



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 03:59 PM EDT

PDB ID : 5W5T / pdb_00005w5t
Title : Agrobacterium tumefaciens ADP-Glucose Pyrophosphorylase bound to activator ethyl pyruvate
Authors : Mascarenhas, R.N.; Hill, B.L.; Ballicora, M.A.; Liu, D.
Deposited on : 2017-06-15
Resolution : 1.76 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

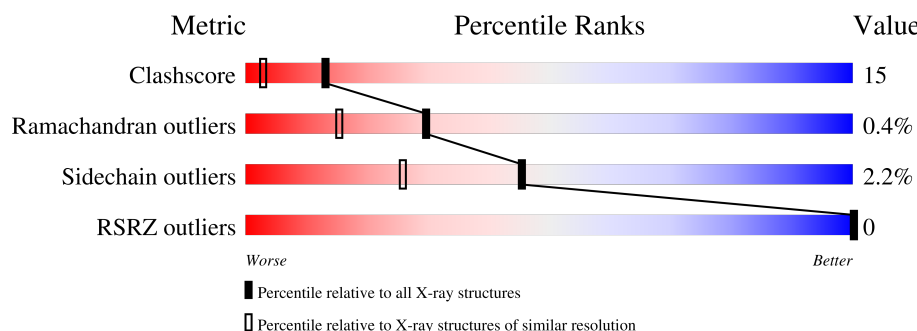
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	415	
1	B	415	
1	C	415	
1	D	415	
1	E	415	
1	F	415	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	415	 72% 26% ..
1	H	415	 76% 22% ..
1	I	415	 74% 23% ..
1	J	415	 77% 20% ..
1	K	415	 69% 28% ..
1	L	415	 74% 23% ..
1	M	415	 77% 21% ..
1	N	415	 77% 21% ..
1	O	415	 73% 24% ..
1	P	415	 73% 26% .
1	Q	415	 76% 21% ..
1	R	415	 79% 19% ..
1	T	415	 75% 23% ..
1	Z	415	 72% 25% ..

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
2	SO4	A	501	-	-	X	-
2	SO4	C	504	-	-	X	-
2	SO4	H	502	-	-	X	-
2	SO4	K	502	-	-	X	-
2	SO4	P	503	-	-	X	-
2	SO4	Q	508	-	-	X	-
2	SO4	R	505	-	-	X	-
2	SO4	R	506	-	-	X	-
3	GOL	A	505	-	-	X	-
3	GOL	K	504	-	-	X	-
3	GOL	R	509	-	-	X	-
4	9X7	A	506	-	X	-	-
4	9X7	F	503	-	X	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	9X7	R	511	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 76418 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 Glucose-1-phosphate adenylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3196	2029	553	601	13			
1	B	412	Total	C	N	O	S	0	2	0
			3241	2057	561	610	13			
1	C	412	Total	C	N	O	S	0	1	0
			3231	2051	558	609	13			
1	D	410	Total	C	N	O	S	0	0	0
			3217	2042	556	606	13			
1	E	411	Total	C	N	O	S	0	1	0
			3222	2045	556	608	13			
1	F	411	Total	C	N	O	S	0	0	0
			3222	2045	557	607	13			
1	G	411	Total	C	N	O	S	0	1	0
			3230	2049	560	608	13			
1	H	410	Total	C	N	O	S	0	1	0
			3221	2045	556	607	13			
1	I	412	Total	C	N	O	S	0	0	0
			3227	2048	558	608	13			
1	J	410	Total	C	N	O	S	0	1	0
			3221	2045	556	607	13			
1	K	408	Total	C	N	O	S	0	0	0
			3207	2036	554	604	13			
1	L	410	Total	C	N	O	S	0	0	0
			3217	2042	556	606	13			
1	M	410	Total	C	N	O	S	0	3	0
			3235	2054	559	607	15			
1	N	411	Total	C	N	O	S	0	1	0
			3226	2048	557	608	13			
1	O	408	Total	C	N	O	S	0	0	0
			3200	2031	553	603	13			
1	P	413	Total	C	N	O	S	0	0	0
			3235	2053	562	607	13			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	410	Total	C	N	O	S	0	1	0
			3223	2046	558	606	13			
1	R	412	Total	C	N	O	S	0	1	0
			3231	2051	558	609	13			
1	Z	408	Total	C	N	O	S	0	1	0
			3208	2034	556	605	13			
1	T	409	Total	C	N	O	S	0	1	0
			3212	2040	554	605	13			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	221	LEU	VAL	conflict	UNP P39669
B	221	LEU	VAL	conflict	UNP P39669
C	221	LEU	VAL	conflict	UNP P39669
D	221	LEU	VAL	conflict	UNP P39669
E	221	LEU	VAL	conflict	UNP P39669
F	221	LEU	VAL	conflict	UNP P39669
G	221	LEU	VAL	conflict	UNP P39669
H	221	LEU	VAL	conflict	UNP P39669
I	221	LEU	VAL	conflict	UNP P39669
J	221	LEU	VAL	conflict	UNP P39669
K	221	LEU	VAL	conflict	UNP P39669
L	221	LEU	VAL	conflict	UNP P39669
M	221	LEU	VAL	conflict	UNP P39669
N	221	LEU	VAL	conflict	UNP P39669
O	221	LEU	VAL	conflict	UNP P39669
P	221	LEU	VAL	conflict	UNP P39669
Q	221	LEU	VAL	conflict	UNP P39669
R	221	LEU	VAL	conflict	UNP P39669
Z	221	LEU	VAL	conflict	UNP P39669
T	221	LEU	VAL	conflict	UNP P39669

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	Q	1	Total	O	S	0	0
			5	4	1		
2	Q	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	Q	1	Total	O	S	0	0
			5	4	1		
2	Q	1	Total	O	S	0	0
			5	4	1		
2	Q	1	Total	O	S	0	0
			5	4	1		
2	Q	1	Total	O	S	0	0
			5	4	1		
2	Q	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	Z	1	Total	O	S	0	0
			5	4	1		
2	Z	1	Total	O	S	0	0
			5	4	1		
2	Z	1	Total	O	S	0	0
			5	4	1		
2	T	1	Total	O	S	0	0
			5	4	1		
2	T	1	Total	O	S	0	0
			5	4	1		
2	T	1	Total	O	S	0	0
			5	4	1		
2	T	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

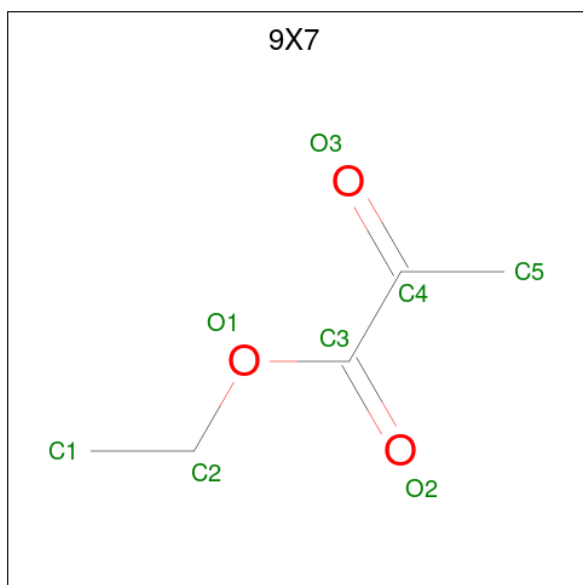
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		
3	M	1	Total	C	O	0	0
			6	3	3		
3	M	1	Total	C	O	0	0
			6	3	3		
3	M	1	Total	C	O	0	0
			6	3	3		
3	M	1	Total	C	O	0	0
			6	3	3		
3	N	1	Total	C	O	0	0
			6	3	3		
3	N	1	Total	C	O	0	0
			6	3	3		
3	O	1	Total	C	O	0	0
			6	3	3		
3	O	1	Total	C	O	0	0
			6	3	3		
3	P	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	P	1	Total	C	O	0	0
			6	3	3		
3	Q	1	Total	C	O	0	0
			6	3	3		
3	Q	1	Total	C	O	0	0
			6	3	3		
3	Q	1	Total	C	O	0	0
			6	3	3		
3	R	1	Total	C	O	0	0
			6	3	3		
3	R	1	Total	C	O	0	0
			6	3	3		
3	R	1	Total	C	O	0	0
			6	3	3		
3	R	1	Total	C	O	0	0
			6	3	3		
3	Z	1	Total	C	O	0	0
			6	3	3		
3	Z	1	Total	C	O	0	0
			6	3	3		
3	T	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is ethyl 2-oxopropanoate (CCD ID: 9X7) (formula: C₅H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 5 3	0	0
4	D	1	Total C O 16 10 6	0	1
4	F	1	Total C O 8 5 3	0	0
4	G	1	Total C O 8 5 3	0	0
4	I	1	Total C O 8 5 3	0	0
4	L	1	Total C O 8 5 3	0	0
4	M	1	Total C O 8 5 3	0	0
4	O	1	Total C O 8 5 3	0	0
4	R	1	Total C O 8 5 3	0	0
4	Z	1	Total C O 8 5 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	568	Total O 568 568	0	0
5	B	560	Total O 560 560	0	0
5	C	622	Total O 622 622	0	0
5	D	543	Total O 543 543	0	0
5	E	562	Total O 562 562	0	0
5	F	575	Total O 575 575	0	0
5	G	551	Total O 551 551	0	0
5	H	483	Total O 483 483	0	0
5	I	542	Total O 542 542	0	0
5	J	637	Total O 637 637	0	0

Continued on next page...

