



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 07:04 am GMT

PDB ID : 1M6V  
Title : Crystal Structure of the G359F (small subunit) Point Mutant of Carbamoyl Phosphate Synthetase  
Authors : Thoden, J.B.; Huang, X.; Raushel, F.M.; Holden, H.M.  
Deposited on : 2002-07-17  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

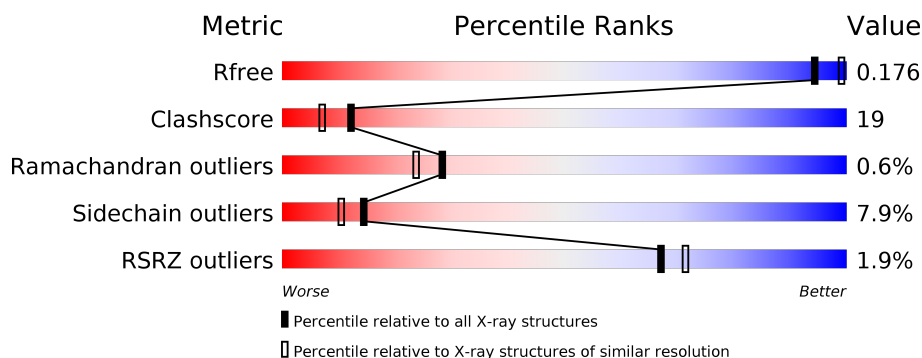
# 1 Overall quality at a glance

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))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (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  $\geq 3$ , 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>0.1%</div> <div>61% 30% 7% .</div> </div>
1	C	1073	<div> <div>2%</div> <div>62% 30% 7% ..</div> </div>
1	E	1073	<div> <div>2%</div> <div>61% 29% 8% ..</div> </div>
1	G	1073	<div> <div>2%</div> <div>52% 37% 8% ..</div> </div>
2	B	382	<div> <div>2%</div> <div>37% 46% 14% ..</div> </div>
2	D	382	<div> <div>0.1%</div> <div>59% 32% 8% .</div> </div>

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Mol	Chain	Length	Quality of chain
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
8	ORN	A	4011	-	-	-	X
8	ORN	C	4031	-	-	-	X
8	ORN	E	4054	-	-	-	X
8	ORN	G	4076	-	-	-	X
9	NET	G	4077	-	-	-	X

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 48206 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 synthetase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1059	Total	C	N	O	S	0	6	0
			8190	5140	1425	1579	46			
1	C	1059	Total	C	N	O	S	0	5	0
			8196	5144	1431	1576	45			
1	E	1059	Total	C	N	O	S	0	6	0
			8189	5141	1426	1576	46			
1	G	1059	Total	C	N	O	S	0	6	0
			8197	5144	1428	1580	45			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	ASN	LEU	SEE REMARK 999	UNP P00968
C	46	ASN	LEU	SEE REMARK 999	UNP P00968
E	46	ASN	LEU	SEE REMARK 999	UNP P00968
G	46	ASN	LEU	SEE REMARK 999	UNP P00968

- Molecule 2 is a protein called carbamoyl-phosphate synthetase small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	375	Total	C	N	O	S	0	1	0
			2871	1812	504	545	10			
2	D	375	Total	C	N	O	S	0	2	0
			2877	1814	507	546	10			
2	F	375	Total	C	N	O	S	0	3	0
			2880	1818	505	546	11			
2	H	375	Total	C	N	O	S	0	1	0
			2871	1812	504	545	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	183	GLN	GLU	SEE REMARK 999	UNP P00907
B	359	PHE	GLY	ENGINEERED	UNP P00907
D	183	GLN	GLU	SEE REMARK 999	UNP P00907
D	359	PHE	GLY	ENGINEERED	UNP P00907
F	183	GLN	GLU	SEE REMARK 999	UNP P00907
F	359	PHE	GLY	ENGINEERED	UNP P00907
H	183	GLN	GLU	SEE REMARK 999	UNP P00907
H	359	PHE	GLY	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

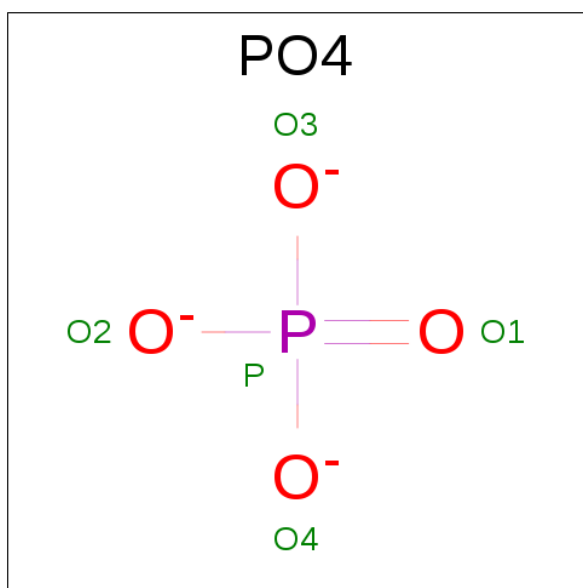
- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	6	Total K 6 6	0	0
4	D	1	Total K 1 1	0	0
4	E	6	Total K 6 6	0	0
4	B	1	Total K 1 1	0	0
4	C	6	Total K 6 6	0	0
4	A	5	Total K 5 5	0	0
4	F	1	Total K 1 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

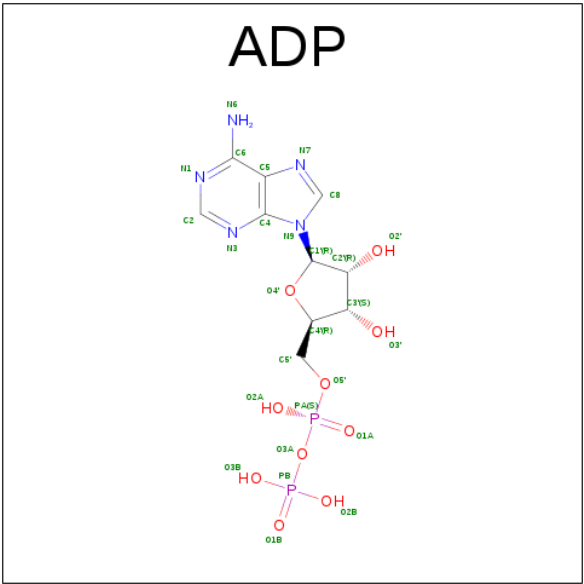
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	6	Total Cl 6 6	0	0
5	D	1	Total Cl 1 1	0	0
5	E	6	Total Cl 6 6	0	0
5	H	1	Total Cl 1 1	0	0
5	B	1	Total Cl 1 1	0	0
5	C	7	Total Cl 7 7	0	0
5	A	5	Total Cl 5 5	0	0
5	F	1	Total Cl 1 1	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



