



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2014 – 05:55 PM BST

PDB ID : 4D8Q
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>

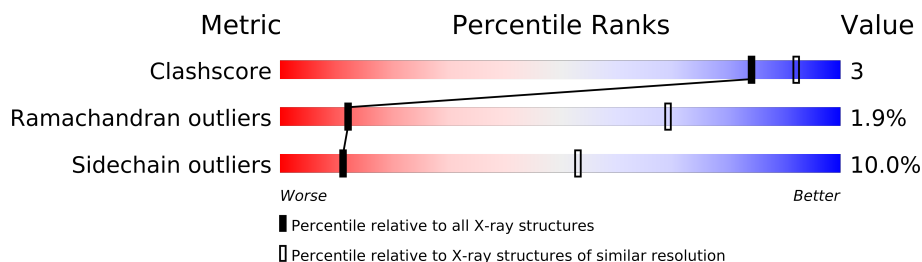
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23004

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))
Clashscore	79885	1100 (4.10-3.50)
Ramachandran outliers	78287	1050 (4.10-3.50)
Sidechain outliers	78261	1042 (4.10-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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.

Note EDS was not executed.

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	
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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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).

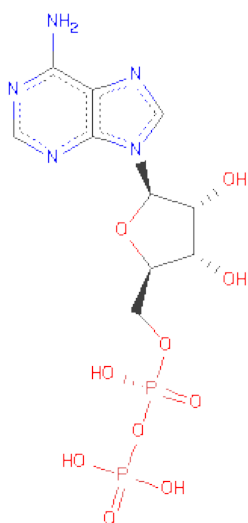
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	P	1	Total Mg 1 1	0	0
9	G	1	Total Mg 1 1	0	0
9	J	1	Total Mg 1 1	0	0
9	D	1	Total Mg 1 1	0	0
9	K	1	Total Mg 1 1	0	0
9	E	1	Total Mg 1 1	0	0
9	H	1	Total Mg 1 1	0	0

Continued on next page...

Continued from previous page...

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: $C_{10}H_{15}N_5O_{10}P_2$).



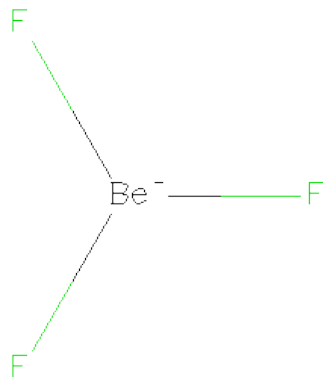
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	F	1	Total	C	N	O	P	
			27	10	5	10	2	0
10	H	1	Total	C	N	O	P	
			27	10	5	10	2	0

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

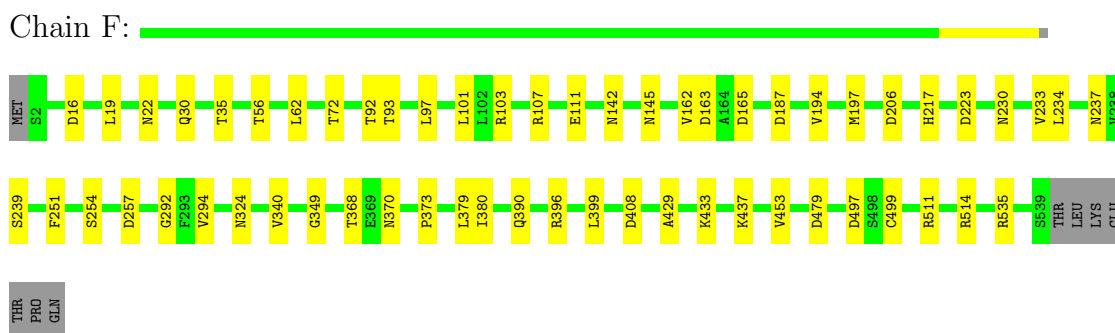
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	I	1	Total 4	Be 1	F 3	0	0
11	K	1	Total 4	Be 1	F 3	0	0

3 Residue-property plots

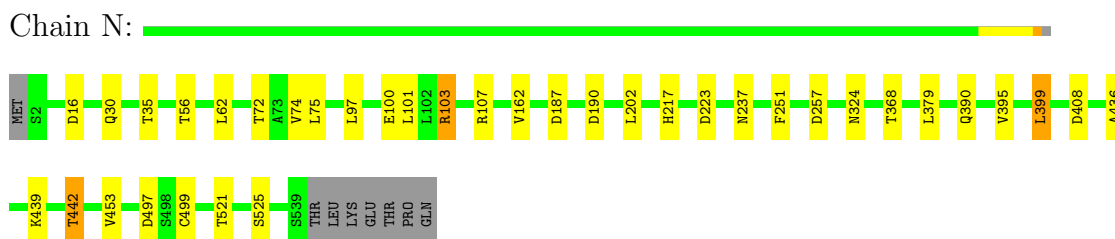
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

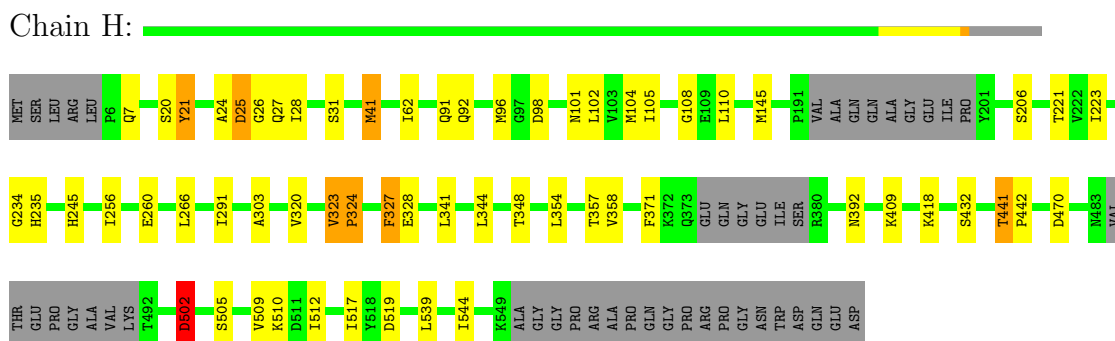
- Molecule 1: T-complex protein 1 subunit zeta



- Molecule 1: T-complex protein 1 subunit zeta

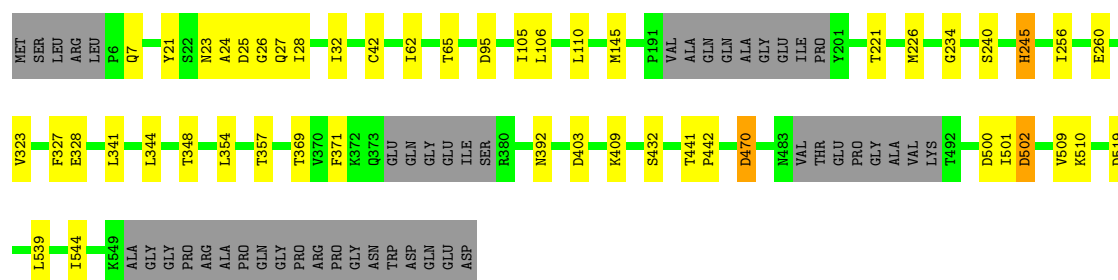


- Molecule 2: T-complex protein 1 subunit theta



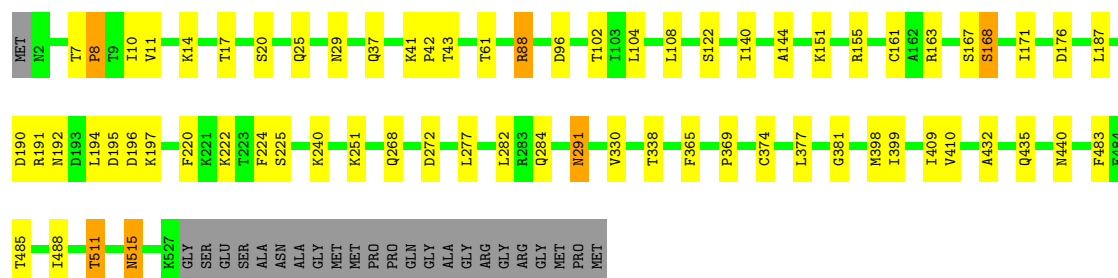
- Molecule 2: T-complex protein 1 subunit theta