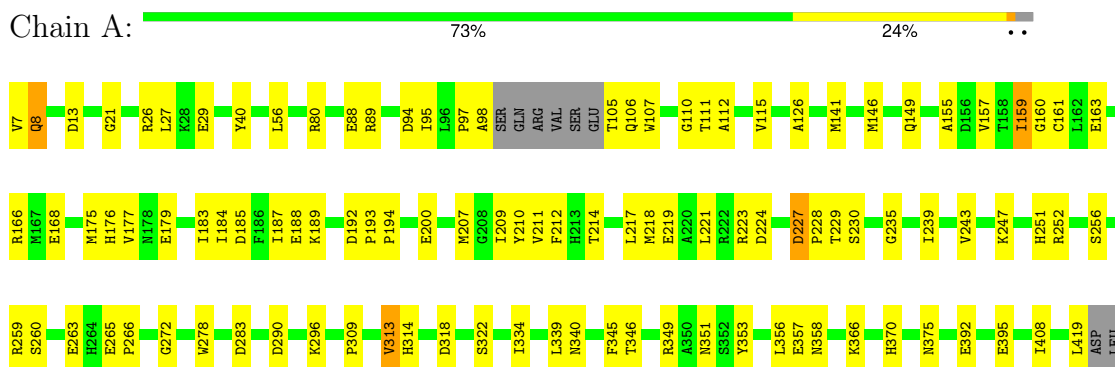
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	K	511	Total 511	O 511	0	0
5	L	535	Total 535	O 535	0	0
5	M	557	Total 557	O 557	0	0
5	N	561	Total 561	O 561	0	0
5	O	528	Total 528	O 528	0	0
5	P	560	Total 560	O 560	0	0
5	Q	667	Total 667	O 667	0	0
5	R	605	Total 605	O 605	0	0
5	Z	542	Total 542	O 542	0	0
5	T	548	Total 548	O 548	0	0

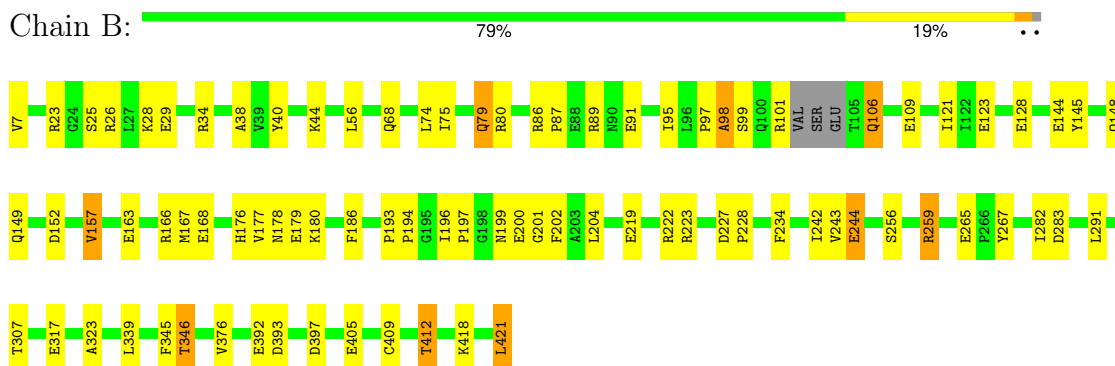
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

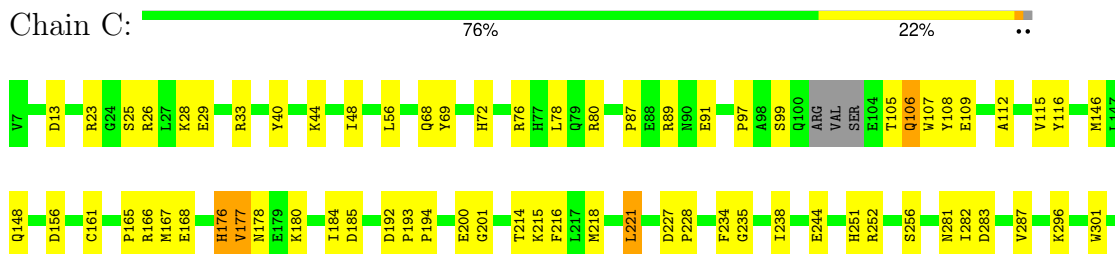
- Molecule 1: Glucose-1-phosphate adenylyltransferase



- Molecule 1: Glucose-1-phosphate adenylyltransferase



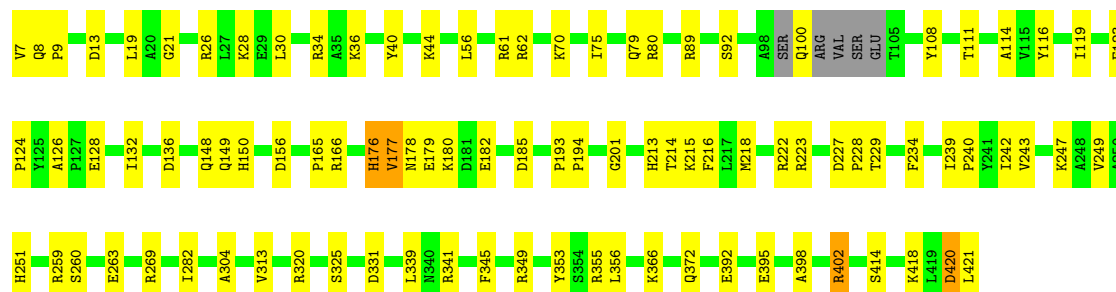
- Molecule 1: Glucose-1-phosphate adenylyltransferase





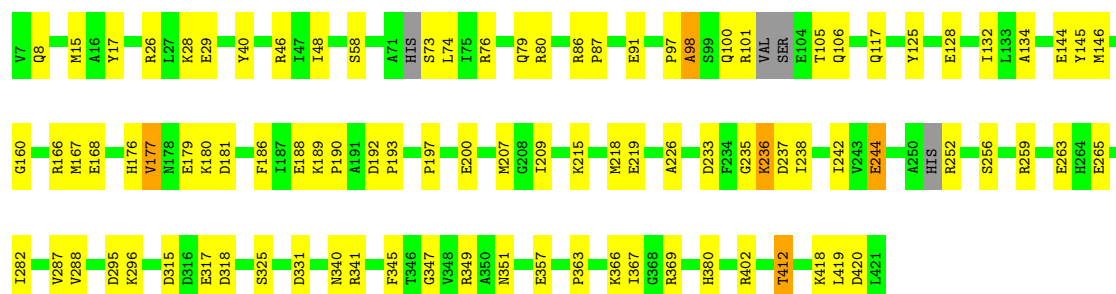
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain D: 76% 22% ..



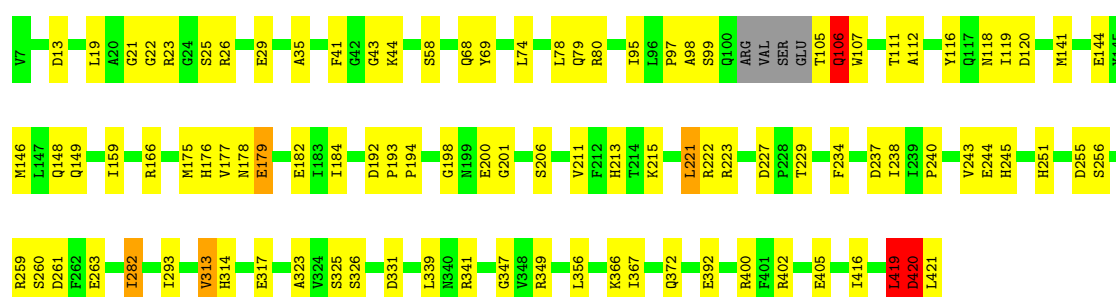
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain E: 76% 21% ..



• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain F: 75% 22% ...



• Molecule 1: Glucose-1-phosphate adenylyltransferase

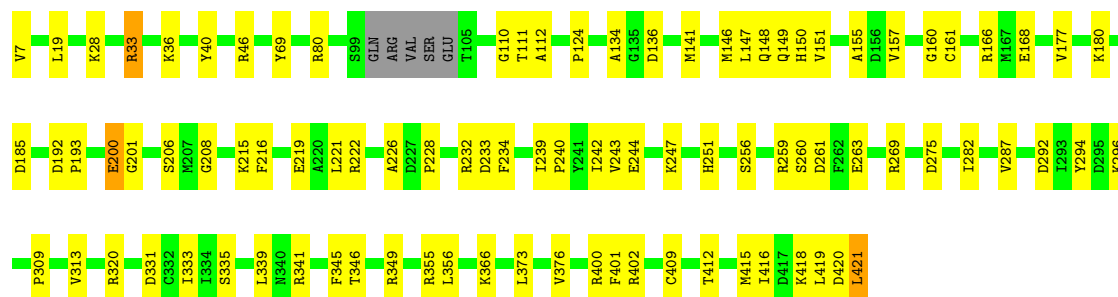
Chain G: 72% 26% ..





