



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:23 PM GMT

PDB ID : 1T36
Title : Crystal structure of E. coli carbamoyl phosphate synthetase small subunit mutant C248D complexed with uridine 5'-monophosphate
Authors : Thoden, J.B.; Huang, X.; Raushel, F.M.; Holden, H.M.
Deposited on : 2004-04-24
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

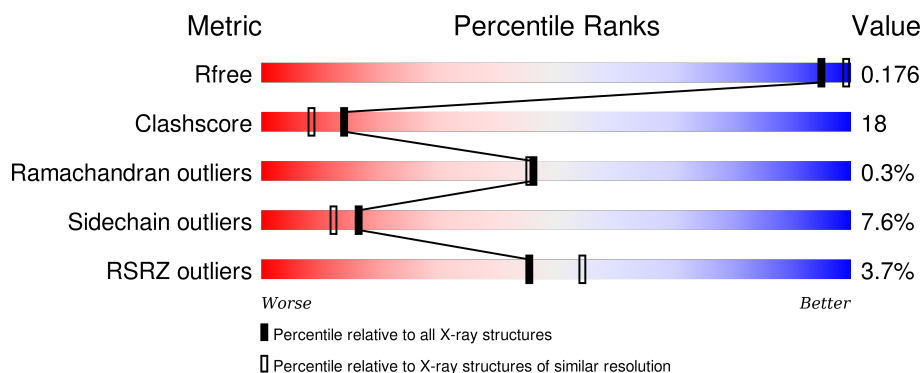
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1073	<div> <div>2%</div> <div>62% 30% 7% .</div> </div>
1	C	1073	<div> <div>3%</div> <div>58% 32% 7% ..</div> </div>
1	E	1073	<div> <div>2%</div> <div>65% 27% 6% ..</div> </div>
1	G	1073	<div> <div>4%</div> <div>52% 37% 9% ..</div> </div>
2	B	382	<div> <div>4%</div> <div>54% 35% 8% ..</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	382	
2	F	382	
2	H	382	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CL	H	384	-	-	-	X
8	ORN	A	1089	-	-	-	X
8	ORN	C	1091	-	-	-	X
8	ORN	E	1091	-	-	-	X
8	ORN	G	1091	-	-	-	X
9	NET	E	1092	-	-	-	X
9	NET	G	1092	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 48757 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Carbamoyl-phosphate synthase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1058	Total	C	N	O	S	0	9	0
			8212	5155	1436	1575	46			
1	C	1058	Total	C	N	O	S	0	8	0
			8197	5146	1426	1579	46			
1	E	1058	Total	C	N	O	S	0	5	0
			8182	5137	1425	1575	45			
1	G	1058	Total	C	N	O	S	0	8	0
			8206	5152	1432	1577	45			

- Molecule 2 is a protein called Carbamoyl-phosphate synthase small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	379	Total	C	N	O	S	0	0	0
			2897	1826	508	554	9			
2	D	379	Total	C	N	O	S	0	1	0
			2904	1830	511	554	9			
2	F	379	Total	C	N	O	S	0	0	0
			2897	1826	508	554	9			
2	H	379	Total	C	N	O	S	0	0	0
			2897	1826	508	554	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	248	ASP	CYS	ENGINEERED	UNP P00907
D	248	ASP	CYS	ENGINEERED	UNP P00907
F	248	ASP	CYS	ENGINEERED	UNP P00907
H	248	ASP	CYS	ENGINEERED	UNP P00907

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	3	Total Mn 3 3	0	0
3	A	3	Total Mn 3 3	0	0
3	C	3	Total Mn 3 3	0	0
3	E	3	Total Mn 3 3	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	5	Total K 5 5	0	0
4	D	1	Total K 1 1	0	0
4	E	5	Total K 5 5	0	0
4	H	1	Total K 1 1	0	0
4	B	1	Total K 1 1	0	0
4	C	4	Total K 4 4	0	0
4	A	4	Total K 4 4	0	0
4	F	1	Total K 1 1	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

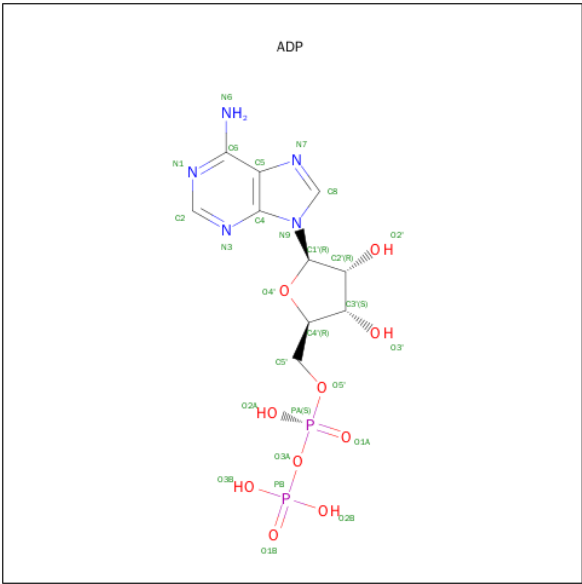


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	E	1	Total	O	P	0	0
			5	4	1		
5	G	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

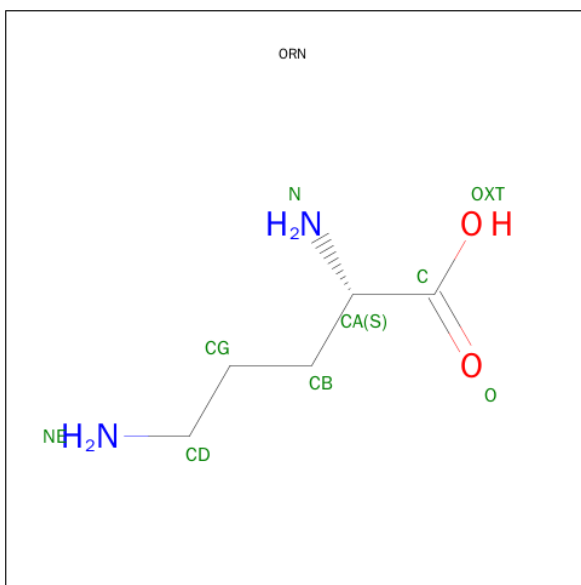
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	6	Total	Cl	0	0
			6	6		
6	D	1	Total	Cl	0	0
			1	1		
6	E	6	Total	Cl	0	0
			6	6		
6	H	2	Total	Cl	0	0
			2	2		
6	C	6	Total	Cl	0	0
			6	6		
6	A	5	Total	Cl	0	0
			5	5		
6	F	1	Total	Cl	0	0
			1	1		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



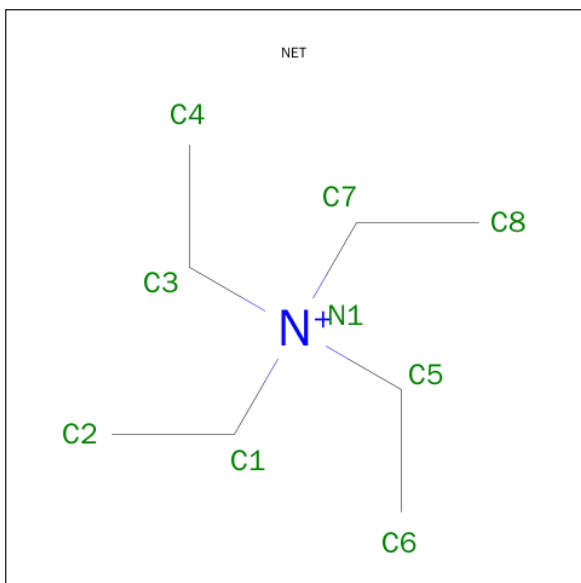
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 8 is L-ORNITHINE (three-letter code: ORN) (formula: $C_5H_{12}N_2O_2$).