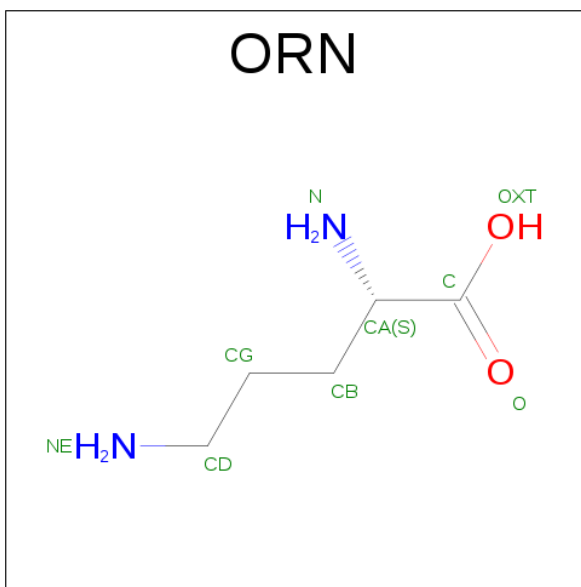
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O P 5 4 1	0	0
6	C	1	Total O P 5 4 1	0	0
6	E	1	Total O P 5 4 1	0	0
6	G	1	Total O P 5 4 1	0	0

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



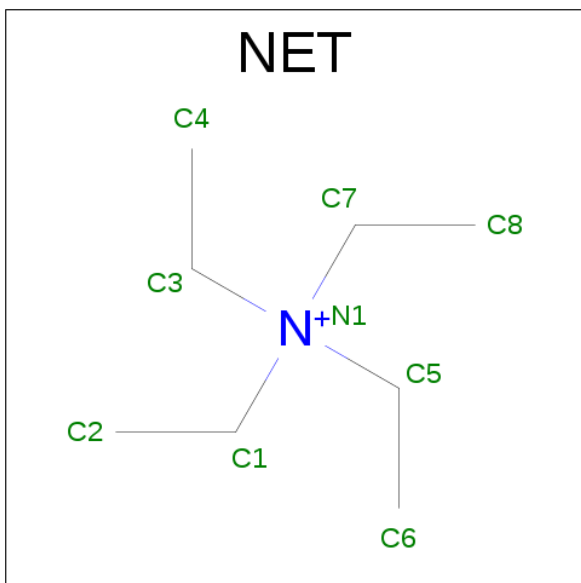
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	G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

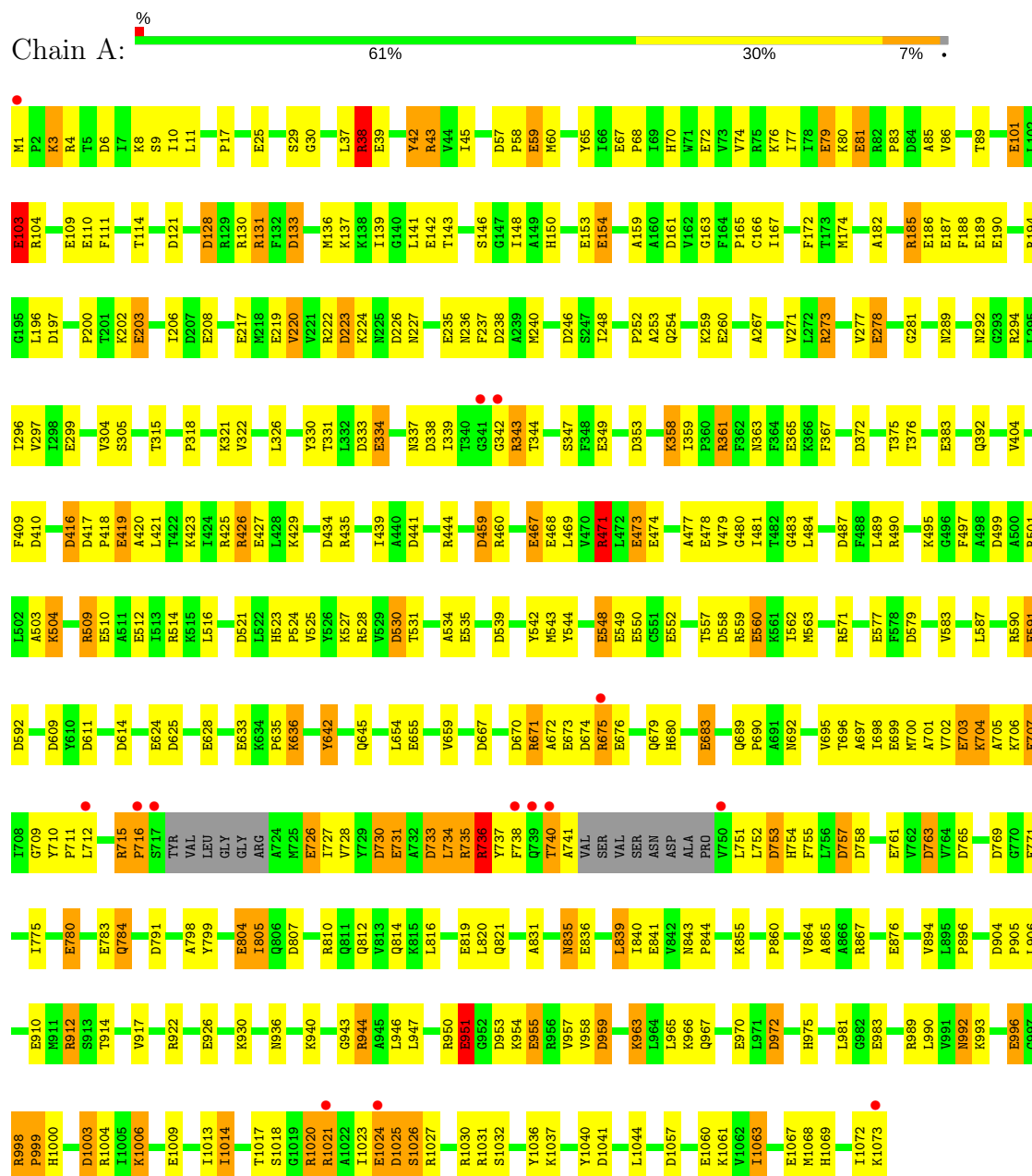
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	793	Total O 793 793	0	0
10	B	130	Total O 130 130	0	0
10	C	681	Total O 681 681	0	0
10	D	177	Total O 177 177	0	0
10	E	813	Total O 813 813	0	0
10	F	205	Total O 205 205	0	0
10	G	645	Total O 645 645	0	0
10	H	117	Total O 117 117	0	0