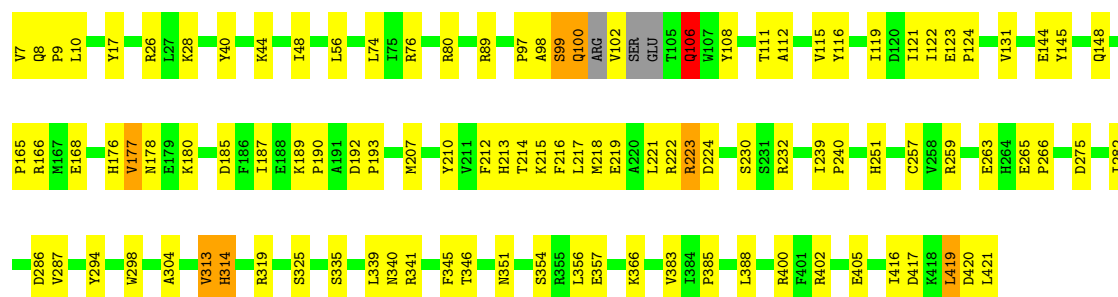
- Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain H: 76% 22%



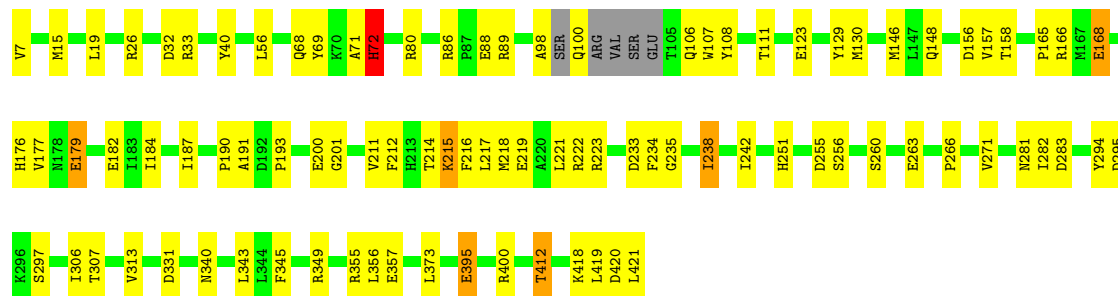
- Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain I: 74% 23%



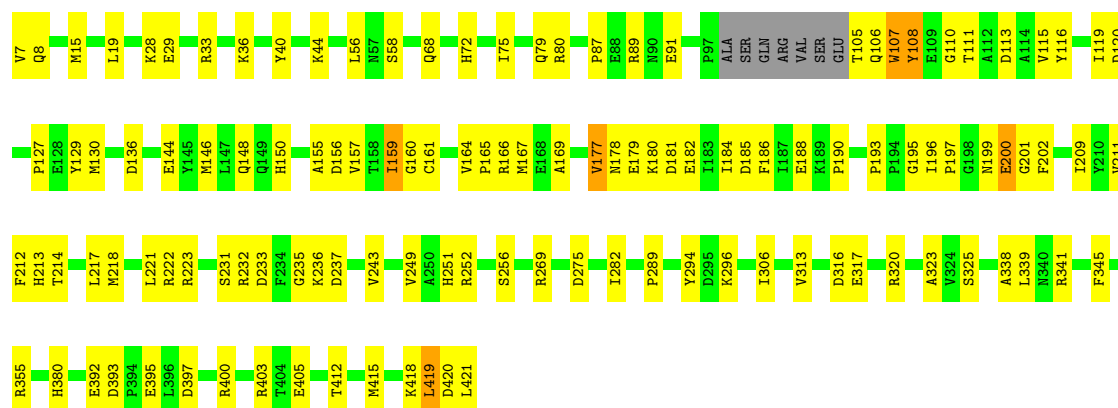
- Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain J: 77% 20%



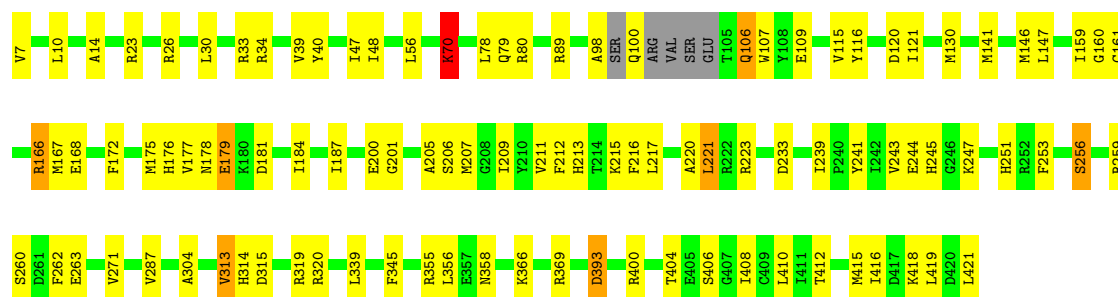
- Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain K:  69% 28% ..



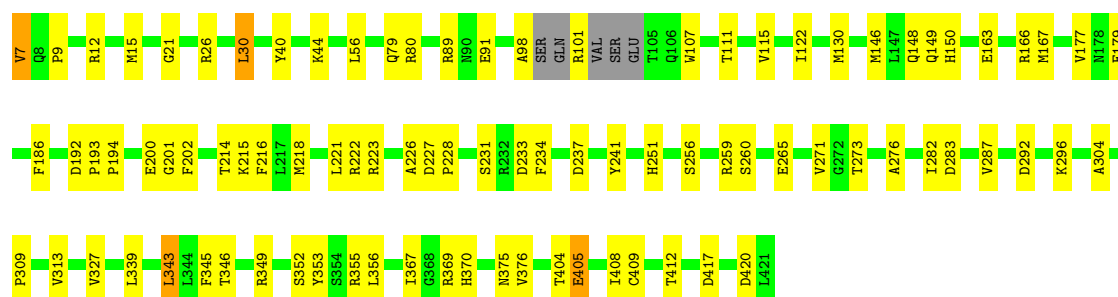
- Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain L:  74% 23% ..



- Molecule 1: Glucose-1-phosphate adenylyltransferase

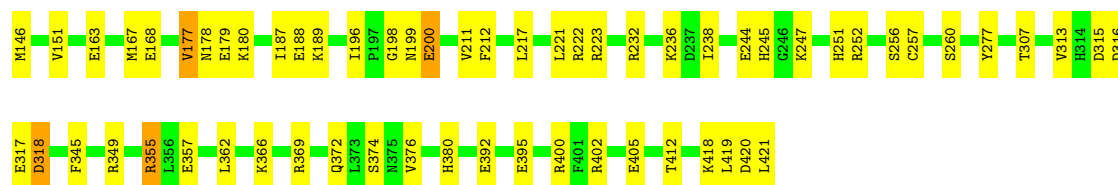
Chain M:  77% 21% ..



- Molecule 1: Glucose-1-phosphate adenylyltransferase

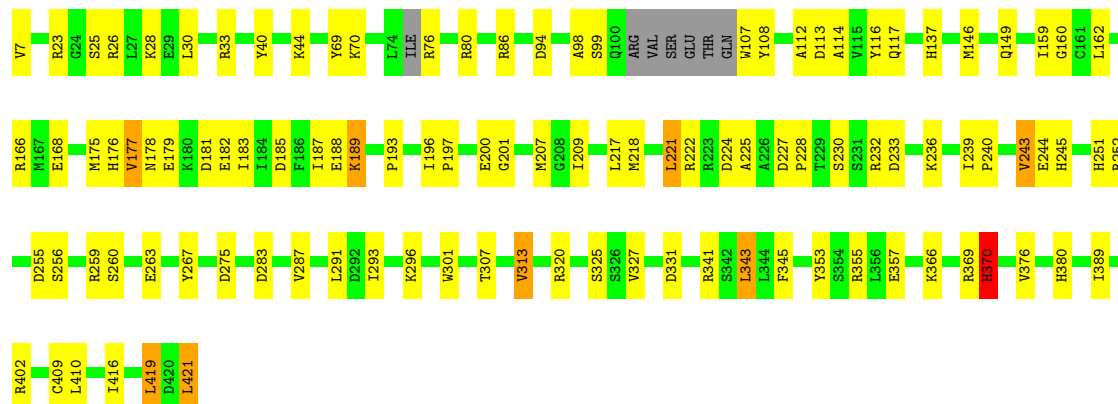
Chain N:  77% 21% ..





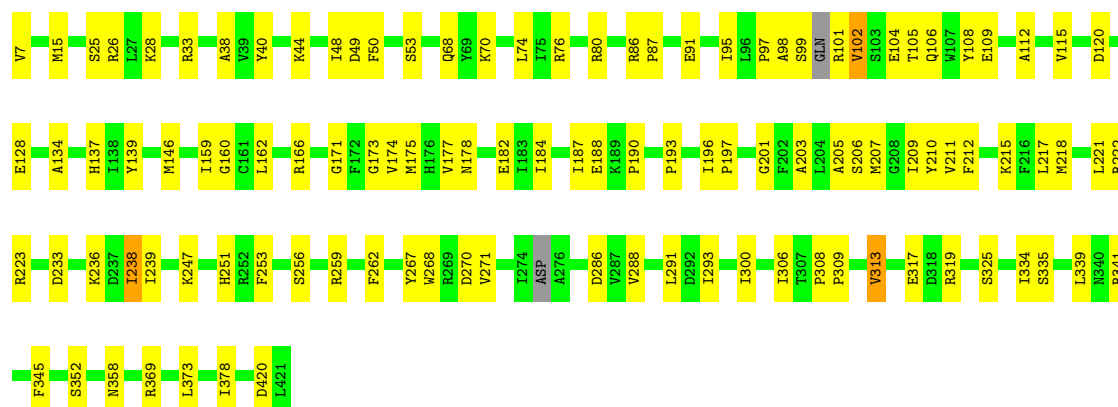
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain O: 73% 24% ..



