:HG	1.97	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
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
7:G:126:ARG:HH22	7:G:129:GLU:HB3	1.76	0.45
4:D:271:ARG:HD2	7:G:137:TYR:CG	2.51	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
4:D:295:ASP:CB	2:J:334:HIS:HE1	2.30	0.45
1:A:283:THR:HG22	1:A:310:SER:H	1.81	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
7:O:126:ARG:HH22	7:O:129:GLU:HB3	1.77	0.45
2:J:175:LEU:HB3	2:J:197:ILE:HG12	1.99	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
3:K:68:MET:HB3	3:K:71:VAL:H	1.81	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
4:L:187:TYR:HE1	4:L:188:LYS:HD3	1.82	0.44
5:E:233:LEU:HD22	6:F:55:TRP:CE3	2.52	0.44
4:D:165:GLU:HA	4:D:168:ILE:HG22	1.99	0.44
1:I:258:VAL:HG11	1:I:289:ALA:HB2	1.99	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
5:M:173:THR:HG22	5:M:261:TYR:CG	2.52	0.44
3:C:68:MET:HB3	3:C:71:VAL:H	1.81	0.44
4:D:378:CYS:HB2	5:E:247:VAL:HG13	1.98	0.44
3:C:94:ARG:HH22	3:C:137:GLN:HE22	1.64	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
2:J:149:PHE:CZ	2:J:193:GLN:HB2	2.53	0.43
1:A:258:VAL:HG11	1:A:289:ALA:HB2	2.00	0.43
2:B:152:ASN:HB3	2:B:175:LEU:HD21	2.00	0.43
7:O:126:ARG:NH2	7:O:129:GLU:HB2	2.34	0.43
4:L:244:ARG:HB3	6:N:147:GLU:HB2	2.01	0.43
5:E:318:LEU:HD23	8:H:200:LEU:HD21	2.01	0.43
7:O:142:ARG:HB2	7:O:156:TYR:HB3	2.00	0.43
7:G:142:ARG:HB2	7:G:156:TYR:HB3	2.00	0.43
2:J:152:ASN:HB3	2:J:175:LEU:HD21	2.01	0.43
5:E:173:THR:HG22	5:E:261:TYR:CG	2.53	0.42
4:D:356:ASP:HB3	4:D:358:ILE:HD12	2.00	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:M:96:PHE:CE1	5:M:120:TYR:CD2	3.08	0.42
1:I:134:ILE:HG22	1:I:138:LEU:HD12	2.01	0.42
5:E:62:LEU:HD11	5:E:181:VAL:HG11	2.02	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
2:J:408:LEU:HD22	4:L:355:ILE:HG12	2.01	0.42
1:I:333:ALA:O	1:I:337:PHE:HB2	2.20	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
6:N:70:GLY:HA3	6:N:125:TYR:CE2	2.54	0.41
3:C:56:LEU:HD11	3:C:100:PHE:HA	2.02	0.41
6:F:258:ARG:HD2	7:G:42:VAL:HG21	2.02	0.41
4:D:396:THR:O	4:D:400:MET:HB2	2.20	0.41
5:M:173:THR:CG2	5:M:261:TYR:CB	2.83	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
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
8:H:129:ILE:HG13	7:O:123:ARG:NH2	2.35	0.41
2:B:381:ASP:OD2	4:L:294:ALA:O	2.39	0.41
3:K:275:LEU:HD22	3:K:302:LEU:HD22	2.02	0.41
4:D:321:PHE:CZ	4:D:352:ILE:HG23	2.51	0.41
3:C:275:LEU:HD22	3:C:302:LEU:HD22	2.02	0.41
3:C:39:LEU:HB3	3:C:58:VAL:HG13	2.02	0.41
3:K:39:LEU:HB3	3:K:58:VAL:HG13	2.02	0.41
7:G:98:HIS:HD2	7:G:135:ALA:HB2	1.86	0.41
7:O:98:HIS:HD2	7:O:135:ALA:HB2	1.86	0.41
4:L:222:ARG:HH22	6:N:179:ALA:HB3	1.86	0.41
6:N:254:HIS:O	6:N:258:ARG:HB2	2.21	0.41
1:I:242:ILE:HG23	1:I:254:VAL:HG13	2.02	0.41
4:L:396:THR:O	4:L:400:MET:HB2	2.21	0.41
5:E:240:LEU:HD13	6:F:164:PRO:HD3	2.03	0.41
6:N:38:SER:HB2	6:N:169:GLU:OE1	2.21	0.40
4:L:153:ARG:NH2	4:L:186:HIS:HB3	2.36	0.40
6:N:39:VAL:HA	6:N:79:ARG:O	2.21	0.40
6:F:254:HIS:O	6:F:258:ARG:HB2	2.22	0.40
6:F:132:ASP:HB2	6:F:133:PRO:CD	2.51	0.40
1:A:242:ILE:HG23	1:A:254:VAL:HG13	2.02	0.40
2:J:423:ALA:HB2	5:M:267:PHE:CE2	2.56	0.40
5:E:318:LEU:HD11	6:F:283:CYS:HA	2.03	0.40
5:E:140:HIS:CG	5:E:143:TYR:CE1	3.10	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