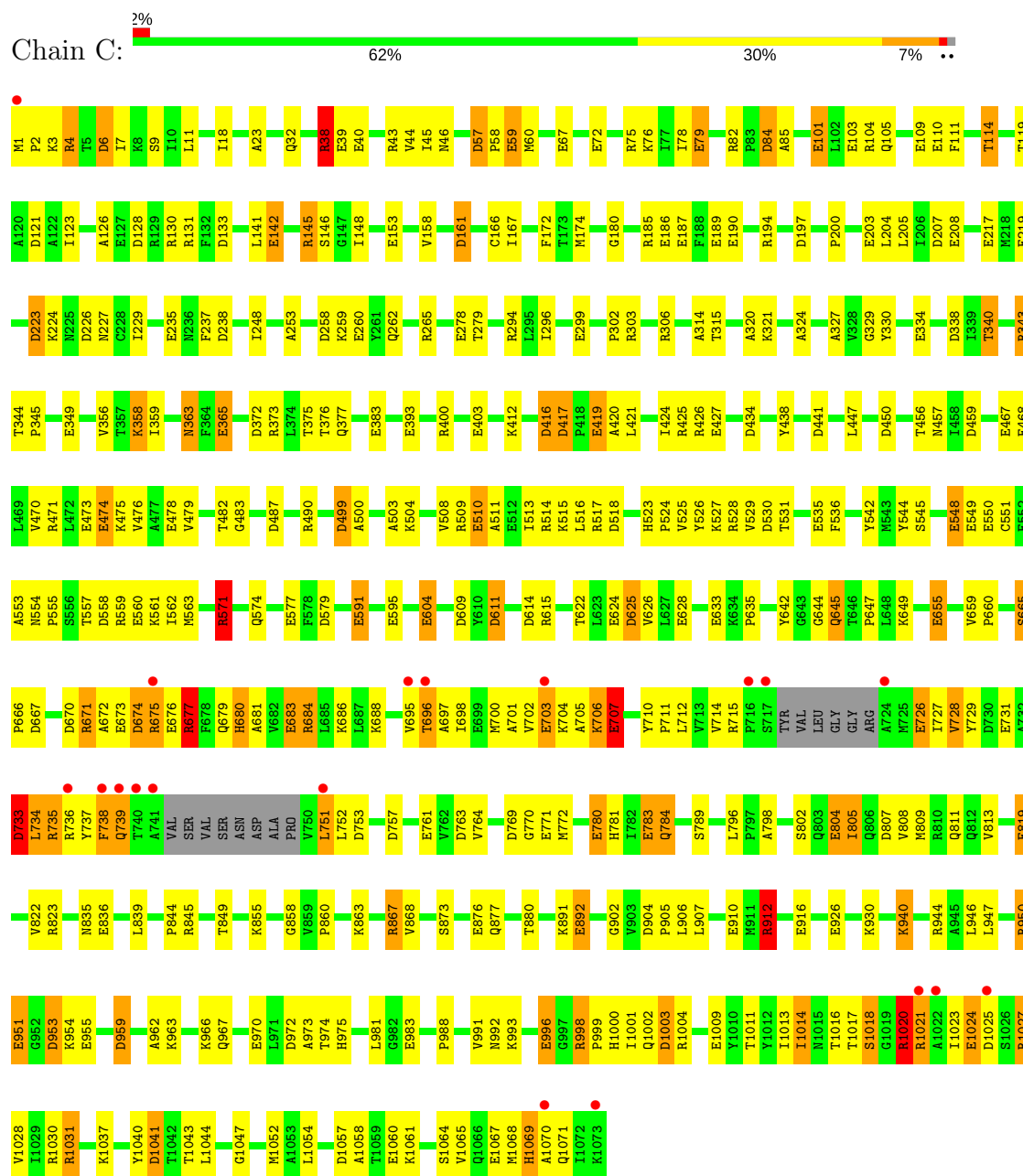
### 3 Residue-property plots

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

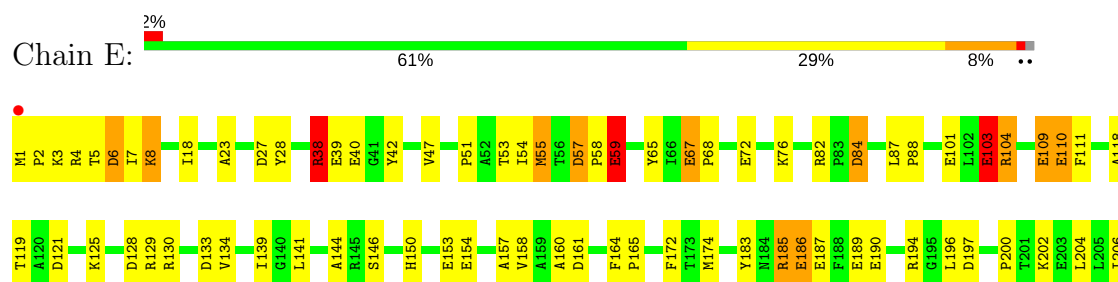
- Molecule 1: carbamoyl phosphate synthetase large chain

