



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 10:45 AM EDT

PDB ID : 3ODM / pdb_00003odm
Title : Archaeal-type phosphoenolpyruvate carboxylase
Authors : Dunten, P.W.
Deposited on : 2010-08-11
Resolution : 2.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

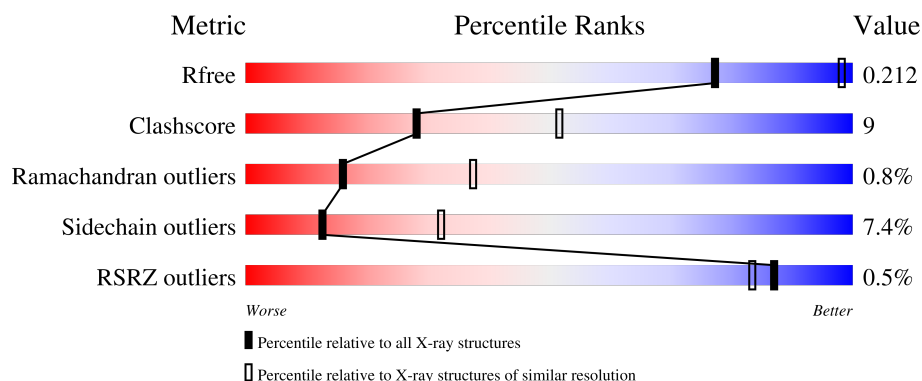
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	560	
1	B	560	
1	C	560	
1	D	560	
1	E	560	

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Mol	Chain	Length	Quality of chain
1	F	560	
1	G	560	
1	H	560	

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	AUC	A	607	-	-	X	-
2	AUC	A	608	-	-	X	-
2	AUC	B	609	-	-	X	-
2	AUC	B	610	-	-	X	-
2	AUC	C	601	-	-	X	-
2	AUC	C	602	-	-	X	-
2	AUC	D	603	-	-	X	-
2	AUC	D	604	-	-	X	-
2	AUC	E	605	-	-	X	-
2	AUC	E	606	-	-	X	-
2	AUC	F	614	-	-	X	-
2	AUC	G	615	-	-	X	-
2	AUC	H	611	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 33563 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 Phosphoenolpyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			4146	2629	696	797	24			
1	B	529	Total	C	N	O	S	0	0	0
			4169	2641	701	803	24			
1	C	530	Total	C	N	O	S	0	0	1
			4171	2645	699	803	24			
1	D	526	Total	C	N	O	S	0	0	0
			4153	2634	697	798	24			
1	E	524	Total	C	N	O	S	0	0	0
			4137	2623	694	796	24			
1	F	529	Total	C	N	O	S	0	0	0
			4160	2637	696	803	24			
1	G	527	Total	C	N	O	S	0	0	0
			4156	2635	698	799	24			
1	H	527	Total	C	N	O	S	0	0	0
			4164	2643	699	798	24			