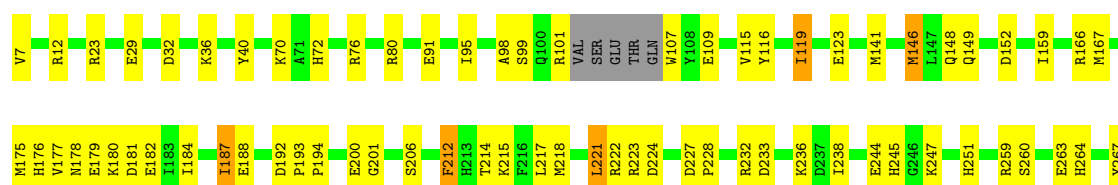
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain P: 73% 26% .



• Molecule 1: Glucose-1-phosphate adenylyltransferase

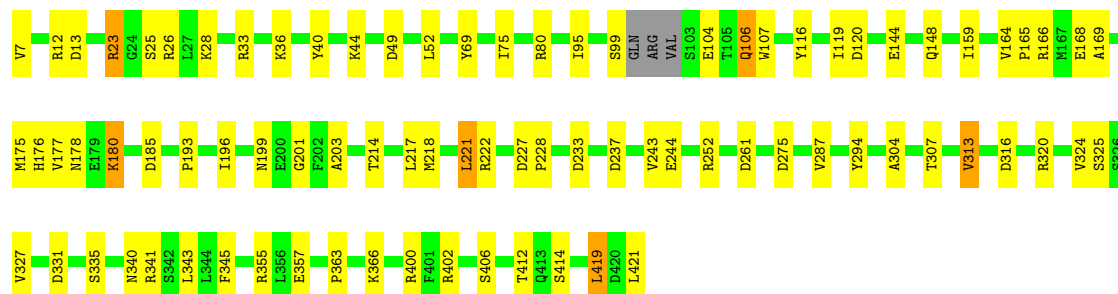
Chain Q: 76% 21% ..





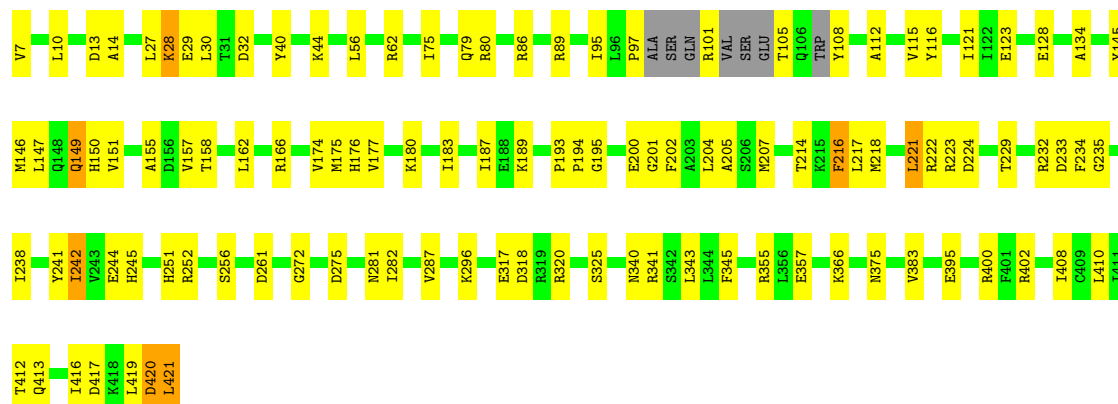
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain R: 79% 19% ..



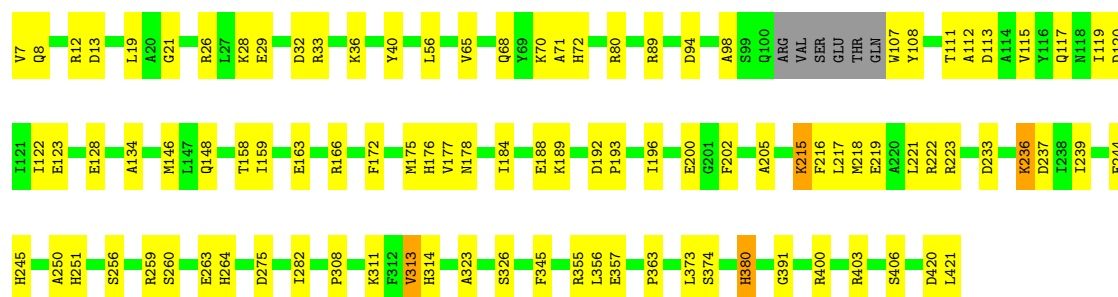
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain Z: 72% 25% ..



• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain T: 75% 23% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	93.78Å 140.15Å 228.85Å 107.81° 101.84° 90.06°	Depositor
Resolution (Å)	41.26 – 1.76 41.26 – 1.76	Depositor EDS
% Data completeness (in resolution range)	91.1 (41.26-1.76) 85.9 (41.26-1.76)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 1.76Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.163 , 0.207 0.155 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.57$, $\langle L^2 \rangle = 0.41$	Xtriage
Estimated twinning fraction	0.477 for h,-k,-h-l 0.470 for -h,k,-k-l 0.469 for -h,-k,h+k+l	Xtriage
Reported twinning fraction	0.500 for h,-k,-h-l	Depositor
Outliers	0 of 974352 reflections	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	76418	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 72.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1345e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GOL, 9X7, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.47	0/3272	0.79	4/4444 (0.1%)
1	B	0.49	0/3323	0.81	1/4514 (0.0%)
1	C	0.50	0/3310	0.82	2/4497 (0.0%)
1	D	0.48	0/3292	0.79	3/4470 (0.1%)
1	E	0.48	0/3297	0.81	1/4475 (0.0%)
1	F	0.47	0/3298	0.79	4/4480 (0.1%)
1	G	0.48	0/3307	0.82	4/4489 (0.1%)
1	H	0.47	0/3300	0.79	1/4483 (0.0%)
1	I	0.48	0/3303	0.84	2/4487 (0.0%)
1	J	0.50	0/3299	0.80	2/4480 (0.0%)
1	K	0.49	0/3283	0.83	6/4459 (0.1%)
1	L	0.50	1/3292 (0.0%)	0.81	2/4470 (0.0%)
1	M	0.47	0/3319	0.79	1/4505 (0.0%)
1	N	0.48	0/3305	0.79	1/4490 (0.0%)
1	O	0.49	0/3275	0.81	4/4447 (0.1%)
1	P	0.49	0/3310	0.79	2/4494 (0.0%)
1	Q	0.50	1/3302 (0.0%)	0.81	3/4485 (0.1%)
1	R	0.49	0/3310	0.79	2/4497 (0.0%)
1	T	0.50	0/3291	0.85	6/4471 (0.1%)
1	Z	0.50	0/3283	0.83	3/4454 (0.1%)
All	All	0.49	2/65971 (0.0%)	0.81	54/89591 (0.1%)

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
1	E	0	1
1	F	0	1
1	I	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	2
1	O	0	1
1	Q	0	1
1	R	0	1
All	All	0	9

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	70	LYS	CD-CE	-5.55	1.35	1.52
1	Q	212	PHE	C-O	-5.03	1.17	1.23

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	420	ASP	N-CA-C	-9.07	102.00	113.43
1	T	72	HIS	N-CA-C	8.97	122.03	111.71
1	Q	420	ASP	N-CA-C	-8.92	102.80	114.31
1	T	420	ASP	N-CA-C	-7.99	102.34	114.16
1	I	100	GLN	N-CA-C	-7.73	103.15	112.58

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	419	LEU	Peptide
1	F	419	LEU	Peptide
1	I	419	LEU	Peptide
1	I	99	SER	Peptide
1	J	212	PHE	Peptide