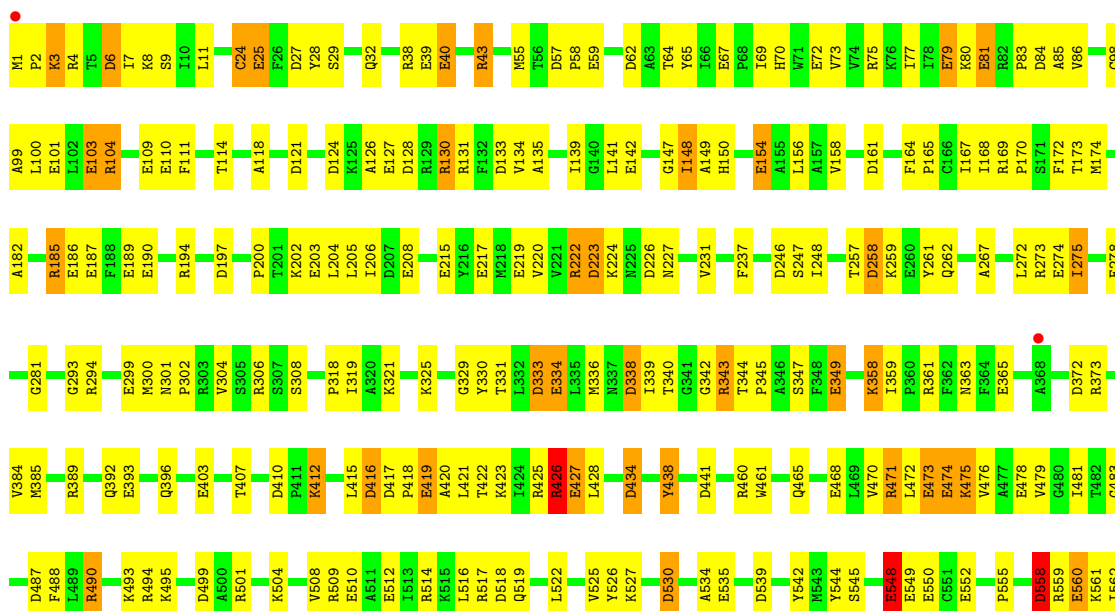


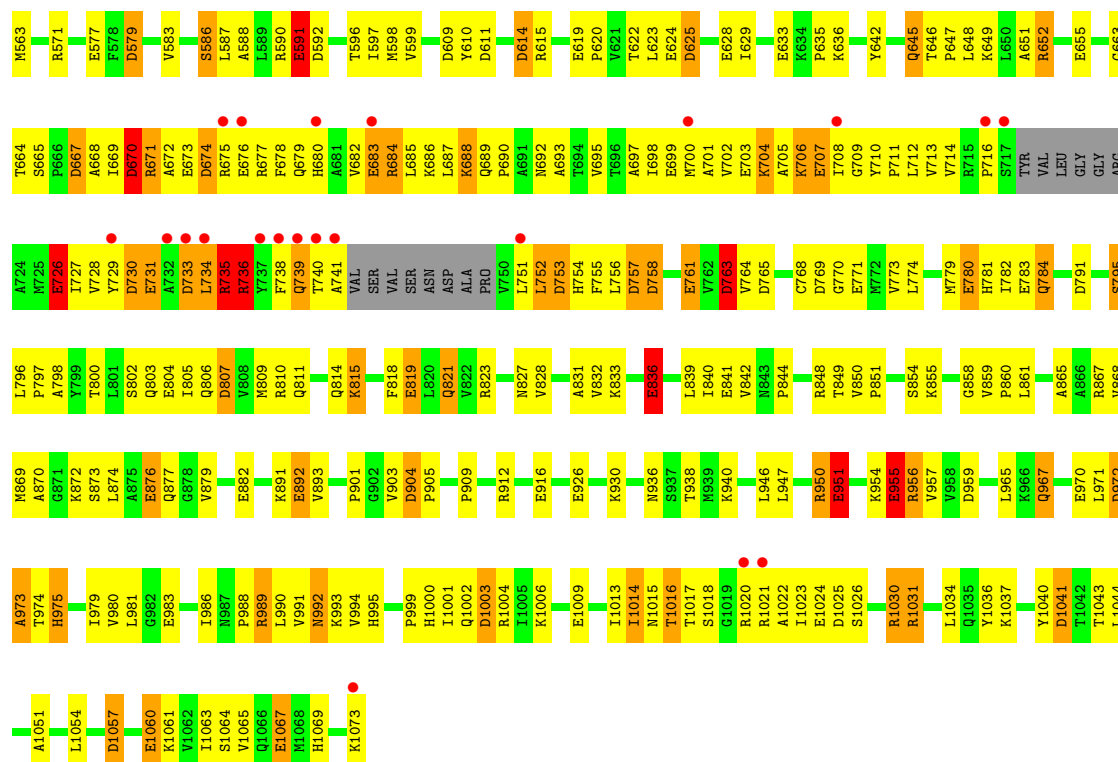
• Molecule 1: carbamoyl phosphate synthetase large chain



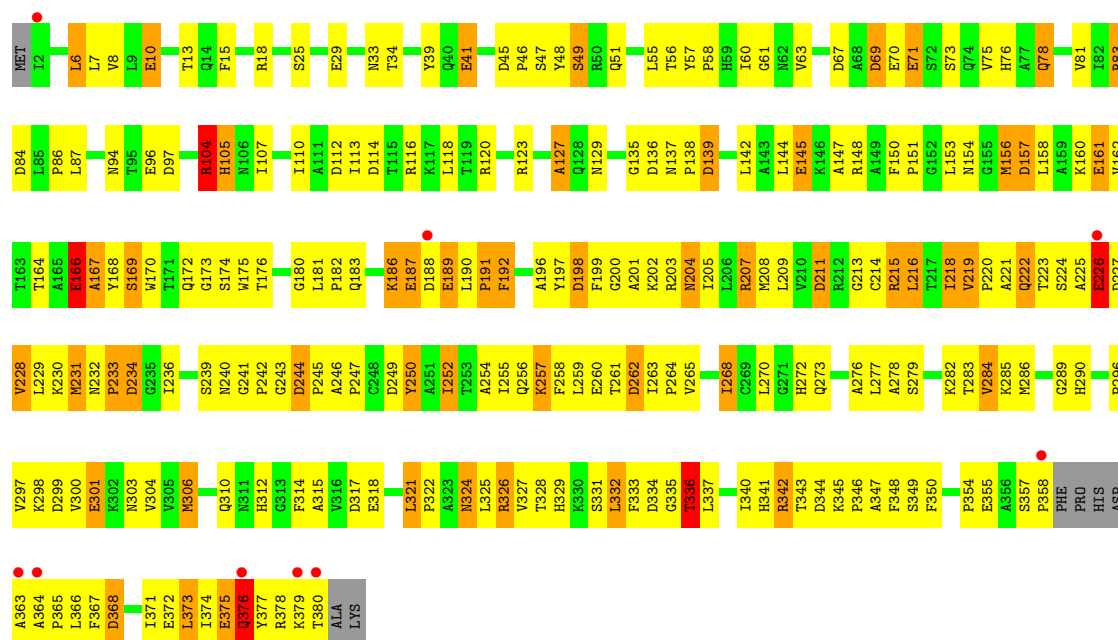
• Molecule 1: carbamoyl phosphate synthetase large chain