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP Q8XLE8
A	-21	GLY	-	expression tag	UNP Q8XLE8
A	-20	HIS	-	expression tag	UNP Q8XLE8
A	-19	HIS	-	expression tag	UNP Q8XLE8
A	-18	HIS	-	expression tag	UNP Q8XLE8
A	-17	HIS	-	expression tag	UNP Q8XLE8
A	-16	HIS	-	expression tag	UNP Q8XLE8
A	-15	HIS	-	expression tag	UNP Q8XLE8
A	-14	HIS	-	expression tag	UNP Q8XLE8
A	-13	HIS	-	expression tag	UNP Q8XLE8
A	-12	HIS	-	expression tag	UNP Q8XLE8
A	-11	HIS	-	expression tag	UNP Q8XLE8
A	-10	SER	-	expression tag	UNP Q8XLE8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	SER	-	expression tag	UNP Q8XLE8
A	-8	GLY	-	expression tag	UNP Q8XLE8
A	-7	HIS	-	expression tag	UNP Q8XLE8
A	-6	ILE	-	expression tag	UNP Q8XLE8
A	-5	ASP	-	expression tag	UNP Q8XLE8
A	-4	ASP	-	expression tag	UNP Q8XLE8
A	-3	ASP	-	expression tag	UNP Q8XLE8
A	-2	ASP	-	expression tag	UNP Q8XLE8
A	-1	LYS	-	expression tag	UNP Q8XLE8
A	0	HIS	-	expression tag	UNP Q8XLE8
B	-22	MET	-	expression tag	UNP Q8XLE8
B	-21	GLY	-	expression tag	UNP Q8XLE8
B	-20	HIS	-	expression tag	UNP Q8XLE8
B	-19	HIS	-	expression tag	UNP Q8XLE8
B	-18	HIS	-	expression tag	UNP Q8XLE8
B	-17	HIS	-	expression tag	UNP Q8XLE8
B	-16	HIS	-	expression tag	UNP Q8XLE8
B	-15	HIS	-	expression tag	UNP Q8XLE8
B	-14	HIS	-	expression tag	UNP Q8XLE8
B	-13	HIS	-	expression tag	UNP Q8XLE8
B	-12	HIS	-	expression tag	UNP Q8XLE8
B	-11	HIS	-	expression tag	UNP Q8XLE8
B	-10	SER	-	expression tag	UNP Q8XLE8
B	-9	SER	-	expression tag	UNP Q8XLE8
B	-8	GLY	-	expression tag	UNP Q8XLE8
B	-7	HIS	-	expression tag	UNP Q8XLE8
B	-6	ILE	-	expression tag	UNP Q8XLE8
B	-5	ASP	-	expression tag	UNP Q8XLE8
B	-4	ASP	-	expression tag	UNP Q8XLE8
B	-3	ASP	-	expression tag	UNP Q8XLE8
B	-2	ASP	-	expression tag	UNP Q8XLE8
B	-1	LYS	-	expression tag	UNP Q8XLE8
B	0	HIS	-	expression tag	UNP Q8XLE8
C	-22	MET	-	expression tag	UNP Q8XLE8
C	-21	GLY	-	expression tag	UNP Q8XLE8
C	-20	HIS	-	expression tag	UNP Q8XLE8
C	-19	HIS	-	expression tag	UNP Q8XLE8
C	-18	HIS	-	expression tag	UNP Q8XLE8
C	-17	HIS	-	expression tag	UNP Q8XLE8
C	-16	HIS	-	expression tag	UNP Q8XLE8
C	-15	HIS	-	expression tag	UNP Q8XLE8
C	-14	HIS	-	expression tag	UNP Q8XLE8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	HIS	-	expression tag	UNP Q8XLE8
C	-12	HIS	-	expression tag	UNP Q8XLE8
C	-11	HIS	-	expression tag	UNP Q8XLE8
C	-10	SER	-	expression tag	UNP Q8XLE8
C	-9	SER	-	expression tag	UNP Q8XLE8
C	-8	GLY	-	expression tag	UNP Q8XLE8
C	-7	HIS	-	expression tag	UNP Q8XLE8
C	-6	ILE	-	expression tag	UNP Q8XLE8
C	-5	ASP	-	expression tag	UNP Q8XLE8
C	-4	ASP	-	expression tag	UNP Q8XLE8
C	-3	ASP	-	expression tag	UNP Q8XLE8
C	-2	ASP	-	expression tag	UNP Q8XLE8
C	-1	LYS	-	expression tag	UNP Q8XLE8
C	0	HIS	-	expression tag	UNP Q8XLE8
D	-22	MET	-	expression tag	UNP Q8XLE8
D	-21	GLY	-	expression tag	UNP Q8XLE8
D	-20	HIS	-	expression tag	UNP Q8XLE8
D	-19	HIS	-	expression tag	UNP Q8XLE8
D	-18	HIS	-	expression tag	UNP Q8XLE8
D	-17	HIS	-	expression tag	UNP Q8XLE8
D	-16	HIS	-	expression tag	UNP Q8XLE8
D	-15	HIS	-	expression tag	UNP Q8XLE8
D	-14	HIS	-	expression tag	UNP Q8XLE8
D	-13	HIS	-	expression tag	UNP Q8XLE8
D	-12	HIS	-	expression tag	UNP Q8XLE8
D	-11	HIS	-	expression tag	UNP Q8XLE8
D	-10	SER	-	expression tag	UNP Q8XLE8
D	-9	SER	-	expression tag	UNP Q8XLE8
D	-8	GLY	-	expression tag	UNP Q8XLE8
D	-7	HIS	-	expression tag	UNP Q8XLE8
D	-6	ILE	-	expression tag	UNP Q8XLE8
D	-5	ASP	-	expression tag	UNP Q8XLE8
D	-4	ASP	-	expression tag	UNP Q8XLE8
D	-3	ASP	-	expression tag	UNP Q8XLE8
D	-2	ASP	-	expression tag	UNP Q8XLE8
D	-1	LYS	-	expression tag	UNP Q8XLE8
D	0	HIS	-	expression tag	UNP Q8XLE8
E	-22	MET	-	expression tag	UNP Q8XLE8
E	-21	GLY	-	expression tag	UNP Q8XLE8
E	-20	HIS	-	expression tag	UNP Q8XLE8
E	-19	HIS	-	expression tag	UNP Q8XLE8
E	-18	HIS	-	expression tag	UNP Q8XLE8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-17	HIS	-	expression tag	UNP Q8XLE8
E	-16	HIS	-	expression tag	UNP Q8XLE8
E	-15	HIS	-	expression tag	UNP Q8XLE8
E	-14	HIS	-	expression tag	UNP Q8XLE8
E	-13	HIS	-	expression tag	UNP Q8XLE8
E	-12	HIS	-	expression tag	UNP Q8XLE8
E	-11	HIS	-	expression tag	UNP Q8XLE8
E	-10	SER	-	expression tag	UNP Q8XLE8
E	-9	SER	-	expression tag	UNP Q8XLE8
E	-8	GLY	-	expression tag	UNP Q8XLE8
E	-7	HIS	-	expression tag	UNP Q8XLE8
E	-6	ILE	-	expression tag	UNP Q8XLE8
E	-5	ASP	-	expression tag	UNP Q8XLE8
E	-4	ASP	-	expression tag	UNP Q8XLE8
E	-3	ASP	-	expression tag	UNP Q8XLE8
E	-2	ASP	-	expression tag	UNP Q8XLE8
E	-1	LYS	-	expression tag	UNP Q8XLE8
E	0	HIS	-	expression tag	UNP Q8XLE8
F	-22	MET	-	expression tag	UNP Q8XLE8
F	-21	GLY	-	expression tag	UNP Q8XLE8
F	-20	HIS	-	expression tag	UNP Q8XLE8
F	-19	HIS	-	expression tag	UNP Q8XLE8
F	-18	HIS	-	expression tag	UNP Q8XLE8
F	-17	HIS	-	expression tag	UNP Q8XLE8
F	-16	HIS	-	expression tag	UNP Q8XLE8
F	-15	HIS	-	expression tag	UNP Q8XLE8
F	-14	HIS	-	expression tag	UNP Q8XLE8
F	-13	HIS	-	expression tag	UNP Q8XLE8
F	-12	HIS	-	expression tag	UNP Q8XLE8
F	-11	HIS	-	expression tag	UNP Q8XLE8
F	-10	SER	-	expression tag	UNP Q8XLE8
F	-9	SER	-	expression tag	UNP Q8XLE8
F	-8	GLY	-	expression tag	UNP Q8XLE8
F	-7	HIS	-	expression tag	UNP Q8XLE8
F	-6	ILE	-	expression tag	UNP Q8XLE8
F	-5	ASP	-	expression tag	UNP Q8XLE8
F	-4	ASP	-	expression tag	UNP Q8XLE8
F	-3	ASP	-	expression tag	UNP Q8XLE8
F	-2	ASP	-	expression tag	UNP Q8XLE8
F	-1	LYS	-	expression tag	UNP Q8XLE8
F	0	HIS	-	expression tag	UNP Q8XLE8
G	-22	MET	-	expression tag	UNP Q8XLE8

