



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 08:20 AM GMT

PDB ID : 4D8R
Title : Molecular architecture of the eukaryotic chaperonin TRiC/CCT derived by a combination of chemical crosslinking and mass-spectrometry, XL-MS
Authors : Leitner, A.; Joachimiak, L.A.; Bracher, A.; Walzthoeni, T.; Chen, B.; Monke-meyer, L.; Pechmann, S.; Holmes, S.; Cong, Y.; Ma, B.; Ludtke, S.; Chiu, W.; Hartl, F.U.; Aebersold, R.; Frydman, J.
Deposited on : 2012-01-11
Resolution : 3.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

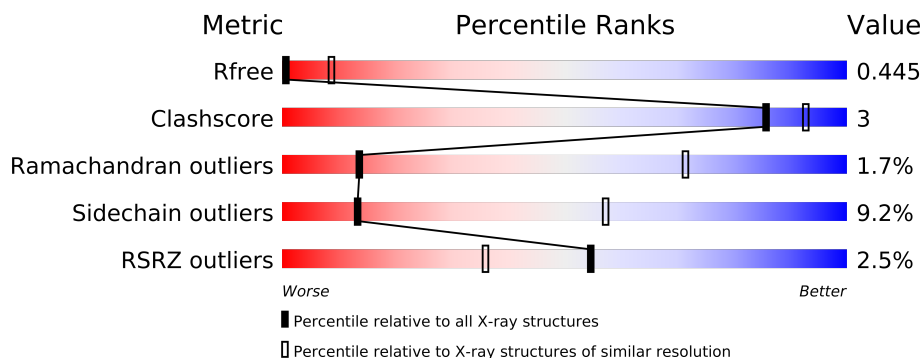
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.80 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}	66092	1162 (4.20-3.40)
Clashscore	79885	1100 (4.10-3.50)
Ramachandran outliers	78287	1050 (4.10-3.50)
Sidechain outliers	78261	1042 (4.10-3.50)
RSRZ outliers	66119	1163 (4.20-3.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	f	546	
1	n	546	
2	h	568	
2	p	568	
3	g	550	
3	o	550	
4	e	562	
4	m	562	
5	b	527	
5	j	527	
6	d	528	
6	l	528	
7	a	559	
7	i	559	

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Mol	Chain	Length	Quality of chain
8	c	590	
8	k	590	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 60040 atoms, of which 0 are hydrogen and 0 are deuterium.

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 T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	f	538	Total	C	N	O	S	0	0	0
			3836	2417	640	765	14			
1	n	538	Total	C	N	O	S	0	0	0
			3836	2417	640	765	14			

- Molecule 2 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	h	521	Total	C	N	O	S	0	0	0
			3619	2286	602	708	23			
2	p	521	Total	C	N	O	S	0	0	0
			3619	2286	602	708	23			

- Molecule 3 is a protein called T-complex protein 1 subunit eta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	g	526	Total	C	N	O	S	0	0	0
			3752	2372	631	730	19			
3	o	526	Total	C	N	O	S	0	0	0
			3752	2372	631	730	19			

- Molecule 4 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	e	535	Total	C	N	O	S	0	0	0
			3798	2391	634	752	21			
4	m	535	Total	C	N	O	S	0	0	0
			3798	2391	634	752	21			

- Molecule 5 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	b	518	Total	C	N	O	S	0	0	0
			3689	2306	623	747	13			
5	j	518	Total	C	N	O	S	0	0	0
			3689	2306	623	747	13			

- Molecule 6 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	d	523	Total	C	N	O	S	0	0	0
			3685	2306	631	731	17			
6	l	523	Total	C	N	O	S	0	0	0
			3685	2306	631	731	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	345	ASP	GLY	ENGINEERED MUTATION	UNP P39078
l	345	ASP	GLY	ENGINEERED MUTATION	UNP P39078

- Molecule 7 is a protein called T-complex protein 1 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	a	539	Total	C	N	O	S	0	0	0
			3770	2369	638	746	17			
7	i	539	Total	C	N	O	S	0	0	0
			3770	2369	638	746	17			

- Molecule 8 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	c	513	Total	C	N	O	S	0	0	0
			3615	2270	620	699	26			
8	k	513	Total	C	N	O	S	0	0	0
			3615	2270	620	699	26			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	1001	GLY	-	SEE REMARK 999	UNP P39077
c	1002	SER	-	SEE REMARK 999	UNP P39077
c	1003	GLY	-	SEE REMARK 999	UNP P39077
c	1004	SER	-	SEE REMARK 999	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
c	1005	GLY	-	SEE REMARK 999	UNP P39077
c	1006	TRP	-	SEE REMARK 999	UNP P39077
c	1007	SER	-	SEE REMARK 999	UNP P39077
c	1008	HIS	-	SEE REMARK 999	UNP P39077
c	1009	PRO	-	SEE REMARK 999	UNP P39077
c	1010	GLN	-	SEE REMARK 999	UNP P39077
c	1011	PHE	-	SEE REMARK 999	UNP P39077
c	1012	GLU	-	SEE REMARK 999	UNP P39077
c	1013	LYS	-	SEE REMARK 999	UNP P39077
c	1014	GLY	-	SEE REMARK 999	UNP P39077
c	1015	SER	-	SEE REMARK 999	UNP P39077
c	1016	GLY	-	SEE REMARK 999	UNP P39077
c	1017	LYS	-	SEE REMARK 999	UNP P39077
c	1018	ARG	-	SEE REMARK 999	UNP P39077
c	1019	ARG	-	SEE REMARK 999	UNP P39077
c	1020	TRP	-	SEE REMARK 999	UNP P39077
c	1021	LYS	-	SEE REMARK 999	UNP P39077
c	1022	LYS	-	SEE REMARK 999	UNP P39077
c	1023	ASN	-	SEE REMARK 999	UNP P39077
c	1024	PHE	-	SEE REMARK 999	UNP P39077
c	1025	ILE	-	SEE REMARK 999	UNP P39077
c	1026	ALA	-	SEE REMARK 999	UNP P39077
c	1027	VAL	-	SEE REMARK 999	UNP P39077
c	1028	SER	-	SEE REMARK 999	UNP P39077
c	1029	ALA	-	SEE REMARK 999	UNP P39077
c	1030	ALA	-	SEE REMARK 999	UNP P39077
c	1031	ASN	-	SEE REMARK 999	UNP P39077
c	1032	ARG	-	SEE REMARK 999	UNP P39077
c	1033	PHE	-	SEE REMARK 999	UNP P39077
c	1034	LYS	-	SEE REMARK 999	UNP P39077
c	1035	LYS	-	SEE REMARK 999	UNP P39077
c	1036	ILE	-	SEE REMARK 999	UNP P39077
c	1037	SER	-	SEE REMARK 999	UNP P39077
c	1038	SER	-	SEE REMARK 999	UNP P39077
c	1039	SER	-	SEE REMARK 999	UNP P39077
c	1040	GLY	-	SEE REMARK 999	UNP P39077
c	1041	ALA	-	SEE REMARK 999	UNP P39077
c	1042	LEU	-	SEE REMARK 999	UNP P39077
c	1043	GLY	-	SEE REMARK 999	UNP P39077
c	1044	SER	-	SEE REMARK 999	UNP P39077
c	1045	GLY	-	SEE REMARK 999	UNP P39077
c	1046	HIS	-	SEE REMARK 999	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
c	1047	HIS	-	SEE REMARK 999	UNP P39077
c	1048	HIS	-	SEE REMARK 999	UNP P39077
c	1049	HIS	-	SEE REMARK 999	UNP P39077
c	1050	HIS	-	SEE REMARK 999	UNP P39077
c	1051	HIS	-	SEE REMARK 999	UNP P39077
c	1052	HIS	-	SEE REMARK 999	UNP P39077
c	1053	HIS	-	SEE REMARK 999	UNP P39077
c	1054	GLY	-	SEE REMARK 999	UNP P39077
c	1055	SER	-	SEE REMARK 999	UNP P39077
c	1056	GLY	-	SEE REMARK 999	UNP P39077
k	1001	GLY	-	SEE REMARK 999	UNP P39077
k	1002	SER	-	SEE REMARK 999	UNP P39077
k	1003	GLY	-	SEE REMARK 999	UNP P39077
k	1004	SER	-	SEE REMARK 999	UNP P39077
k	1005	GLY	-	SEE REMARK 999	UNP P39077
k	1006	TRP	-	SEE REMARK 999	UNP P39077
k	1007	SER	-	SEE REMARK 999	UNP P39077
k	1008	HIS	-	SEE REMARK 999	UNP P39077
k	1009	PRO	-	SEE REMARK 999	UNP P39077
k	1010	GLN	-	SEE REMARK 999	UNP P39077
k	1011	PHE	-	SEE REMARK 999	UNP P39077
k	1012	GLU	-	SEE REMARK 999	UNP P39077
k	1013	LYS	-	SEE REMARK 999	UNP P39077
k	1014	GLY	-	SEE REMARK 999	UNP P39077
k	1015	SER	-	SEE REMARK 999	UNP P39077
k	1016	GLY	-	SEE REMARK 999	UNP P39077
k	1017	LYS	-	SEE REMARK 999	UNP P39077
k	1018	ARG	-	SEE REMARK 999	UNP P39077
k	1019	ARG	-	SEE REMARK 999	UNP P39077
k	1020	TRP	-	SEE REMARK 999	UNP P39077
k	1021	LYS	-	SEE REMARK 999	UNP P39077
k	1022	LYS	-	SEE REMARK 999	UNP P39077
k	1023	ASN	-	SEE REMARK 999	UNP P39077
k	1024	PHE	-	SEE REMARK 999	UNP P39077
k	1025	ILE	-	SEE REMARK 999	UNP P39077
k	1026	ALA	-	SEE REMARK 999	UNP P39077
k	1027	VAL	-	SEE REMARK 999	UNP P39077
k	1028	SER	-	SEE REMARK 999	UNP P39077
k	1029	ALA	-	SEE REMARK 999	UNP P39077
k	1030	ALA	-	SEE REMARK 999	UNP P39077
k	1031	ASN	-	SEE REMARK 999	UNP P39077
k	1032	ARG	-	SEE REMARK 999	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
k	1033	PHE	-	SEE REMARK 999	UNP P39077
k	1034	LYS	-	SEE REMARK 999	UNP P39077
k	1035	LYS	-	SEE REMARK 999	UNP P39077
k	1036	ILE	-	SEE REMARK 999	UNP P39077
k	1037	SER	-	SEE REMARK 999	UNP P39077
k	1038	SER	-	SEE REMARK 999	UNP P39077
k	1039	SER	-	SEE REMARK 999	UNP P39077
k	1040	GLY	-	SEE REMARK 999	UNP P39077
k	1041	ALA	-	SEE REMARK 999	UNP P39077
k	1042	LEU	-	SEE REMARK 999	UNP P39077
k	1043	GLY	-	SEE REMARK 999	UNP P39077
k	1044	SER	-	SEE REMARK 999	UNP P39077
k	1045	GLY	-	SEE REMARK 999	UNP P39077
k	1046	HIS	-	SEE REMARK 999	UNP P39077
k	1047	HIS	-	SEE REMARK 999	UNP P39077
k	1048	HIS	-	SEE REMARK 999	UNP P39077
k	1049	HIS	-	SEE REMARK 999	UNP P39077
k	1050	HIS	-	SEE REMARK 999	UNP P39077
k	1051	HIS	-	SEE REMARK 999	UNP P39077
k	1052	HIS	-	SEE REMARK 999	UNP P39077
k	1053	HIS	-	SEE REMARK 999	UNP P39077
k	1054	GLY	-	SEE REMARK 999	UNP P39077
k	1055	SER	-	SEE REMARK 999	UNP P39077
k	1056	GLY	-	SEE REMARK 999	UNP P39077