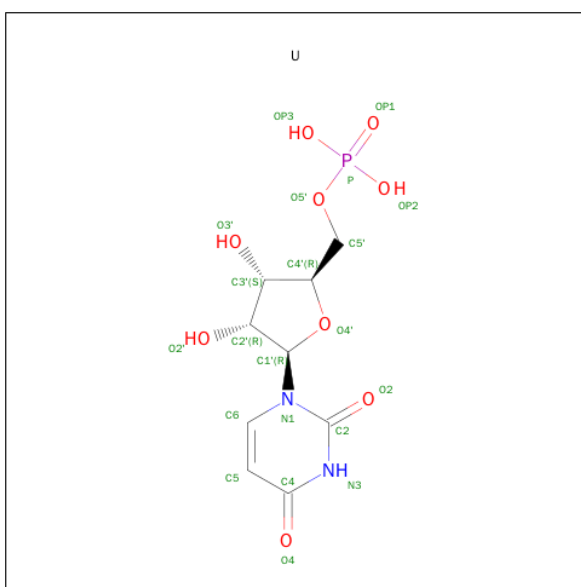
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			9	5	2	2		
8	C	1	Total	C	N	O	0	0
			9	5	2	2		
8	E	1	Total	C	N	O	0	0
			9	5	2	2		
8	G	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 9 is TETRAETHYLAMMONIUM ION (three-letter code: NET) (formula: $C_8H_{20}N$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C N 9 8 1	0	0
9	C	1	Total C N 9 8 1	0	0
9	E	1	Total C N 9 8 1	0	0
9	G	1	Total C N 9 8 1	0	0

- Molecule 10 is URIDINE-5'-MONOPHOSPHATE (three-letter code: U) (formula: $C_9H_{13}N_2O_9P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C N O P 21 9 2 9 1	0	0
10	C	1	Total C N O P 21 9 2 9 1	0	0
10	E	1	Total C N O P 21 9 2 9 1	0	0
10	G	1	Total C N O P 21 9 2 9 1	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	851	Total O 851 851	0	0

Continued on next page...

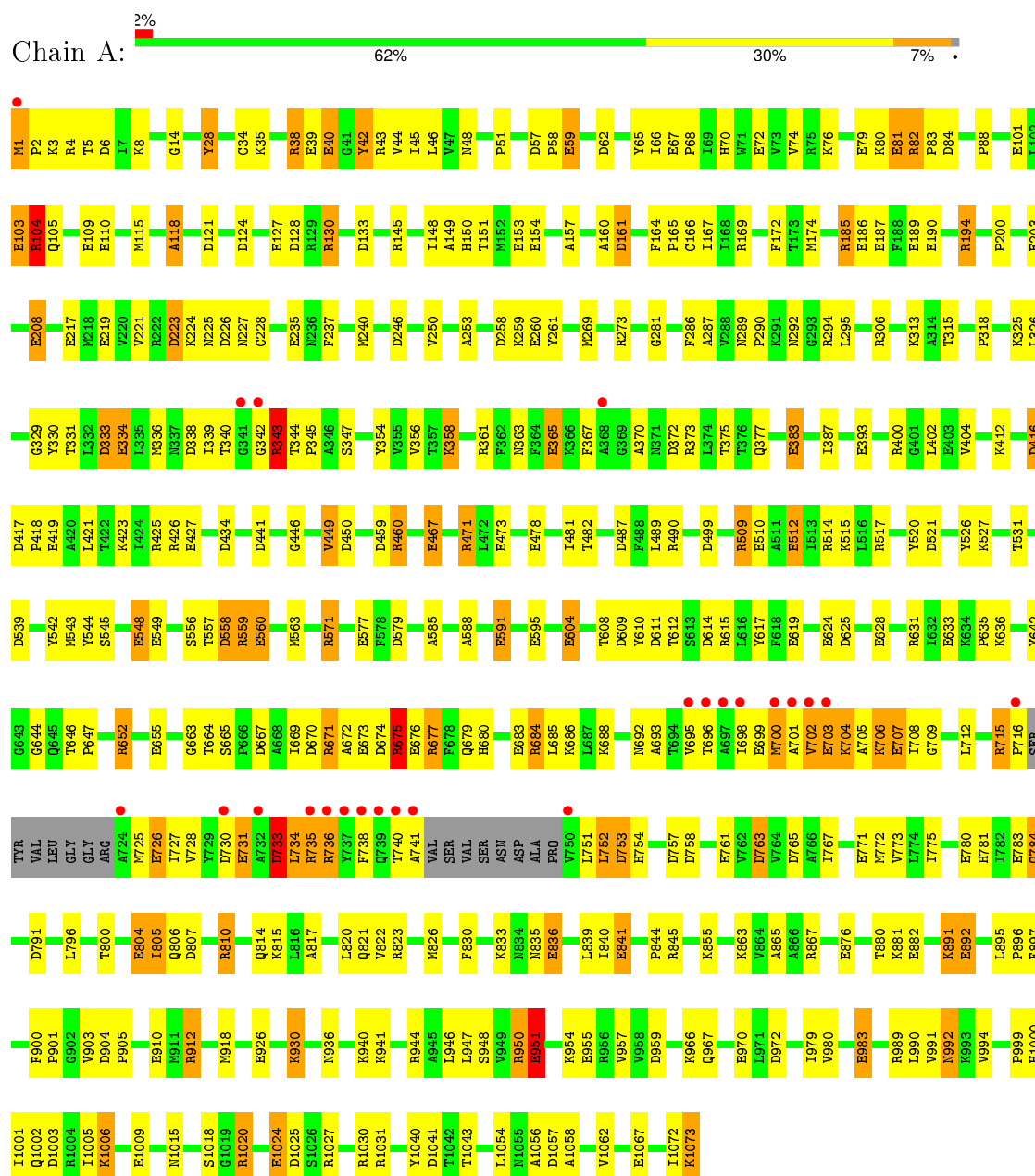
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	161	Total 161	O 161	0	0
11	C	819	Total 819	O 819	0	0
11	D	221	Total 221	O 221	0	0
11	E	832	Total 832	O 832	0	0
11	F	200	Total 200	O 200	0	0
11	G	705	Total 705	O 705	0	0
11	H	118	Total 118	O 118	0	0