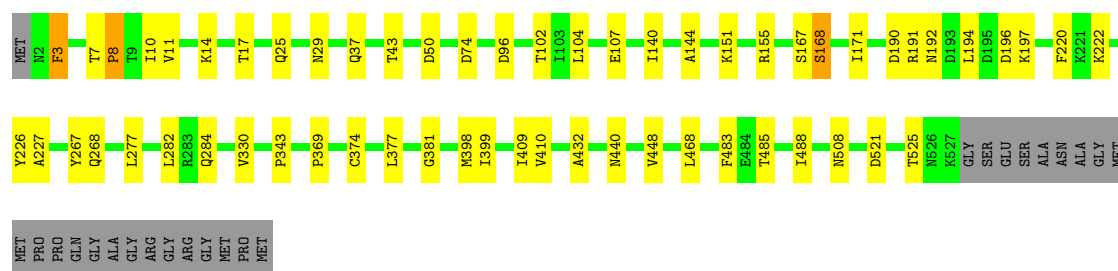
- Molecule 3: T-complex protein 1 subunit eta

Chain G:



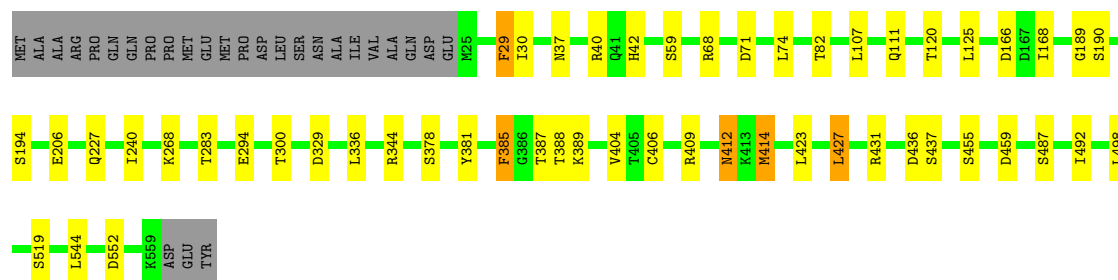
- Molecule 3: T-complex protein 1 subunit eta

Chain O:



- Molecule 4: T-complex protein 1 subunit epsilon

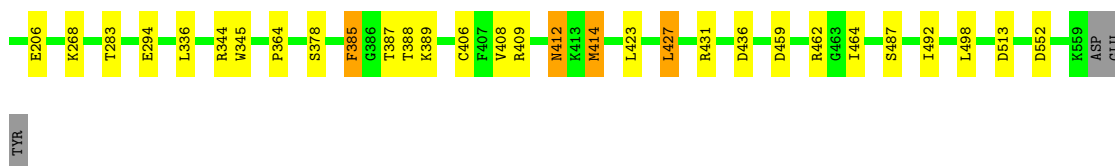
Chain E:



- Molecule 4: T-complex protein 1 subunit epsilon

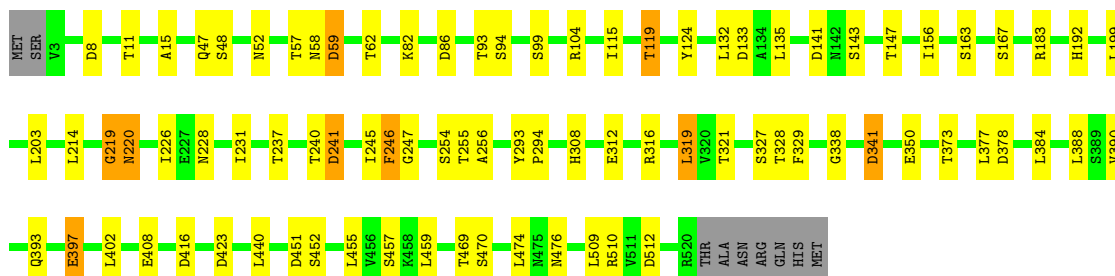
Chain M:





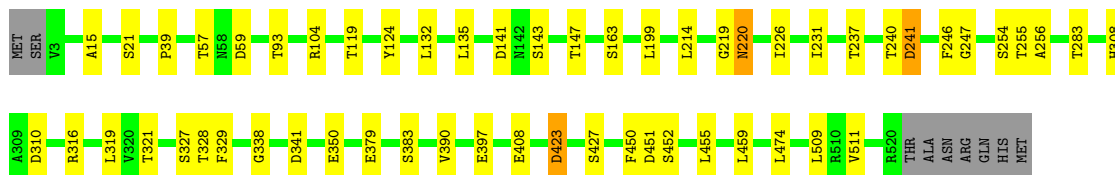
- Molecule 5: T-complex protein 1 subunit beta

Chain B:



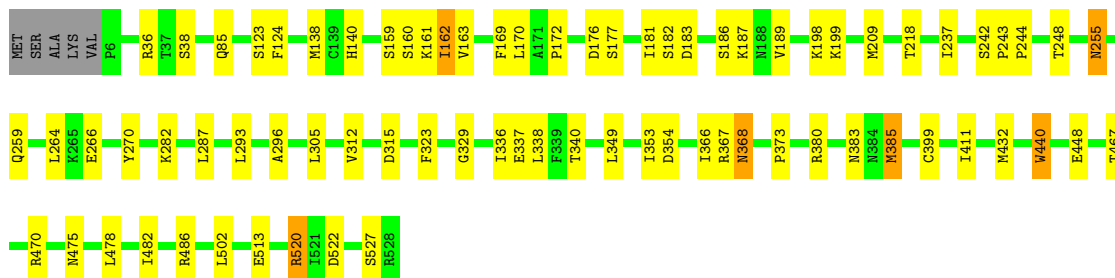
- Molecule 5: T-complex protein 1 subunit beta

Chain J:



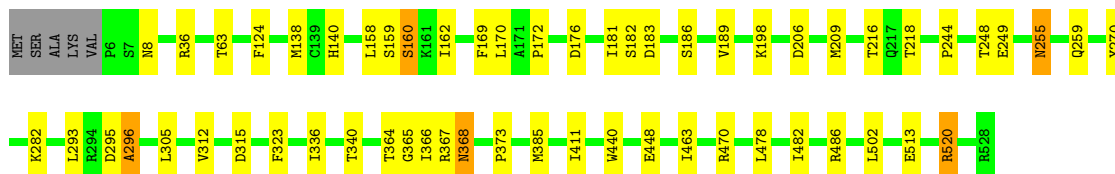
- Molecule 6: T-complex protein 1 subunit delta

Chain D:



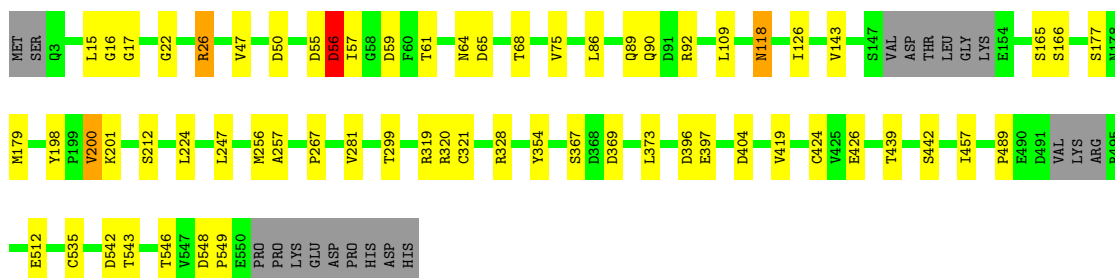
- Molecule 6: T-complex protein 1 subunit delta

Chain L:



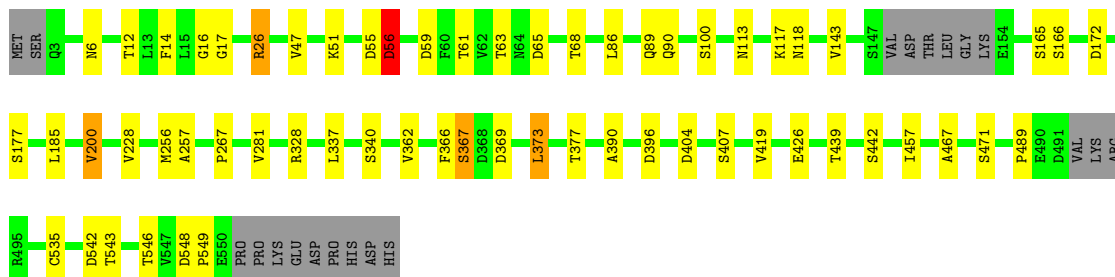
- Molecule 7: T-complex protein 1 subunit alpha

Chain A:



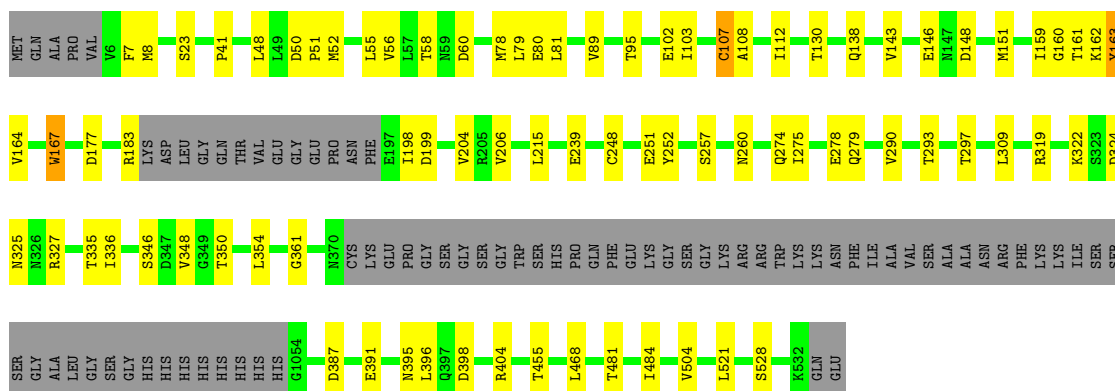
• Molecule 7: T-complex protein 1 subunit alpha