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

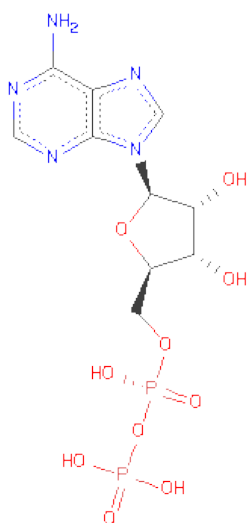
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	p	1	Total Mg 1 1	0	0
9	g	1	Total Mg 1 1	0	0
9	j	1	Total Mg 1 1	0	0
9	d	1	Total Mg 1 1	0	0
9	k	1	Total Mg 1 1	0	0
9	e	1	Total Mg 1 1	0	0
9	h	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	b	1	Total	Mg	0	0
			1	1		
9	i	1	Total	Mg	0	0
			1	1		
9	c	1	Total	Mg	0	0
			1	1		
9	a	1	Total	Mg	0	0
			1	1		
9	n	1	Total	Mg	0	0
			1	1		
9	o	1	Total	Mg	0	0
			1	1		
9	l	1	Total	Mg	0	0
			1	1		
9	f	1	Total	Mg	0	0
			1	1		
9	m	1	Total	Mg	0	0
			1	1		

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



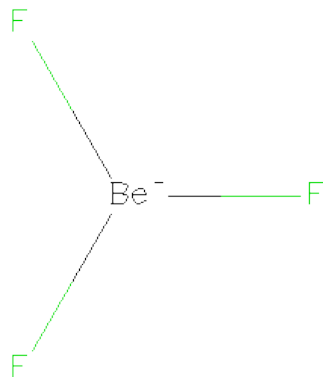
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	f	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	h	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	g	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	e	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	b	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	d	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	a	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	c	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	n	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	p	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	o	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	m	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	j	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	l	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	i	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	k	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 11 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	f	1	Total	Be	F	0	0
			4	1	3		
11	h	1	Total	Be	F	0	0
			4	1	3		
11	g	1	Total	Be	F	0	0
			4	1	3		
11	e	1	Total	Be	F	0	0
			4	1	3		
11	b	1	Total	Be	F	0	0
			4	1	3		
11	d	1	Total	Be	F	0	0
			4	1	3		
11	a	1	Total	Be	F	0	0
			4	1	3		
11	c	1	Total	Be	F	0	0
			4	1	3		
11	n	1	Total	Be	F	0	0
			4	1	3		
11	p	1	Total	Be	F	0	0
			4	1	3		
11	o	1	Total	Be	F	0	0
			4	1	3		
11	m	1	Total	Be	F	0	0
			4	1	3		
11	j	1	Total	Be	F	0	0
			4	1	3		
11	l	1	Total	Be	F	0	0
			4	1	3		

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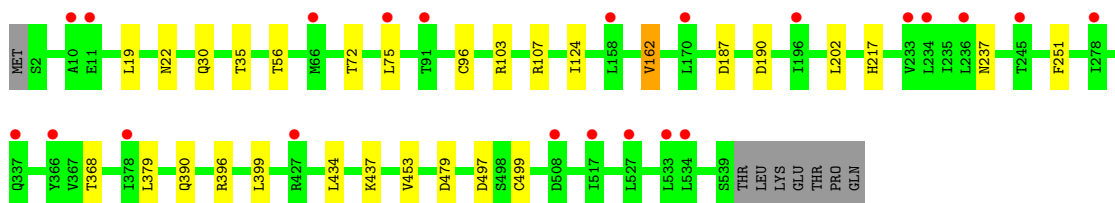
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	i	1	Total 4	Be 1	F 3	0	0
11	k	1	Total 4	Be 1	F 3	0	0

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.

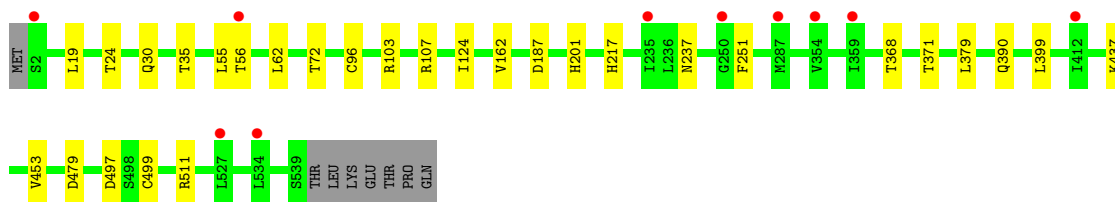
- Molecule 1: T-complex protein 1 subunit zeta

Chain f: 



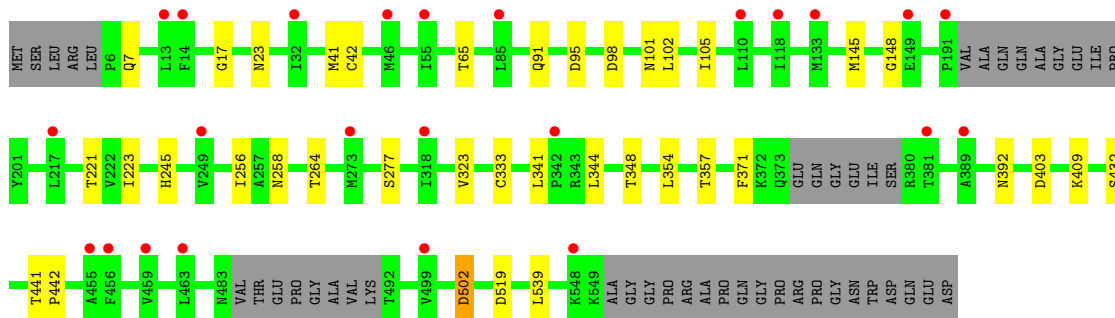
- Molecule 1: T-complex protein 1 subunit zeta

Chain n: 



- Molecule 2: T-complex protein 1 subunit theta

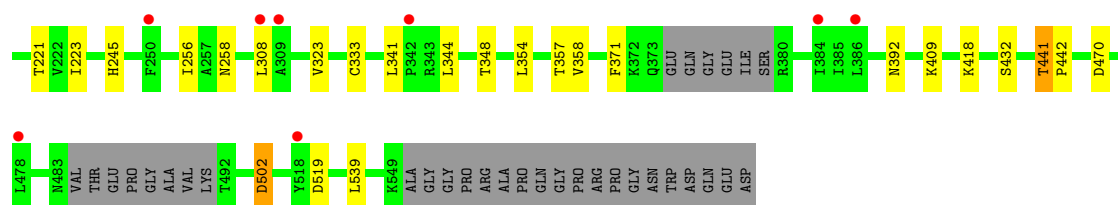
Chain h: 



- Molecule 2: T-complex protein 1 subunit theta

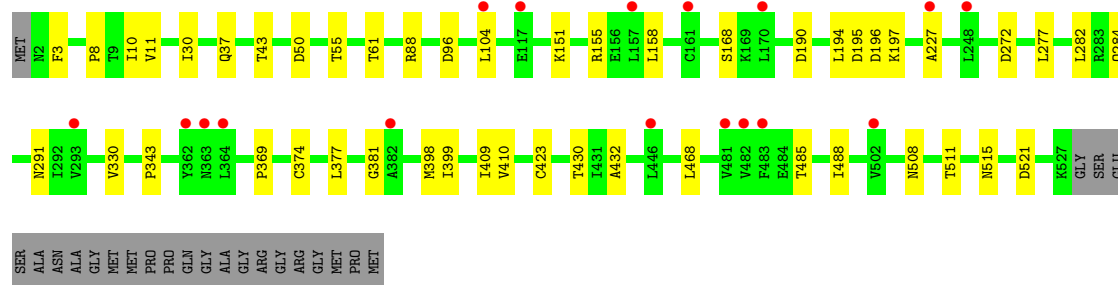
Chain p: 





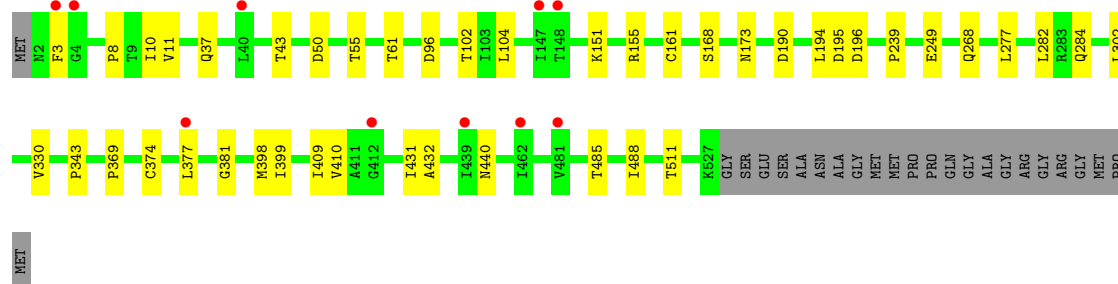
• Molecule 3: T-complex protein 1 subunit eta

Chain g:



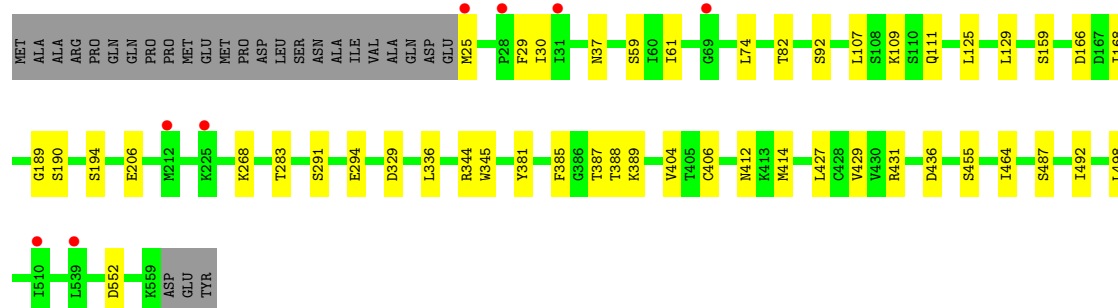
• Molecule 3: T-complex protein 1 subunit eta