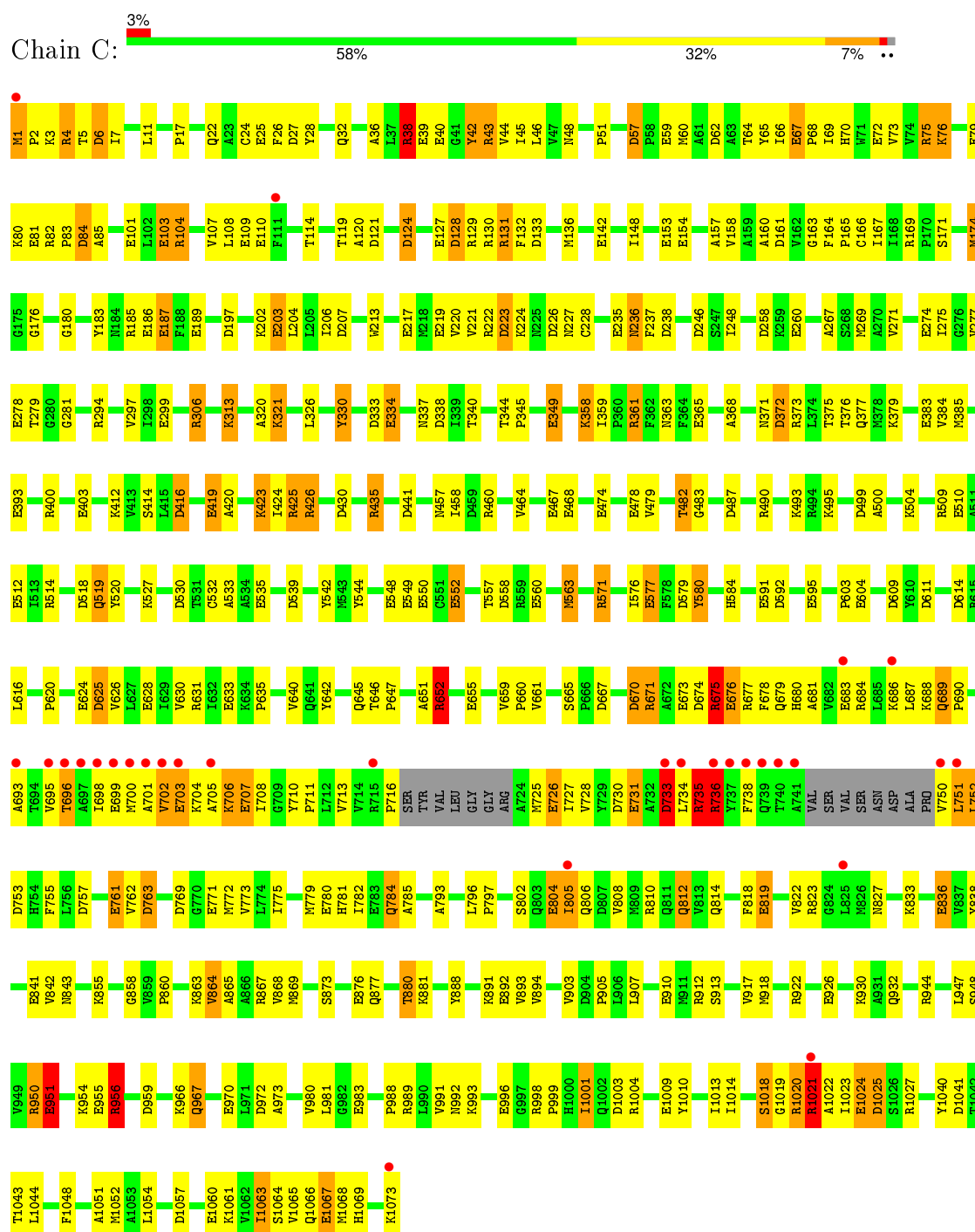
3 Residue-property plots

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.

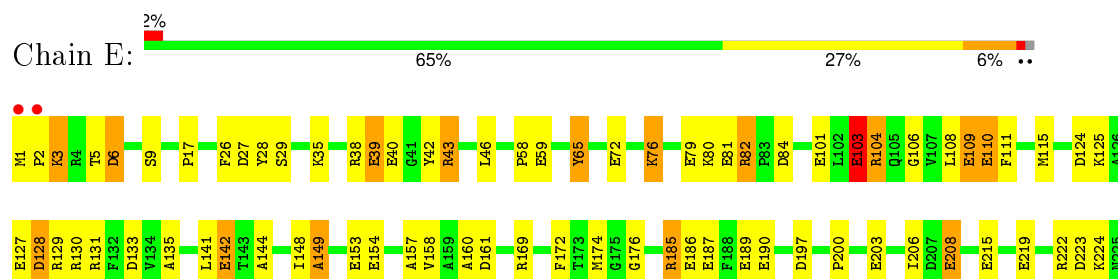
- Molecule 1: Carbamoyl-phosphate synthase large chain