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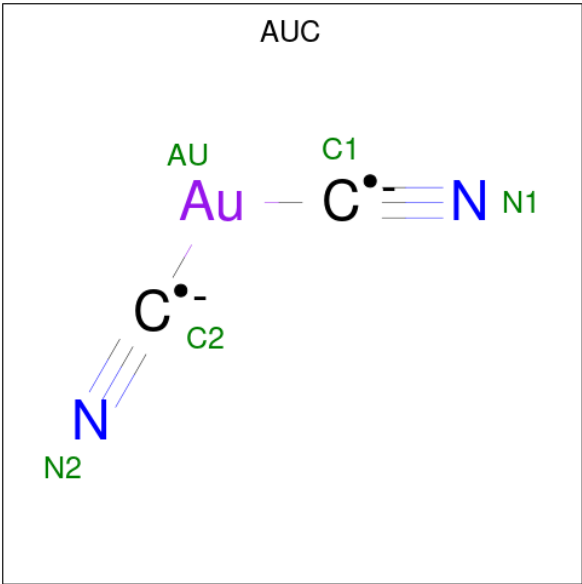
Chain	Residue	Modelled	Actual	Comment	Reference
G	-21	GLY	-	expression tag	UNP Q8XLE8
G	-20	HIS	-	expression tag	UNP Q8XLE8
G	-19	HIS	-	expression tag	UNP Q8XLE8
G	-18	HIS	-	expression tag	UNP Q8XLE8
G	-17	HIS	-	expression tag	UNP Q8XLE8
G	-16	HIS	-	expression tag	UNP Q8XLE8
G	-15	HIS	-	expression tag	UNP Q8XLE8
G	-14	HIS	-	expression tag	UNP Q8XLE8
G	-13	HIS	-	expression tag	UNP Q8XLE8
G	-12	HIS	-	expression tag	UNP Q8XLE8
G	-11	HIS	-	expression tag	UNP Q8XLE8
G	-10	SER	-	expression tag	UNP Q8XLE8
G	-9	SER	-	expression tag	UNP Q8XLE8
G	-8	GLY	-	expression tag	UNP Q8XLE8
G	-7	HIS	-	expression tag	UNP Q8XLE8
G	-6	ILE	-	expression tag	UNP Q8XLE8
G	-5	ASP	-	expression tag	UNP Q8XLE8
G	-4	ASP	-	expression tag	UNP Q8XLE8
G	-3	ASP	-	expression tag	UNP Q8XLE8
G	-2	ASP	-	expression tag	UNP Q8XLE8
G	-1	LYS	-	expression tag	UNP Q8XLE8
G	0	HIS	-	expression tag	UNP Q8XLE8
H	-22	MET	-	expression tag	UNP Q8XLE8
H	-21	GLY	-	expression tag	UNP Q8XLE8
H	-20	HIS	-	expression tag	UNP Q8XLE8
H	-19	HIS	-	expression tag	UNP Q8XLE8
H	-18	HIS	-	expression tag	UNP Q8XLE8
H	-17	HIS	-	expression tag	UNP Q8XLE8
H	-16	HIS	-	expression tag	UNP Q8XLE8
H	-15	HIS	-	expression tag	UNP Q8XLE8
H	-14	HIS	-	expression tag	UNP Q8XLE8
H	-13	HIS	-	expression tag	UNP Q8XLE8
H	-12	HIS	-	expression tag	UNP Q8XLE8
H	-11	HIS	-	expression tag	UNP Q8XLE8
H	-10	SER	-	expression tag	UNP Q8XLE8
H	-9	SER	-	expression tag	UNP Q8XLE8
H	-8	GLY	-	expression tag	UNP Q8XLE8
H	-7	HIS	-	expression tag	UNP Q8XLE8
H	-6	ILE	-	expression tag	UNP Q8XLE8
H	-5	ASP	-	expression tag	UNP Q8XLE8
H	-4	ASP	-	expression tag	UNP Q8XLE8
H	-3	ASP	-	expression tag	UNP Q8XLE8