Chain o:



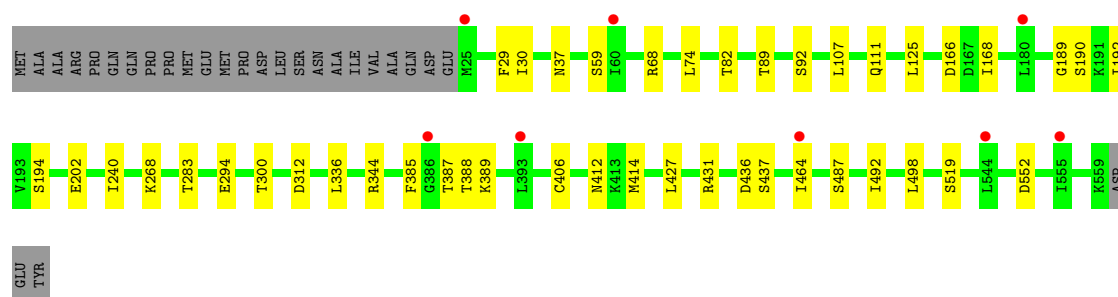
• Molecule 4: T-complex protein 1 subunit epsilon

Chain e:



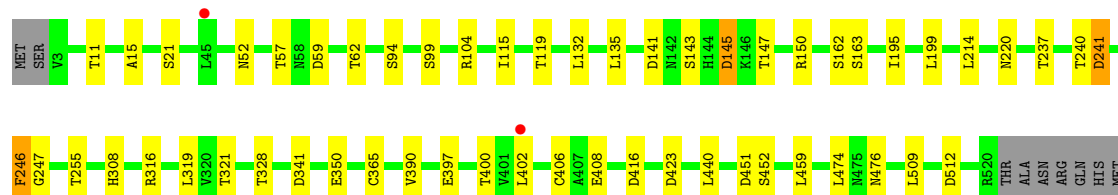
• Molecule 4: T-complex protein 1 subunit epsilon

Chain m:



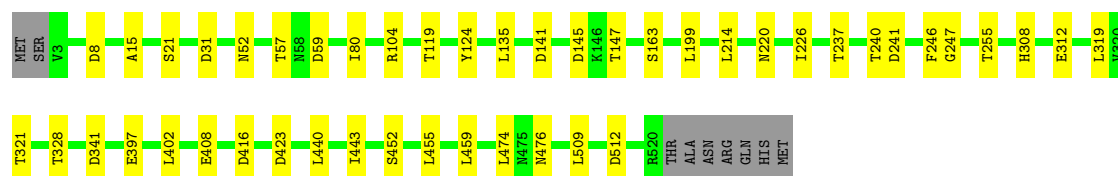
- Molecule 5: T-complex protein 1 subunit beta

Chain b:



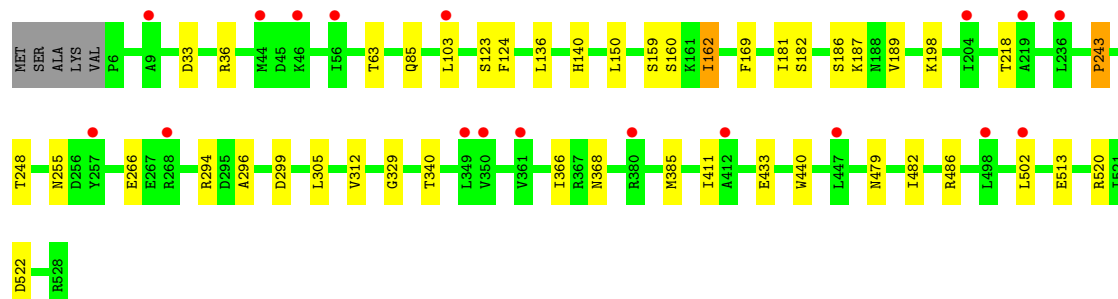
- Molecule 5: T-complex protein 1 subunit beta

Chain j:



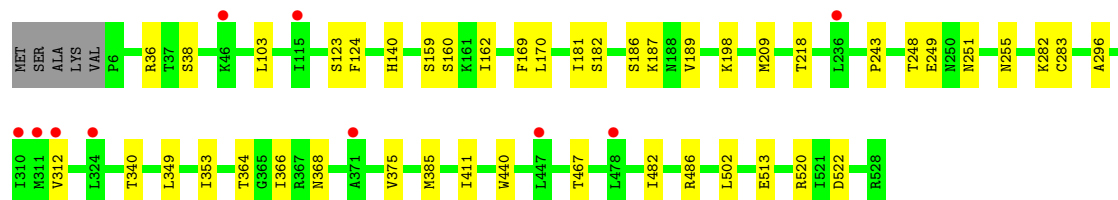
- Molecule 6: T-complex protein 1 subunit delta

Chain d:



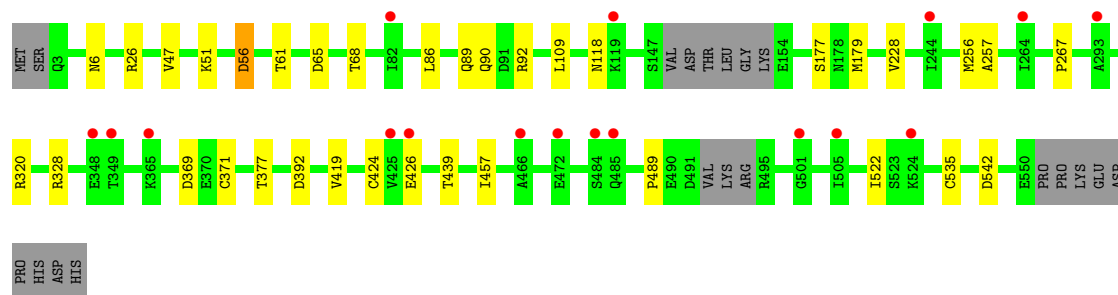
- Molecule 6: T-complex protein 1 subunit delta

Chain l:



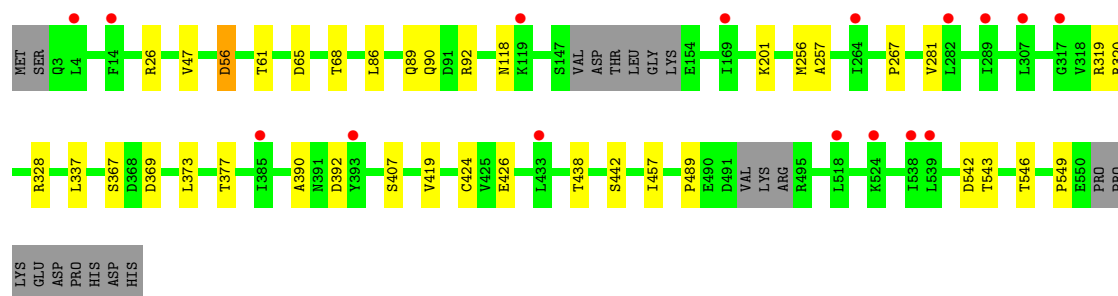
- Molecule 7: T-complex protein 1 subunit alpha

Chain a:



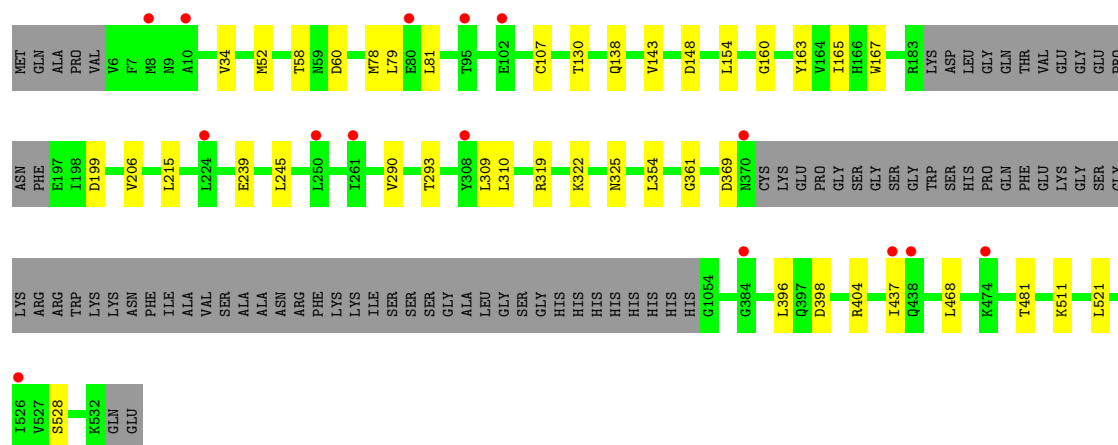
- Molecule 7: T-complex protein 1 subunit alpha

Chain i:



- Molecule 8: T-complex protein 1 subunit gamma

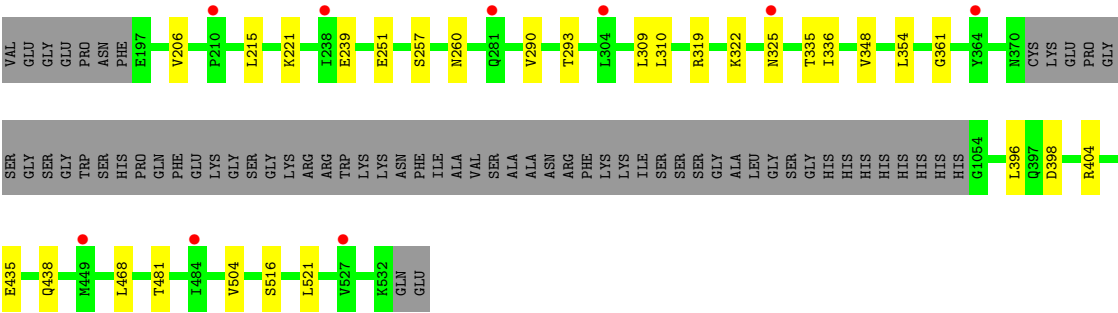
Chain c:



- Molecule 8: T-complex protein 1 subunit gamma

Chain k:





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	159.10Å 162.54Å 268.10Å 85.23° 81.15° 61.17°	Depositor
Resolution (Å)	30.00 – 3.80 30.01 – 3.80	Depositor EDS
% Data completeness (in resolution range)	91.6 (30.00-3.80) 91.5 (30.01-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 3.75Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.257 , 0.305 0.437 , 0.445	Depositor DCC
R_{free} test set	10463 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	116.0	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 52.9	EDS
Estimated twinning fraction	0.024 for -h,-h+k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 209266 reflections	Xtriage
F_o, F_c correlation	0.67	EDS
Total number of atoms	60040	wwPDB-VP
Average B, all atoms (Å ²)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BEF, ADP