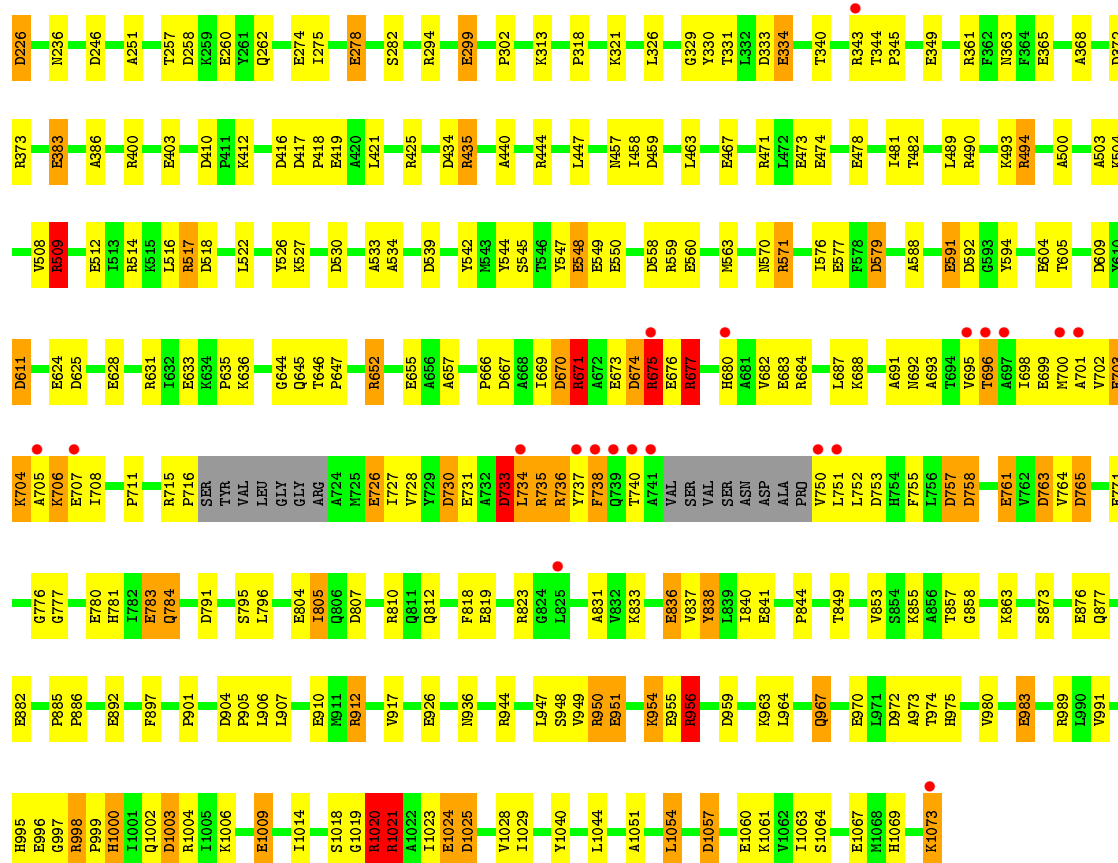


- Molecule 1: Carbamoyl-phosphate synthase large chain

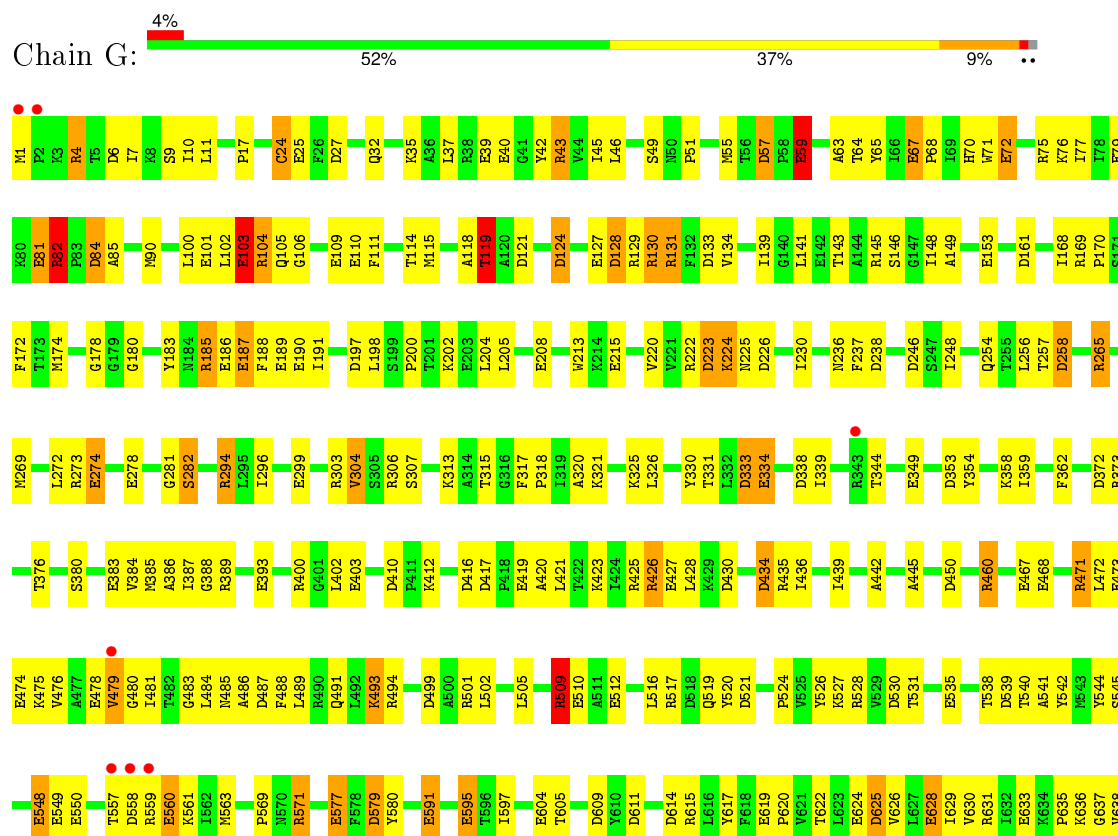


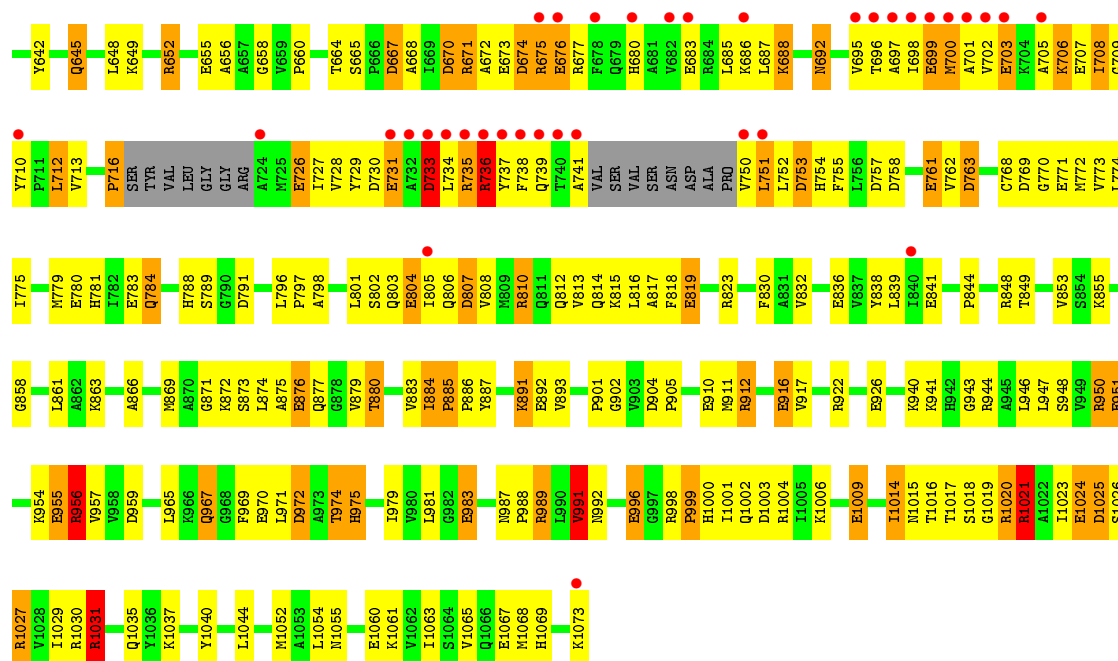
• Molecule 1: Carbamoyl-phosphate synthase large chain