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	3196	0	3104	93	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3241	0	3150	87	0
1	C	3231	0	3132	98	0
1	D	3217	0	3120	90	0
1	E	3222	0	3129	93	0
1	F	3222	0	3123	87	0
1	G	3230	0	3135	114	0
1	H	3221	0	3128	96	0
1	I	3227	0	3125	91	0
1	J	3221	0	3127	87	0
1	K	3207	0	3114	121	0
1	L	3217	0	3120	111	0
1	M	3235	0	3152	83	0
1	N	3226	0	3130	89	0
1	O	3200	0	3101	101	0
1	P	3235	0	3135	104	0
1	Q	3223	0	3133	88	1
1	R	3231	0	3132	83	1
1	T	3212	0	3120	89	0
1	Z	3208	0	3122	110	0
2	A	20	0	0	3	0
2	B	15	0	0	1	0
2	C	20	0	0	5	0
2	D	20	0	0	1	0
2	E	15	0	0	1	0
2	F	10	0	0	0	0
2	G	15	0	0	3	0
2	H	10	0	0	4	0
2	I	20	0	0	2	0
2	J	15	0	0	1	0
2	K	15	0	0	2	0
2	L	20	0	0	1	0
2	M	15	0	0	0	0
2	N	15	0	0	0	0
2	O	25	0	0	2	0
2	P	20	0	0	3	0
2	Q	40	0	0	5	0
2	R	30	0	0	6	0
2	T	20	0	0	1	0
2	Z	15	0	0	0	0
3	A	6	0	8	4	0
3	B	18	0	24	3	0
3	C	24	0	32	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	18	0	24	2	0
3	E	6	0	8	1	0
3	G	12	0	16	2	0
3	H	6	0	8	1	0
3	I	18	0	24	5	0
3	J	24	0	32	7	0
3	K	12	0	16	6	0
3	L	12	0	16	1	0
3	M	24	0	32	7	0
3	N	12	0	16	3	0
3	O	12	0	16	1	0
3	P	12	0	16	1	0
3	Q	18	0	24	5	0
3	R	24	0	32	7	0
3	T	6	0	8	0	0
3	Z	12	0	16	3	0
4	A	8	0	0	2	0
4	D	16	0	0	1	0
4	F	8	0	0	0	0
4	G	8	0	0	0	0
4	I	8	0	0	0	0
4	L	8	0	0	0	0
4	M	8	0	0	1	0
4	O	8	0	0	1	0
4	R	8	0	0	2	0
4	Z	8	0	0	1	0
5	A	568	0	0	44	3
5	B	560	0	0	53	0
5	C	622	0	0	46	1
5	D	543	0	0	51	2
5	E	562	0	0	55	14
5	F	575	0	0	49	11
5	G	551	0	0	61	8
5	H	483	0	0	66	8
5	I	542	0	0	42	1
5	J	637	0	0	54	2
5	K	511	0	0	66	4
5	L	535	0	0	52	3
5	M	557	0	0	45	3
5	N	561	0	0	55	3
5	O	528	0	0	51	11
5	P	560	0	0	59	7

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Q	667	0	0	53	14
5	R	605	0	0	42	9
5	T	548	0	0	47	1
5	Z	542	0	0	51	1
All	All	76418	0	62900	1913	54

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 15.

The worst 5 of 1913 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)
1:Z:207:MET:SD	5:Z:1085:HOH:O	1.98	1.19
1:P:207:MET:SD	5:P:988:HOH:O	2.08	1.10
1:D:7:VAL:N	5:D:602:HOH:O	1.87	1.07
1:O:207:MET:SD	5:O:989:HOH:O	2.17	1.02
1:L:23:ARG:HG2	5:L:606:HOH:O	1.57	1.01

The worst 5 of 54 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)
5:D:685:HOH:O	5:P:674:HOH:O[1_455]	1.78	0.42
5:F:791:HOH:O	5:Q:952:HOH:O[1_565]	1.78	0.42
5:E:981:HOH:O	5:M:969:HOH:O[1_655]	1.81	0.39
5:L:1026:HOH:O	5:N:871:HOH:O[1_444]	1.81	0.39
5:E:981:HOH:O	5:M:629:HOH:O[1_655]	1.84	0.36

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	403/415 (97%)	387 (96%)	16 (4%)	0	100	100
1	B	410/415 (99%)	391 (95%)	18 (4%)	1 (0%)	43	27
1	C	409/415 (99%)	393 (96%)	14 (3%)	2 (0%)	24	11
1	D	405/415 (98%)	387 (96%)	18 (4%)	0	100	100
1	E	404/415 (97%)	387 (96%)	16 (4%)	1 (0%)	43	27
1	F	407/415 (98%)	387 (95%)	16 (4%)	4 (1%)	12	3
1	G	406/415 (98%)	392 (97%)	14 (3%)	0	100	100
1	H	407/415 (98%)	390 (96%)	16 (4%)	1 (0%)	43	27
1	I	408/415 (98%)	393 (96%)	13 (3%)	2 (0%)	24	11
1	J	406/415 (98%)	392 (97%)	13 (3%)	1 (0%)	43	27
1	K	404/415 (97%)	383 (95%)	18 (4%)	3 (1%)	18	7
1	L	405/415 (98%)	388 (96%)	14 (4%)	3 (1%)	18	7
1	M	408/415 (98%)	392 (96%)	15 (4%)	1 (0%)	43	27
1	N	408/415 (98%)	391 (96%)	16 (4%)	1 (0%)	43	27
1	O	402/415 (97%)	384 (96%)	16 (4%)	2 (0%)	24	11
1	P	407/415 (98%)	389 (96%)	13 (3%)	5 (1%)	10	2
1	Q	407/415 (98%)	394 (97%)	10 (2%)	3 (1%)	18	7
1	R	409/415 (99%)	394 (96%)	14 (3%)	1 (0%)	43	27
1	T	406/415 (98%)	393 (97%)	12 (3%)	1 (0%)	43	27
1	Z	402/415 (97%)	386 (96%)	16 (4%)	0	100	100
All	All	8123/8300 (98%)	7793 (96%)	298 (4%)	32 (0%)	30	15

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	98	ALA
1	E	98	ALA
1	F	106	GLN
1	L	106	GLN
1	O	370	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	336/347 (97%)	332 (99%)	4 (1%)	63	49
1	B	341/347 (98%)	327 (96%)	14 (4%)	27	8
1	C	339/347 (98%)	335 (99%)	4 (1%)	63	49
1	D	338/347 (97%)	334 (99%)	4 (1%)	63	49
1	E	338/347 (97%)	330 (98%)	8 (2%)	43	23
1	F	338/347 (97%)	330 (98%)	8 (2%)	43	23
1	G	339/347 (98%)	330 (97%)	9 (3%)	39	19
1	H	339/347 (98%)	330 (97%)	9 (3%)	39	19
1	I	338/347 (97%)	331 (98%)	7 (2%)	47	27
1	J	339/347 (98%)	329 (97%)	10 (3%)	37	17
1	K	338/347 (97%)	332 (98%)	6 (2%)	51	33
1	L	338/347 (97%)	330 (98%)	8 (2%)	43	23
1	M	342/347 (99%)	332 (97%)	10 (3%)	37	17
1	N	339/347 (98%)	327 (96%)	12 (4%)	32	12
1	O	336/347 (97%)	326 (97%)	10 (3%)	36	16
1	P	338/347 (97%)	333 (98%)	5 (2%)	57	41
1	Q	339/347 (98%)	329 (97%)	10 (3%)	37	17
1	R	339/347 (98%)	331 (98%)	8 (2%)	43	23
1	T	338/347 (97%)	334 (99%)	4 (1%)	63	49
1	Z	339/347 (98%)	330 (97%)	9 (3%)	39	19
All	All	6771/6940 (98%)	6612 (98%)	159 (2%)	45	24

5 of 159 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	187	ILE
1	R	313	VAL
1	O	313	VAL
1	Q	167	MET
1	Z	242	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
1	R	372	GLN
1	Z	213	HIS
1	T	148	GLN
1	G	314	HIS
1	G	176	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

132 ligands are modelled in this entry.