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-2	ASP	-	expression tag	UNP Q8XLE8
H	-1	LYS	-	expression tag	UNP Q8XLE8
H	0	HIS	-	expression tag	UNP Q8XLE8

- Molecule 2 is GOLD (I) CYANIDE ION (CCD ID: AUC) (formula: C₂AuN₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	Au	C	N	0	0
			5	1	2	2		
2	A	1	Total	Au			0	0
			1	1				
2	A	1	Total	Au			0	0
			1	1				
2	A	1	Total	Au	C	N	0	0
			5	1	2	2		
2	B	1	Total	Au			0	0
			1	1				
2	B	1	Total	Au			0	0
			1	1				
2	B	1	Total	Au	C	N	0	0
			5	1	2	2		
2	B	1	Total	Au			0	0
			1	1				
2	B	1	Total	Au			0	0
			1	1				
2	B	1	Total	Au			0	0
			1	1				

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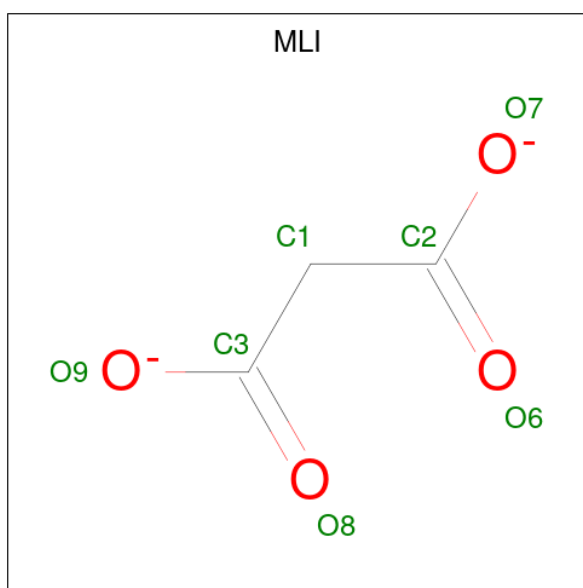
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Au 1 1	0	0
2	C	1	Total Au 1 1	0	0
2	C	1	Total Au C N 5 1 2 2	0	0
2	C	1	Total Au 1 1	0	0
2	C	1	Total Au 1 1	0	0
2	D	1	Total Au C N 5 1 2 2	0	0
2	D	1	Total Au 1 1	0	0
2	D	1	Total Au 1 1	0	0
2	D	1	Total Au 1 1	0	0
2	E	1	Total Au 1 1	0	0
2	E	1	Total Au C N 5 1 2 2	0	0
2	E	1	Total Au 1 1	0	0
2	E	1	Total Au 1 1	0	0
2	F	1	Total Au 1 1	0	0
2	F	1	Total Au 1 1	0	0
2	F	1	Total Au C N 5 1 2 2	0	0
2	F	1	Total Au 1 1	0	0
2	F	1	Total Au 1 1	0	0
2	F	1	Total Au 1 1	0	0
2	G	1	Total Au C N 5 1 2 2	0	0
2	G	1	Total Au 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Au	0	0
			1	1		
2	H	1	Total	Au	0	0
			5	1	2	2
2	H	1	Total	Au	0	0
			1	1		
2	H	1	Total	Au	0	0
			1	1		
2	H	1	Total	Au	0	0
			1	1		

- Molecule 3 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C O	0	0
			7	3 4		
3	C	1	Total	C O	0	0
			7	3 4		
3	D	1	Total	C O	0	0
			7	3 4		
3	E	1	Total	C O	0	0
			7	3 4		
3	H	1	Total	C O	0	0
			7	3 4		