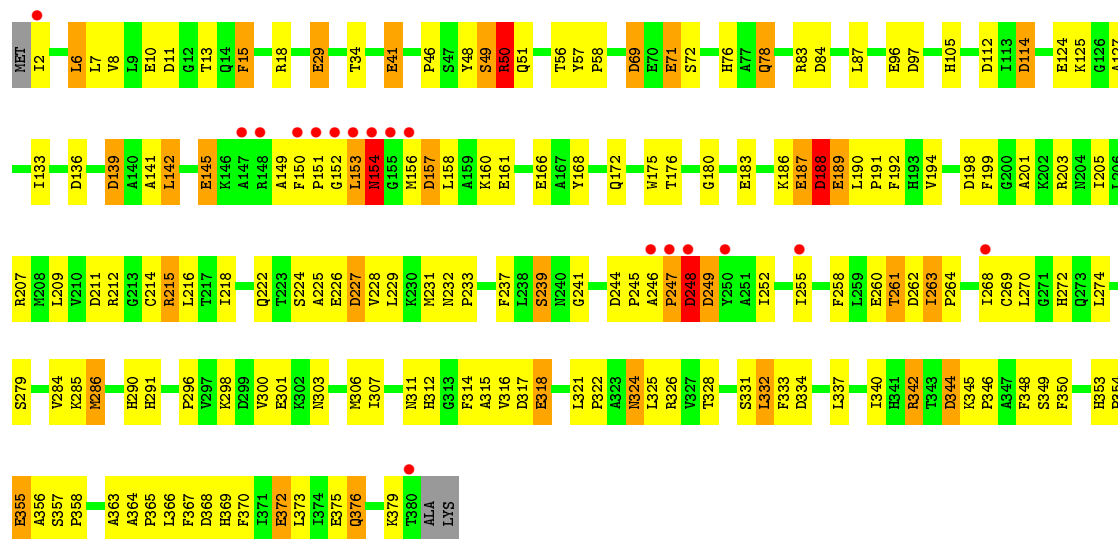


● Molecule 1: Carbamoyl-phosphate synthase large chain

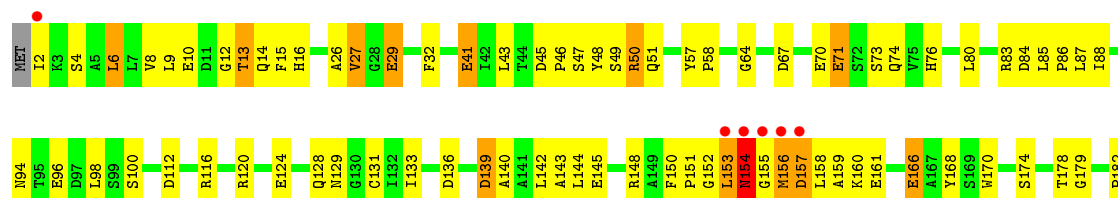


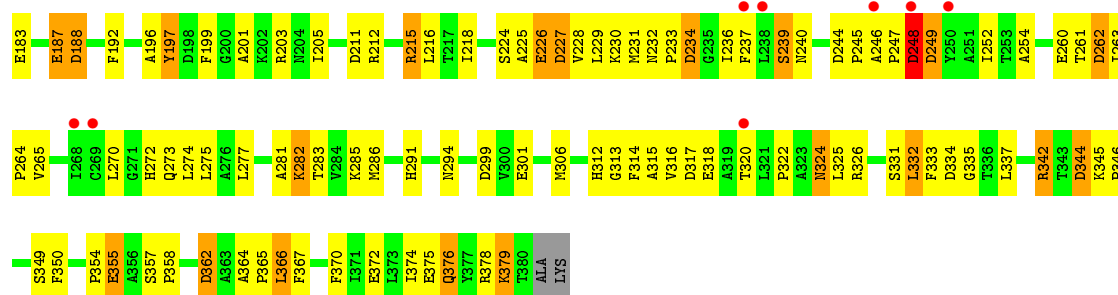


• Molecule 2: Carbamoyl-phosphate synthase small chain

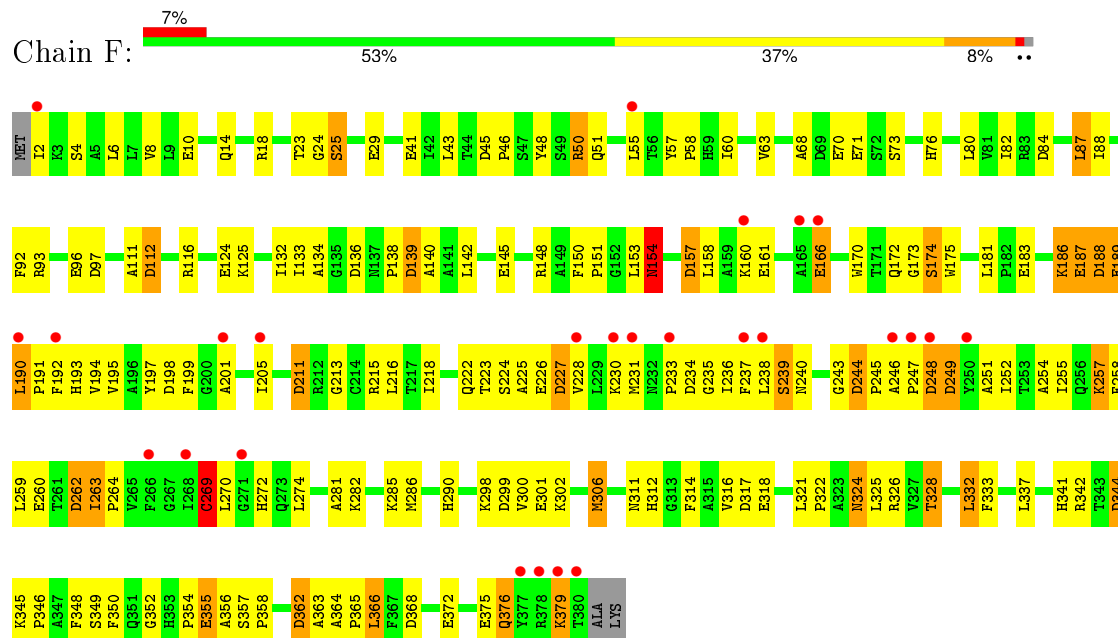


• Molecule 2: Carbamoyl-phosphate synthase small chain

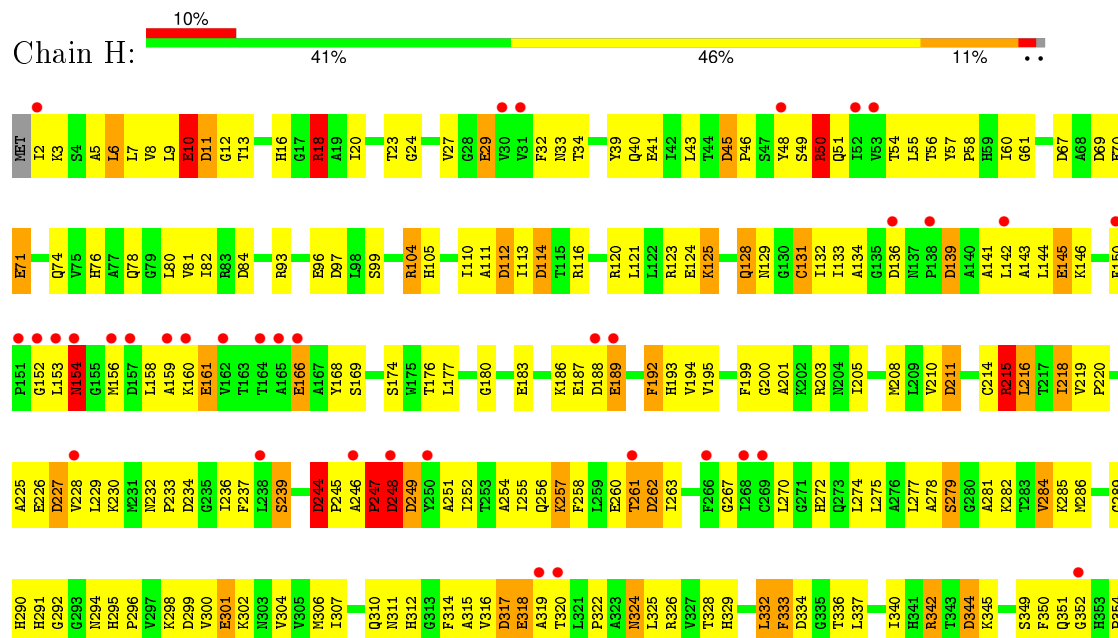




• Molecule 2: Carbamoyl-phosphate synthase small chain



• Molecule 2: Carbamoyl-phosphate synthase small chain



E355	
H361	
D362	
A363	
A364	
P365	
L366	
F367	
D368	
H369	
F370	
L371	
E372	
L373	
I374	
E375	
Q376	
Y377	
R378	
K379	
T380	
ALA	
LYS	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	152.50Å 164.90Å 333.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 29.70 – 2.10	Depositor EDS
% Data completeness (in resolution range)	90.0 (30.00-2.10) 88.6 (29.70-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.88 (at 2.10Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.176 , 0.209 0.175 , 0.176	Depositor DCC
R_{free} test set	42730 reflections (11.03%)	DCC
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 119.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 430082 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	48757	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, CL, K, MN, ORN, NET, PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.05	68/8374 (0.8%)	1.50	137/11315 (1.2%)
1	C	1.06	81/8355 (1.0%)	1.48	127/11293 (1.1%)
1	E	1.06	74/8328 (0.9%)	1.50	128/11257 (1.1%)
1	G	1.05	74/8368 (0.9%)	1.50	148/11308 (1.3%)
2	B	0.94	19/2959 (0.6%)	1.46	43/4019 (1.1%)
2	D	0.97	17/2970 (0.6%)	1.48	45/4033 (1.1%)
2	F	0.97	19/2959 (0.6%)	1.45	41/4019 (1.0%)
2	H	0.94	20/2959 (0.7%)	1.42	37/4019 (0.9%)
All	All	1.03	372/45272 (0.8%)	1.49	706/61263 (1.2%)

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
2	B	1	0
2	D	1	0
2	F	1	0
All	All	3	0

The worst 5 of 372 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	372	GLU	CD-OE2	8.39	1.34	1.25
2	H	166	GLU	CD-OE2	8.34	1.34	1.25
2	D	145	GLU	CD-OE2	8.28	1.34	1.25
1	G	1009[A]	GLU	CD-OE2	8.21	1.34	1.25
1	G	1009[B]	GLU	CD-OE2	8.21	1.34	1.25

The worst 5 of 706 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	514	ARG	NE-CZ-NH2	-15.12	112.74	120.30
1	A	944	ARG	NE-CZ-NH1	14.25	127.42	120.30
1	C	514	ARG	NE-CZ-NH2	-14.00	113.30	120.30
1	A	104	ARG	NE-CZ-NH1	13.43	127.02	120.30
1	A	652	ARG	NE-CZ-NH1	13.13	126.87	120.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	154	ASN	CA
2	D	154	ASN	CA
2	F	154	ASN	CA