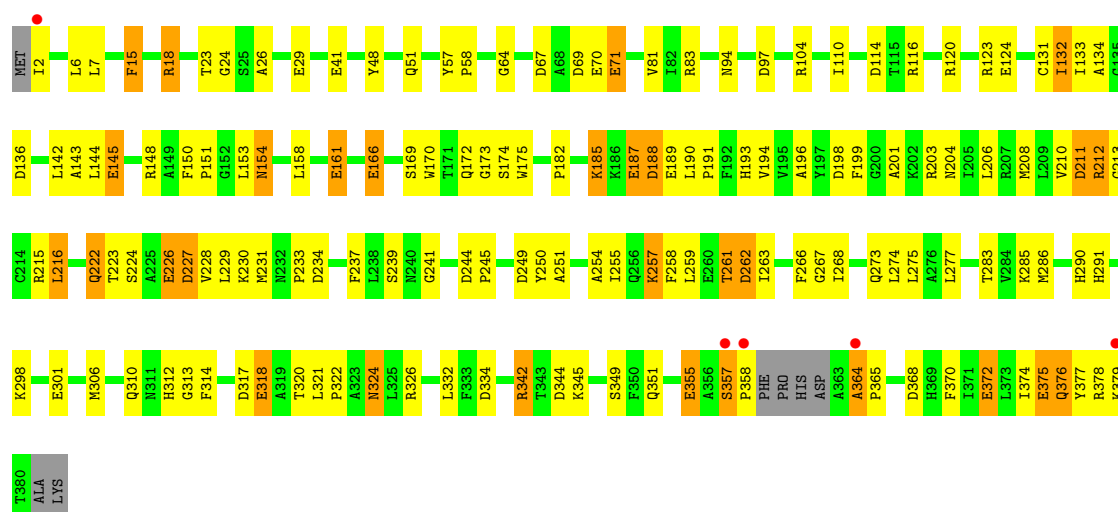


• Molecule 2: carbamoyl-phosphate synthetase small chain

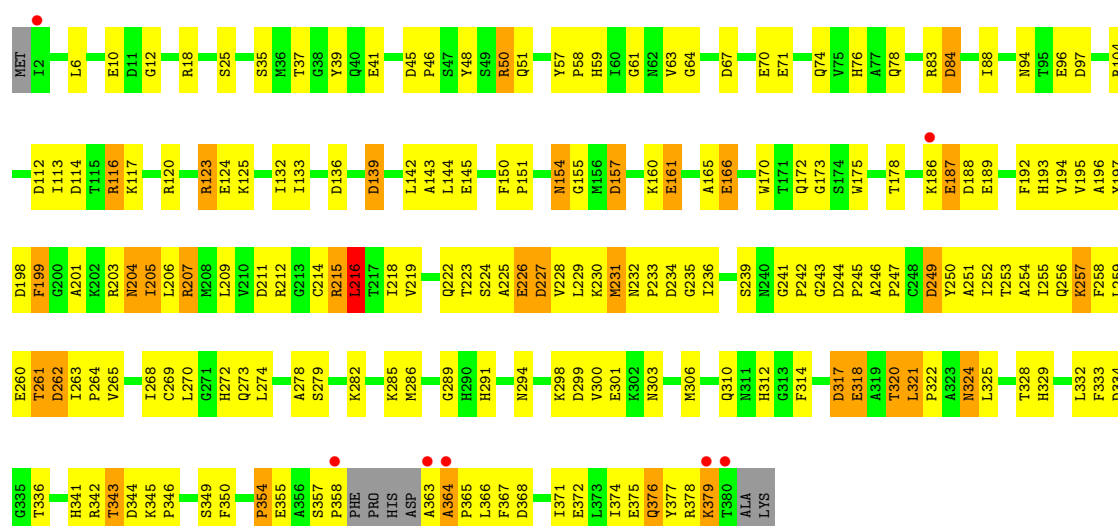


• Molecule 2: carbamoyl-phosphate synthetase small chain

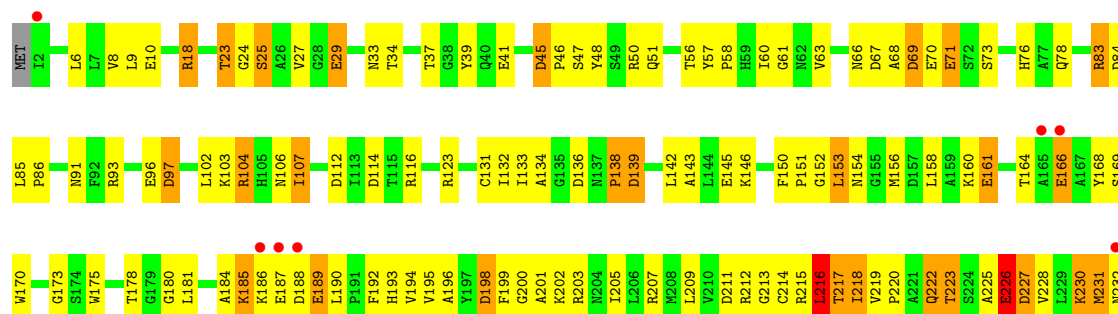


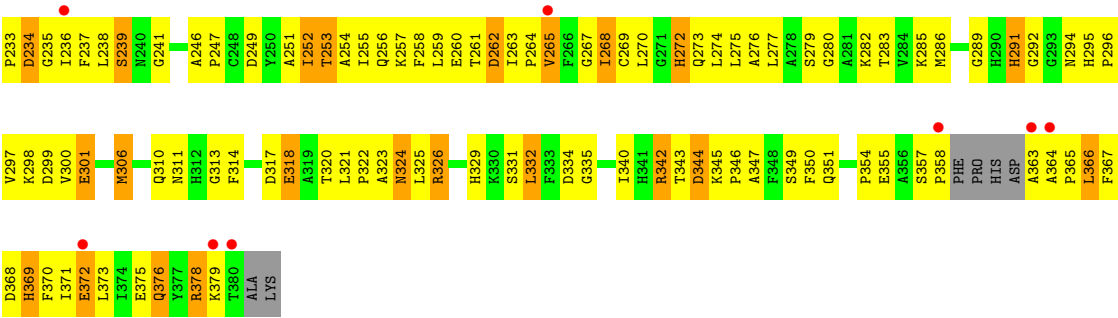


• Molecule 2: carbamoyl-phosphate synthetase small chain



• Molecule 2: carbamoyl-phosphate synthetase small chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.50Å 164.20Å 331.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 19.93 – 2.09	Depositor EDS
% Data completeness (in resolution range)	92.4 (30.00-2.10) 92.0 (19.93-2.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.78 (at 2.09Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.174 , 0.245 0.176 , 0.176	Depositor DCC
$R_{free}$ test set	44042 reflections (11.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.4	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 104.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	48206	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality ⓘ