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	f	0.34	0/3886	0.52	1/5318 (0.0%)
1	n	0.35	0/3886	0.54	0/5318
2	h	0.35	0/3661	0.52	0/5005
2	p	0.36	0/3661	0.54	0/5005
3	g	0.37	0/3803	0.53	0/5194
3	o	0.38	0/3803	0.53	0/5194
4	e	0.36	0/3849	0.51	0/5252
4	m	0.36	0/3849	0.53	0/5252
5	b	0.35	0/3726	0.54	0/5077
5	j	0.40	1/3726 (0.0%)	0.55	0/5077
6	d	0.35	0/3723	0.53	0/5089
6	l	0.36	0/3723	0.54	0/5089
7	a	0.35	0/3805	0.53	0/5196
7	i	0.35	0/3805	0.53	0/5196
8	c	0.35	0/3657	0.55	0/5003
8	k	0.34	0/3657	0.56	1/5003 (0.0%)
All	All	0.36	1/60220 (0.0%)	0.53	2/82268 (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
6	d	0	1
6	l	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	j	452	SER	CB-OG	7.94	1.52	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
8	k	79	LEU	CA-CB-CG	5.19	127.24	115.30
1	f	434	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	d	243	PRO	Peptide
6	l	243	PRO	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	f	3836	0	0	0	0
1	n	3836	0	0	0	0
2	h	3619	0	0	0	0
2	p	3619	0	0	0	0
3	g	3752	0	0	0	0
3	o	3752	0	0	0	0
4	e	3798	0	0	0	0
4	m	3798	0	0	0	0
5	b	3689	0	0	0	0
5	j	3689	0	0	0	0
6	d	3685	0	0	0	0
6	l	3685	0	0	0	0
7	a	3770	0	0	0	0
7	i	3770	0	0	0	0
8	c	3615	0	0	0	0
8	k	3615	0	0	0	0
9	a	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	b	1	0	0	0	0
9	c	1	0	0	0	0
9	d	1	0	0	0	0
9	e	1	0	0	0	0
9	f	1	0	0	0	0
9	g	1	0	0	0	0
9	h	1	0	0	0	0
9	i	1	0	0	0	0
9	j	1	0	0	0	0
9	k	1	0	0	0	0
9	l	1	0	0	0	0
9	m	1	0	0	0	0
9	n	1	0	0	0	0
9	o	1	0	0	0	0
9	p	1	0	0	0	0
10	a	27	0	0	0	0
10	b	27	0	0	0	0
10	c	27	0	0	0	0
10	d	27	0	0	0	0
10	e	27	0	0	0	0
10	f	27	0	0	0	0
10	g	27	0	0	0	0
10	h	27	0	0	0	0
10	i	27	0	0	0	0
10	j	27	0	0	0	0
10	k	27	0	0	0	0
10	l	27	0	0	0	0
10	m	27	0	0	0	0
10	n	27	0	0	0	0
10	o	27	0	0	0	0
10	p	27	0	0	0	0
11	a	4	0	0	0	0
11	b	4	0	0	0	0
11	c	4	0	0	0	0
11	d	4	0	0	0	0
11	e	4	0	0	0	0
11	f	4	0	0	0	0
11	g	4	0	0	0	0
11	h	4	0	0	0	0
11	i	4	0	0	0	0
11	j	4	0	0	0	0
11	k	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	l	4	0	0	0	0
11	m	4	0	0	0	0
11	n	4	0	0	0	0
11	o	4	0	0	0	0
11	p	4	0	0	0	0
All	All	60040	0	0	0	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

There are no clashes within the asymmetric unit.

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	f	536/546 (98%)	484 (90%)	49 (9%)	3 (1%)	33	86
1	n	536/546 (98%)	486 (91%)	48 (9%)	2 (0%)	43	90
2	h	513/568 (90%)	460 (90%)	46 (9%)	7 (1%)	16	74
2	p	513/568 (90%)	450 (88%)	53 (10%)	10 (2%)	12	69
3	g	524/550 (95%)	477 (91%)	38 (7%)	9 (2%)	14	71
3	o	524/550 (95%)	472 (90%)	41 (8%)	11 (2%)	11	67
4	e	533/562 (95%)	500 (94%)	27 (5%)	6 (1%)	21	79
4	m	533/562 (95%)	492 (92%)	33 (6%)	8 (2%)	15	73
5	b	516/527 (98%)	461 (89%)	41 (8%)	14 (3%)	8	62
5	j	516/527 (98%)	459 (89%)	47 (9%)	10 (2%)	12	69
6	d	521/528 (99%)	473 (91%)	34 (6%)	14 (3%)	8	62
6	l	521/528 (99%)	469 (90%)	41 (8%)	11 (2%)	11	67
7	a	533/559 (95%)	482 (90%)	43 (8%)	8 (2%)	15	73
7	i	533/559 (95%)	484 (91%)	37 (7%)	12 (2%)	10	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	c	507/590 (86%)	456 (90%)	44 (9%)	7 (1%)	16	74
8	k	507/590 (86%)	448 (88%)	50 (10%)	9 (2%)	13	70
All	All	8366/8860 (94%)	7553 (90%)	672 (8%)	141 (2%)	14	71

All (141) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	h	323	VAL
2	h	442	PRO
2	h	502	ASP
3	g	8	PRO
4	e	389	LYS
5	b	15	ALA
5	b	163	SER
5	b	220	ASN
5	b	255	THR
5	b	328	THR
6	d	368	ASN
8	c	163	TYR
2	p	323	VAL
2	p	442	PRO
2	p	502	ASP
3	o	8	PRO
4	m	190	SER
4	m	389	LYS
5	j	15	ALA
5	j	163	SER
5	j	220	ASN
5	j	255	THR
5	j	328	THR
6	l	282	LYS
6	l	368	ASN
8	k	163	TYR
3	g	168	SER
3	g	381	GLY
4	e	189	GLY
4	e	190	SER
5	b	59	ASP
5	b	145	ASP
5	b	246	PHE
6	d	182	SER

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Mol	Chain	Res	Type
6	d	189	VAL
7	a	56	ASP
7	a	65	ASP
7	a	256	MET
7	a	257	ALA
8	c	160	GLY
8	c	239	GLU
3	o	168	SER
3	o	381	GLY
4	m	194	SER
5	j	247	GLY
6	l	160	SER
6	l	182	SER
6	l	189	VAL
6	l	296	ALA
7	i	56	ASP
7	i	201	LYS
7	i	256	MET
7	i	257	ALA
8	k	160	GLY
1	f	437	LYS
2	h	23	ASN
3	g	151	LYS
3	g	227	ALA
5	b	162	SER
5	b	451	ASP
6	d	160	SER
6	d	186	SER
6	d	433	GLU
8	c	319	ARG
8	c	361	GLY
2	p	7	GLN
2	p	23	ASN
3	o	190	ASP
3	o	432	ALA
4	m	189	GLY
4	m	437	SER
5	j	59	ASP
6	l	187	LYS
6	l	249	GLU
7	i	65	ASP
7	i	118	ASN

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Mol	Chain	Res	Type
7	i	367	SER
7	i	390	ALA
7	i	549	PRO
8	k	60	ASP
8	k	221	LYS
8	k	239	GLU
8	k	319	ARG
8	k	361	GLY
1	f	202	LEU
2	h	7	GLN
2	h	148	GLY
3	g	190	ASP
3	g	432	ALA
4	e	194	SER
4	e	345	TRP
5	b	143	SER
6	d	159	SER
6	d	162	ILE
6	d	187	LYS
6	d	296	ALA
6	d	479	ASN
7	a	369	ASP
8	c	60	ASP
8	c	511	LYS
1	n	201	HIS
2	p	148	GLY
4	m	202	GLU
4	m	268	LYS
6	l	186	SER
7	i	267	PRO
7	i	369	ASP
8	k	80	GLU
4	e	268	LYS
5	b	241	ASP
5	b	350	GLU
6	d	294	ARG
7	a	267	PRO
2	p	153	LYS
3	o	151	LYS
3	o	249	GLU
5	j	145	ASP
5	j	312	GLU

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Mol	Chain	Res	Type
3	g	343	PRO
5	b	247	GLY
7	a	118	ASN
7	a	489	PRO
1	n	437	LYS
2	p	418	LYS
3	o	343	PRO
5	j	241	ASP
6	l	159	SER
8	k	435	GLU
3	g	369	PRO
7	i	489	PRO
1	f	162	VAL
3	o	431	ILE
2	h	17	GLY
6	d	329	GLY
3	o	239	PRO
2	p	17	GLY
2	p	441	THR
3	o	369	PRO
6	l	353	ILE
6	d	243	PRO
4	m	192	ILE

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	f	380/463 (82%)	354 (93%)	26 (7%)	22	71
1	n	380/463 (82%)	353 (93%)	27 (7%)	21	70
2	h	352/473 (74%)	320 (91%)	32 (9%)	14	58
2	p	352/473 (74%)	315 (90%)	37 (10%)	10	50
3	g	373/454 (82%)	334 (90%)	39 (10%)	10	50
3	o	373/454 (82%)	340 (91%)	33 (9%)	14	60
4	e	382/483 (79%)	340 (89%)	42 (11%)	9	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	m	382/483 (79%)	346 (91%)	36 (9%)	13	56
5	b	374/441 (85%)	330 (88%)	44 (12%)	8	43
5	j	374/441 (85%)	339 (91%)	35 (9%)	13	56
6	d	374/454 (82%)	342 (91%)	32 (9%)	15	61
6	l	374/454 (82%)	341 (91%)	33 (9%)	14	60
7	a	375/471 (80%)	347 (92%)	28 (8%)	19	67
7	i	375/471 (80%)	348 (93%)	27 (7%)	21	69
8	c	359/497 (72%)	325 (90%)	34 (10%)	12	55
8	k	359/497 (72%)	320 (89%)	39 (11%)	9	48
All	All	5938/7472 (80%)	5394 (91%)	544 (9%)	13	57

All (544) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	f	19	LEU
1	f	22	ASN
1	f	30	GLN
1	f	35	THR
1	f	56	THR
1	f	72	THR
1	f	75	LEU
1	f	96	CYS
1	f	103	ARG
1	f	107	ARG
1	f	124	ILE
1	f	162	VAL
1	f	187	ASP
1	f	190	ASP
1	f	217	HIS
1	f	237	ASN
1	f	251	PHE
1	f	368	THR
1	f	379	LEU
1	f	390	GLN
1	f	396	ARG
1	f	399	LEU
1	f	453	VAL
1	f	479	ASP
1	f	497	ASP