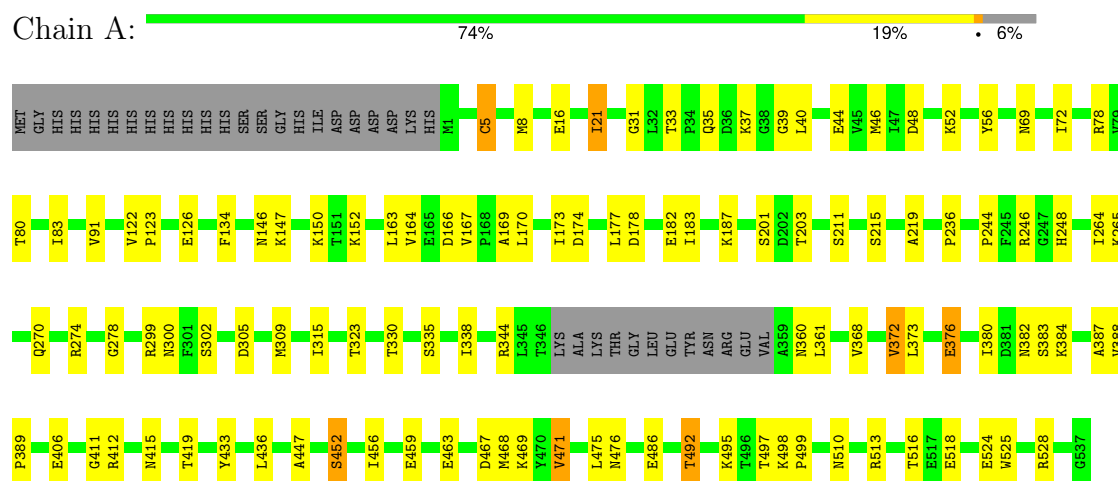
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	34	Total 34	O 34	0	0
4	B	26	Total 26	O 26	0	0
4	C	23	Total 23	O 23	0	0
4	D	22	Total 22	O 22	0	0
4	E	26	Total 26	O 26	0	0
4	F	21	Total 21	O 21	0	0
4	G	19	Total 19	O 19	0	0
4	H	29	Total 29	O 29	0	0

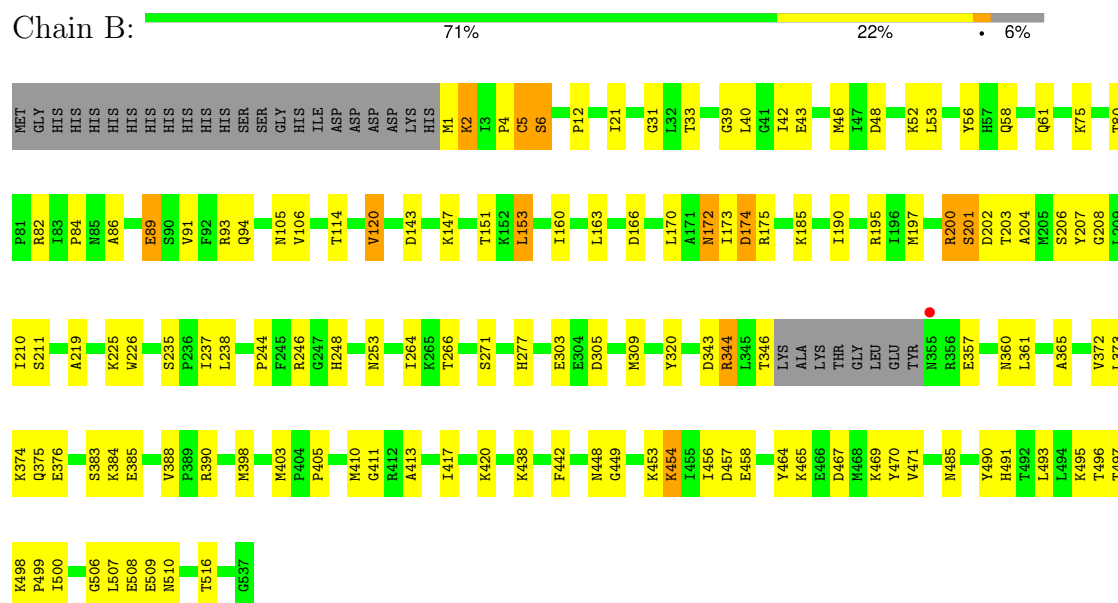
3 Residue-property plots

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.

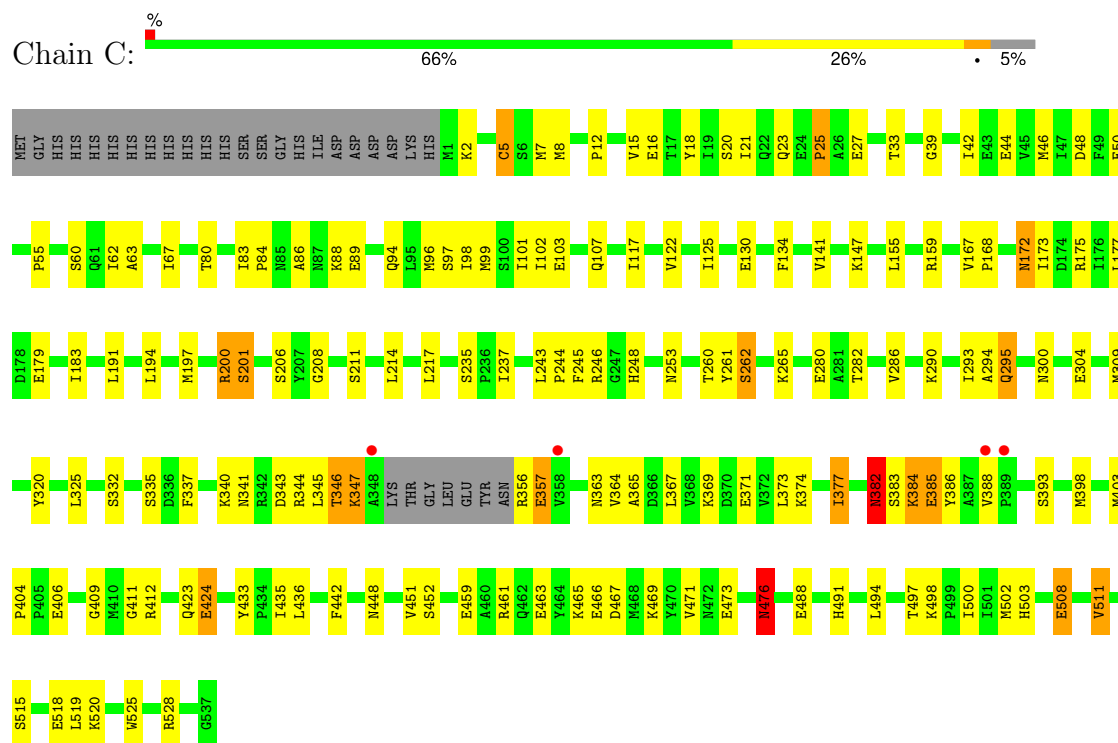
• Molecule 1: Phosphoenolpyruvate carboxylase