### 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	1.07	77/8340 (0.9%)	1.42	118/11273 (1.0%)
1	C	1.05	74/8350 (0.9%)	1.44	124/11288 (1.1%)
1	E	1.06	67/8339 (0.8%)	1.45	136/11272 (1.2%)
1	G	1.04	72/8351 (0.9%)	1.46	139/11291 (1.2%)
2	B	0.94	18/2934 (0.6%)	1.40	39/3981 (1.0%)
2	D	0.96	16/2944 (0.5%)	1.44	41/3996 (1.0%)
2	F	0.94	16/2951 (0.5%)	1.40	42/4003 (1.0%)
2	H	0.93	18/2934 (0.6%)	1.40	42/3981 (1.1%)
All	All	1.03	358/45143 (0.8%)	1.43	681/61085 (1.1%)

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	H	1	0

The worst 5 of 358 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	683	GLU	CD-OE2	9.30	1.35	1.25
1	C	1009	GLU	CD-OE2	8.99	1.35	1.25
1	E	804	GLU	CD-OE2	8.31	1.34	1.25
1	C	955	GLU	CD-OE2	8.07	1.34	1.25
1	A	876	GLU	CD-OE2	8.00	1.34	1.25

The worst 5 of 681 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	490	ARG	NE-CZ-NH1	12.98	126.79	120.30
1	C	517	ARG	NE-CZ-NH2	-12.62	113.99	120.30
1	E	185	ARG	NE-CZ-NH1	11.06	125.83	120.30
1	G	43	ARG	NE-CZ-NH2	-10.61	115.00	120.30
1	G	579	ASP	CB-CG-OD2	-10.16	109.15	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	H	216	LEU	CA

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8190	0	8213	225	0
1	C	8196	0	8236	225	0
1	E	8189	0	8219	254	0
1	G	8197	0	8218	334	0
2	B	2871	0	2850	213	0
2	D	2877	0	2852	108	0
2	F	2880	0	2859	156	0
2	H	2871	0	2850	199	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	5	0	0	1	0
4	B	1	0	0	0	0
4	C	6	0	0	0	0
4	D	1	0	0	0	0
4	E	6	0	0	0	0
4	F	1	0	0	0	0
4	G	6	0	0	0	0
5	A	5	0	0	0	0
5	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	7	0	0	1	0
5	D	1	0	0	1	0
5	E	6	0	0	0	0
5	F	1	0	0	0	0
5	G	6	0	0	1	0
5	H	1	0	0	0	0
6	A	5	0	0	0	0
6	C	5	0	0	0	0
6	E	5	0	0	0	0
6	G	5	0	0	0	0
7	A	54	0	24	3	0
7	C	54	0	24	1	0
7	E	54	0	24	1	0
7	G	54	0	24	0	0
8	A	9	0	11	0	0
8	C	9	0	11	2	0
8	E	9	0	11	1	0
8	G	9	0	11	2	0
9	A	9	0	20	3	0
9	C	9	0	20	1	0
9	E	9	0	20	0	0
9	G	9	0	20	0	0
10	A	793	0	0	23	0
10	B	130	0	0	3	0
10	C	681	0	0	13	0
10	D	177	0	0	2	0
10	E	813	0	0	20	0
10	F	205	0	0	9	0
10	G	645	0	0	17	0
10	H	117	0	0	6	0
All	All	48206	0	44517	1694	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

The worst 5 of 1694 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)
4:A:4009:K:K	10:A:4434:HOH:O	1.26	1.26
2:H:133:ILE:HD12	2:H:143:ALA:HB2	1.28	1.15
2:D:187:GLU:HG2	2:D:215:ARG:HD2	1.25	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:GLU:HG2	2:B:215:ARG:HD2	1.30	1.11
1:G:695:VAL:HG11	1:G:701:ALA:HB2	1.32	1.10

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1059/1073 (99%)	993 (94%)	63 (6%)	3 (0%)	44	44
1	C	1060/1073 (99%)	997 (94%)	59 (6%)	4 (0%)	38	35
1	E	1059/1073 (99%)	1008 (95%)	46 (4%)	5 (0%)	32	28
1	G	1060/1073 (99%)	989 (93%)	64 (6%)	7 (1%)	25	20
2	B	372/382 (97%)	334 (90%)	31 (8%)	7 (2%)	9	4
2	D	373/382 (98%)	351 (94%)	21 (6%)	1 (0%)	44	44
2	F	374/382 (98%)	360 (96%)	11 (3%)	3 (1%)	22	17
2	H	372/382 (97%)	324 (87%)	40 (11%)	8 (2%)	8	3
All	All	5729/5820 (98%)	5356 (94%)	335 (6%)	38 (1%)	28	20

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	167	ALA
1	G	558	ASP
1	G	739	GLN
2	H	185	LYS
2	H	223	THR

### 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	871/878 (99%)	810 (93%)	61 (7%)	18	14
1	C	872/878 (99%)	820 (94%)	52 (6%)	22	19
1	E	871/878 (99%)	807 (93%)	64 (7%)	16	13
1	G	872/878 (99%)	798 (92%)	74 (8%)	12	8
2	B	306/311 (98%)	267 (87%)	39 (13%)	5	2
2	D	307/311 (99%)	288 (94%)	19 (6%)	21	18
2	F	308/311 (99%)	279 (91%)	29 (9%)	10	6
2	H	306/311 (98%)	270 (88%)	36 (12%)	6	3
All	All	4713/4756 (99%)	4339 (92%)	374 (8%)	14	10

5 of 374 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	376	GLN
1	E	733	ASP
2	H	107	ILE
1	E	38	ARG
1	E	509	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1055	ASN
1	E	457	ASN
2	H	78	GLN
2	D	14	GLN
2	D	324	ASN