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Mol	Chain	Res	Type
1	f	499	CYS
2	h	41	MET
2	h	42	CYS
2	h	65	THR
2	h	91	GLN
2	h	95	ASP
2	h	98	ASP
2	h	101	ASN
2	h	102	LEU
2	h	105	ILE
2	h	145	MET
2	h	221	THR
2	h	223	ILE
2	h	245	HIS
2	h	256	ILE
2	h	258	ASN
2	h	264	THR
2	h	277	SER
2	h	333	CYS
2	h	341	LEU
2	h	344	LEU
2	h	348	THR
2	h	354	LEU
2	h	357	THR
2	h	371	PHE
2	h	392	ASN
2	h	403	ASP
2	h	409	LYS
2	h	432	SER
2	h	441	THR
2	h	502	ASP
2	h	519	ASP
2	h	539	LEU
3	g	3	PHE
3	g	10	ILE
3	g	11	VAL
3	g	30	ILE
3	g	37	GLN
3	g	43	THR
3	g	50	ASP
3	g	55	THR
3	g	61	THR

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Mol	Chain	Res	Type
3	g	88	ARG
3	g	96	ASP
3	g	104	LEU
3	g	155	ARG
3	g	158	LEU
3	g	194	LEU
3	g	195	ASP
3	g	196	ASP
3	g	197	LYS
3	g	272	ASP
3	g	277	LEU
3	g	282	LEU
3	g	284	GLN
3	g	291	ASN
3	g	330	VAL
3	g	374	CYS
3	g	377	LEU
3	g	398	MET
3	g	399	ILE
3	g	409	ILE
3	g	410	VAL
3	g	423	CYS
3	g	430	THR
3	g	468	LEU
3	g	485	THR
3	g	488	ILE
3	g	508	ASN
3	g	511	THR
3	g	515	ASN
3	g	521	ASP
4	e	25	MET
4	e	29	PHE
4	e	30	ILE
4	e	37	ASN
4	e	59	SER
4	e	61	ILE
4	e	74	LEU
4	e	82	THR
4	e	92	SER
4	e	107	LEU
4	e	109	LYS
4	e	111	GLN

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Mol	Chain	Res	Type
4	e	125	LEU
4	e	129	LEU
4	e	159	SER
4	e	166	ASP
4	e	168	ILE
4	e	206	GLU
4	e	283	THR
4	e	291	SER
4	e	294	GLU
4	e	329	ASP
4	e	336	LEU
4	e	344	ARG
4	e	381	TYR
4	e	385	PHE
4	e	387	THR
4	e	388	THR
4	e	404	VAL
4	e	406	CYS
4	e	412	ASN
4	e	414	MET
4	e	427	LEU
4	e	429	VAL
4	e	431	ARG
4	e	436	ASP
4	e	455	SER
4	e	464	ILE
4	e	487	SER
4	e	492	ILE
4	e	498	LEU
4	e	552	ASP
5	b	11	THR
5	b	21	SER
5	b	52	ASN
5	b	57	THR
5	b	62	THR
5	b	94	SER
5	b	99	SER
5	b	104	ARG
5	b	115	ILE
5	b	119	THR
5	b	132	LEU
5	b	135	LEU

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Mol	Chain	Res	Type
5	b	141	ASP
5	b	145	ASP
5	b	147	THR
5	b	150	ARG
5	b	195	ILE
5	b	199	LEU
5	b	214	LEU
5	b	237	THR
5	b	240	THR
5	b	241	ASP
5	b	246	PHE
5	b	308	HIS
5	b	316	ARG
5	b	319	LEU
5	b	321	THR
5	b	341	ASP
5	b	365	CYS
5	b	390	VAL
5	b	397	GLU
5	b	400	THR
5	b	402	LEU
5	b	406	CYS
5	b	408	GLU
5	b	416	ASP
5	b	423	ASP
5	b	440	LEU
5	b	452	SER
5	b	459	LEU
5	b	474	LEU
5	b	476	ASN
5	b	509	LEU
5	b	512	ASP
6	d	33	ASP
6	d	36	ARG
6	d	63	THR
6	d	85	GLN
6	d	103	LEU
6	d	123	SER
6	d	124	PHE
6	d	136	LEU
6	d	140	HIS
6	d	150	LEU

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Mol	Chain	Res	Type
6	d	162	ILE
6	d	169	PHE
6	d	181	ILE
6	d	198	LYS
6	d	218	THR
6	d	248	THR
6	d	255	ASN
6	d	266	GLU
6	d	299	ASP
6	d	305	LEU
6	d	312	VAL
6	d	340	THR
6	d	366	ILE
6	d	385	MET
6	d	411	ILE
6	d	440	TRP
6	d	482	ILE
6	d	486	ARG
6	d	502	LEU
6	d	513	GLU
6	d	520	ARG
6	d	522	ASP
7	a	6	ASN
7	a	26	ARG
7	a	47	VAL
7	a	51	LYS
7	a	56	ASP
7	a	61	THR
7	a	68	THR
7	a	86	LEU
7	a	89	GLN
7	a	90	GLN
7	a	92	ARG
7	a	109	LEU
7	a	177	SER
7	a	179	MET
7	a	228	VAL
7	a	320	ARG
7	a	328	ARG
7	a	371	CYS
7	a	377	THR
7	a	392	ASP

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Mol	Chain	Res	Type
7	a	419	VAL
7	a	424	CYS
7	a	426	GLU
7	a	439	THR
7	a	457	ILE
7	a	522	ILE
7	a	535	CYS
7	a	542	ASP
8	c	34	VAL
8	c	52	MET
8	c	58	THR
8	c	78	MET
8	c	79	LEU
8	c	81	LEU
8	c	107	CYS
8	c	130	THR
8	c	138	GLN
8	c	143	VAL
8	c	148	ASP
8	c	154	LEU
8	c	165	ILE
8	c	167	TRP
8	c	199	ASP
8	c	206	VAL
8	c	215	LEU
8	c	245	LEU
8	c	290	VAL
8	c	293	THR
8	c	309	LEU
8	c	310	LEU
8	c	322	LYS
8	c	325	ASN
8	c	354	LEU
8	c	369	ASP
8	c	396	LEU
8	c	398	ASP
8	c	404	ARG
8	c	437	ILE
8	c	468	LEU
8	c	481	THR
8	c	521	LEU
8	c	528	SER

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Mol	Chain	Res	Type
1	n	19	LEU
1	n	24	THR
1	n	30	GLN
1	n	35	THR
1	n	55	LEU
1	n	56	THR
1	n	62	LEU
1	n	72	THR
1	n	96	CYS
1	n	103	ARG
1	n	107	ARG
1	n	124	ILE
1	n	162	VAL
1	n	187	ASP
1	n	217	HIS
1	n	237	ASN
1	n	251	PHE
1	n	368	THR
1	n	371	THR
1	n	379	LEU
1	n	390	GLN
1	n	399	LEU
1	n	453	VAL
1	n	479	ASP
1	n	497	ASP
1	n	499	CYS
1	n	511	ARG
2	p	21	TYR
2	p	25	ASP
2	p	31	SER
2	p	32	ILE
2	p	41	MET
2	p	42	CYS
2	p	45	SER
2	p	62	ILE
2	p	65	THR
2	p	98	ASP
2	p	101	ASN
2	p	102	LEU
2	p	105	ILE
2	p	113	VAL
2	p	145	MET

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Mol	Chain	Res	Type
2	p	221	THR
2	p	223	ILE
2	p	245	HIS
2	p	256	ILE
2	p	258	ASN
2	p	308	LEU
2	p	333	CYS
2	p	341	LEU
2	p	344	LEU
2	p	348	THR
2	p	354	LEU
2	p	357	THR
2	p	358	VAL
2	p	371	PHE
2	p	392	ASN
2	p	409	LYS
2	p	432	SER
2	p	441	THR
2	p	470	ASP
2	p	502	ASP
2	p	519	ASP
2	p	539	LEU
3	o	3	PHE
3	o	10	ILE
3	o	11	VAL
3	o	37	GLN
3	o	43	THR
3	o	50	ASP
3	o	55	THR
3	o	61	THR
3	o	96	ASP
3	o	102	THR
3	o	104	LEU
3	o	155	ARG
3	o	161	CYS
3	o	173	ASN
3	o	194	LEU
3	o	195	ASP
3	o	196	ASP
3	o	268	GLN
3	o	277	LEU
3	o	282	LEU

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Mol	Chain	Res	Type
3	o	284	GLN
3	o	302	LEU
3	o	330	VAL
3	o	374	CYS
3	o	377	LEU
3	o	398	MET
3	o	399	ILE
3	o	409	ILE
3	o	410	VAL
3	o	440	ASN
3	o	485	THR
3	o	488	ILE
3	o	511	THR
4	m	29	PHE
4	m	30	ILE
4	m	37	ASN
4	m	59	SER
4	m	68	ARG
4	m	74	LEU
4	m	82	THR
4	m	89	THR
4	m	92	SER
4	m	107	LEU
4	m	111	GLN
4	m	125	LEU
4	m	166	ASP
4	m	168	ILE
4	m	240	ILE
4	m	283	THR
4	m	294	GLU
4	m	300	THR
4	m	312	ASP
4	m	336	LEU
4	m	344	ARG
4	m	385	PHE
4	m	387	THR
4	m	388	THR
4	m	406	CYS
4	m	412	ASN
4	m	414	MET
4	m	427	LEU
4	m	431	ARG

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Mol	Chain	Res	Type
4	m	436	ASP
4	m	464	ILE
4	m	487	SER
4	m	492	ILE
4	m	498	LEU
4	m	519	SER
4	m	552	ASP
5	j	8	ASP
5	j	21	SER
5	j	31	ASP
5	j	52	ASN
5	j	57	THR
5	j	80	ILE
5	j	104	ARG
5	j	119	THR
5	j	124	TYR
5	j	135	LEU
5	j	141	ASP
5	j	147	THR
5	j	199	LEU
5	j	214	LEU
5	j	226	ILE
5	j	237	THR
5	j	240	THR
5	j	246	PHE
5	j	308	HIS
5	j	319	LEU
5	j	321	THR
5	j	341	ASP
5	j	397	GLU
5	j	402	LEU
5	j	408	GLU
5	j	416	ASP
5	j	423	ASP
5	j	440	LEU
5	j	443	ILE
5	j	455	LEU
5	j	459	LEU
5	j	474	LEU
5	j	476	ASN
5	j	509	LEU
5	j	512	ASP

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Mol	Chain	Res	Type
6	l	36	ARG
6	l	38	SER
6	l	103	LEU
6	l	123	SER
6	l	124	PHE
6	l	140	HIS
6	l	162	ILE
6	l	169	PHE
6	l	170	LEU
6	l	181	ILE
6	l	198	LYS
6	l	209	MET
6	l	218	THR
6	l	248	THR
6	l	251	ASN
6	l	255	ASN
6	l	283	CYS
6	l	312	VAL
6	l	340	THR
6	l	349	LEU
6	l	364	THR
6	l	366	ILE
6	l	375	VAL
6	l	385	MET
6	l	411	ILE
6	l	440	TRP
6	l	467	THR
6	l	482	ILE
6	l	486	ARG
6	l	502	LEU
6	l	513	GLU
6	l	520	ARG
6	l	522	ASP
7	i	26	ARG
7	i	47	VAL
7	i	56	ASP
7	i	61	THR
7	i	68	THR
7	i	86	LEU
7	i	89	GLN
7	i	90	GLN
7	i	92	ARG