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	$\# Z > 2$
3	GOL	Q	511	-	5,5,5	0.31	0	5,5,5	0.80	0
2	SO4	A	502	-	4,4,4	0.23	0	6,6,6	0.12	0
3	GOL	R	509	-	5,5,5	0.45	0	5,5,5	0.93	0
4	9X7	A	506	-	7,7,7	2.72	2 (28%)	6,8,8	4.00	3 (50%)
2	SO4	R	503	-	4,4,4	0.26	0	6,6,6	0.25	0
2	SO4	Q	508	-	4,4,4	0.26	0	6,6,6	0.29	0
3	GOL	K	505	-	5,5,5	0.33	0	5,5,5	0.41	0
3	GOL	Q	510	-	5,5,5	0.46	0	5,5,5	0.49	0
2	SO4	Q	507	-	4,4,4	0.22	0	6,6,6	0.10	0
3	GOL	J	504	-	5,5,5	0.47	0	5,5,5	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	I	506	-	5,5,5	0.40	0	5,5,5	0.32	0
2	SO4	B	502	-	4,4,4	0.22	0	6,6,6	0.29	0
3	GOL	B	506	-	5,5,5	0.43	0	5,5,5	0.31	0
4	9X7	I	508	-	7,7,7	2.51	2 (28%)	6,8,8	2.52	1 (16%)
2	SO4	E	501	-	4,4,4	0.26	0	6,6,6	0.22	0
2	SO4	P	502	-	4,4,4	0.27	0	6,6,6	0.23	0
4	9X7	D	508[B]	-	7,7,7	2.43	2 (28%)	6,8,8	3.16	3 (50%)
4	9X7	L	507	-	7,7,7	2.58	2 (28%)	6,8,8	3.08	2 (33%)
3	GOL	J	506	-	5,5,5	0.47	0	5,5,5	0.82	0
2	SO4	L	503	-	4,4,4	0.24	0	6,6,6	0.18	0
4	9X7	R	511	-	7,7,7	2.71	2 (28%)	6,8,8	3.23	3 (50%)
3	GOL	I	507	-	5,5,5	0.47	0	5,5,5	0.51	0
2	SO4	I	501	-	4,4,4	0.28	0	6,6,6	0.27	0
2	SO4	D	504	-	4,4,4	0.24	0	6,6,6	0.19	0
3	GOL	O	507	-	5,5,5	0.42	0	5,5,5	0.45	0
2	SO4	Z	502	-	4,4,4	0.19	0	6,6,6	0.23	0
3	GOL	P	505	-	5,5,5	0.51	0	5,5,5	0.70	0
3	GOL	D	507	-	5,5,5	0.43	0	5,5,5	0.56	0
3	GOL	L	506	-	5,5,5	0.33	0	5,5,5	0.39	0
3	GOL	M	507	-	5,5,5	0.46	0	5,5,5	0.51	0
2	SO4	R	506	-	4,4,4	0.26	0	6,6,6	0.24	0
3	GOL	R	507	-	5,5,5	0.48	0	5,5,5	0.86	0
4	9X7	F	503	-	7,7,7	2.68	2 (28%)	6,8,8	2.64	2 (33%)
2	SO4	Q	504	-	4,4,4	0.26	0	6,6,6	0.23	0
2	SO4	C	504	-	4,4,4	0.27	0	6,6,6	0.20	0
3	GOL	C	506	-	5,5,5	0.43	0	5,5,5	0.64	0
2	SO4	T	504	-	4,4,4	0.25	0	6,6,6	0.11	0
2	SO4	E	503	-	4,4,4	0.29	0	6,6,6	0.12	0
2	SO4	C	503	-	4,4,4	0.28	0	6,6,6	0.07	0
3	GOL	P	506	-	5,5,5	0.38	0	5,5,5	0.68	0
4	9X7	G	506	-	7,7,7	2.69	2 (28%)	6,8,8	3.06	1 (16%)
2	SO4	K	501	-	4,4,4	0.21	0	6,6,6	0.35	0
2	SO4	L	504	-	4,4,4	0.22	0	6,6,6	0.16	0
3	GOL	L	505	-	5,5,5	0.43	0	5,5,5	0.29	0
2	SO4	O	501	-	4,4,4	0.24	0	6,6,6	0.17	0
2	SO4	P	503	-	4,4,4	0.28	0	6,6,6	0.29	0
3	GOL	E	504	-	5,5,5	0.42	0	5,5,5	0.79	0
3	GOL	C	505	-	5,5,5	0.63	0	5,5,5	0.71	0
2	SO4	G	502	-	4,4,4	0.24	0	6,6,6	0.21	0
2	SO4	N	503	-	4,4,4	0.23	0	6,6,6	0.20	0
3	GOL	C	508	-	5,5,5	0.43	0	5,5,5	0.58	0
3	GOL	G	504	-	5,5,5	0.41	0	5,5,5	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	O	503	-	4,4,4	0.30	0	6,6,6	0.09	0
3	GOL	A	505	-	5,5,5	0.58	0	5,5,5	0.66	0
2	SO4	R	504	-	4,4,4	0.25	0	6,6,6	0.20	0
2	SO4	Z	503	-	4,4,4	0.28	0	6,6,6	0.20	0
2	SO4	G	501	-	4,4,4	0.23	0	6,6,6	0.29	0
2	SO4	Q	503	-	4,4,4	0.29	0	6,6,6	0.17	0
2	SO4	O	505	-	4,4,4	0.28	0	6,6,6	0.15	0
2	SO4	R	501	-	4,4,4	0.20	0	6,6,6	0.31	0
2	SO4	H	502	-	4,4,4	0.18	0	6,6,6	0.24	0
2	SO4	A	504	-	4,4,4	0.22	0	6,6,6	0.19	0
3	GOL	D	506	-	5,5,5	0.38	0	5,5,5	0.26	0
2	SO4	Q	502	-	4,4,4	0.23	0	6,6,6	0.26	0
2	SO4	M	502	-	4,4,4	0.26	0	6,6,6	0.21	0
2	SO4	D	502	-	4,4,4	0.21	0	6,6,6	0.42	0
2	SO4	K	503	-	4,4,4	0.23	0	6,6,6	0.20	0
2	SO4	L	501	-	4,4,4	0.26	0	6,6,6	0.13	0
2	SO4	Z	501	-	4,4,4	0.26	0	6,6,6	0.18	0
3	GOL	M	504	-	5,5,5	0.46	0	5,5,5	0.34	0
2	SO4	R	505	-	4,4,4	0.24	0	6,6,6	0.14	0
2	SO4	A	501	-	4,4,4	0.27	0	6,6,6	0.22	0
3	GOL	N	504	-	5,5,5	0.48	0	5,5,5	0.71	0
2	SO4	D	501	-	4,4,4	0.23	0	6,6,6	0.11	0
3	GOL	B	505	-	5,5,5	0.46	0	5,5,5	0.65	0
3	GOL	R	510	-	5,5,5	0.36	0	5,5,5	1.13	0
2	SO4	M	503	-	4,4,4	0.26	0	6,6,6	0.20	0
3	GOL	R	508	-	5,5,5	0.32	0	5,5,5	0.49	0
2	SO4	I	504	-	4,4,4	0.27	0	6,6,6	0.09	0
2	SO4	K	502	-	4,4,4	0.25	0	6,6,6	0.21	0
3	GOL	Z	505	-	5,5,5	0.48	0	5,5,5	0.54	0
2	SO4	B	503	-	4,4,4	0.27	0	6,6,6	0.23	0
2	SO4	I	502	-	4,4,4	0.26	0	6,6,6	0.20	0
2	SO4	J	503	-	4,4,4	0.22	0	6,6,6	0.28	0
2	SO4	G	503	-	4,4,4	0.28	0	6,6,6	0.12	0
3	GOL	J	505	-	5,5,5	0.45	0	5,5,5	0.71	0
2	SO4	E	502	-	4,4,4	0.22	0	6,6,6	0.26	0
2	SO4	F	502	-	4,4,4	0.23	0	6,6,6	0.31	0
2	SO4	P	501	-	4,4,4	0.21	0	6,6,6	0.17	0
3	GOL	J	507	-	5,5,5	0.33	0	5,5,5	0.62	0
3	GOL	T	505	-	5,5,5	0.41	0	5,5,5	0.42	0
2	SO4	Q	501	-	4,4,4	0.24	0	6,6,6	0.29	0
2	SO4	T	502	-	4,4,4	0.22	0	6,6,6	0.18	0
2	SO4	D	503	-	4,4,4	0.27	0	6,6,6	0.13	0
3	GOL	I	505	-	5,5,5	0.48	0	5,5,5	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	C	507	-	5,5,5	0.47	0	5,5,5	0.51	0
3	GOL	O	506	-	5,5,5	0.36	0	5,5,5	0.19	0
3	GOL	M	506	-	5,5,5	0.43	0	5,5,5	0.28	0
3	GOL	H	503	-	5,5,5	0.39	0	5,5,5	0.50	0
2	SO4	N	501	-	4,4,4	0.21	0	6,6,6	0.33	0
2	SO4	H	501	-	4,4,4	0.21	0	6,6,6	0.26	0
2	SO4	F	501	-	4,4,4	0.21	0	6,6,6	0.14	0
2	SO4	O	502	-	4,4,4	0.26	0	6,6,6	0.25	0
4	9X7	Z	506	-	7,7,7	2.59	2 (28%)	6,8,8	3.07	3 (50%)
2	SO4	Q	505	-	4,4,4	0.21	0	6,6,6	0.14	0
2	SO4	Q	506	-	4,4,4	0.21	0	6,6,6	0.17	0
2	SO4	P	504	-	4,4,4	0.21	0	6,6,6	0.19	0
3	GOL	K	504	-	5,5,5	0.43	0	5,5,5	0.79	0
4	9X7	D	508[A]	-	7,7,7	2.69	2 (28%)	6,8,8	2.58	1 (16%)
3	GOL	D	505	-	5,5,5	0.51	0	5,5,5	0.57	0
2	SO4	R	502	-	4,4,4	0.23	0	6,6,6	0.15	0
2	SO4	J	501	-	4,4,4	0.25	0	6,6,6	0.27	0
4	9X7	O	508	-	7,7,7	2.75	2 (28%)	6,8,8	4.00	3 (50%)
2	SO4	O	504	-	4,4,4	0.19	0	6,6,6	0.05	0
2	SO4	L	502	-	4,4,4	0.25	0	6,6,6	0.21	0
3	GOL	N	505	-	5,5,5	0.39	0	5,5,5	0.66	0
2	SO4	N	502	-	4,4,4	0.24	0	6,6,6	0.16	0
2	SO4	B	501	-	4,4,4	0.22	0	6,6,6	0.29	0
2	SO4	T	503	-	4,4,4	0.21	0	6,6,6	0.15	0
3	GOL	Z	504	-	5,5,5	0.53	0	5,5,5	0.75	0
3	GOL	Q	509	-	5,5,5	0.38	0	5,5,5	0.43	0
2	SO4	M	501	-	4,4,4	0.23	0	6,6,6	0.35	0
3	GOL	B	504	-	5,5,5	0.39	0	5,5,5	0.30	0
2	SO4	I	503	-	4,4,4	0.29	0	6,6,6	0.10	0
3	GOL	M	505	-	5,5,5	0.45	0	5,5,5	0.79	0
2	SO4	J	502	-	4,4,4	0.36	0	6,6,6	0.24	0
2	SO4	A	503	-	4,4,4	0.28	0	6,6,6	0.14	0
2	SO4	C	502	-	4,4,4	0.20	0	6,6,6	0.31	0
2	SO4	C	501	-	4,4,4	0.26	0	6,6,6	0.26	0
4	9X7	M	508	-	7,7,7	2.61	2 (28%)	6,8,8	2.91	2 (33%)
3	GOL	G	505	-	5,5,5	0.42	0	5,5,5	0.15	0
2	SO4	T	501	-	4,4,4	0.25	0	6,6,6	0.35	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
3	GOL	Q	511	-	-	3/4/4/4	-
3	GOL	P	505	-	-	3/4/4/4	-
3	GOL	D	507	-	-	1/4/4/4	-
3	GOL	L	506	-	-	2/4/4/4	-
3	GOL	D	506	-	-	0/4/4/4	-
3	GOL	M	507	-	-	0/4/4/4	-
3	GOL	R	509	-	-	3/4/4/4	-
4	9X7	Z	506	-	-	3/7/7/7	-
4	9X7	F	503	-	-	5/7/7/7	-
3	GOL	R	507	-	-	2/4/4/4	-
3	GOL	M	504	-	-	0/4/4/4	-
4	9X7	A	506	-	-	4/7/7/7	-
3	GOL	G	505	-	-	2/4/4/4	-
3	GOL	N	504	-	-	2/4/4/4	-
3	GOL	C	506	-	-	2/4/4/4	-
3	GOL	R	510	-	-	1/4/4/4	-
3	GOL	B	505	-	-	0/4/4/4	-
4	9X7	D	508[A]	-	-	2/7/7/7	-
3	GOL	D	505	-	-	2/4/4/4	-
3	GOL	P	506	-	-	4/4/4/4	-
4	9X7	G	506	-	-	2/7/7/7	-
3	GOL	K	505	-	-	2/4/4/4	-
3	GOL	R	508	-	-	3/4/4/4	-
3	GOL	Q	510	-	-	4/4/4/4	-
4	9X7	O	508	-	-	2/7/7/7	-
3	GOL	J	504	-	-	2/4/4/4	-
3	GOL	Z	505	-	-	4/4/4/4	-
3	GOL	I	506	-	-	4/4/4/4	-
3	GOL	L	505	-	-	4/4/4/4	-
3	GOL	N	505	-	-	0/4/4/4	-
3	GOL	B	506	-	-	2/4/4/4	-
4	9X7	I	508	-	-	4/7/7/7	-
3	GOL	E	504	-	-	2/4/4/4	-
3	GOL	J	505	-	-	1/4/4/4	-
3	GOL	C	505	-	-	1/4/4/4	-
3	GOL	Z	504	-	-	2/4/4/4	-
4	9X7	L	507	-	-	4/7/7/7	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	9X7	D	508[B]	-	-	2/7/7/7	-
3	GOL	Q	509	-	-	4/4/4/4	-
3	GOL	J	507	-	-	2/4/4/4	-
3	GOL	T	505	-	-	4/4/4/4	-
3	GOL	J	506	-	-	2/4/4/4	-
3	GOL	C	508	-	-	2/4/4/4	-
3	GOL	G	504	-	-	1/4/4/4	-
3	GOL	B	504	-	-	1/4/4/4	-
3	GOL	I	505	-	-	2/4/4/4	-
3	GOL	A	505	-	-	3/4/4/4	-
4	9X7	R	511	-	-	5/7/7/7	-
3	GOL	M	505	-	-	4/4/4/4	-
3	GOL	C	507	-	-	2/4/4/4	-
3	GOL	O	506	-	-	0/4/4/4	-
3	GOL	I	507	-	-	4/4/4/4	-
3	GOL	O	507	-	-	2/4/4/4	-
3	GOL	M	506	-	-	4/4/4/4	-
4	9X7	M	508	-	-	3/7/7/7	-
3	GOL	H	503	-	-	2/4/4/4	-
3	GOL	K	504	-	-	1/4/4/4	-