Chain I:



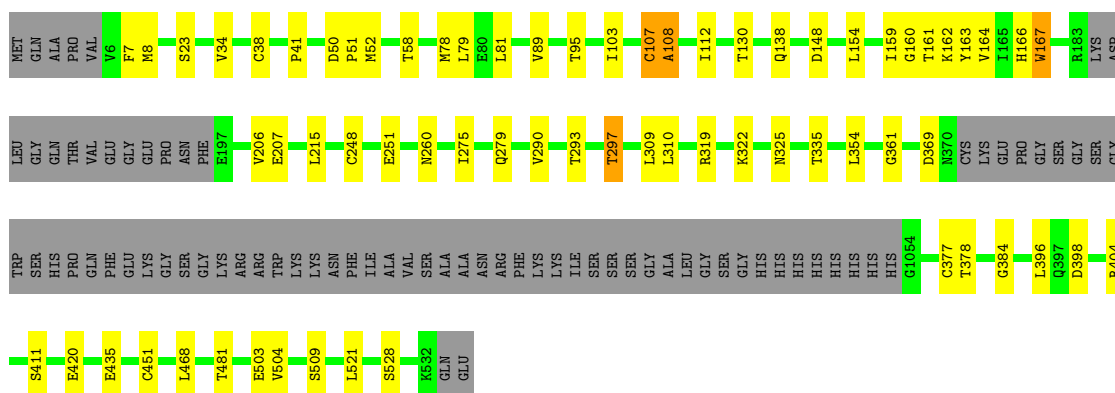
• Molecule 8: T-complex protein 1 subunit gamma

Chain C:



• Molecule 8: T-complex protein 1 subunit gamma

Chain K:



4 Data and refinement statistics

EDS was not executed - this section will therefore be incomplete.

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	Depositor
% Data completeness (in resolution range)	91.6 (30.00-3.80)	Depositor
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	Depositor
Wilson B-factor (Å ²)	116.0	Xtriage
Anisotropy	0.040	Xtriage
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
Total number of atoms	60040	wwPDB-VP
Average B, all atoms (Å ²)	141.0	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	0.35	0/3886	0.55	0/5318
1	N	0.34	0/3886	0.53	0/5318
2	H	0.35	0/3661	0.55	0/5005
2	P	0.36	0/3661	0.54	0/5005
3	G	0.36	0/3803	0.53	0/5194
3	O	0.36	0/3803	0.51	0/5194
4	E	0.34	0/3849	0.52	0/5252
4	M	0.34	0/3849	0.52	0/5252
5	B	0.36	0/3726	0.56	0/5077
5	J	0.35	0/3726	0.54	0/5077
6	D	0.36	0/3723	0.56	0/5089
6	L	0.34	0/3723	0.52	0/5089
7	A	0.36	0/3805	0.54	0/5196
7	I	0.35	0/3805	0.53	0/5196
8	C	0.38	0/3657	0.57	0/5003
8	K	0.35	0/3657	0.55	0/5003
All	All	0.35	0/60220	0.54	0/82268

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
1	F	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	194	VAL	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	9	0
1	N	3836	0	0	5	0
2	H	3619	0	0	14	0
2	P	3619	0	0	8	0
3	G	3752	0	0	13	0
3	O	3752	0	0	11	0
4	E	3798	0	0	6	0
4	M	3798	0	0	6	0
5	B	3689	0	0	17	0
5	J	3689	0	0	6	0
6	D	3685	0	0	18	0
6	L	3685	0	0	11	0
7	A	3770	0	0	14	0
7	I	3770	0	0	11	0
8	C	3615	0	0	16	0
8	K	3615	0	0	11	0
9	A	1	0	0	0	0
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	P	1	0	0	0	0
10	A	27	0	0	0	0
10	B	27	0	0	1	0
10	C	27	0	0	1	0
10	D	27	0	0	1	0
10	E	27	0	0	1	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	1	0
10	K	27	0	0	1	0
10	L	27	0	0	0	0
10	M	27	0	0	1	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	1	0
11	D	4	0	0	1	0
11	E	4	0	0	1	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	1	0
11	K	4	0	0	1	0
11	L	4	0	0	0	0
11	M	4	0	0	1	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	175	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.