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Mol	Chain	Res	Type
7	i	281	VAL
7	i	319	ARG
7	i	320	ARG
7	i	328	ARG
7	i	337	LEU
7	i	373	LEU
7	i	377	THR
7	i	392	ASP
7	i	407	SER
7	i	419	VAL
7	i	424	CYS
7	i	426	GLU
7	i	438	THR
7	i	442	SER
7	i	457	ILE
7	i	542	ASP
7	i	543	THR
7	i	546	THR
8	k	23	SER
8	k	34	VAL
8	k	52	MET
8	k	58	THR
8	k	78	MET
8	k	79	LEU
8	k	81	LEU
8	k	102	GLU
8	k	107	CYS
8	k	130	THR
8	k	138	GLN
8	k	143	VAL
8	k	148	ASP
8	k	154	LEU
8	k	167	TRP
8	k	206	VAL
8	k	215	LEU
8	k	251	GLU
8	k	257	SER
8	k	260	ASN
8	k	290	VAL
8	k	293	THR
8	k	309	LEU
8	k	310	LEU

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Mol	Chain	Res	Type
8	k	322	LYS
8	k	325	ASN
8	k	335	THR
8	k	336	ILE
8	k	348	VAL
8	k	354	LEU
8	k	396	LEU
8	k	398	ASP
8	k	404	ARG
8	k	438	GLN
8	k	468	LEU
8	k	481	THR
8	k	504	VAL
8	k	516	SER
8	k	521	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 48 ligands modelled in this entry, 16 are monoatomic - leaving 32 for Mogul analysis.

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	$\# Z > 2$
10	ADP	a	602	9,11	29,29,29	1.08	2 (6%)	45,45,45	1.83	8 (17%)
11	BEF	a	603	10	0,3,3	0.00	-	0,3,3	0.00	-
10	ADP	b	602	11,9	29,29,29	1.13	2 (6%)	45,45,45	1.70	8 (17%)
11	BEF	b	603	10	0,3,3	0.00	-	0,3,3	0.00	-
10	ADP	c	602	11,9	29,29,29	1.05	2 (6%)	45,45,45	1.72	7 (15%)
11	BEF	c	603	10	0,3,3	0.00	-	0,3,3	0.00	-
10	ADP	d	602	11,9	29,29,29	1.08	2 (6%)	45,45,45	1.77	8 (17%)
11	BEF	d	603	10	0,3,3	0.00	-	0,3,3	0.00	-
10	ADP	e	602	11,9	29,29,29	1.05	2 (6%)	45,45,45	1.81	8 (17%)
11	BEF	e	603	10	0,3,3	0.00	-	0,3,3	0.00	-
10	ADP	f	602	11,9	29,29,29	1.10	1 (3%)	45,45,45	1.89	8 (17%)
11	BEF	f	603	10	0,3,3	0.00	-	0,3,3	0.00	-
10	ADP	g	602	9	29,29,29	1.10	2 (6%)	45,45,45	1.83	9 (20%)
11	BEF	g	603	-	0,3,3	0.00	-	0,3,3	0.00	-
10	ADP	h	602	9	29,29,29	1.05	2 (6%)	45,45,45	1.79	7 (15%)
11	BEF	h	603	-	0,3,3	0.00	-	0,3,3	0.00	-
10	ADP	i	602	11,9	29,29,29	1.04	2 (6%)	45,45,45	1.85	8 (17%)
11	BEF	i	603	10	0,3,3	0.00	-	0,3,3	0.00	-
10	ADP	j	602	11,9	29,29,29	1.17	2 (6%)	45,45,45	1.74	8 (17%)
11	BEF	j	603	10	0,3,3	0.00	-	0,3,3	0.00	-
10	ADP	k	602	11,9	29,29,29	1.05	2 (6%)	45,45,45	1.84	7 (15%)
11	BEF	k	603	10	0,3,3	0.00	-	0,3,3	0.00	-
10	ADP	l	602	11,9	29,29,29	1.05	2 (6%)	45,45,45	1.83	8 (17%)
11	BEF	l	603	10	0,3,3	0.00	-	0,3,3	0.00	-
10	ADP	m	602	9,11	29,29,29	1.09	2 (6%)	45,45,45	1.83	7 (15%)
11	BEF	m	603	10	0,3,3	0.00	-	0,3,3	0.00	-
10	ADP	n	602	11,9	29,29,29	1.09	2 (6%)	45,45,45	1.77	8 (17%)
11	BEF	n	603	10	0,3,3	0.00	-	0,3,3	0.00	-
10	ADP	o	602	9	29,29,29	1.09	2 (6%)	45,45,45	1.94	9 (20%)
11	BEF	o	603	-	0,3,3	0.00	-	0,3,3	0.00	-
10	ADP	p	602	9	29,29,29	1.03	2 (6%)	45,45,45	1.93	8 (17%)
11	BEF	p	603	-	0,3,3	0.00	-	0,3,3	0.00	-

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
10	ADP	a	602	9,11	-	0/16/32/32	0/1/3/3
11	BEF	a	603	10	-	0/0/0/0	0/0/0/0
10	ADP	b	602	11,9	-	0/16/32/32	0/1/3/3
11	BEF	b	603	10	-	0/0/0/0	0/0/0/0
10	ADP	c	602	11,9	-	0/16/32/32	0/1/3/3
11	BEF	c	603	10	-	0/0/0/0	0/0/0/0
10	ADP	d	602	11,9	-	0/16/32/32	0/1/3/3
11	BEF	d	603	10	-	0/0/0/0	0/0/0/0
10	ADP	e	602	11,9	-	0/16/32/32	0/1/3/3
11	BEF	e	603	10	-	0/0/0/0	0/0/0/0
10	ADP	f	602	11,9	-	0/16/32/32	0/1/3/3
11	BEF	f	603	10	-	0/0/0/0	0/0/0/0
10	ADP	g	602	9	-	0/16/32/32	0/1/3/3
11	BEF	g	603	-	-	0/0/0/0	0/0/0/0
10	ADP	h	602	9	-	0/16/32/32	0/1/3/3
11	BEF	h	603	-	-	0/0/0/0	0/0/0/0
10	ADP	i	602	11,9	-	0/16/32/32	0/1/3/3
11	BEF	i	603	10	-	0/0/0/0	0/0/0/0
10	ADP	j	602	11,9	-	0/16/32/32	0/1/3/3
11	BEF	j	603	10	-	0/0/0/0	0/0/0/0
10	ADP	k	602	11,9	-	0/16/32/32	0/1/3/3
11	BEF	k	603	10	-	0/0/0/0	0/0/0/0
10	ADP	l	602	11,9	-	0/16/32/32	0/1/3/3
11	BEF	l	603	10	-	0/0/0/0	0/0/0/0
10	ADP	m	602	9,11	-	0/16/32/32	0/1/3/3
11	BEF	m	603	10	-	0/0/0/0	0/0/0/0
10	ADP	n	602	11,9	-	0/16/32/32	0/1/3/3
11	BEF	n	603	10	-	0/0/0/0	0/0/0/0
10	ADP	o	602	9	-	0/16/32/32	0/1/3/3
11	BEF	o	603	-	-	0/0/0/0	0/0/0/0
10	ADP	p	602	9	-	0/16/32/32	0/1/3/3
11	BEF	p	603	-	-	0/0/0/0	0/0/0/0

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	f	602	ADP	C5-C4	3.42	1.48	1.40
10	m	602	ADP	C5-C4	3.38	1.48	1.40
10	n	602	ADP	C5-C4	3.37	1.48	1.40
10	b	602	ADP	C5-C4	3.33	1.48	1.40
10	k	602	ADP	C5-C4	3.30	1.47	1.40
10	j	602	ADP	C5-C4	3.27	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	l	602	ADP	C5-C4	3.26	1.47	1.40
10	c	602	ADP	C5-C4	3.23	1.47	1.40
10	g	602	ADP	C5-C4	3.22	1.47	1.40
10	i	602	ADP	C5-C4	3.17	1.47	1.40
10	o	602	ADP	C5-C4	3.16	1.47	1.40
10	e	602	ADP	C5-C4	3.15	1.47	1.40
10	a	602	ADP	C5-C4	3.12	1.47	1.40
10	p	602	ADP	C5-C4	3.09	1.47	1.40
10	d	602	ADP	C5-C4	3.05	1.47	1.40
10	h	602	ADP	C5-C4	3.05	1.47	1.40
10	j	602	ADP	C4-N9	-2.92	1.33	1.37
10	d	602	ADP	C4-N9	-2.92	1.33	1.37
10	b	602	ADP	C4-N9	-2.72	1.33	1.37
10	c	602	ADP	C4-N9	-2.64	1.33	1.37
10	a	602	ADP	C4-N9	-2.63	1.33	1.37
10	e	602	ADP	C4-N9	-2.59	1.34	1.37
10	k	602	ADP	C4-N9	-2.44	1.34	1.37
10	l	602	ADP	C4-N9	-2.44	1.34	1.37
10	g	602	ADP	C4-N9	-2.42	1.34	1.37
10	h	602	ADP	C4-N9	-2.38	1.34	1.37
10	n	602	ADP	C4-N9	-2.30	1.34	1.37
10	o	602	ADP	C4-N9	-2.21	1.34	1.37
10	p	602	ADP	C4-N9	-2.19	1.34	1.37
10	i	602	ADP	C4-N9	-2.16	1.34	1.37
10	m	602	ADP	C4-N9	-2.08	1.34	1.37