### 5.3.3 RNA ⓘ

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, 66 are monoatomic - leaving 20 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$
7	ADP	A	4001	3	25,29,29	1.12	3 (12%)	24,45,45	1.48	2 (8%)
6	PO4	A	4006	3	4,4,4	1.78	1 (25%)	6,6,6	1.22	1 (16%)
7	ADP	A	4007	3,4	25,29,29	1.01	2 (8%)	24,45,45	1.11	1 (4%)
8	ORN	A	4011	-	3,8,8	0.52	0	2,9,9	0.47	0
9	NET	A	4012	-	8,8,8	0.54	0	10,10,10	0.69	0
7	ADP	C	4021	3	25,29,29	1.53	5 (20%)	24,45,45	1.37	4 (16%)
6	PO4	C	4026	3	4,4,4	2.28	3 (75%)	6,6,6	0.91	0
7	ADP	C	4027	3,4	25,29,29	1.49	4 (16%)	24,45,45	1.11	1 (4%)
8	ORN	C	4031	-	3,8,8	0.45	0	2,9,9	0.41	0
9	NET	C	4032	-	8,8,8	0.55	0	10,10,10	0.67	0
7	ADP	E	4044	3	25,29,29	1.00	1 (4%)	24,45,45	1.13	2 (8%)
6	PO4	E	4049	3	4,4,4	2.05	2 (50%)	6,6,6	0.66	0
7	ADP	E	4050	3,4	25,29,29	1.28	4 (16%)	24,45,45	1.09	2 (8%)
8	ORN	E	4054	-	3,8,8	0.69	0	2,9,9	0.94	0
9	NET	E	4055	-	8,8,8	0.63	0	10,10,10	0.60	0
7	ADP	G	4066	3	25,29,29	1.43	5 (20%)	24,45,45	1.38	4 (16%)
6	PO4	G	4071	3	4,4,4	1.94	1 (25%)	6,6,6	0.95	0
7	ADP	G	4072	3,4	25,29,29	1.58	4 (16%)	24,45,45	1.17	1 (4%)
8	ORN	G	4076	-	3,8,8	0.46	0	2,9,9	0.30	0
9	NET	G	4077	-	8,8,8	0.63	0	10,10,10	0.64	0

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
7	ADP	A	4001	3	-	0/12/32/32	0/3/3/3
6	PO4	A	4006	3	-	0/0/0/0	0/0/0/0
7	ADP	A	4007	3,4	-	0/12/32/32	0/3/3/3
8	ORN	A	4011	-	-	0/4/8/8	0/0/0/0
9	NET	A	4012	-	-	0/12/12/12	0/0/0/0
7	ADP	C	4021	3	-	0/12/32/32	0/3/3/3
6	PO4	C	4026	3	-	0/0/0/0	0/0/0/0
7	ADP	C	4027	3,4	-	0/12/32/32	0/3/3/3
8	ORN	C	4031	-	-	0/4/8/8	0/0/0/0
9	NET	C	4032	-	-	0/12/12/12	0/0/0/0
7	ADP	E	4044	3	-	0/12/32/32	0/3/3/3
6	PO4	E	4049	3	-	0/0/0/0	0/0/0/0
7	ADP	E	4050	3,4	-	0/12/32/32	0/3/3/3
8	ORN	E	4054	-	-	0/4/8/8	0/0/0/0
9	NET	E	4055	-	-	0/12/12/12	0/0/0/0
7	ADP	G	4066	3	-	0/12/32/32	0/3/3/3
6	PO4	G	4071	3	-	0/0/0/0	0/0/0/0
7	ADP	G	4072	3,4	-	0/12/32/32	0/3/3/3
8	ORN	G	4076	-	-	0/4/8/8	0/0/0/0
9	NET	G	4077	-	-	0/12/12/12	0/0/0/0

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	4072	ADP	O4'-C1'	-3.37	1.36	1.41
6	C	4026	PO4	P-O2	-3.13	1.43	1.54
7	C	4021	ADP	O4'-C1'	-2.85	1.37	1.41
7	G	4066	ADP	O4'-C1'	-2.75	1.37	1.41
6	G	4071	PO4	P-O2	-2.74	1.44	1.54

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	4066	ADP	C1'-N9-C4	-2.57	122.20	126.64
7	A	4001	ADP	N6-C6-N1	-2.47	113.86	118.77
6	A	4006	PO4	O2-P-O1	-2.34	101.01	110.97
7	C	4021	ADP	N6-C6-N1	-2.30	114.21	118.77
7	E	4044	ADP	O3'-C3'-C2'	2.05	118.39	111.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	4001	ADP	1	0
7	A	4007	ADP	2	0
9	A	4012	NET	3	0
7	C	4027	ADP	1	0
8	C	4031	ORN	2	0
9	C	4032	NET	1	0
7	E	4050	ADP	1	0
8	E	4054	ORN	1	0
8	G	4076	ORN	2	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 [i](#)

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1059/1073 (98%)	-0.56	14 (1%) 77 81	14, 29, 71, 100	0
1	C	1059/1073 (98%)	-0.51	19 (1%) 69 73	14, 31, 76, 100	0
1	E	1059/1073 (98%)	-0.57	19 (1%) 69 73	13, 27, 75, 100	0
1	G	1059/1073 (98%)	-0.38	23 (2%) 62 67	17, 36, 81, 100	0
2	B	375/382 (98%)	-0.09	9 (2%) 59 64	21, 48, 84, 100	0
2	D	375/382 (98%)	-0.40	5 (1%) 77 81	17, 33, 71, 100	0
2	F	375/382 (98%)	-0.34	7 (1%) 67 71	16, 36, 76, 100	0
2	H	375/382 (98%)	0.04	15 (4%) 39 46	26, 52, 90, 100	0
All	All	5736/5820 (98%)	-0.42	111 (1%) 67 71	13, 33, 79, 100	0

The worst 5 of 111 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	9.7
1	C	1	MET	7.4
1	E	1	MET	7.0
1	G	1	MET	6.9
2	D	358	PRO	6.8