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8212	0	8255	231	0
1	C	8197	0	8225	254	0
1	E	8182	0	8216	209	0
1	G	8206	0	8247	340	0
2	B	2897	0	2860	147	0
2	D	2904	0	2869	133	0
2	F	2897	0	2860	128	0
2	H	2897	0	2860	213	0
3	A	3	0	0	0	0
3	C	3	0	0	0	0
3	E	3	0	0	0	0
3	G	3	0	0	0	0
4	A	4	0	0	0	0
4	B	1	0	0	0	0
4	C	4	0	0	0	0
4	D	1	0	0	0	0
4	E	5	0	0	0	0
4	F	1	0	0	0	0
4	G	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1	0	0	0	0
5	A	5	0	0	0	0
5	C	10	0	0	1	0
5	E	5	0	0	0	0
5	G	5	0	0	0	0
6	A	5	0	0	1	0
6	C	6	0	0	0	0
6	D	1	0	0	0	0
6	E	6	0	0	1	0
6	F	1	0	0	0	0
6	G	6	0	0	2	0
6	H	2	0	0	0	0
7	A	54	0	24	2	0
7	C	54	0	24	0	0
7	E	54	0	24	3	0
7	G	54	0	24	0	0
8	A	9	0	11	0	0
8	C	9	0	11	1	0
8	E	9	0	11	2	0
8	G	9	0	11	1	0
9	A	9	0	20	1	0
9	C	9	0	20	1	0
9	E	9	0	20	2	0
9	G	9	0	20	2	0
10	A	21	0	11	1	0
10	C	21	0	11	2	0
10	E	21	0	11	2	0
10	G	21	0	11	1	0
11	A	851	0	0	29	1
11	B	161	0	0	5	0
11	C	819	0	0	23	1
11	D	221	0	0	5	0
11	E	832	0	0	24	0
11	F	200	0	0	2	0
11	G	705	0	0	28	0
11	H	118	0	0	5	0
All	All	48757	0	44656	1643	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

The worst 5 of 1643 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:27:VAL:HG22	2:H:131:CYS:HB2	1.13	1.10
2:D:227:ASP:HA	2:D:230:LYS:HD2	1.25	1.07
1:G:784:GLN:NE2	1:G:784:GLN:H	1.53	1.05
2:H:133:ILE:HD12	2:H:143:ALA:HB2	1.41	1.03
1:A:38:ARG:HH11	1:A:38:ARG:HG3	1.25	1.00

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1848:HOH:O	11:C:1912:HOH:O[4_555]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1061/1073 (99%)	1015 (96%)	44 (4%)	2 (0%)	52	53
1	C	1060/1073 (99%)	1005 (95%)	54 (5%)	1 (0%)	56	58
1	E	1057/1073 (98%)	1013 (96%)	42 (4%)	2 (0%)	52	53
1	G	1061/1073 (99%)	996 (94%)	59 (6%)	6 (1%)	30	24
2	B	377/382 (99%)	348 (92%)	26 (7%)	3 (1%)	24	17
2	D	378/382 (99%)	354 (94%)	23 (6%)	1 (0%)	46	45
2	F	377/382 (99%)	355 (94%)	21 (6%)	1 (0%)	46	45
2	H	377/382 (99%)	346 (92%)	27 (7%)	4 (1%)	17	11
All	All	5748/5820 (99%)	5432 (94%)	296 (5%)	20 (0%)	46	45

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	154	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	154	ASN
1	E	738	PHE
1	G	485	ASN
1	G	975	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	874/878 (100%)	811 (93%)	63 (7%)	18	14
1	C	873/878 (99%)	809 (93%)	64 (7%)	17	13
1	E	870/878 (99%)	818 (94%)	52 (6%)	24	20
1	G	874/878 (100%)	800 (92%)	74 (8%)	13	9
2	B	308/310 (99%)	283 (92%)	25 (8%)	15	10
2	D	309/310 (100%)	283 (92%)	26 (8%)	14	9
2	F	308/310 (99%)	276 (90%)	32 (10%)	9	5
2	H	308/310 (99%)	278 (90%)	30 (10%)	10	6
All	All	4724/4752 (99%)	4358 (92%)	366 (8%)	16	12