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	h	602	ADP	N3-C2-N1	-6.64	123.15	128.71
10	p	602	ADP	N3-C2-N1	-6.63	123.17	128.71
10	o	602	ADP	N3-C2-N1	-6.53	123.25	128.71
10	a	602	ADP	N3-C2-N1	-6.51	123.27	128.71
10	l	602	ADP	N3-C2-N1	-6.49	123.28	128.71
10	i	602	ADP	N3-C2-N1	-6.42	123.34	128.71
10	g	602	ADP	N3-C2-N1	-6.38	123.38	128.71
10	n	602	ADP	N3-C2-N1	-6.31	123.43	128.71
10	m	602	ADP	N3-C2-N1	-6.28	123.46	128.71
10	d	602	ADP	N3-C2-N1	-6.26	123.47	128.71
10	f	602	ADP	N3-C2-N1	-6.20	123.53	128.71
10	k	602	ADP	N3-C2-N1	-6.11	123.60	128.71
10	j	602	ADP	N3-C2-N1	-6.11	123.60	128.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	e	602	ADP	N3-C2-N1	-6.04	123.66	128.71
10	b	602	ADP	N3-C2-N1	-5.81	123.85	128.71
10	m	602	ADP	N3-C4-N9	5.71	135.73	125.43
10	c	602	ADP	N3-C2-N1	-5.68	123.96	128.71
10	p	602	ADP	N3-C4-N9	5.63	135.59	125.43
10	h	602	ADP	N3-C4-N9	5.48	135.33	125.43
10	f	602	ADP	N3-C4-N9	5.43	135.25	125.43
10	j	602	ADP	N3-C4-N9	5.38	135.15	125.43
10	g	602	ADP	N3-C4-N9	5.36	135.10	125.43
10	o	602	ADP	N3-C4-N9	5.35	135.10	125.43
10	e	602	ADP	N3-C4-N9	5.33	135.06	125.43
10	i	602	ADP	N3-C4-N9	5.31	135.03	125.43
10	d	602	ADP	N3-C4-N9	5.26	134.94	125.43
10	l	602	ADP	N3-C4-N9	5.24	134.89	125.43
10	c	602	ADP	N3-C4-N9	5.23	134.87	125.43
10	k	602	ADP	N3-C4-N9	5.22	134.86	125.43
10	b	602	ADP	N3-C4-N9	5.21	134.83	125.43
10	a	602	ADP	N3-C4-N9	5.18	134.79	125.43
10	n	602	ADP	N3-C4-N9	5.16	134.76	125.43
10	f	602	ADP	O4'-C1'-N9	4.74	112.84	108.44
10	p	602	ADP	O4'-C1'-N9	4.06	112.22	108.44
10	o	602	ADP	O4'-C1'-N9	3.97	112.14	108.44
10	k	602	ADP	PA-O3A-PB	-3.79	120.58	131.68
10	e	602	ADP	C4-C5-N7	-3.67	106.38	109.52
10	a	602	ADP	C4-C5-N7	-3.67	106.38	109.52
10	p	602	ADP	C4-C5-N7	-3.63	106.41	109.52
10	n	602	ADP	C4-C5-N7	-3.63	106.41	109.52
10	f	602	ADP	C4-C5-N7	-3.56	106.47	109.52
10	i	602	ADP	C5-C4-N3	-3.55	117.97	125.70
10	b	602	ADP	C4-C5-N7	-3.54	106.49	109.52
10	g	602	ADP	C3'-C2'-C1'	3.54	106.45	100.91
10	i	602	ADP	C4-C5-N7	-3.53	106.50	109.52
10	o	602	ADP	C4-C5-N7	-3.53	106.50	109.52
10	f	602	ADP	C5-C4-N3	-3.52	118.03	125.70
10	p	602	ADP	C5-C4-N3	-3.51	118.05	125.70
10	m	602	ADP	C5-C4-N3	-3.51	118.06	125.70
10	c	602	ADP	C4-C5-N7	-3.49	106.53	109.52
10	o	602	ADP	C5-C4-N3	-3.49	118.11	125.70
10	i	602	ADP	C3'-C2'-C1'	3.46	106.32	100.91
10	m	602	ADP	C4-C5-N7	-3.45	106.57	109.52
10	h	602	ADP	C4-C5-N7	-3.45	106.57	109.52
10	o	602	ADP	C3'-C2'-C1'	3.42	106.26	100.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	k	602	ADP	C4-C5-N7	-3.40	106.61	109.52
10	h	602	ADP	C5-C4-N3	-3.39	118.31	125.70
10	e	602	ADP	C5-C4-N3	-3.35	118.40	125.70
10	l	602	ADP	C3'-C2'-C1'	3.35	106.14	100.91
10	g	602	ADP	C5-C4-N3	-3.33	118.44	125.70
10	d	602	ADP	C4-C5-N7	-3.33	106.67	109.52
10	l	602	ADP	C4-C5-N7	-3.33	106.67	109.52
10	k	602	ADP	C5-C4-N3	-3.29	118.53	125.70
10	a	602	ADP	C5-C4-N3	-3.28	118.55	125.70
10	n	602	ADP	C5-C4-N3	-3.27	118.59	125.70
10	c	602	ADP	C5-C4-N3	-3.26	118.61	125.70
10	l	602	ADP	C5-C4-N3	-3.22	118.69	125.70
10	b	602	ADP	C5-C4-N3	-3.21	118.71	125.70
10	c	602	ADP	PA-O3A-PB	-3.17	122.39	131.68
10	m	602	ADP	C3'-C2'-C1'	3.14	105.82	100.91
10	e	602	ADP	C3'-C2'-C1'	3.11	105.77	100.91
10	g	602	ADP	C4-C5-N7	-3.07	106.89	109.52
10	k	602	ADP	C3'-C2'-C1'	3.06	105.69	100.91
10	j	602	ADP	C5-C4-N3	-3.05	119.05	125.70
10	d	602	ADP	C5-C4-N3	-3.05	119.06	125.70
10	p	602	ADP	C3'-C2'-C1'	3.01	105.62	100.91
10	f	602	ADP	C3'-C2'-C1'	2.98	105.57	100.91
10	e	602	ADP	PA-O3A-PB	-2.89	123.19	131.68
10	i	602	ADP	PA-O3A-PB	-2.78	123.54	131.68
10	b	602	ADP	C3'-C2'-C1'	2.77	105.25	100.91
10	o	602	ADP	PA-O3A-PB	-2.77	123.56	131.68
10	a	602	ADP	PA-O3A-PB	-2.77	123.57	131.68
10	p	602	ADP	C2-N3-C4	2.74	121.82	114.01
10	d	602	ADP	C8-N9-C4	2.74	108.99	106.90
10	i	602	ADP	C2-N3-C4	2.73	121.79	114.01
10	o	602	ADP	C2-N3-C4	2.71	121.74	114.01
10	h	602	ADP	C3'-C2'-C1'	2.71	105.15	100.91
10	h	602	ADP	C2-N3-C4	2.69	121.67	114.01
10	g	602	ADP	O4'-C1'-N9	2.68	110.94	108.44
10	j	602	ADP	C4-C5-N7	-2.68	107.23	109.52
10	m	602	ADP	C2-N3-C4	2.66	121.58	114.01
10	a	602	ADP	C2-N3-C4	2.64	121.53	114.01
10	l	602	ADP	PA-O3A-PB	-2.62	124.00	131.68
10	f	602	ADP	C2-N3-C4	2.61	121.45	114.01
10	j	602	ADP	C3'-C2'-C1'	2.60	104.98	100.91
10	i	602	ADP	O4'-C1'-N9	2.60	110.86	108.44
10	c	602	ADP	C3'-C2'-C1'	2.57	104.93	100.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	d	602	ADP	C3'-C2'-C1'	2.56	104.92	100.91
10	g	602	ADP	PA-O3A-PB	-2.56	124.18	131.68
10	p	602	ADP	PA-O3A-PB	-2.56	124.19	131.68
10	e	602	ADP	C2-N3-C4	2.55	121.28	114.01
10	l	602	ADP	C2-N3-C4	2.55	121.26	114.01
10	n	602	ADP	C2-N3-C4	2.54	121.24	114.01
10	g	602	ADP	C2-N3-C4	2.53	121.20	114.01
10	d	602	ADP	PA-O3A-PB	-2.51	124.32	131.68
10	a	602	ADP	C3'-C2'-C1'	2.49	104.81	100.91
10	n	602	ADP	C3'-C2'-C1'	2.49	104.80	100.91
10	k	602	ADP	C2-N3-C4	2.48	121.08	114.01
10	d	602	ADP	C2-N3-C4	2.43	120.92	114.01
10	m	602	ADP	C4'-O4'-C1'	2.42	112.38	109.75
10	b	602	ADP	C2-N3-C4	2.38	120.79	114.01
10	o	602	ADP	C4'-O4'-C1'	2.35	112.30	109.75
10	j	602	ADP	C2-N3-C4	2.34	120.66	114.01
10	c	602	ADP	C2-N3-C4	2.32	120.63	114.01
10	f	602	ADP	PA-O3A-PB	-2.29	124.98	131.68
10	j	602	ADP	C8-N9-C4	2.27	108.63	106.90
10	n	602	ADP	PA-O3A-PB	-2.25	125.08	131.68
10	b	602	ADP	PA-O3A-PB	-2.13	125.43	131.68
10	g	602	ADP	C4'-O4'-C1'	2.13	112.06	109.75
10	n	602	ADP	O4'-C1'-N9	2.10	110.40	108.44
10	a	602	ADP	O4'-C1'-N9	2.07	110.37	108.44
10	j	602	ADP	PA-O3A-PB	-2.05	125.67	131.68
10	b	602	ADP	C4'-O4'-C1'	2.04	111.97	109.75
10	l	602	ADP	C4'-O4'-C1'	2.04	111.97	109.75
10	h	602	ADP	PA-O3A-PB	-2.03	125.72	131.68
10	e	602	ADP	C4'-O4'-C1'	2.02	111.95	109.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	f	538/546 (98%)	0.46	22 (4%)	35	24	132, 160, 198, 229	0
1	n	538/546 (98%)	0.41	10 (1%)	64	42	112, 129, 161, 201	0
2	h	521/568 (91%)	0.52	24 (4%)	31	22	133, 160, 194, 273	0
2	p	521/568 (91%)	0.39	14 (2%)	52	34	101, 140, 177, 203	0
3	g	526/550 (95%)	0.41	17 (3%)	45	30	115, 141, 181, 238	0
3	o	526/550 (95%)	0.41	10 (1%)	64	42	99, 128, 174, 247	0
4	e	535/562 (95%)	0.37	8 (1%)	70	48	100, 124, 173, 249	0
4	m	535/562 (95%)	0.37	8 (1%)	70	48	94, 113, 161, 235	0
5	b	518/527 (98%)	0.33	2 (0%)	90	79	100, 116, 141, 176	0
5	j	518/527 (98%)	0.32	0	100	100	90, 110, 131, 155	0
6	d	523/528 (99%)	0.40	18 (3%)	43	29	112, 136, 166, 182	0
6	l	523/528 (99%)	0.35	10 (1%)	64	42	103, 129, 170, 196	0
7	a	539/559 (96%)	0.47	17 (3%)	45	30	112, 135, 177, 208	0
7	i	539/559 (96%)	0.41	16 (2%)	48	31	101, 132, 185, 212	0
8	c	513/590 (86%)	0.49	15 (2%)	49	32	121, 143, 186, 223	0
8	k	513/590 (86%)	0.47	17 (3%)	44	29	114, 131, 176, 246	0
All	All	8426/8860 (95%)	0.41	208 (2%)	54	36	90, 133, 180, 273	0