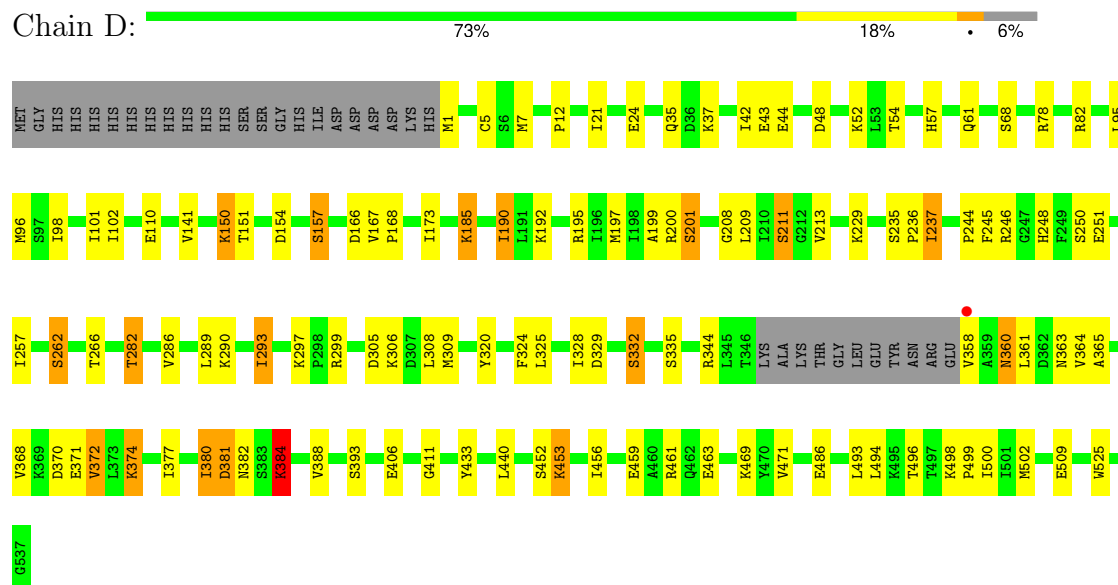
• Molecule 1: Phosphoenolpyruvate carboxylase



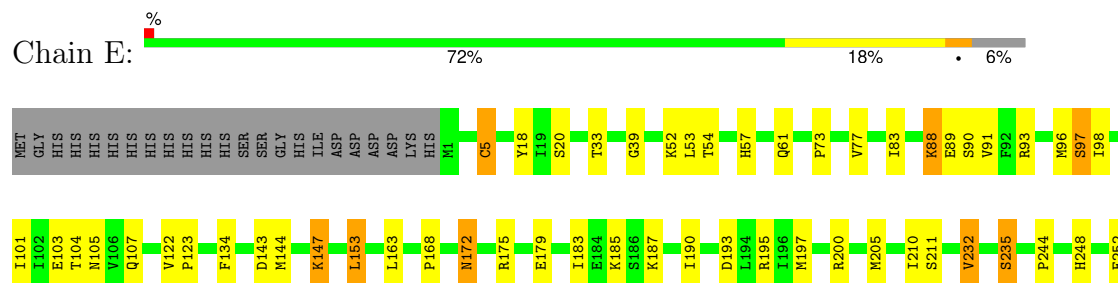
• Molecule 1: Phosphoenolpyruvate carboxylase