All (175) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:A:16:GLY:O	7:A:548:ASP:N	2.11	0.83
7:I:16:GLY:O	7:I:548:ASP:N	2.19	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:P:24:ALA:O	2:P:28:ILE:N	2.21	0.72
8:C:162:LYS:O	8:C:164:VAL:N	2.28	0.66
7:A:26:ARG:CG	7:A:26:ARG:NH1	2.58	0.66
10:K:602:ADP:O3B	11:K:603:BEF:F2	2.05	0.65
2:H:24:ALA:O	2:H:28:ILE:N	2.29	0.65
2:P:509:VAL:CG1	2:P:510:LYS:N	2.61	0.64
6:D:353:ILE:CG2	6:D:354:ASP:N	2.61	0.64
2:H:509:VAL:CG1	2:H:510:LYS:N	2.61	0.63
6:D:138:MET:SD	6:D:478:LEU:CD2	2.87	0.63
2:H:27:GLN:NE2	2:H:544:ILE:CD1	2.62	0.62
5:B:82:LYS:NZ	5:B:86:ASP:OD2	2.32	0.62
4:E:412:ASN:ND2	4:E:414:MET:SD	2.72	0.62
8:K:159:ILE:O	8:K:161:THR:N	2.33	0.61
8:C:146:GLU:OE2	8:C:183:ARG:NH1	2.34	0.60
8:K:162:LYS:O	8:K:164:VAL:N	2.35	0.59
10:J:602:ADP:O3B	11:J:603:BEF:F3	2.10	0.58
7:I:26:ARG:NH1	7:I:26:ARG:CG	2.65	0.58
8:C:159:ILE:O	8:C:161:THR:N	2.37	0.57
6:L:448:GLU:OE1	6:L:470:ARG:NH2	2.37	0.57
4:E:40:ARG:NH1	4:E:42:HIS:ND1	2.52	0.57
4:E:423:LEU:O	4:E:427:LEU:N	2.39	0.56
8:C:324:ASP:OD1	8:C:327:ARG:NH2	2.39	0.55
8:C:167:TRP:CD1	8:C:167:TRP:N	2.74	0.55
5:J:219:GLY:O	5:J:220:ASN:CB	2.54	0.54
3:G:7:THR:O	3:G:8:PRO:O	2.26	0.54
3:O:25:GLN:OE1	3:O:29:ASN:ND2	2.41	0.54
6:L:520:ARG:CG	6:L:520:ARG:NH2	2.71	0.54
7:A:17:GLY:CA	7:A:546:THR:O	2.56	0.54
5:B:119:THR:OG1	6:L:8:ASN:OD1	2.25	0.54
10:C:602:ADP:O3B	11:C:603:BEF:F2	2.15	0.54
7:I:55:ASP:N	7:I:59:ASP:O	2.41	0.53
3:G:25:GLN:OE1	3:G:29:ASN:ND2	2.42	0.53
7:A:55:ASP:O	7:A:56:ASP:CB	2.56	0.53
8:K:103:ILE:O	8:K:107:CYS:CB	2.57	0.53
3:G:163:ARG:NH2	3:G:176:ASP:OD1	2.42	0.53
7:I:17:GLY:CA	7:I:546:THR:O	2.57	0.52
2:P:327:PHE:CG	2:P:328:GLU:N	2.77	0.52
1:F:233:VAL:N	1:F:349:GLY:O	2.42	0.52
4:M:385:PHE:O	4:M:409:ARG:NH2	2.42	0.52
3:O:167:SER:O	3:O:168:SER:CB	2.57	0.52
3:G:224:PHE:CD2	3:G:225:SER:N	2.77	0.52
7:I:165:SER:O	7:I:166:SER:CB	2.57	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:D:367:ARG:O	6:D:368:ASN:CB	2.58	0.52
4:M:412:ASN:ND2	4:M:414:MET:SD	2.82	0.52
3:G:167:SER:O	3:G:168:SER:CB	2.58	0.52
6:L:367:ARG:O	6:L:368:ASN:CB	2.57	0.51
1:F:254:SER:CB	2:H:266:LEU:O	2.58	0.51
4:M:423:LEU:O	4:M:427:LEU:N	2.43	0.51
7:A:15:LEU:C	7:A:17:GLY:N	2.62	0.51
1:N:97:LEU:O	1:N:101:LEU:CB	2.58	0.51
10:E:602:ADP:O3B	11:E:603:BEF:F2	2.18	0.51
1:F:97:LEU:O	1:F:101:LEU:CB	2.59	0.51
6:D:432:MET:SD	6:D:440:TRP:CZ3	3.04	0.51
5:B:393:GLN:O	5:B:397:GLU:N	2.44	0.51
1:F:429:ALA:O	1:F:433:LYS:N	2.43	0.50
5:B:219:GLY:O	5:B:220:ASN:CB	2.59	0.50
4:E:385:PHE:O	4:E:409:ARG:NH2	2.45	0.50
6:D:244:PRO:CD	6:D:270:TYR:CE2	2.95	0.50
5:J:254:SER:O	5:J:256:ALA:N	2.44	0.50
8:C:48:LEU:N	8:C:56:VAL:O	2.45	0.49
5:B:228:ASN:N	5:B:341:ASP:O	2.46	0.49
6:L:255:ASN:N	6:L:259:GLN:OE1	2.46	0.49
5:B:377:LEU:O	5:B:378:ASP:C	2.51	0.49
6:D:520:ARG:CG	6:D:520:ARG:NH2	2.76	0.48
6:D:199:LYS:O	6:D:380:ARG:NH1	2.46	0.48
8:K:108:ALA:O	8:K:112:ILE:N	2.47	0.48
7:I:12:THR:CB	7:I:14:PHE:CE2	2.96	0.48
7:A:165:SER:O	7:A:166:SER:CB	2.61	0.48
5:J:327:SER:O	5:J:329:PHE:N	2.47	0.48
7:A:55:ASP:CB	7:A:59:ASP:O	2.62	0.48
1:N:100:GLU:OE1	1:N:103:ARG:NH1	2.47	0.47
3:G:220:PHE:C	3:G:222:LYS:N	2.68	0.47
2:H:104:MET:O	2:H:108:GLY:N	2.47	0.47
2:H:25:ASP:C	2:H:27:GLN:N	2.68	0.47
8:C:248:CYS:O	8:C:297:THR:CG2	2.63	0.47
7:A:143:VAL:O	7:A:143:VAL:CG1	2.62	0.47
5:J:231:ILE:N	5:J:338:GLY:O	2.48	0.46
8:C:50:ASP:CB	8:C:51:PRO:CD	2.94	0.46
7:A:15:LEU:O	7:A:17:GLY:N	2.49	0.46
5:B:254:SER:O	5:B:256:ALA:N	2.49	0.46
7:A:198:TYR:CD2	7:A:198:TYR:N	2.84	0.46
1:N:395:VAL:O	1:N:399:LEU:N	2.49	0.46
6:L:172:PRO:O	6:L:176:ASP:N	2.49	0.45
8:C:108:ALA:O	8:C:112:ILE:N	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:231:ILE:N	5:B:338:GLY:O	2.49	0.45
1:N:439:LYS:O	1:N:442:THR:CG2	2.64	0.45
3:G:88:ARG:CG	3:G:88:ARG:NH1	2.79	0.45
6:D:162:ILE:O	6:D:162:ILE:CG1	2.64	0.45
6:L:323:PHE:CD1	6:L:323:PHE:C	2.90	0.45
3:G:240:LYS:N	3:G:291:ASN:OD1	2.49	0.45
10:D:602:ADP:O3B	11:D:603:BEF:F2	2.24	0.45
5:B:192:HIS:CD2	5:B:319:LEU:CD1	3.00	0.45
4:E:29:PHE:CD2	4:E:29:PHE:N	2.83	0.45
3:O:107:GLU:CG	3:O:448:VAL:CG2	2.95	0.45
8:C:198:ILE:CG2	8:C:199:ASP:N	2.80	0.44
2:H:323:VAL:O	2:H:324:PRO:C	2.56	0.44
3:O:226:TYR:O	3:O:227:ALA:C	2.55	0.44
3:O:3:PHE:N	3:O:3:PHE:CD2	2.81	0.44
6:L:244:PRO:CD	6:L:270:TYR:CE2	3.00	0.44
8:K:377:CYS:SG	8:K:378:THR:N	2.90	0.44
6:D:448:GLU:OE1	6:D:470:ARG:NH2	2.51	0.44
7:I:55:ASP:O	7:I:56:ASP:CB	2.66	0.44
5:B:58:ASN:O	5:B:59:ASP:C	2.56	0.44
3:O:220:PHE:C	3:O:222:LYS:N	2.70	0.44
5:B:47:GLN:O	6:D:527:SER:N	2.51	0.44
6:D:161:LYS:O	6:D:163:VAL:N	2.50	0.44
8:C:391:GLU:O	8:C:395:ASN:ND2	2.50	0.44
8:C:274:GLN:O	8:C:278:GLU:N	2.51	0.43
6:D:323:PHE:C	6:D:323:PHE:CD1	2.91	0.43
7:A:56:ASP:OD1	7:A:56:ASP:C	2.56	0.43
2:P:21:TYR:N	2:P:21:TYR:CD2	2.86	0.43
5:B:203:LEU:N	6:D:513:GLU:OE2	2.51	0.43
6:L:158:LEU:O	6:L:160:SER:N	2.51	0.43
2:P:500:ASP:OD1	2:P:501:ILE:N	2.51	0.43
2:H:25:ASP:O	2:H:27:GLN:N	2.52	0.43
2:P:240:SER:CA	2:P:245:HIS:NE2	2.82	0.43
8:K:50:ASP:CB	8:K:51:PRO:CD	2.96	0.43
4:E:71:ASP:N	5:B:510:ARG:O	2.52	0.43
6:L:295:ASP:O	6:L:296:ALA:CB	2.67	0.43
3:O:14:LYS:O	3:O:17:THR:OG1	2.35	0.43
7:A:56:ASP:OD1	7:A:57:ILE:N	2.52	0.43
8:K:411:SER:OG	8:K:503:GLU:OE1	2.36	0.43
3:O:191:ARG:O	3:O:192:ASN:C	2.58	0.43
8:K:167:TRP:CD1	8:K:167:TRP:N	2.86	0.43
2:P:106:LEU:O	2:P:110:LEU:N	2.52	0.43
2:H:512:ILE:CG2	2:H:517:ILE:O	2.67	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:M:61:ILE:O	4:M:64:SER:N	2.52	0.43
8:C:103:ILE:O	8:C:107:CYS:CB	2.67	0.43
3:G:191:ARG:O	3:G:192:ASN:C	2.57	0.43
8:K:248:CYS:O	8:K:297:THR:CG2	2.67	0.42
10:M:602:ADP:O3B	11:M:603:BEF:F2	2.27	0.42
2:H:327:PHE:CG	2:H:328:GLU:N	2.86	0.42
7:I:366:PHE:O	7:I:367:SER:C	2.58	0.42
6:D:255:ASN:N	6:D:259:GLN:OE1	2.52	0.42
7:I:143:VAL:O	7:I:143:VAL:CG1	2.67	0.42
7:I:113:ASN:O	7:I:117:LYS:N	2.52	0.42
5:B:327:SER:O	5:B:329:PHE:N	2.53	0.42
4:M:73:ILE:CG2	5:J:511:VAL:CG1	2.97	0.42
8:C:7:PHE:CG	8:C:8:MET:N	2.87	0.42
3:G:140:ILE:O	3:G:144:ALA:N	2.52	0.42
5:B:94:SER:N	10:B:602:ADP:O2B	2.52	0.42
8:K:275:ILE:O	8:K:279:GLN:N	2.53	0.42
2:P:25:ASP:C	2:P:27:GLN:N	2.73	0.42
2:H:234:GLY:O	2:H:235:HIS:CG	2.73	0.42
1:N:521:THR:O	1:N:525:SER:CB	2.68	0.42
8:C:252:TYR:CD2	8:C:252:TYR:N	2.88	0.42
3:G:41:LYS:N	3:G:42:PRO:CD	2.83	0.41
5:J:379:GLU:O	5:J:383:SER:N	2.54	0.41
3:G:511:THR:O	3:G:515:ASN:N	2.53	0.41
2:H:502:ASP:OD1	2:H:505:SER:N	2.53	0.41
8:K:7:PHE:CG	8:K:8:MET:N	2.88	0.41
3:O:74:ASP:O	4:M:33:LYS:N	2.54	0.41
6:D:237:ILE:N	6:D:287:LEU:O	2.54	0.41
2:H:21:TYR:CD2	2:H:21:TYR:N	2.88	0.41
7:A:55:ASP:N	7:A:59:ASP:O	2.54	0.41
8:C:275:ILE:O	8:C:279:GLN:N	2.54	0.41
3:O:7:THR:O	3:O:8:PRO:O	2.38	0.41
1:F:197:MET:O	1:F:380:ILE:N	2.54	0.41
1:F:93:THR:O	1:F:97:LEU:CB	2.69	0.41
6:D:385:MET:N	6:D:385:MET:SD	2.94	0.41
6:L:138:MET:SD	6:L:478:LEU:CD2	3.09	0.41
5:B:384:LEU:O	5:B:388:LEU:N	2.54	0.40
5:B:293:TYR:CB	5:B:294:PRO:CD	2.98	0.40
7:A:50:ASP:OD1	7:A:64:ASN:CB	2.68	0.40
1:F:234:LEU:N	1:F:294:VAL:O	2.53	0.40
1:F:142:ASN:O	1:F:145:ASN:ND2	2.54	0.40
6:D:172:PRO:O	6:D:176:ASP:N	2.54	0.40
2:H:234:GLY:O	2:H:235:HIS:ND1	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:I:362:VAL:O	7:I:373:LEU:N	2.53	0.40
3:G:14:LYS:O	3:G:17:THR:OG1	2.39	0.40
1:F:230:ASN:O	1:F:292:GLY:N	2.54	0.40
3:O:140:ILE:O	3:O:144:ALA:N	2.54	0.40
6:D:336:ILE:C	6:D:338:LEU:N	2.75	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	F	536/546 (98%)	477 (89%)	56 (10%)	3 (1%)	33	86
1	N	536/546 (98%)	483 (90%)	51 (10%)	2 (0%)	43	90
2	H	513/568 (90%)	445 (87%)	57 (11%)	11 (2%)	11	67
2	P	513/568 (90%)	458 (89%)	47 (9%)	8 (2%)	14	72
3	G	524/550 (95%)	467 (89%)	48 (9%)	9 (2%)	14	71
3	O	524/550 (95%)	479 (91%)	36 (7%)	9 (2%)	14	71
4	E	533/562 (95%)	482 (90%)	45 (8%)	6 (1%)	21	79
4	M	533/562 (95%)	494 (93%)	31 (6%)	8 (2%)	15	73
5	B	516/527 (98%)	452 (88%)	48 (9%)	16 (3%)	7	59
5	J	516/527 (98%)	460 (89%)	42 (8%)	14 (3%)	8	62
6	D	521/528 (99%)	457 (88%)	46 (9%)	18 (4%)	6	56
6	L	521/528 (99%)	474 (91%)	33 (6%)	14 (3%)	8	62
7	A	533/559 (95%)	470 (88%)	50 (9%)	13 (2%)	9	64
7	I	533/559 (95%)	483 (91%)	36 (7%)	14 (3%)	8	62
8	C	507/590 (86%)	445 (88%)	54 (11%)	8 (2%)	14	72
8	K	507/590 (86%)	454 (90%)	43 (8%)	10 (2%)	11	68
All	All	8366/8860 (94%)	7480 (89%)	723 (9%)	163 (2%)	12	69