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	508	9X7	O1-C3	6.79	1.46	1.33
4	A	506	9X7	O1-C3	6.68	1.46	1.33
4	R	511	9X7	O1-C3	6.65	1.46	1.33
4	D	508[A]	9X7	O1-C3	6.54	1.45	1.33
4	G	506	9X7	O1-C3	6.52	1.45	1.33

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	508	9X7	O1-C3-C4	8.72	123.01	111.38
4	A	506	9X7	O1-C3-C4	8.64	122.90	111.38
4	R	511	9X7	O1-C3-C4	6.95	120.64	111.38
4	G	506	9X7	O1-C3-C4	6.85	120.52	111.38
4	L	507	9X7	O1-C3-C4	6.75	120.39	111.38

There are no chirality outliers.

5 of 134 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	505	GOL	C1-C2-C3-O3
3	A	505	GOL	O2-C2-C3-O3
3	B	506	GOL	O1-C1-C2-O2
3	B	506	GOL	O1-C1-C2-C3
3	C	506	GOL	O1-C1-C2-C3

There are no ring outliers.

62 monomers are involved in 109 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Q	511	GOL	2	0
3	R	509	GOL	6	0
4	A	506	9X7	2	0
2	R	503	SO4	1	0
2	Q	508	SO4	3	0
3	K	505	GOL	2	0
3	Q	510	GOL	2	0
3	I	506	GOL	2	0
3	B	506	GOL	2	0
2	E	501	SO4	1	0
3	J	506	GOL	3	0
4	R	511	9X7	2	0
3	D	507	GOL	2	0
3	M	507	GOL	2	0
2	R	506	SO4	3	0
3	R	507	GOL	1	0
2	Q	504	SO4	1	0
2	C	504	SO4	4	0
3	P	506	GOL	1	0
3	L	505	GOL	1	0
2	P	503	SO4	2	0
3	E	504	GOL	1	0
2	G	502	SO4	1	0
2	O	503	SO4	1	0
3	A	505	GOL	4	0
2	G	501	SO4	1	0
2	Q	503	SO4	1	0
2	O	505	SO4	1	0
2	H	502	SO4	4	0
2	A	504	SO4	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	502	SO4	1	0
2	L	501	SO4	1	0
3	M	504	GOL	1	0
2	R	505	SO4	2	0
2	A	501	SO4	2	0
3	B	505	GOL	1	0
2	I	504	SO4	1	0
2	K	502	SO4	2	0
3	Z	505	GOL	3	0
2	B	503	SO4	1	0
2	I	502	SO4	1	0
2	G	503	SO4	1	0
3	J	505	GOL	2	0
3	J	507	GOL	2	0
3	I	505	GOL	3	0
3	C	507	GOL	2	0
3	O	506	GOL	1	0
3	M	506	GOL	3	0
3	H	503	GOL	1	0
4	Z	506	9X7	1	0
2	P	504	SO4	1	0
3	K	504	GOL	4	0
4	D	508[A]	9X7	1	0
4	O	508	9X7	1	0
3	N	505	GOL	3	0
2	T	503	SO4	1	0
3	Q	509	GOL	1	0
3	M	505	GOL	1	0
2	J	502	SO4	1	0
2	C	502	SO4	1	0
4	M	508	9X7	1	0
3	G	505	GOL	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 ⓘ

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	407/415 (98%)	-1.46	0 100 100	11, 22, 44, 66	0
1	B	412/415 (99%)	-1.47	0 100 100	10, 21, 43, 72	2 (0%)
1	C	412/415 (99%)	-1.49	0 100 100	8, 19, 39, 78	1 (0%)
1	D	410/415 (98%)	-1.48	0 100 100	12, 21, 39, 75	0
1	E	411/415 (99%)	-1.45	0 100 100	11, 22, 44, 72	1 (0%)
1	F	411/415 (99%)	-1.46	0 100 100	10, 22, 43, 74	0
1	G	411/415 (99%)	-1.42	0 100 100	11, 22, 46, 72	1 (0%)
1	H	410/415 (98%)	-1.43	0 100 100	12, 23, 46, 66	1 (0%)
1	I	412/415 (99%)	-1.45	0 100 100	10, 21, 43, 72	0
1	J	410/415 (98%)	-1.50	0 100 100	9, 18, 34, 70	1 (0%)
1	K	408/415 (98%)	-1.40	0 100 100	11, 23, 46, 75	0
1	L	410/415 (98%)	-1.44	0 100 100	12, 22, 43, 68	0
1	M	410/415 (98%)	-1.48	0 100 100	9, 21, 41, 72	3 (0%)
1	N	411/415 (99%)	-1.44	0 100 100	11, 22, 44, 74	1 (0%)
1	O	408/415 (98%)	-1.44	0 100 100	11, 23, 43, 65	0
1	P	413/415 (99%)	-1.44	0 100 100	10, 22, 43, 84	0
1	Q	410/415 (98%)	-1.49	0 100 100	9, 18, 37, 63	1 (0%)
1	R	412/415 (99%)	-1.50	0 100 100	8, 18, 38, 85	1 (0%)
1	T	409/415 (98%)	-1.46	0 100 100	11, 21, 44, 63	1 (0%)
1	Z	408/415 (98%)	-1.45	0 100 100	12, 22, 43, 72	1 (0%)
All	All	8205/8300 (98%)	-1.46	0 100 100	8, 21, 43, 85	15 (0%)