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
8	ORN	E	4054	9/9	0.95	0.14	6.10	17,28,35,38	0
8	ORN	G	4076	9/9	0.96	0.12	4.03	22,30,47,60	0
8	ORN	C	4031	9/9	0.96	0.12	2.40	19,26,46,57	0
9	NET	G	4077	9/9	0.96	0.10	2.34	23,28,36,42	0
8	ORN	A	4011	9/9	0.97	0.10	2.30	15,23,32,38	0
9	NET	E	4055	9/9	0.98	0.07	1.88	12,19,31,35	0
9	NET	A	4012	9/9	0.98	0.08	1.56	12,19,26,28	0
9	NET	C	4032	9/9	0.98	0.07	0.52	15,21,28,30	0
4	K	C	4034	1/1	0.96	0.10	0.12	51,51,51,51	0
7	ADP	G	4066	27/27	0.98	0.08	0.09	9,22,31,38	0
5	CL	H	4085	1/1	0.98	0.09	0.04	52,52,52,52	0
5	CL	G	4083	1/1	0.98	0.10	-0.05	58,58,58,58	0
7	ADP	C	4021	27/27	0.99	0.07	-0.16	12,19,24,45	0
6	PO4	A	4006	5/5	0.99	0.07	-0.40	16,22,28,30	0
7	ADP	A	4001	27/27	0.99	0.07	-0.42	12,22,32,38	0
7	ADP	G	4072	27/27	0.96	0.08	-0.52	30,43,80,95	0
7	ADP	C	4027	27/27	0.98	0.08	-0.57	16,33,62,83	0
7	ADP	E	4050	27/27	0.97	0.08	-0.59	19,33,50,58	0
6	PO4	C	4026	5/5	0.99	0.07	-0.64	14,15,19,24	0
7	ADP	E	4044	27/27	0.99	0.07	-0.67	8,20,25,28	0
6	PO4	G	4071	5/5	0.99	0.06	-0.85	15,16,17,32	0
7	ADP	A	4007	27/27	0.99	0.06	-0.87	14,28,48,77	0
5	CL	A	4017	1/1	0.99	0.05	-1.34	39,39,39,39	0
5	CL	E	4062	1/1	0.98	0.05	-1.44	48,48,48,48	0
6	PO4	E	4049	5/5	0.99	0.05	-1.83	17,17,21,25	0
4	K	E	4048	1/1	1.00	0.07	-1.91	23,23,23,23	0
3	MN	G	4067	1/1	1.00	0.04	-1.92	25,25,25,25	0
3	MN	E	4045	1/1	1.00	0.05	-2.16	24,24,24,24	0
4	K	G	4070	1/1	0.99	0.06	-2.38	30,30,30,30	0
5	CL	C	4039	1/1	0.98	0.04	-2.40	45,45,45,45	0
4	K	G	4069	1/1	0.99	0.04	-2.40	24,24,24,24	0
4	K	A	4005	1/1	1.00	0.05	-2.43	25,25,25,25	0
5	CL	F	4064	1/1	1.00	0.04	-2.45	33,33,33,33	0
3	MN	A	4002	1/1	1.00	0.04	-2.75	21,21,21,21	0
4	K	G	4075	1/1	1.00	0.04	-2.89	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	K	C	4025	1/1	0.98	0.05	-3.29	25,25,25,25	0
5	CL	B	4019	1/1	0.99	0.03	-3.37	33,33,33,33	0
4	K	A	4010	1/1	1.00	0.04	-3.91	21,21,21,21	0
4	K	E	4047	1/1	1.00	0.03	-3.99	19,19,19,19	0
4	K	A	4004	1/1	1.00	0.03	-4.02	20,20,20,20	0
4	K	E	4053	1/1	1.00	0.02	-4.37	23,23,23,23	0
4	K	C	4030	1/1	0.99	0.03	-4.44	26,26,26,26	0
4	K	C	4024	1/1	1.00	0.02	-4.71	19,19,19,19	0
3	MN	C	4022	1/1	1.00	0.04	-4.86	21,21,21,21	0
5	CL	G	4084	1/1	0.97	0.10	-	76,76,76,76	0
5	CL	A	4020	1/1	0.97	0.06	-	45,45,45,45	0
3	MN	C	4028	1/1	0.99	0.03	-	39,39,39,39	0
3	MN	C	4023	1/1	1.00	0.04	-	24,24,24,24	0
5	CL	A	4018	1/1	0.88	0.10	-	58,58,58,58	0
4	K	A	4009	1/1	0.99	0.06	-	80,80,80,80	0
3	MN	E	4046	1/1	1.00	0.03	-	21,21,21,21	0
5	CL	G	4081	1/1	0.93	0.20	-	75,75,75,75	0
5	CL	G	4086	1/1	0.98	0.05	-	47,47,47,47	0
4	K	F	4058	1/1	0.99	0.04	-	39,39,39,39	0
5	CL	G	4082	1/1	0.99	0.06	-	39,39,39,39	0
3	MN	E	4051	1/1	0.99	0.02	-	36,36,36,36	0
5	CL	A	4015	1/1	1.00	0.03	-	23,23,23,23	0
5	CL	C	4040	1/1	0.94	0.08	-	59,59,59,59	0
5	CL	G	4080	1/1	1.00	0.03	-	23,23,23,23	0
5	CL	D	4043	1/1	0.75	0.15	-	80,80,80,80	0
4	K	G	4074	1/1	0.90	0.10	-	86,86,86,86	0
5	CL	E	4065	1/1	0.99	0.11	-	46,46,46,46	0
4	K	G	4078	1/1	0.97	0.07	-	53,53,53,53	0
4	K	D	4035	1/1	0.98	0.04	-	34,34,34,34	0
5	CL	E	4061	1/1	0.99	0.05	-	41,41,41,41	0
4	K	C	4033	1/1	0.98	0.06	-	55,55,55,55	0
4	K	A	4013	1/1	0.96	0.05	-	55,55,55,55	0
5	CL	E	4059	1/1	1.00	0.04	-	24,24,24,24	0
5	CL	C	4041	1/1	0.99	0.04	-	27,27,27,27	0
3	MN	A	4003	1/1	1.00	0.04	-	21,21,21,21	0
5	CL	C	4037	1/1	0.66	0.18	-	81,81,81,81	0
5	CL	C	4036	1/1	0.99	0.04	-	26,26,26,26	0
4	K	C	4029	1/1	0.97	0.05	-	76,76,76,76	0
5	CL	E	4060	1/1	0.95	0.11	-	56,56,56,56	0
5	CL	C	4042	1/1	0.98	0.07	-	45,45,45,45	0
3	MN	A	4008	1/1	1.00	0.02	-	28,28,28,28	0
5	CL	A	4016	1/1	0.98	0.04	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	K	B	4014	1/1	0.97	0.07	-	42,42,42,42	0
4	K	E	4056	1/1	0.98	0.05	-	42,42,42,42	0
4	K	E	4052	1/1	0.98	0.04	-	61,61,61,61	0
3	MN	G	4073	1/1	1.00	0.02	-	49,49,49,49	0
5	CL	C	4038	1/1	0.99	0.03	-	33,33,33,33	0
5	CL	E	4063	1/1	0.97	0.08	-	59,59,59,59	0
3	MN	G	4068	1/1	1.00	0.03	-	22,22,22,22	0
4	K	G	4079	1/1	0.99	0.12	-	49,49,49,49	0
4	K	E	4057	1/1	0.95	0.06	-	55,55,55,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.