All (208) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	o	4	GLY	4.9
4	m	25	MET	4.9
8	c	384	GLY	4.4
4	e	25	MET	4.3
3	g	362	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
1	n	250	GLY	4.1
3	g	157	LEU	4.0
7	a	349	THR	4.0
8	k	304	LEU	3.9
1	f	11	GLU	3.7
3	o	412	GLY	3.7
4	e	69	GLY	3.6
7	i	4	LEU	3.5
7	a	425	VAL	3.5
1	n	527	LEU	3.5
6	d	44	MET	3.5
3	g	364	LEU	3.5
8	k	6	VAL	3.4
4	e	510	ILE	3.4
2	p	201	TYR	3.3
2	h	110	LEU	3.3
2	p	386	LEU	3.3
2	h	149	GLU	3.3
6	l	371	ALA	3.3
7	a	348	GLU	3.2
6	d	350	VAL	3.2
8	k	8	MET	3.1
7	a	485	GLN	3.1
2	h	13	LEU	3.1
7	a	472	GLU	3.1
7	a	505	ILE	3.1
7	a	524	LYS	3.0
5	b	45	LEU	3.0
3	g	104	LEU	3.0
2	h	456	PHE	3.0
4	m	464	ILE	2.9
7	a	466	ALA	2.9
1	n	534	LEU	2.9
3	o	147	ILE	2.9
1	f	517	ILE	2.9
2	p	167	ILE	2.9
8	k	49	LEU	2.9
8	k	210	PRO	2.8
2	h	389	ALA	2.8
1	f	233	VAL	2.8
6	d	361	VAL	2.8
4	m	180	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	h	217	LEU	2.7
4	e	212	MET	2.7
3	o	3	PHE	2.7
8	c	474	LYS	2.7
2	h	46	MET	2.6
3	g	482	VAL	2.6
1	f	236	LEU	2.6
1	f	158	LEU	2.6
7	a	484	SER	2.6
6	l	312	VAL	2.6
6	l	478	LEU	2.6
8	c	80	GLU	2.6
6	l	115	ILE	2.6
3	o	439	ILE	2.6
3	g	382	ALA	2.6
1	f	508	ASP	2.5
2	h	548	LYS	2.5
8	k	281	GLN	2.5
8	k	364	TYR	2.5
6	d	412	ALA	2.5
1	f	533	LEU	2.5
8	c	8	MET	2.5
8	k	449	MET	2.5
2	h	14	PHE	2.5
6	l	311	MET	2.5
2	h	499	VAL	2.5
7	i	264	ILE	2.5
7	i	538	ILE	2.5
6	d	349	LEU	2.5
2	h	459	VAL	2.5
6	l	310	ILE	2.5
3	o	148	THR	2.5
2	h	133	MET	2.5
1	n	359	ILE	2.4
1	n	56	THR	2.4
2	p	6	PRO	2.4
1	f	66	MET	2.4
3	g	161	CYS	2.4
1	n	287	MET	2.4
8	c	437	ILE	2.4
8	k	70	VAL	2.4
2	h	191	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
7	a	244	ILE	2.4
2	h	463	LEU	2.4
7	a	264	ILE	2.4
8	c	526	ILE	2.4
1	f	337	GLN	2.4
8	k	238	ILE	2.4
3	g	502	VAL	2.3
1	f	278	ILE	2.3
7	i	393	TYR	2.3
7	i	169	ILE	2.3
4	m	393	LEU	2.3
5	b	402	LEU	2.3
6	d	219	ALA	2.3
1	n	354	VAL	2.3
7	a	119	LYS	2.3
3	o	462	ILE	2.3
6	l	447	LEU	2.3
7	i	14	PHE	2.3
3	g	446	LEU	2.3
8	c	224	LEU	2.3
1	f	170	LEU	2.3
8	c	308	TYR	2.3
3	g	481	VAL	2.3
1	f	378	ILE	2.3
1	n	235	ILE	2.2
6	d	56	ILE	2.2
8	c	261	ILE	2.2
7	a	293	ALA	2.2
3	g	117	GLU	2.2
1	f	427	ARG	2.2
6	d	447	LEU	2.2
6	d	502	LEU	2.2
1	f	196	ILE	2.2
4	m	386	GLY	2.2
4	e	225	LYS	2.2
1	f	534	LEU	2.2
4	e	539	LEU	2.2
7	i	539	LEU	2.2
1	n	2	SER	2.2
2	h	249	VAL	2.2
8	k	163	TYR	2.2
7	a	501	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
8	k	125	LEU	2.2
6	d	9	ALA	2.2
7	i	524	LYS	2.2
1	f	75	LEU	2.2
1	f	234	LEU	2.2
8	k	325	ASN	2.2
2	p	7	GLN	2.2
2	h	455	ALA	2.2
3	g	170	LEU	2.2
8	k	14	ARG	2.2
8	c	438	GLN	2.2
1	f	366	TYR	2.2
2	h	85	LEU	2.2
2	h	118	ILE	2.2
8	c	102	GLU	2.1
7	i	317	GLY	2.1
6	d	498	LEU	2.1
8	k	159	ILE	2.1
1	f	10	ALA	2.1
4	m	60	ILE	2.1
7	i	433	LEU	2.1
3	g	227	ALA	2.1
2	p	384	ILE	2.1
7	i	307	LEU	2.1
7	i	518	LEU	2.1
2	h	273	MET	2.1
7	a	82	ILE	2.1
2	p	309	ALA	2.1
6	d	257	TYR	2.1
6	l	46	LYS	2.1
4	e	28	PRO	2.1
2	p	478	LEU	2.1
2	p	518	TYR	2.1
1	n	412	ILE	2.1
7	i	282	LEU	2.1
1	f	91	THR	2.1
2	p	35	ILE	2.1
6	d	46	LYS	2.1
2	h	318	ILE	2.1
8	c	95	THR	2.1
2	p	250	PHE	2.1
6	d	268	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
6	d	380	ARG	2.1
3	o	40	LEU	2.1
2	p	117	LEU	2.1
4	m	555	ILE	2.1
2	p	308	LEU	2.1
3	g	248	LEU	2.1
7	i	289	ILE	2.1
2	p	342	PRO	2.1
3	o	377	LEU	2.1
7	a	426	GLU	2.0
8	c	250	LEU	2.0
7	i	119	LYS	2.0
2	h	55	ILE	2.0
8	c	10	ALA	2.0
8	c	370	ASN	2.0
6	d	103	LEU	2.0
6	d	236	LEU	2.0
8	k	527	VAL	2.0
1	f	527	LEU	2.0
2	h	342	PRO	2.0
3	g	363	ASN	2.0
8	k	484	ILE	2.0
2	h	381	THR	2.0
6	l	324	LEU	2.0
3	g	293	VAL	2.0
3	o	481	VAL	2.0
7	i	385	ILE	2.0
6	d	204	ILE	2.0
7	a	365	LYS	2.0
1	f	245	THR	2.0
4	m	544	LEU	2.0
2	h	32	ILE	2.0
4	e	31	ILE	2.0
3	g	483	PHE	2.0
6	l	236	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
9	MG	i	601	1/1	0.49	1.07	111,111,111,111	0
11	BEF	g	603	4/4	0.26	0.25	128,132,132,134	0
11	BEF	j	603	4/4	0.26	0.01	93,94,94,96	0
10	ADP	i	602	27/27	0.33	-0.09	113,121,126,127	0
10	ADP	h	602	27/27	0.34	-0.10	152,159,166,167	0
10	ADP	f	602	27/27	0.35	-0.13	149,154,159,160	0
10	ADP	k	602	27/27	0.31	-0.17	115,117,120,121	0
10	ADP	b	602	27/27	0.30	-0.22	104,109,115,115	0
10	ADP	m	602	27/27	0.29	-0.26	102,106,108,109	0
10	ADP	e	602	27/27	0.26	-0.32	117,124,127,128	0
9	MG	h	601	1/1	0.23	-0.33	151,151,151,151	0
11	BEF	m	603	4/4	0.23	-0.36	99,100,101,103	0
10	ADP	d	602	27/27	0.27	-0.39	125,135,149,151	0
11	BEF	p	603	4/4	0.25	-0.41	130,132,133,133	0
10	ADP	j	602	27/27	0.28	-0.43	94,100,106,107	0
10	ADP	a	602	27/27	0.26	-0.43	126,139,146,148	0
11	BEF	b	603	4/4	0.23	-0.50	103,105,105,107	0
10	ADP	o	602	27/27	0.28	-0.50	119,128,133,134	0
10	ADP	n	602	27/27	0.30	-0.59	112,116,123,124	0
10	ADP	l	602	27/27	0.24	-0.60	117,129,144,145	0
10	ADP	g	602	27/27	0.27	-0.61	132,141,149,150	0
10	ADP	p	602	27/27	0.26	-0.62	133,145,154,156	0
11	BEF	f	603	4/4	0.20	-0.73	152,152,154,156	0
11	BEF	h	603	4/4	0.17	-0.83	55,55,55,55	0
10	ADP	c	602	27/27	0.23	-0.92	134,138,142,143	0
11	BEF	i	603	4/4	0.18	-0.94	104,105,105,106	0
11	BEF	o	603	4/4	0.19	-0.98	116,118,119,119	0
9	MG	o	601	1/1	0.18	-0.98	115,115,115,115	0
11	BEF	e	603	4/4	0.18	-0.99	114,114,116,118	0
11	BEF	l	603	4/4	0.18	-1.05	107,110,111,111	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	MG	b	601	1/1	0.21	-1.07	97,97,97,97	0
11	BEF	d	603	4/4	0.19	-1.26	116,120,121,121	0
9	MG	c	601	1/1	0.17	-1.35	129,129,129,129	0
11	BEF	k	603	4/4	0.16	-1.43	110,111,111,112	0
9	MG	j	601	1/1	0.15	-1.46	88,88,88,88	0
9	MG	d	601	1/1	0.16	-1.47	115,115,115,115	0
9	MG	l	601	1/1	0.13	-1.59	107,107,107,107	0
9	MG	g	601	1/1	0.24	-1.65	129,129,129,129	0
11	BEF	a	603	4/4	0.12	-1.75	118,120,121,121	0
11	BEF	n	603	4/4	0.19	-1.80	115,115,116,118	0
9	MG	f	601	1/1	0.20	-1.84	143,143,143,143	0
11	BEF	c	603	4/4	0.15	-1.85	126,127,127,129	0
9	MG	n	601	1/1	0.18	-2.15	108,108,108,108	0
9	MG	p	601	1/1	0.17	-2.17	131,131,131,131	0
9	MG	k	601	1/1	0.17	-2.25	111,111,111,111	0
9	MG	e	601	1/1	0.14	-2.31	102,102,102,102	0
9	MG	m	601	1/1	0.13	-2.33	84,84,84,84	0
9	MG	a	601	1/1	0.12	-2.52	126,126,126,126	0

6.5 Other polymers ⓘ

There are no such residues in this entry.