All (163) 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
6	D	159	SER
6	D	160	SER
6	D	368	ASN
7	A	257	ALA
8	C	163	TYR
8	C	239	GLU
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	160	SER
6	L	182	SER
6	L	368	ASN
7	I	257	ALA
8	K	163	TYR
2	H	26	GLY
3	G	151	LYS
3	G	168	SER
3	G	381	GLY
3	G	432	ALA
4	E	189	GLY
4	E	190	SER
4	E	194	SER
5	B	246	PHE
5	B	328	THR
5	B	451	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	D	183	ASP
6	D	189	VAL
6	D	282	LYS
6	D	296	ALA
7	A	56	ASP
7	A	65	ASP
7	A	200	VAL
7	A	201	LYS
7	A	256	MET
8	C	60	ASP
8	C	319	ARG
8	C	361	GLY
3	O	151	LYS
3	O	168	SER
3	O	432	ALA
4	M	345	TRP
6	L	186	SER
6	L	296	ALA
7	I	56	ASP
7	I	65	ASP
7	I	256	MET
7	I	367	SER
7	I	369	ASP
8	K	160	GLY
8	K	166	HIS
8	K	319	ARG
8	K	361	GLY
1	F	437	LYS
2	H	7	GLN
2	H	303	ALA
4	E	268	LYS
5	B	219	GLY
5	B	350	GLU
6	D	182	SER
6	D	186	SER
6	D	187	LYS
6	D	337	GLU
7	A	369	ASP
1	N	202	LEU
1	N	436	ALA
3	O	190	ASP
3	O	381	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	M	364	PRO
5	J	143	SER
5	J	310	ASP
5	J	451	ASP
6	L	159	SER
6	L	189	VAL
6	L	282	LYS
6	L	293	LEU
6	L	315	ASP
7	I	549	PRO
1	F	163	ASP
2	H	41	MET
2	H	96	MET
3	G	369	PRO
5	B	59	ASP
5	B	133	ASP
5	B	143	SER
6	D	293	LEU
6	D	329	GLY
7	A	118	ASN
7	A	367	SER
8	C	160	GLY
2	P	23	ASN
3	O	171	ILE
4	M	189	GLY
5	J	59	ASP
5	J	247	GLY
5	J	423	ASP
6	L	183	ASP
7	I	340	SER
7	I	390	ALA
7	I	467	ALA
1	F	373	PRO
2	H	418	LYS
3	G	251	LYS
4	E	437	SER
5	B	312	GLU
6	D	162	ILE
6	D	315	ASP
8	C	41	PRO
8	C	80	GLU
2	P	7	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	470	ASP
4	M	194	SER
4	M	268	LYS
4	M	462	ARG
5	J	350	GLU
6	L	249	GLU
7	I	118	ASN
3	G	171	ILE
3	G	190	ASP
5	B	241	ASP
5	B	470	SER
6	D	243	PRO
7	A	489	PRO
5	J	241	ASP
8	K	41	PRO
8	K	108	ALA
8	K	207	GLU
8	K	435	GLU
7	A	267	PRO
7	A	549	PRO
2	P	26	GLY
5	J	39	PRO
6	L	373	PRO
6	D	373	PRO
3	O	369	PRO
6	L	365	GLY
2	H	324	PRO
5	B	247	GLY
7	A	22	GLY
7	I	489	PRO
2	H	441	THR
6	D	242	SER
2	P	234	GLY
3	O	343	PRO
7	I	200	VAL
7	I	267	PRO
8	K	384	GLY

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%)	342 (90%)	38 (10%)	11	53
1	N	380/463 (82%)	352 (93%)	28 (7%)	20	67
2	H	352/473 (74%)	314 (89%)	38 (11%)	9	49
2	P	352/473 (74%)	323 (92%)	29 (8%)	17	63
3	G	373/454 (82%)	332 (89%)	41 (11%)	9	48
3	O	373/454 (82%)	340 (91%)	33 (9%)	14	60
4	E	382/483 (79%)	340 (89%)	42 (11%)	9	48
4	M	382/483 (79%)	346 (91%)	36 (9%)	13	56
5	B	374/441 (85%)	325 (87%)	49 (13%)	6	38
5	J	374/441 (85%)	340 (91%)	34 (9%)	14	58
6	D	374/454 (82%)	340 (91%)	34 (9%)	14	58
6	L	374/454 (82%)	344 (92%)	30 (8%)	17	64
7	A	375/471 (80%)	335 (89%)	40 (11%)	10	49
7	I	375/471 (80%)	341 (91%)	34 (9%)	14	58
8	C	359/497 (72%)	312 (87%)	47 (13%)	6	38
8	K	359/497 (72%)	318 (89%)	41 (11%)	8	45
All	All	5938/7472 (80%)	5344 (90%)	594 (10%)	11	53