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	415/480 (86%)	395 (95%)	16 (4%)	4 (1%)	19	65
1	I	415/480 (86%)	395 (95%)	17 (4%)	3 (1%)	26	71
2	B	399/447 (89%)	365 (92%)	24 (6%)	10 (2%)	7	48
2	J	399/447 (89%)	365 (92%)	24 (6%)	10 (2%)	7	48
3	C	399/427 (93%)	360 (90%)	26 (6%)	13 (3%)	5	43
3	K	399/427 (93%)	360 (90%)	25 (6%)	14 (4%)	4	42
4	D	404/410 (98%)	399 (99%)	2 (0%)	3 (1%)	26	71
4	L	404/410 (98%)	400 (99%)	1 (0%)	3 (1%)	26	71
5	E	294/327 (90%)	283 (96%)	8 (3%)	3 (1%)	19	65
5	M	294/327 (90%)	283 (96%)	9 (3%)	2 (1%)	26	71
6	F	277/331 (84%)	267 (96%)	8 (3%)	2 (1%)	26	71
6	N	275/331 (83%)	264 (96%)	8 (3%)	3 (1%)	17	64
7	G	206/222 (93%)	195 (95%)	8 (4%)	3 (2%)	13	58
7	O	206/222 (93%)	195 (95%)	8 (4%)	3 (2%)	13	58
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%)	13	58

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 ⓘ

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%)	86	93
1	I	365/415 (88%)	360 (99%)	5 (1%)	74	89
2	B	367/406 (90%)	359 (98%)	8 (2%)	60	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	367/406 (90%)	358 (98%)	9 (2%)	55	82
3	C	358/378 (95%)	347 (97%)	11 (3%)	47	78
3	K	358/378 (95%)	348 (97%)	10 (3%)	51	80
4	D	347/348 (100%)	334 (96%)	13 (4%)	41	75
4	L	347/348 (100%)	342 (99%)	5 (1%)	74	89
5	E	255/278 (92%)	246 (96%)	9 (4%)	43	77
5	M	255/278 (92%)	247 (97%)	8 (3%)	47	78
6	F	251/277 (91%)	245 (98%)	6 (2%)	57	83
6	N	251/277 (91%)	247 (98%)	4 (2%)	70	88
7	G	174/184 (95%)	168 (97%)	6 (3%)	44	77
7	O	174/184 (95%)	168 (97%)	6 (3%)	44	77
8	H	144/174 (83%)	138 (96%)	6 (4%)	36	72
8	P	144/174 (83%)	138 (96%)	6 (4%)	36	72
All	All	4522/4920 (92%)	4407 (98%)	115 (2%)	55	82

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

Some 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 carbohydrates 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](#)