5 of 366 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	239	SER
1	E	696	THR
2	H	6	LEU
2	D	306	MET
1	E	185	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	324	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	987	ASN
2	H	51	GLN
1	E	105	GLN
1	E	689	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 86 ligands modelled in this entry, 61 are monoatomic - leaving 25 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	$\# Z > 2$
5	PO4	A	1078	3	4,4,4	1.29	0	6,6,6	0.35	0
7	ADP	A	1087	3	22,29,29	1.17	2 (9%)	27,45,45	0.78	0
7	ADP	A	1088	3	22,29,29	0.98	0	27,45,45	0.95	1 (3%)
8	ORN	A	1089	-	5,8,8	0.67	0	3,9,9	1.17	0
9	NET	A	1090	-	8,8,8	0.67	0	10,10,10	0.60	0
10	U	A	1091	-	16,22,22	1.57	4 (25%)	21,33,33	3.02	2 (9%)
5	PO4	C	1078	3	4,4,4	1.65	1 (25%)	6,6,6	0.31	0
5	PO4	C	1088	-	4,4,4	1.83	1 (25%)	6,6,6	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ADP	C	1089	3	22,29,29	1.26	3 (13%)	27,45,45	1.48	4 (14%)
7	ADP	C	1090	3	22,29,29	1.07	2 (9%)	27,45,45	1.11	1 (3%)
8	ORN	C	1091	-	5,8,8	0.58	0	3,9,9	0.27	0
9	NET	C	1092	-	8,8,8	0.46	0	10,10,10	0.70	0
10	U	C	1093	-	16,22,22	1.54	3 (18%)	21,33,33	3.07	3 (14%)
5	PO4	E	1078	3	4,4,4	1.82	2 (50%)	6,6,6	0.34	0
7	ADP	E	1089	3	22,29,29	1.20	2 (9%)	27,45,45	1.15	3 (11%)
7	ADP	E	1090	3	22,29,29	1.26	3 (13%)	27,45,45	1.30	4 (14%)
8	ORN	E	1091	-	5,8,8	0.60	0	3,9,9	0.47	0
9	NET	E	1092	-	8,8,8	0.36	0	10,10,10	0.70	0
10	U	E	1093	-	16,22,22	1.62	4 (25%)	21,33,33	3.56	5 (23%)
5	PO4	G	1078	3	4,4,4	1.65	1 (25%)	6,6,6	0.31	0
7	ADP	G	1089	3	22,29,29	1.37	3 (13%)	27,45,45	1.40	4 (14%)
7	ADP	G	1090	3	22,29,29	1.26	3 (13%)	27,45,45	1.16	4 (14%)
8	ORN	G	1091	-	5,8,8	0.48	0	3,9,9	0.24	0
9	NET	G	1092	-	8,8,8	0.67	0	10,10,10	0.42	0
10	U	G	1093	-	16,22,22	1.63	4 (25%)	21,33,33	3.45	5 (23%)

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
5	PO4	A	1078	3	-	0/0/0/0	0/0/0/0
7	ADP	A	1087	3	-	0/12/32/32	0/3/3/3
7	ADP	A	1088	3	-	0/12/32/32	0/3/3/3
8	ORN	A	1089	-	-	0/4/8/8	0/0/0/0
9	NET	A	1090	-	-	0/12/12/12	0/0/0/0
10	U	A	1091	-	-	0/6/26/26	0/2/2/2
5	PO4	C	1078	3	-	0/0/0/0	0/0/0/0
5	PO4	C	1088	-	-	0/0/0/0	0/0/0/0
7	ADP	C	1089	3	-	0/12/32/32	0/3/3/3
7	ADP	C	1090	3	-	0/12/32/32	0/3/3/3
8	ORN	C	1091	-	-	0/4/8/8	0/0/0/0
9	NET	C	1092	-	-	0/12/12/12	0/0/0/0
10	U	C	1093	-	-	0/6/26/26	0/2/2/2
5	PO4	E	1078	3	-	0/0/0/0	0/0/0/0
7	ADP	E	1089	3	-	0/12/32/32	0/3/3/3
7	ADP	E	1090	3	-	0/12/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ORN	E	1091	-	-	0/4/8/8	0/0/0/0
9	NET	E	1092	-	-	0/12/12/12	0/0/0/0
10	U	E	1093	-	-	0/6/26/26	0/2/2/2
5	PO4	G	1078	3	-	0/0/0/0	0/0/0/0
7	ADP	G	1089	3	-	0/12/32/32	0/3/3/3
7	ADP	G	1090	3	-	0/12/32/32	0/3/3/3
8	ORN	G	1091	-	-	0/4/8/8	0/0/0/0
9	NET	G	1092	-	-	0/12/12/12	0/0/0/0
10	U	G	1093	-	-	0/6/26/26	0/2/2/2

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	1089	ADP	O4'-C1'	-3.28	1.37	1.41
10	A	1091	U	C6-C5	-2.96	1.31	1.38
10	E	1093	U	C6-C5	-2.90	1.31	1.38
10	C	1093	U	C6-C5	-2.87	1.31	1.38
10	G	1093	U	C6-C5	-2.80	1.32	1.38

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	E	1093	U	OP3-P-O5'	-4.53	93.51	106.56
10	E	1093	U	C5-C4-N3	-4.08	112.66	123.12
7	E	1090	ADP	O3A-PA-O5'	-4.02	92.28	102.94
10	G	1093	U	C5-C4-N3	-3.99	112.89	123.12
10	G	1093	U	OP3-P-O5'	-3.97	95.14	106.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1087	ADP	1	0
7	A	1088	ADP	1	0
9	A	1090	NET	1	0
10	A	1091	U	1	0
5	C	1078	PO4	1	0
8	C	1091	ORN	1	0
9	C	1092	NET	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	1093	U	2	0
7	E	1089	ADP	1	0
7	E	1090	ADP	2	0
8	E	1091	ORN	2	0
9	E	1092	NET	2	0
10	E	1093	U	2	0
8	G	1091	ORN	1	0
9	G	1092	NET	2	0
10	G	1093	U	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	1058/1073 (98%)	-0.37	24 (2%)	64	70	17, 33, 73, 100	0
1	C	1058/1073 (98%)	-0.24	30 (2%)	56	64	18, 35, 81, 100	0
1	E	1058/1073 (98%)	-0.31	22 (2%)	67	72	17, 31, 75, 100	0
1	G	1058/1073 (98%)	-0.06	42 (3%)	42	51	20, 42, 84, 100	0
2	B	379/382 (99%)	0.08	17 (4%)	37	46	21, 48, 87, 100	0
2	D	379/382 (99%)	0.01	14 (3%)	45	54	21, 40, 78, 100	0
2	F	379/382 (99%)	0.22	26 (6%)	20	27	20, 47, 92, 100	0
2	H	379/382 (99%)	0.54	39 (10%)	9	12	33, 63, 97, 100	0
All	All	5748/5820 (98%)	-0.12	214 (3%)	45	54	17, 38, 84, 100	0

The worst 5 of 214 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	8.6
1	E	1	MET	8.2
1	A	1	MET	7.6
1	G	1	MET	7.0
1	A	738	PHE	5.7