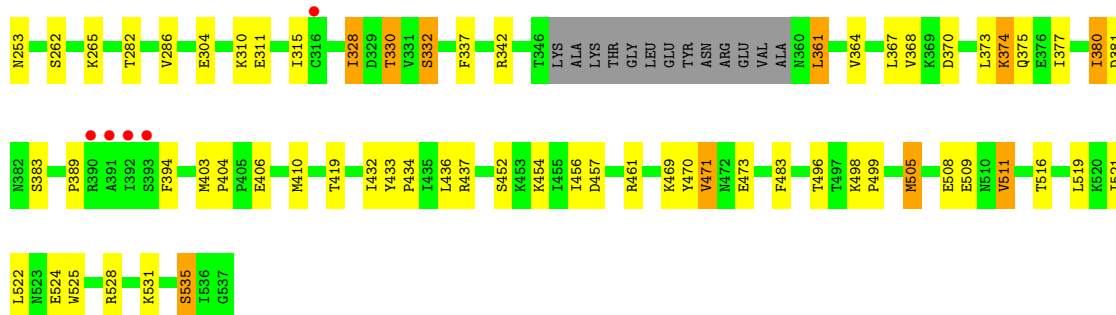


- Molecule 1: Phosphoenolpyruvate carboxylase



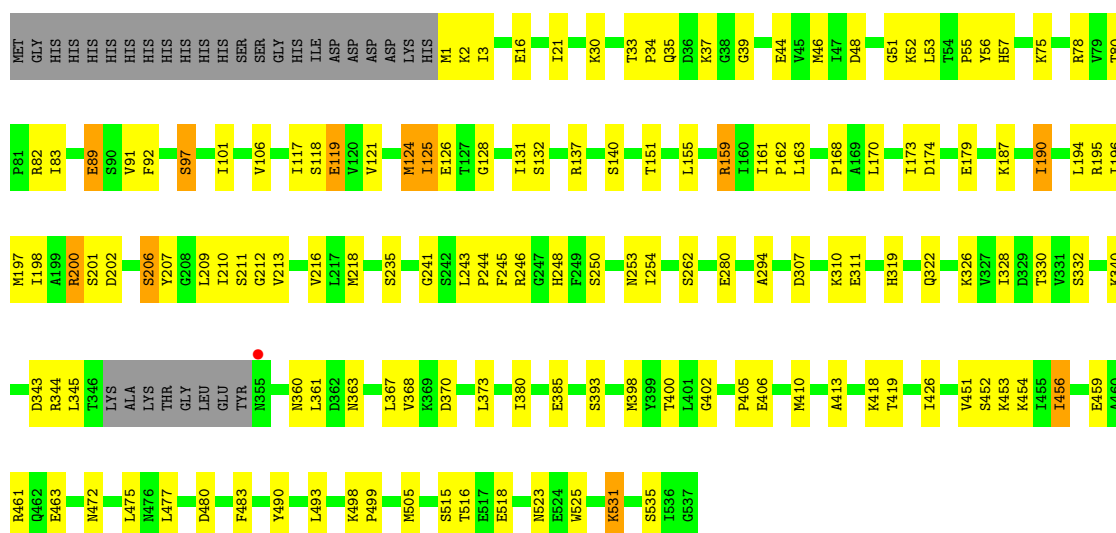
- Molecule 1: Phosphoenolpyruvate carboxylase





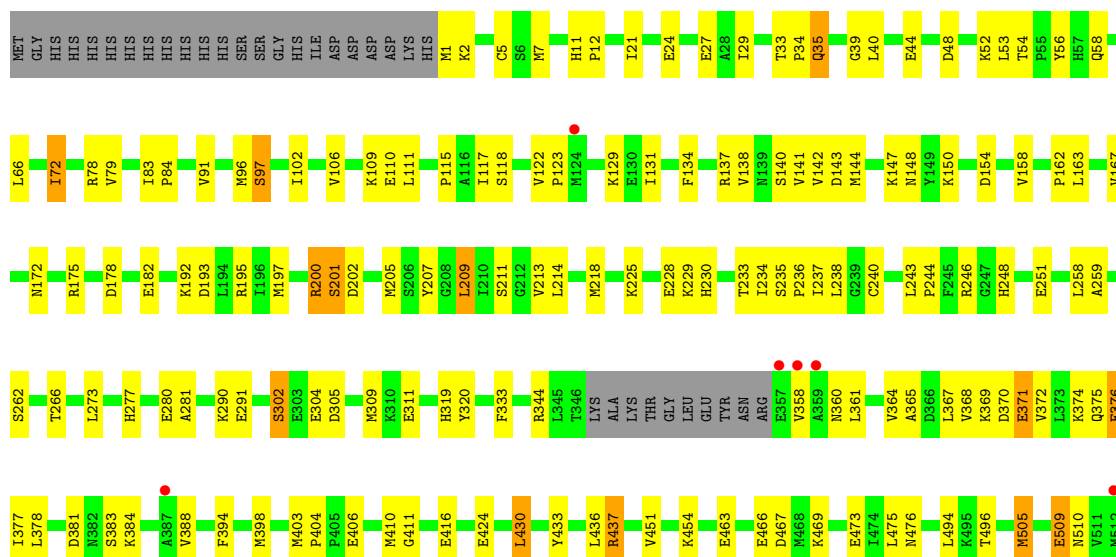
● Molecule 1: Phosphoenolpyruvate carboxylase