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	419/480 (87%)	0.24	25 (5%) 25 17	152, 242, 277, 283	0
1	I	419/480 (87%)	0.10	12 (2%) 55 43	140, 208, 264, 271	0
2	B	403/447 (90%)	0.26	32 (7%) 15 11	147, 264, 281, 288	0
2	J	403/447 (90%)	0.22	18 (4%) 37 28	134, 243, 264, 276	0
3	C	401/427 (93%)	0.13	16 (3%) 42 32	149, 205, 267, 276	0
3	K	401/427 (93%)	0.12	10 (2%) 61 49	121, 179, 260, 268	0
4	D	406/410 (99%)	0.25	14 (3%) 49 38	139, 227, 276, 281	0
4	L	406/410 (99%)	0.36	33 (8%) 15 11	162, 249, 287, 292	0
5	E	298/327 (91%)	0.04	5 (1%) 73 63	132, 172, 222, 242	0
5	M	298/327 (91%)	0.16	15 (5%) 32 24	148, 206, 242, 258	0
6	F	281/331 (84%)	0.07	6 (2%) 67 56	132, 181, 230, 244	0
6	N	281/331 (84%)	0.08	10 (3%) 46 36	132, 213, 247, 259	0
7	G	208/222 (93%)	0.01	4 (1%) 70 60	152, 211, 255, 264	0
7	O	208/222 (93%)	0.04	6 (2%) 55 43	175, 226, 268, 272	0
8	H	173/213 (81%)	0.02	4 (2%) 64 53	165, 200, 231, 241	0
8	P	173/213 (81%)	-0.04	2 (1%) 81 73	160, 193, 228, 239	0
All	All	5178/5714 (90%)	0.15	212 (4%) 41 31	121, 212, 275, 292	0

All (212) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	8	THR	12.6
2	B	142	ALA	9.1
5	M	85	VAL	7.7
2	B	204	MET	6.8
4	L	2	ALA	6.8