All (594) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	16	ASP
1	F	19	LEU
1	F	22	ASN
1	F	30	GLN
1	F	35	THR
1	F	56	THR
1	F	62	LEU
1	F	72	THR
1	F	92	THR
1	F	103	ARG
1	F	107	ARG
1	F	111	GLU
1	F	162	VAL
1	F	165	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	187	ASP
1	F	206	ASP
1	F	217	HIS
1	F	223	ASP
1	F	237	ASN
1	F	239	SER
1	F	251	PHE
1	F	257	ASP
1	F	324	ASN
1	F	340	VAL
1	F	368	THR
1	F	370	ASN
1	F	379	LEU
1	F	390	GLN
1	F	396	ARG
1	F	399	LEU
1	F	408	ASP
1	F	453	VAL
1	F	479	ASP
1	F	497	ASP
1	F	499	CYS
1	F	511	ARG
1	F	514	ARG
1	F	535	ARG
2	H	20	SER
2	H	21	TYR
2	H	25	ASP
2	H	31	SER
2	H	41	MET
2	H	62	ILE
2	H	91	GLN
2	H	92	GLN
2	H	98	ASP
2	H	101	ASN
2	H	102	LEU
2	H	105	ILE
2	H	110	LEU
2	H	145	MET
2	H	206	SER
2	H	221	THR
2	H	223	ILE
2	H	245	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	256	ILE
2	H	260	GLU
2	H	291	ILE
2	H	320	VAL
2	H	327	PHE
2	H	341	LEU
2	H	344	LEU
2	H	348	THR
2	H	354	LEU
2	H	357	THR
2	H	358	VAL
2	H	371	PHE
2	H	392	ASN
2	H	409	LYS
2	H	432	SER
2	H	441	THR
2	H	470	ASP
2	H	502	ASP
2	H	519	ASP
2	H	539	LEU
3	G	10	ILE
3	G	11	VAL
3	G	20	SER
3	G	37	GLN
3	G	43	THR
3	G	61	THR
3	G	88	ARG
3	G	96	ASP
3	G	102	THR
3	G	104	LEU
3	G	108	LEU
3	G	122	SER
3	G	155	ARG
3	G	161	CYS
3	G	187	LEU
3	G	194	LEU
3	G	195	ASP
3	G	196	ASP
3	G	197	LYS
3	G	268	GLN
3	G	272	ASP
3	G	277	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	282	LEU
3	G	284	GLN
3	G	291	ASN
3	G	330	VAL
3	G	338	THR
3	G	365	PHE
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	435	GLN
3	G	440	ASN
3	G	483	PHE
3	G	485	THR
3	G	488	ILE
3	G	511	THR
3	G	515	ASN
4	E	29	PHE
4	E	30	ILE
4	E	37	ASN
4	E	59	SER
4	E	68	ARG
4	E	74	LEU
4	E	82	THR
4	E	107	LEU
4	E	111	GLN
4	E	120	THR
4	E	125	LEU
4	E	166	ASP
4	E	168	ILE
4	E	206	GLU
4	E	227	GLN
4	E	240	ILE
4	E	283	THR
4	E	294	GLU
4	E	300	THR
4	E	329	ASP
4	E	336	LEU
4	E	344	ARG
4	E	378	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	431	ARG
4	E	436	ASP
4	E	455	SER
4	E	459	ASP
4	E	487	SER
4	E	492	ILE
4	E	498	LEU
4	E	519	SER
4	E	544	LEU
4	E	552	ASP
5	B	8	ASP
5	B	11	THR
5	B	48	SER
5	B	52	ASN
5	B	57	THR
5	B	62	THR
5	B	93	THR
5	B	99	SER
5	B	104	ARG
5	B	115	ILE
5	B	119	THR
5	B	124	TYR
5	B	132	LEU
5	B	135	LEU
5	B	141	ASP
5	B	147	THR
5	B	156	ILE
5	B	167	SER
5	B	183	ARG
5	B	199	LEU
5	B	214	LEU
5	B	226	ILE
5	B	237	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	B	240	THR
5	B	241	ASP
5	B	245	ILE
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	373	THR
5	B	390	VAL
5	B	397	GLU
5	B	402	LEU
5	B	408	GLU
5	B	416	ASP
5	B	423	ASP
5	B	440	LEU
5	B	452	SER
5	B	455	LEU
5	B	457	SER
5	B	459	LEU
5	B	469	THR
5	B	474	LEU
5	B	476	ASN
5	B	509	LEU
5	B	512	ASP
6	D	36	ARG
6	D	38	SER
6	D	85	GLN
6	D	123	SER
6	D	124	PHE
6	D	140	HIS
6	D	169	PHE
6	D	170	LEU
6	D	177	SER
6	D	181	ILE
6	D	198	LYS
6	D	209	MET
6	D	218	THR
6	D	248	THR
6	D	255	ASN
6	D	264	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	D	266	GLU
6	D	305	LEU
6	D	312	VAL
6	D	340	THR
6	D	349	LEU
6	D	366	ILE
6	D	383	ASN
6	D	385	MET
6	D	399	CYS
6	D	411	ILE
6	D	440	TRP
6	D	467	THR
6	D	475	ASN
6	D	482	ILE
6	D	486	ARG
6	D	502	LEU
6	D	520	ARG
6	D	522	ASP
7	A	26	ARG
7	A	47	VAL
7	A	56	ASP
7	A	61	THR
7	A	68	THR
7	A	75	VAL
7	A	86	LEU
7	A	89	GLN
7	A	90	GLN
7	A	92	ARG
7	A	109	LEU
7	A	118	ASN
7	A	126	ILE
7	A	177	SER
7	A	179	MET
7	A	200	VAL
7	A	212	SER
7	A	224	LEU
7	A	247	LEU
7	A	281	VAL
7	A	299	THR
7	A	319	ARG
7	A	320	ARG
7	A	321	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	A	328	ARG
7	A	354	TYR
7	A	373	LEU
7	A	396	ASP
7	A	397	GLU
7	A	404	ASP
7	A	419	VAL
7	A	424	CYS
7	A	426	GLU
7	A	439	THR
7	A	442	SER
7	A	457	ILE
7	A	512	GLU
7	A	535	CYS
7	A	542	ASP
7	A	543	THR
8	C	23	SER
8	C	52	MET
8	C	55	LEU
8	C	58	THR
8	C	78	MET
8	C	79	LEU
8	C	81	LEU
8	C	89	VAL
8	C	95	THR
8	C	102	GLU
8	C	107	CYS
8	C	130	THR
8	C	138	GLN
8	C	143	VAL
8	C	148	ASP
8	C	151	MET
8	C	163	TYR
8	C	167	TRP
8	C	177	ASP
8	C	204	VAL
8	C	206	VAL
8	C	215	LEU
8	C	251	GLU
8	C	257	SER
8	C	260	ASN
8	C	290	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	C	293	THR
8	C	309	LEU
8	C	322	LYS
8	C	325	ASN
8	C	335	THR
8	C	336	ILE
8	C	346	SER
8	C	348	VAL
8	C	350	THR
8	C	354	LEU
8	C	387	ASP
8	C	396	LEU
8	C	398	ASP
8	C	404	ARG
8	C	455	THR
8	C	468	LEU
8	C	481	THR
8	C	484	ILE
8	C	504	VAL
8	C	521	LEU
8	C	528	SER
1	N	16	ASP
1	N	30	GLN
1	N	35	THR
1	N	56	THR
1	N	62	LEU
1	N	72	THR
1	N	74	VAL
1	N	75	LEU
1	N	103	ARG
1	N	107	ARG
1	N	162	VAL
1	N	187	ASP
1	N	190	ASP
1	N	217	HIS
1	N	223	ASP
1	N	237	ASN
1	N	251	PHE
1	N	257	ASP
1	N	324	ASN
1	N	368	THR
1	N	379	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	390	GLN
1	N	399	LEU
1	N	408	ASP
1	N	442	THR
1	N	453	VAL
1	N	497	ASP
1	N	499	CYS
2	P	32	ILE
2	P	42	CYS
2	P	62	ILE
2	P	65	THR
2	P	95	ASP
2	P	105	ILE
2	P	145	MET
2	P	221	THR
2	P	226	MET
2	P	245	HIS
2	P	256	ILE
2	P	260	GLU
2	P	341	LEU
2	P	344	LEU
2	P	348	THR
2	P	354	LEU
2	P	357	THR
2	P	369	THR
2	P	371	PHE
2	P	392	ASN
2	P	403	ASP
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
2	P	544	ILE
3	O	3	PHE
3	O	10	ILE
3	O	11	VAL
3	O	37	GLN
3	O	43	THR
3	O	50	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	O	96	ASP
3	O	102	THR
3	O	104	LEU
3	O	155	ARG
3	O	194	LEU
3	O	196	ASP
3	O	197	LYS
3	O	267	TYR
3	O	268	GLN
3	O	277	LEU
3	O	282	LEU
3	O	284	GLN
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	468	LEU
3	O	483	PHE
3	O	485	THR
3	O	488	ILE
3	O	508	ASN
3	O	521	ASP
3	O	525	THR
4	M	25	MET
4	M	29	PHE
4	M	30	ILE
4	M	37	ASN
4	M	74	LEU
4	M	82	THR
4	M	92	SER
4	M	107	LEU
4	M	111	GLN
4	M	125	LEU
4	M	129	LEU
4	M	166	ASP
4	M	168	ILE
4	M	206	GLU
4	M	283	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	M	294	GLU
4	M	336	LEU
4	M	344	ARG
4	M	378	SER
4	M	385	PHE
4	M	387	THR
4	M	388	THR
4	M	406	CYS
4	M	408	VAL
4	M	412	ASN
4	M	414	MET
4	M	427	LEU
4	M	431	ARG
4	M	436	ASP
4	M	459	ASP
4	M	464	ILE
4	M	487	SER
4	M	492	ILE
4	M	498	LEU
4	M	513	ASP
4	M	552	ASP
5	J	21	SER
5	J	57	THR
5	J	93	THR
5	J	104	ARG
5	J	119	THR
5	J	124	TYR
5	J	132	LEU
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	241	ASP
5	J	246	PHE
5	J	283	THR
5	J	308	HIS
5	J	316	ARG
5	J	319	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	J	321	THR
5	J	341	ASP
5	J	390	VAL
5	J	397	GLU
5	J	408	GLU
5	J	423	ASP
5	J	427	SER
5	J	450	PHE
5	J	452	SER
5	J	455	LEU
5	J	459	LEU
5	J	474	LEU
5	J	509	LEU
6	L	36	ARG
6	L	63	THR
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	206	ASP
6	L	209	MET
6	L	216	THR
6	L	218	THR
6	L	248	THR
6	L	255	ASN
6	L	305	LEU
6	L	312	VAL
6	L	336	ILE
6	L	340	THR
6	L	364	THR
6	L	366	ILE
6	L	385	MET
6	L	411	ILE
6	L	440	TRP
6	L	463	ILE
6	L	482	ILE
6	L	486	ARG
6	L	502	LEU
6	L	513	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	L	520	ARG
7	I	6	ASN
7	I	26	ARG
7	I	47	VAL
7	I	51	LYS
7	I	56	ASP
7	I	61	THR
7	I	63	THR
7	I	68	THR
7	I	86	LEU
7	I	89	GLN
7	I	90	GLN
7	I	100	SER
7	I	172	ASP
7	I	177	SER
7	I	185	LEU
7	I	200	VAL
7	I	228	VAL
7	I	281	VAL
7	I	328	ARG
7	I	337	LEU
7	I	373	LEU
7	I	377	THR
7	I	396	ASP
7	I	404	ASP
7	I	407	SER
7	I	419	VAL
7	I	426	GLU
7	I	439	THR
7	I	442	SER
7	I	457	ILE
7	I	471	SER
7	I	535	CYS
7	I	542	ASP
7	I	543	THR
8	K	23	SER
8	K	34	VAL
8	K	38	CYS
8	K	52	MET
8	K	58	THR
8	K	78	MET
8	K	79	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	K	81	LEU
8	K	89	VAL
8	K	95	THR
8	K	107	CYS
8	K	130	THR
8	K	138	GLN
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	260	ASN
8	K	290	VAL
8	K	293	THR
8	K	297	THR
8	K	309	LEU
8	K	310	LEU
8	K	322	LYS
8	K	325	ASN
8	K	335	THR
8	K	354	LEU
8	K	369	ASP
8	K	396	LEU
8	K	398	ASP
8	K	404	ARG
8	K	420	GLU
8	K	451	CYS
8	K	468	LEU
8	K	481	THR
8	K	504	VAL
8	K	509	SER
8	K	521	LEU
8	K	528	SER