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
9	NET	E	1092	9/9	0.98	0.18	4.79	15,23,27,28	0
8	ORN	C	1091	9/9	0.97	0.19	4.10	20,29,35,39	0
9	NET	G	1092	9/9	0.99	0.13	3.58	18,28,29,37	0
8	ORN	A	1089	9/9	0.95	0.18	3.37	24,29,36,37	0
6	CL	H	384	1/1	0.95	0.13	3.15	67,67,67,67	0
8	ORN	E	1091	9/9	0.97	0.13	2.97	16,25,37,40	0
8	ORN	G	1091	9/9	0.96	0.17	2.70	28,33,36,63	0
9	NET	C	1092	9/9	0.99	0.13	1.94	16,21,23,29	0
9	NET	A	1090	9/9	0.98	0.10	1.92	18,23,28,38	0
10	U	C	1093	21/21	0.95	0.12	0.21	33,51,83,89	0
10	U	G	1093	21/21	0.94	0.12	-0.06	31,57,80,85	0
7	ADP	E	1089	27/27	0.99	0.12	-0.10	15,26,34,36	0
6	CL	E	1086	1/1	0.99	0.07	-0.14	41,41,41,41	0
10	U	A	1091	21/21	0.96	0.10	-0.17	28,58,80,81	0
4	K	G	1077	1/1	0.99	0.10	-0.19	38,38,38,38	0
7	ADP	C	1089	27/27	0.99	0.10	-0.30	16,23,31,44	0
4	K	E	1077	1/1	0.99	0.12	-0.35	30,30,30,30	0
7	ADP	G	1089	27/27	0.99	0.11	-0.36	17,27,35,41	0
10	U	E	1093	21/21	0.96	0.10	-0.40	37,54,80,89	0
4	K	C	1077	1/1	0.99	0.11	-0.44	27,27,27,27	0
7	ADP	A	1087	27/27	0.99	0.09	-0.49	16,22,31,38	0
7	ADP	C	1090	27/27	0.98	0.08	-0.65	26,42,61,77	0
6	CL	F	384	1/1	1.00	0.06	-0.70	32,32,32,32	0
7	ADP	G	1090	27/27	0.98	0.09	-0.72	29,47,80,89	0
4	K	A	1080	1/1	0.99	0.08	-0.81	29,29,29,29	0
4	K	C	1080	1/1	0.99	0.08	-0.88	36,36,36,36	0
7	ADP	A	1088	27/27	0.99	0.07	-0.89	20,33,47,60	0
7	ADP	E	1090	27/27	0.99	0.06	-1.04	23,35,48,56	0
6	CL	D	384	1/1	0.99	0.07	-1.08	34,34,34,34	0
6	CL	C	1085	1/1	1.00	0.07	-1.31	39,39,39,39	0
6	CL	G	1086	1/1	0.92	0.07	-1.53	54,54,54,54	0
4	K	A	1077	1/1	0.99	0.08	-1.54	27,27,27,27	0
5	PO4	G	1078	5/5	0.99	0.07	-1.55	17,24,31,35	0
5	PO4	A	1078	5/5	0.99	0.08	-1.73	17,21,24,29	0
4	K	G	1080	1/1	0.99	0.07	-1.74	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	PO4	E	1078	5/5	0.99	0.08	-1.76	19,22,26,27	0
6	CL	A	1085	1/1	0.99	0.06	-1.78	39,39,39,39	0
4	K	E	1080	1/1	0.99	0.06	-1.79	27,27,27,27	0
5	PO4	C	1078	5/5	0.99	0.09	-1.80	16,22,24,25	0
4	K	E	1076	1/1	0.99	0.09	-1.81	25,25,25,25	0
4	K	G	1076	1/1	1.00	0.09	-2.24	28,28,28,28	0
3	MN	A	1074	1/1	1.00	0.07	-2.24	25,25,25,25	0
3	MN	C	1074	1/1	1.00	0.08	-2.30	27,27,27,27	0
3	MN	G	1074	1/1	1.00	0.07	-2.30	31,31,31,31	0
3	MN	E	1074	1/1	1.00	0.09	-2.53	27,27,27,27	0
4	K	C	1076	1/1	1.00	0.07	-2.61	22,22,22,22	0
4	K	A	1076	1/1	1.00	0.07	-2.72	21,21,21,21	0
6	CL	C	1083	1/1	0.91	0.16	-	77,77,77,77	0
4	K	E	1081	1/1	0.95	0.06	-	42,42,42,42	0
4	K	B	383	1/1	0.98	0.07	-	45,45,45,45	0
6	CL	G	1087	1/1	0.98	0.08	-	81,81,81,81	0
4	K	E	1083	1/1	0.98	0.05	-	58,58,58,58	0
6	CL	G	1082	1/1	0.99	0.10	-	29,29,29,29	0
6	CL	C	1084	1/1	0.96	0.08	-	43,43,43,43	0
4	K	C	1082	1/1	0.96	0.06	-	44,44,44,44	0
3	MN	G	1079	1/1	0.99	0.05	-	47,47,47,47	0
4	K	D	383	1/1	0.99	0.03	-	34,34,34,34	0
6	CL	G	1085	1/1	0.98	0.06	-	46,46,46,46	0
4	K	G	1083	1/1	0.99	0.06	-	52,52,52,52	0
3	MN	A	1079	1/1	1.00	0.05	-	37,37,37,37	0
6	CL	G	1088	1/1	0.97	0.17	-	67,67,67,67	0
4	K	F	383	1/1	0.99	0.07	-	36,36,36,36	0
6	CL	E	1085	1/1	0.98	0.05	-	49,49,49,49	0
4	K	G	1081	1/1	0.97	0.06	-	46,46,46,46	0
3	MN	C	1079	1/1	0.99	0.05	-	46,46,46,46	0
6	CL	C	1081	1/1	0.99	0.10	-	29,29,29,29	0
6	CL	G	1084	1/1	0.83	0.22	-	72,72,72,72	0
6	CL	A	1081	1/1	0.99	0.08	-	28,28,28,28	0
3	MN	G	1075	1/1	1.00	0.08	-	28,28,28,28	0
5	PO4	C	1088	5/5	0.92	0.21	-	80,80,80,80	0
6	CL	E	1082	1/1	1.00	0.14	-	24,24,24,24	0
6	CL	E	1087	1/1	0.94	0.06	-	54,54,54,54	0
6	CL	C	1087	1/1	0.99	0.15	-	63,63,63,63	0
6	CL	A	1084	1/1	0.99	0.05	-	40,40,40,40	0
3	MN	C	1075	1/1	0.99	0.07	-	25,25,25,25	0
6	CL	E	1088	1/1	0.99	0.10	-	44,44,44,44	0
6	CL	H	385	1/1	0.84	0.07	-	82,82,82,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	K	A	1082	1/1	0.98	0.04	-	41,41,41,41	0
4	K	H	383	1/1	0.97	0.11	-	64,64,64,64	0
6	CL	A	1086	1/1	0.96	0.06	-	56,56,56,56	0
3	MN	A	1075	1/1	1.00	0.06	-	23,23,23,23	0
6	CL	A	1083	1/1	0.91	0.10	-	66,66,66,66	0
3	MN	E	1079	1/1	1.00	0.05	-	41,41,41,41	0
3	MN	E	1075	1/1	1.00	0.08	-	27,27,27,27	0
6	CL	C	1086	1/1	0.95	0.11	-	67,67,67,67	0
6	CL	E	1084	1/1	0.82	0.15	-	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.