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	M	504	6/6	0.98	0.06	27,29,31,34	0
3	GOL	P	505	6/6	0.98	0.06	20,31,39,39	0
2	SO4	D	504	5/5	0.99	0.03	43,51,53,53	0
2	SO4	E	503	5/5	0.99	0.04	33,34,45,48	0
2	SO4	G	503	5/5	0.99	0.04	47,50,54,57	0
2	SO4	I	504	5/5	0.99	0.03	56,56,57,58	0
2	SO4	J	503	5/5	0.99	0.03	42,43,49,55	0
2	SO4	K	503	5/5	0.99	0.03	37,44,48,54	0
2	SO4	L	503	5/5	0.99	0.04	32,38,46,49	0
2	SO4	O	505	5/5	0.99	0.06	28,33,36,36	0
2	SO4	P	504	5/5	0.99	0.02	30,33,35,37	0
2	SO4	Q	506	5/5	0.99	0.10	30,34,37,42	0
2	SO4	Q	508	5/5	0.99	0.03	53,58,60,66	0
2	SO4	R	505	5/5	0.99	0.04	53,60,62,66	0
2	SO4	T	504	5/5	0.99	0.03	43,45,46,48	0
3	GOL	A	505	6/6	0.99	0.03	31,32,43,46	0
3	GOL	B	504	6/6	0.99	0.03	39,42,43,44	0
3	GOL	B	506	6/6	0.99	0.03	26,34,36,39	0
3	GOL	C	505	6/6	0.99	0.03	21,22,25,26	0
3	GOL	C	506	6/6	0.99	0.03	24,26,30,37	0
3	GOL	C	507	6/6	0.99	0.03	20,27,33,35	0
3	GOL	C	508	6/6	0.99	0.03	33,35,38,39	0
3	GOL	D	505	6/6	0.99	0.04	28,32,37,40	0
3	GOL	D	507	6/6	0.99	0.03	21,22,32,37	0
3	GOL	E	504	6/6	0.99	0.04	20,37,48,50	0
3	GOL	G	504	6/6	0.99	0.03	23,24,27,28	0
3	GOL	H	503	6/6	0.99	0.03	35,38,44,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	I	505	6/6	0.99	0.03	25,27,28,36	0
3	GOL	I	507	6/6	0.99	0.03	23,26,30,32	0
3	GOL	J	504	6/6	0.99	0.03	26,29,35,40	0
3	GOL	J	505	6/6	0.99	0.04	18,21,29,31	0
3	GOL	J	506	6/6	0.99	0.04	22,32,42,47	0
3	GOL	J	507	6/6	0.99	0.05	22,26,30,38	0
3	GOL	K	504	6/6	0.99	0.04	24,33,33,40	0
3	GOL	L	506	6/6	0.99	0.06	25,26,35,44	0
2	SO4	C	504	5/5	0.99	0.03	47,51,52,59	0
3	GOL	M	506	6/6	0.99	0.04	26,31,32,33	0
3	GOL	M	507	6/6	0.99	0.05	22,29,32,35	0
3	GOL	N	504	6/6	0.99	0.03	24,26,28,35	0
3	GOL	N	505	6/6	0.99	0.02	31,32,39,43	0
3	GOL	O	506	6/6	0.99	0.04	31,40,41,42	0
2	SO4	D	503	5/5	0.99	0.03	36,40,47,50	0
3	GOL	P	506	6/6	0.99	0.03	31,35,39,40	0
3	GOL	Q	509	6/6	0.99	0.03	24,27,34,41	0
3	GOL	Q	511	6/6	0.99	0.04	34,40,41,45	0
3	GOL	R	507	6/6	0.99	0.03	17,28,32,35	0
3	GOL	R	509	6/6	0.99	0.03	18,25,28,30	0
3	GOL	R	510	6/6	0.99	0.03	21,22,25,26	0
3	GOL	Z	505	6/6	0.99	0.03	29,35,44,48	0
3	GOL	T	505	6/6	0.99	0.03	27,29,37,44	0
4	9X7	A	506	8/8	0.99	0.04	15,25,34,37	0
4	9X7	D	508[A]	8/8	0.99	0.04	12,13,22,27	8
4	9X7	D	508[B]	8/8	0.99	0.04	10,14,22,27	8
4	9X7	F	503	8/8	0.99	0.04	20,23,30,32	0
4	9X7	G	506	8/8	0.99	0.05	15,20,39,39	0
4	9X7	I	508	8/8	0.99	0.03	13,16,30,32	0
4	9X7	L	507	8/8	0.99	0.04	16,19,43,46	0
4	9X7	O	508	8/8	0.99	0.05	27,32,44,50	0
4	9X7	R	511	8/8	0.99	0.04	23,27,42,45	0
4	9X7	Z	506	8/8	0.99	0.03	14,24,42,47	0
2	SO4	Q	507	5/5	1.00	0.02	26,26,29,34	0
2	SO4	D	502	5/5	1.00	0.02	20,22,25,25	0
2	SO4	R	501	5/5	1.00	0.01	18,18,22,23	0
2	SO4	R	502	5/5	1.00	0.01	17,18,21,21	0
2	SO4	R	503	5/5	1.00	0.03	15,22,27,31	0
2	SO4	R	504	5/5	1.00	0.07	27,29,33,35	0
2	SO4	A	502	5/5	1.00	0.02	21,28,29,31	0
2	SO4	R	506	5/5	1.00	0.02	35,38,42,42	0
2	SO4	Z	501	5/5	1.00	0.02	20,24,27,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	Z	502	5/5	1.00	0.01	18,20,27,27	0
2	SO4	Z	503	5/5	1.00	0.05	21,28,36,36	0
2	SO4	T	501	5/5	1.00	0.01	17,19,19,24	0
2	SO4	T	502	5/5	1.00	0.02	19,20,23,26	0
2	SO4	T	503	5/5	1.00	0.03	22,29,32,37	0
2	SO4	A	503	5/5	1.00	0.02	19,30,33,36	0
2	SO4	E	501	5/5	1.00	0.02	20,21,21,24	0
2	SO4	E	502	5/5	1.00	0.01	23,25,26,27	0
3	GOL	B	505	6/6	1.00	0.03	16,25,32,44	0
2	SO4	A	504	5/5	1.00	0.02	34,38,40,42	0
2	SO4	F	501	5/5	1.00	0.02	18,18,20,23	0
2	SO4	F	502	5/5	1.00	0.01	20,20,25,26	0
2	SO4	G	501	5/5	1.00	0.02	20,22,27,27	0
2	SO4	G	502	5/5	1.00	0.01	23,24,26,26	0
2	SO4	B	501	5/5	1.00	0.02	22,23,24,25	0
3	GOL	D	506	6/6	1.00	0.01	17,18,22,23	0
2	SO4	H	501	5/5	1.00	0.01	17,20,22,22	0
2	SO4	H	502	5/5	1.00	0.04	20,25,28,29	0
2	SO4	I	501	5/5	1.00	0.02	18,21,24,25	0
3	GOL	G	505	6/6	1.00	0.04	16,35,41,45	0
2	SO4	I	502	5/5	1.00	0.02	17,19,25,26	0
2	SO4	I	503	5/5	1.00	0.05	22,26,35,45	0
3	GOL	I	506	6/6	1.00	0.03	25,36,41,41	0
2	SO4	B	502	5/5	1.00	0.01	18,19,20,21	0
2	SO4	J	501	5/5	1.00	0.01	16,18,19,22	0
2	SO4	J	502	5/5	1.00	0.01	16,21,22,22	0
2	SO4	B	503	5/5	1.00	0.03	25,29,32,33	0
2	SO4	K	501	5/5	1.00	0.01	20,22,23,23	0
2	SO4	K	502	5/5	1.00	0.01	19,21,25,26	0
3	GOL	K	505	6/6	1.00	0.02	23,29,33,33	0
3	GOL	L	505	6/6	1.00	0.02	19,27,34,35	0
2	SO4	C	501	5/5	1.00	0.01	17,19,21,24	0
2	SO4	L	501	5/5	1.00	0.03	19,21,23,24	0
3	GOL	M	505	6/6	1.00	0.03	24,32,36,41	0
2	SO4	L	502	5/5	1.00	0.01	19,19,23,24	0
2	SO4	C	502	5/5	1.00	0.01	20,20,22,24	0
2	SO4	L	504	5/5	1.00	0.03	37,39,42,43	0
2	SO4	M	501	5/5	1.00	0.01	17,19,20,24	0
2	SO4	M	502	5/5	1.00	0.01	16,17,19,20	0
3	GOL	O	507	6/6	1.00	0.02	25,32,38,42	0
2	SO4	M	503	5/5	1.00	0.04	21,32,35,36	0
2	SO4	N	501	5/5	1.00	0.02	26,27,28,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	N	502	5/5	1.00	0.02	21,23,24,25	0
3	GOL	Q	510	6/6	1.00	0.03	25,27,28,32	0
2	SO4	N	503	5/5	1.00	0.03	22,24,29,34	0
2	SO4	O	501	5/5	1.00	0.02	23,26,27,32	0
3	GOL	R	508	6/6	1.00	0.03	34,36,40,40	0
2	SO4	O	502	5/5	1.00	0.01	19,21,23,25	0
2	SO4	O	503	5/5	1.00	0.05	24,26,37,44	0
3	GOL	Z	504	6/6	1.00	0.03	21,25,29,31	0
2	SO4	O	504	5/5	1.00	0.02	37,38,40,41	0
2	SO4	C	503	5/5	1.00	0.04	24,27,35,37	0
2	SO4	P	501	5/5	1.00	0.01	21,21,22,24	0
2	SO4	P	502	5/5	1.00	0.01	22,22,24,26	0
2	SO4	P	503	5/5	1.00	0.01	20,21,28,32	0
2	SO4	A	501	5/5	1.00	0.02	23,26,27,28	0
2	SO4	Q	501	5/5	1.00	0.01	15,18,20,22	0
2	SO4	Q	502	5/5	1.00	0.02	17,19,20,21	0
2	SO4	Q	503	5/5	1.00	0.04	24,28,41,42	0
4	9X7	M	508	8/8	1.00	0.03	18,23,38,44	0
2	SO4	Q	504	5/5	1.00	0.03	17,23,26,28	0
2	SO4	Q	505	5/5	1.00	0.02	41,43,46,46	0
2	SO4	D	501	5/5	1.00	0.03	20,22,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.