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	1.05	2 (6%)	45,45,45	1.87	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	1.10	2 (6%)	45,45,45	1.76	10 (22%)
11	BEF	B	603	10	0,3,3	0.00	-	0,3,3	0.00	-
10	ADP	C	602	11,9	29,29,29	1.08	2 (6%)	45,45,45	1.80	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	1.03	2 (6%)	45,45,45	1.85	8 (17%)
11	BEF	D	603	10	0,3,3	0.00	-	0,3,3	0.00	-
10	ADP	E	602	9,11	29,29,29	1.06	2 (6%)	45,45,45	1.87	10 (22%)
11	BEF	E	603	10	0,3,3	0.00	-	0,3,3	0.00	-
10	ADP	F	602	11,9	29,29,29	1.11	2 (6%)	45,45,45	1.67	6 (13%)
11	BEF	F	603	10	0,3,3	0.00	-	0,3,3	0.00	-
10	ADP	G	602	9	29,29,29	1.02	2 (6%)	45,45,45	1.89	8 (17%)
11	BEF	G	603	-	0,3,3	0.00	-	0,3,3	0.00	-
10	ADP	H	602	9	29,29,29	1.07	2 (6%)	45,45,45	1.77	8 (17%)
11	BEF	H	603	-	0,3,3	0.00	-	0,3,3	0.00	-
10	ADP	I	602	9,11	29,29,29	1.07	2 (6%)	45,45,45	1.84	7 (15%)
11	BEF	I	603	10	0,3,3	0.00	-	0,3,3	0.00	-
10	ADP	J	602	11,9	29,29,29	1.08	2 (6%)	45,45,45	1.81	7 (15%)
11	BEF	J	603	10	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	ADP	K	602	11,9	29,29,29	1.11	2 (6%)	45,45,45	1.79	9 (20%)
11	BEF	K	603	10	0,3,3	0.00	-	0,3,3	0.00	-
10	ADP	L	602	11,9	29,29,29	1.06	2 (6%)	45,45,45	1.83	9 (20%)
11	BEF	L	603	10	0,3,3	0.00	-	0,3,3	0.00	-
10	ADP	M	602	11,9	29,29,29	1.08	2 (6%)	45,45,45	1.83	8 (17%)
11	BEF	M	603	10	0,3,3	0.00	-	0,3,3	0.00	-
10	ADP	N	602	9,11	29,29,29	1.09	2 (6%)	45,45,45	1.78	7 (15%)
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	1.84	8 (17%)
11	BEF	O	603	-	0,3,3	0.00	-	0,3,3	0.00	-
10	ADP	P	602	9	29,29,29	1.05	2 (6%)	45,45,45	1.82	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	9,11	-	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	9,11	-	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	11,9	-	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	9,11	-	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 (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	602	ADP	C5-C4	3.29	1.47	1.40
10	C	602	ADP	C5-C4	3.25	1.47	1.40
10	K	602	ADP	C4-N9	-3.23	1.33	1.37
10	N	602	ADP	C5-C4	3.23	1.47	1.40
10	G	602	ADP	C5-C4	3.22	1.47	1.40
10	L	602	ADP	C5-C4	3.17	1.47	1.40
10	P	602	ADP	C5-C4	3.16	1.47	1.40
10	H	602	ADP	C5-C4	3.16	1.47	1.40
10	O	602	ADP	C5-C4	3.15	1.47	1.40
10	F	602	ADP	C5-C4	3.15	1.47	1.40
10	J	602	ADP	C5-C4	3.14	1.47	1.40
10	E	602	ADP	C5-C4	3.12	1.47	1.40
10	M	602	ADP	C5-C4	3.10	1.47	1.40
10	K	602	ADP	C5-C4	3.09	1.47	1.40
10	I	602	ADP	C5-C4	3.06	1.47	1.40
10	D	602	ADP	C5-C4	3.02	1.47	1.40
10	B	602	ADP	C5-C4	2.99	1.47	1.40
10	I	602	ADP	C4-N9	-2.88	1.33	1.37
10	C	602	ADP	C4-N9	-2.86	1.33	1.37
10	M	602	ADP	C4-N9	-2.82	1.33	1.37
10	B	602	ADP	C4-N9	-2.79	1.33	1.37
10	H	602	ADP	C4-N9	-2.76	1.33	1.37
10	E	602	ADP	C4-N9	-2.75	1.33	1.37
10	N	602	ADP	C4-N9	-2.71	1.33	1.37
10	F	602	ADP	C4-N9	-2.64	1.33	1.37
10	L	602	ADP	C4-N9	-2.59	1.34	1.37
10	D	602	ADP	C4-N9	-2.45	1.34	1.37
10	P	602	ADP	C4-N9	-2.41	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	602	ADP	C4-N9	-2.40	1.34	1.37
10	O	602	ADP	C4-N9	-2.29	1.34	1.37
10	A	602	ADP	C4-N9	-2.24	1.34	1.37
10	G	602	ADP	C4-N9	-2.16	1.34	1.37