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Mol	Chain	Res	Type	RSRZ
4	D	19	HIS	6.6
7	G	9	GLY	6.5
2	B	298	GLU	6.4
4	D	15	SER	6.4
2	J	142	ALA	6.2
2	B	291	ILE	6.1
2	B	143	LYS	6.1
4	L	19	HIS	5.9
4	L	20	LYS	5.8
5	M	198	GLU	5.8
6	N	249	GLU	5.4
4	L	136	GLN	5.3
1	A	309	ALA	5.3
7	O	8	THR	5.3
4	L	135	GLY	5.3
1	A	201	HIS	5.0
7	G	12	GLN	5.0
3	C	34	LEU	4.8
4	L	12	LEU	4.8
2	B	230	HIS	4.6
1	I	309	ALA	4.6
2	J	143	LYS	4.6
2	B	292	ASN	4.5
4	L	133	GLU	4.5
1	I	207	HIS	4.3
7	O	12	GLN	4.3
3	K	94	ARG	4.2
4	L	137	LYS	4.2
4	L	99	PHE	4.2
6	N	207	THR	4.1
2	J	338	MET	4.1
4	L	134	THR	4.1
4	L	3	ALA	4.0
4	L	176	ASN	4.0
2	J	230	HIS	4.0
2	B	200	LEU	4.0
1	A	223	ARG	3.9
3	C	53	GLU	3.9
4	D	132	LEU	3.9
3	C	54	HIS	3.8
2	B	201	GLU	3.8
6	F	218	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
6	N	169	GLU	3.7
6	F	313	TYR	3.7
1	I	162	LEU	3.6
4	D	20	LYS	3.6
3	K	54	HIS	3.6
6	N	183	PHE	3.6
3	C	48	ALA	3.5
3	C	156	LYS	3.5
4	L	56	ASN	3.5
4	D	14	ASN	3.4
4	L	175	GLN	3.4
1	A	197	ILE	3.4
5	M	89	THR	3.4
4	L	169	ASN	3.4
1	A	227	TYR	3.3
1	A	315	ASP	3.3
1	I	274	ARG	3.2
1	I	201	HIS	3.2
2	B	198	TYR	3.2
4	L	88	THR	3.2
2	J	77	LYS	3.2
6	F	219	GLU	3.2
5	M	297	GLU	3.2
8	H	166	LYS	3.2
2	B	297	GLN	3.1
1	A	330	GLY	3.1
4	L	58	SER	3.1
2	B	81	LYS	3.0
4	L	57	VAL	3.0
1	I	88	ALA	3.0
1	A	230	SER	3.0
4	D	99	PHE	3.0
4	L	16	SER	3.0
6	F	249	GLU	2.9
2	J	64	LYS	2.9
2	J	172	LEU	2.9
4	D	23	ALA	2.9
4	D	61	ILE	2.9
5	M	189	TYR	2.9
6	N	89	LEU	2.9
1	I	189	LYS	2.8
5	M	296	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	314	CYS	2.8
1	A	87	TYR	2.8
2	B	296	SER	2.7
5	M	90	MET	2.7
1	A	500	ILE	2.7
4	D	2	ALA	2.7
7	O	43	PHE	2.7
8	H	29	GLY	2.7
4	L	100	GLU	2.7
5	M	29	TYR	2.7
2	J	35	GLN	2.6
4	L	168	ILE	2.6
5	E	333	ILE	2.6
5	M	283	GLY	2.6
8	H	165	ARG	2.6
2	B	246	LEU	2.6
1	A	191	ASN	2.6
7	O	87	PRO	2.6
3	C	46	LEU	2.6
8	H	167	PRO	2.6
2	B	144	ASN	2.6
1	I	163	ASP	2.6
2	B	203	GLN	2.6
2	B	165	TYR	2.6
4	L	15	SER	2.6
4	D	12	LEU	2.5
2	B	408	LEU	2.5
7	O	86	PRO	2.5
2	B	199	ALA	2.5
5	E	106	ARG	2.5
4	D	347	ARG	2.5
2	B	112	ILE	2.5
3	C	116	GLN	2.5
4	L	171	ALA	2.5
2	J	107	TYR	2.5
5	E	110	GLN	2.5
3	K	48	ALA	2.5
5	E	29	TYR	2.5
4	L	98	SER	2.5
2	J	279	TYR	2.5
5	M	84	LYS	2.5
2	J	306	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
7	G	46	LEU	2.5
3	C	17	ALA	2.4
4	D	133	GLU	2.4
6	N	170	SER	2.4
3	C	114	ARG	2.4
7	O	9	GLY	2.4
3	C	142	HIS	2.4
1	A	331	LEU	2.4
1	A	196	SER	2.4
2	B	67	TRP	2.4
1	A	189	LYS	2.4
2	J	108	SER	2.4
1	A	300	LYS	2.4
4	L	14	ASN	2.4
6	N	124	TRP	2.3
2	B	442	LEU	2.3
8	P	167	PRO	2.3
2	B	205	TYR	2.3
3	C	157	PRO	2.3
3	C	99	THR	2.3
2	B	77	LYS	2.3
2	B	339	ASP	2.3
5	M	86	ASP	2.3
4	L	296	GLY	2.3
2	J	176	HIS	2.2
4	D	27	ARG	2.2
2	B	443	ALA	2.2
2	B	78	ILE	2.2
3	C	131	MET	2.2
6	N	69	ILE	2.2
1	I	126	PHE	2.2
2	B	176	HIS	2.2
3	K	41	HIS	2.2
4	L	17	GLY	2.2
3	C	391	LYS	2.2
2	J	278	LYS	2.2
1	I	213	ASP	2.2
2	J	80	PHE	2.2
2	B	293	PRO	2.2
6	F	309	PHE	2.2
4	L	124	ALA	2.2
4	D	170	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	J	141	ASP	2.2
1	A	161	ALA	2.1
3	K	69	PRO	2.1
6	F	183	PHE	2.1
4	L	13	MET	2.1
5	M	202	GLU	2.1
1	A	316	PHE	2.1
5	E	74	ASN	2.1
3	K	43	ASP	2.1
1	I	319	LEU	2.1
2	J	169	GLN	2.1
4	L	21	ASP	2.1
4	L	127	LEU	2.1
1	A	204	LEU	2.1
1	A	162	LEU	2.1
2	J	225	LYS	2.1
3	K	45	VAL	2.1
1	A	190	GLY	2.1
1	A	328	TYR	2.1
2	B	409	LEU	2.1
3	K	44	THR	2.1
1	A	346	VAL	2.1
3	C	132	GLN	2.1
5	M	197	ASP	2.1
3	K	53	GLU	2.1
2	B	195	LEU	2.0
5	M	232	SER	2.0
1	A	79	ASN	2.0
4	L	1	MET	2.0
1	A	390	LEU	2.0
6	N	163	LEU	2.0
5	M	164	PRO	2.0
6	N	173	ASP	2.0
4	L	148	TYR	2.0
2	B	410	GLU	2.0
8	P	79	GLN	2.0
3	C	18	GLN	2.0
1	I	87	TYR	2.0
3	K	87	THR	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
9	ZN	M	999	1/1	0.98	0.13	-1.76	173,173,173,173	0
9	ZN	E	999	1/1	0.99	0.14	-1.84	138,138,138,138	0

6.5 Other polymers [i](#)

There are no such residues in this entry.