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	602	ADP	N3-C2-N1	-6.76	123.06	128.71
10	E	602	ADP	N3-C2-N1	-6.66	123.14	128.71
10	I	602	ADP	N3-C2-N1	-6.58	123.21	128.71
10	O	602	ADP	N3-C2-N1	-6.46	123.31	128.71
10	H	602	ADP	N3-C2-N1	-6.46	123.31	128.71
10	P	602	ADP	N3-C2-N1	-6.43	123.33	128.71
10	G	602	ADP	N3-C2-N1	-6.36	123.39	128.71
10	N	602	ADP	N3-C2-N1	-6.33	123.42	128.71
10	F	602	ADP	N3-C2-N1	-6.27	123.47	128.71
10	K	602	ADP	N3-C2-N1	-6.20	123.53	128.71
10	D	602	ADP	N3-C2-N1	-6.17	123.55	128.71
10	L	602	ADP	N3-C2-N1	-6.16	123.56	128.71
10	A	602	ADP	N3-C2-N1	-6.11	123.60	128.71
10	B	602	ADP	N3-C2-N1	-6.10	123.61	128.71
10	J	602	ADP	N3-C2-N1	-6.08	123.62	128.71
10	C	602	ADP	N3-C2-N1	-5.96	123.72	128.71
10	G	602	ADP	N3-C4-N9	5.70	135.73	125.43
10	P	602	ADP	N3-C4-N9	5.48	135.33	125.43
10	E	602	ADP	N3-C4-N9	5.40	135.19	125.43
10	D	602	ADP	N3-C4-N9	5.40	135.18	125.43
10	J	602	ADP	N3-C4-N9	5.40	135.17	125.43
10	O	602	ADP	N3-C4-N9	5.33	135.05	125.43
10	B	602	ADP	N3-C4-N9	5.32	135.04	125.43
10	C	602	ADP	N3-C4-N9	5.28	134.96	125.43
10	H	602	ADP	N3-C4-N9	5.27	134.96	125.43
10	M	602	ADP	N3-C4-N9	5.26	134.94	125.43
10	F	602	ADP	N3-C4-N9	5.20	134.81	125.43
10	L	602	ADP	N3-C4-N9	5.14	134.72	125.43
10	A	602	ADP	N3-C4-N9	5.13	134.70	125.43
10	I	602	ADP	N3-C4-N9	5.13	134.69	125.43
10	N	602	ADP	N3-C4-N9	5.10	134.64	125.43
10	K	602	ADP	N3-C4-N9	4.97	134.41	125.43
10	A	602	ADP	C4-C5-N7	-4.04	106.06	109.52
10	C	602	ADP	PA-O3A-PB	-3.86	120.37	131.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	602	ADP	C4-C5-N7	-3.80	106.26	109.52
10	O	602	ADP	C4-C5-N7	-3.75	106.31	109.52
10	L	602	ADP	C4-C5-N7	-3.71	106.34	109.52
10	P	602	ADP	C4-C5-N7	-3.69	106.36	109.52
10	D	602	ADP	C4-C5-N7	-3.68	106.37	109.52
10	N	602	ADP	C4-C5-N7	-3.68	106.37	109.52
10	G	602	ADP	C4-C5-N7	-3.55	106.48	109.52
10	J	602	ADP	C5-C4-N3	-3.51	118.07	125.70
10	G	602	ADP	C5-C4-N3	-3.49	118.11	125.70
10	I	602	ADP	C4-C5-N7	-3.48	106.54	109.52
10	M	602	ADP	C4-C5-N7	-3.48	106.55	109.52
10	O	602	ADP	C5-C4-N3	-3.47	118.15	125.70
10	G	602	ADP	C3'-C2'-C1'	3.46	106.33	100.91
10	J	602	ADP	C3'-C2'-C1'	3.47	106.33	100.91
10	I	602	ADP	PA-O3A-PB	-3.45	121.56	131.68
10	D	602	ADP	C5-C4-N3	-3.43	118.23	125.70
10	O	602	ADP	C3'-C2'-C1'	3.39	106.21	100.91
10	P	602	ADP	C5-C4-N3	-3.39	118.32	125.70
10	H	602	ADP	C4-C5-N7	-3.35	106.65	109.52
10	K	602	ADP	PA-O3A-PB	-3.34	121.90	131.68
10	D	602	ADP	O4'-C1'-N9	3.33	111.54	108.44
10	A	602	ADP	C5-C4-N3	-3.31	118.49	125.70
10	K	602	ADP	C4-C5-N7	-3.29	106.70	109.52
10	F	602	ADP	C4-C5-N7	-3.26	106.73	109.52
10	C	602	ADP	C5-C4-N3	-3.25	118.62	125.70
10	B	602	ADP	C4-C5-N7	-3.24	106.75	109.52
10	B	602	ADP	C5-C4-N3	-3.22	118.69	125.70
10	L	602	ADP	C5-C4-N3	-3.22	118.69	125.70
10	N	602	ADP	C5-C4-N3	-3.22	118.70	125.70
10	I	602	ADP	C5-C4-N3	-3.21	118.71	125.70
10	L	602	ADP	C3'-C2'-C1'	3.19	105.91	100.91
10	E	602	ADP	C5-C4-N3	-3.18	118.78	125.70
10	H	602	ADP	C5-C4-N3	-3.18	118.78	125.70
10	M	602	ADP	C5-C4-N3	-3.18	118.78	125.70
10	C	602	ADP	C4-C5-N7	-3.17	106.80	109.52
10	A	602	ADP	C3'-C2'-C1'	3.16	105.85	100.91
10	G	602	ADP	PA-O3A-PB	-3.15	122.43	131.68
10	F	602	ADP	C5-C4-N3	-3.11	118.92	125.70
10	E	602	ADP	C4-C5-N7	-3.11	106.86	109.52
10	H	602	ADP	C3'-C2'-C1'	3.10	105.75	100.91
10	A	602	ADP	PA-O3A-PB	-3.06	122.72	131.68
10	P	602	ADP	C3'-C2'-C1'	3.03	105.65	100.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	E	602	ADP	C3'-C2'-C1'	3.00	105.60	100.91
10	K	602	ADP	C5-C4-N3	-2.98	119.20	125.70
10	M	602	ADP	C3'-C2'-C1'	2.96	105.53	100.91
10	C	602	ADP	C3'-C2'-C1'	2.86	105.39	100.91
10	E	602	ADP	PA-O3A-PB	-2.85	123.31	131.68
10	A	602	ADP	O4'-C1'-N9	2.81	111.06	108.44
10	N	602	ADP	C3'-C2'-C1'	2.75	105.21	100.91
10	G	602	ADP	C2-N3-C4	2.68	121.65	114.01
10	O	602	ADP	C2-N3-C4	2.68	121.64	114.01
10	J	602	ADP	C2-N3-C4	2.66	121.60	114.01
10	D	602	ADP	C2-N3-C4	2.65	121.56	114.01
10	P	602	ADP	C2-N3-C4	2.63	121.51	114.01
10	M	602	ADP	C2-N3-C4	2.62	121.47	114.01
10	A	602	ADP	C2-N3-C4	2.61	121.43	114.01
10	I	602	ADP	C2-N3-C4	2.59	121.38	114.01
10	I	602	ADP	C3'-C2'-C1'	2.58	104.94	100.91
10	L	602	ADP	PA-O3A-PB	-2.58	124.12	131.68
10	D	602	ADP	C3'-C2'-C1'	2.58	104.94	100.91
10	E	602	ADP	C2-N3-C4	2.53	121.20	114.01
10	B	602	ADP	O4'-C1'-N9	-2.52	106.09	108.44
10	D	602	ADP	PA-O3A-PB	-2.52	124.29	131.68
10	N	602	ADP	C2-N3-C4	2.51	121.16	114.01
10	H	602	ADP	C2-N3-C4	2.51	121.15	114.01
10	L	602	ADP	C2-N3-C4	2.50	121.14	114.01
10	B	602	ADP	C2-N3-C4	2.50	121.12	114.01
10	F	602	ADP	C2-N3-C4	2.48	121.07	114.01
10	C	602	ADP	C2-N3-C4	2.46	121.01	114.01
10	N	602	ADP	PA-O3A-PB	-2.43	124.54	131.68
10	J	602	ADP	C4'-O4'-C1'	2.42	112.38	109.75
10	K	602	ADP	C2-N3-C4	2.40	120.85	114.01
10	O	602	ADP	C4'-O4'-C1'	2.39	112.34	109.75
10	E	602	ADP	C4'-O4'-C1'	2.36	112.31	109.75
10	P	602	ADP	PA-O3A-PB	-2.34	124.82	131.68
10	K	602	ADP	C3'-C2'-C1'	2.30	104.50	100.91
10	M	602	ADP	C8-N9-C4	2.25	108.62	106.90
10	G	602	ADP	C8-N9-C4	2.22	108.60	106.90
10	B	602	ADP	PA-O3A-PB	-2.18	125.29	131.68
10	B	602	ADP	C8-N9-C4	2.16	108.55	106.90
10	O	602	ADP	PA-O3A-PB	-2.15	125.37	131.68
10	E	602	ADP	C2'-C3'-C4'	2.14	106.93	102.65
10	H	602	ADP	PA-O3A-PB	-2.14	125.40	131.68
10	E	602	ADP	C8-N9-C4	2.12	108.52	106.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	602	ADP	C8-N9-C4	2.12	108.52	106.90
10	H	602	ADP	C8-N9-C4	2.09	108.49	106.90
10	L	602	ADP	O4'-C1'-N9	2.08	110.38	108.44
10	F	602	ADP	C8-N9-C4	2.08	108.49	106.90
10	K	602	ADP	C8-N9-C4	2.08	108.48	106.90
10	K	602	ADP	C2'-C3'-C4'	2.04	106.73	102.65
10	B	602	ADP	C3'-C2'-C1'	2.03	104.09	100.91
10	L	602	ADP	C4'-O4'-C1'	2.02	111.94	109.75
10	B	602	ADP	C4'-O4'-C1'	2.02	111.94	109.75
10	M	602	ADP	PA-O3A-PB	-2.01	125.77	131.68

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.