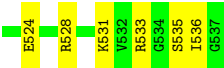
Chain F: 69% 24% 6%



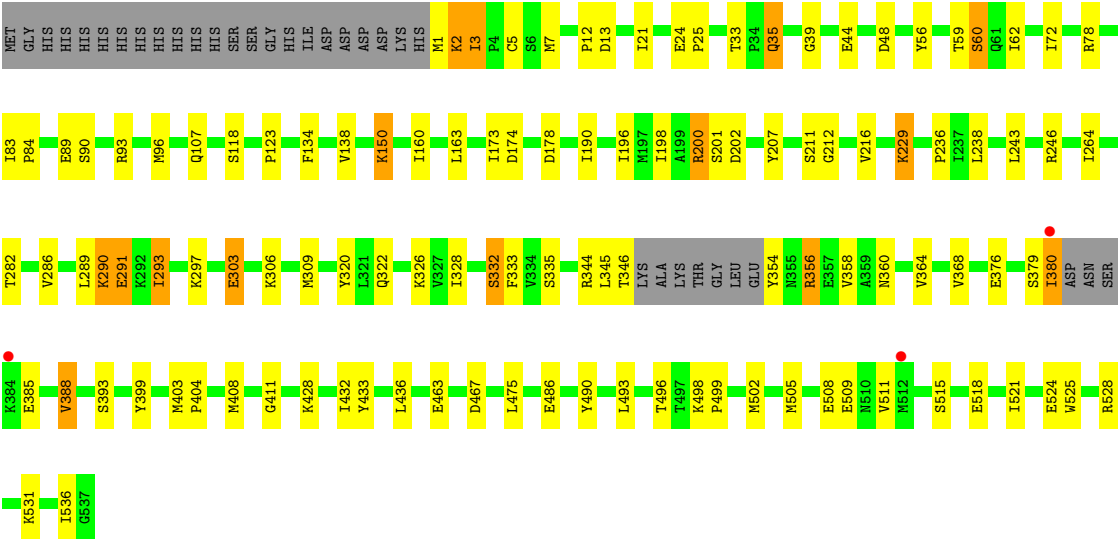
● Molecule 1: Phosphoenolpyruvate carboxylase

Chain G: 65% 27% 6%





● Molecule 1: Phosphoenolpyruvate carboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.42Å 161.58Å 279.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.84 – 2.95 56.84 – 2.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (56.84-2.95) 99.8 (56.84-2.95)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.178 , 0.223 0.177 , 0.212	Depositor DCC
R_{free} test set	1135 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	67.1	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	33563	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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, 0.333 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: AUC, MLI

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	0.78	0/4214	0.99	6/5678 (0.1%)
1	B	0.68	0/4237	0.99	4/5711 (0.1%)
1	C	0.74	0/4239	0.97	4/5712 (0.1%)
1	D	0.76	0/4221	0.96	5/5688 (0.1%)
1	E	0.77	0/4205	0.99	4/5667 (0.1%)
1	F	0.67	0/4228	0.94	1/5700 (0.0%)
1	G	0.69	0/4224	1.00	4/5692 (0.1%)
1	H	0.73	0/4232	1.00	8/5702 (0.1%)
All	All	0.73	0/33800	0.98	36/45550 (0.1%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	388	VAL	N-CA-C	7.78	115.32	108.63
1	C	383	SER	N-CA-C	7.17	119.20	107.23
1	G	360	ASN	N-CA-C	7.10	120.30	110.35
1	C	382	ASN	N-CA-C	6.94	118.59	110.41
1	A	72	ILE	N-CA-C	6.37	113.36	107.56
1	D	211	SER	N-CA-C	-6.33	104.29	111.07
1	A	83	ILE	CA-C-N	-6.31	113.78	120.03
1	A	83	ILE	C-N-CA	-6.31	113.78	120.03
1	H	385	GLU	N-CA-C	6.29	119.20	109.07
1	A	360	ASN	N-CA-C	6.25	118.93	108.73
1	E	511	VAL	N-CA-C	-6.19	103.86	110.36
1	H	72	ILE	N-CA-C	6.18	113.67	107.55
1	E	433	TYR	CA-C-N	6.00	126.16	119.32
1	E	433	TYR	C-N-CA	6.00	126.16	119.32
1	C	15	VAL	N-CA-C	5.92	116.13	110.74
1	F	328	ILE	N-CA-C	5.79	117.23	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	360	ASN	N-CA-C	5.78	118.15	108.96
1	D	24	GLU	CA-C-N	-5.74	112.59	118.85
1	D	24	GLU	C-N-CA	-5.74	112.59	118.85
1	A	278	GLY	N-CA-C	5.65	117.80	112.04
1	G	259	ALA	N-CA-C	-5.63	104.78	111.03
1	H	360	ASN	N-CA-C	5.55	119.31	107.70
1	A	150	LYS	N-CA-C	-5.54	105.16	111.14
1	B	271	SER	N-CA-C	5.52	117.38	111.36
1	C	42	ILE	N-CA-C	-5.46	104.09	110.05
1	G	368	VAL	N-CA-C	5.40	115.94	110.05
1	D	500	ILE	CB-CA-C	-5.39	104.96	112.02
1	H	89	GLU	N-CA-C	5.36	113.90	108.75
1	B	253	ASN	N-CA-C	5.29	119.43	112.92
1	G	72	ILE	N-CA-C	5.25	113.65	107.77
1	E	328	ILE	N-CA-C	5.20	116.55	110.62
1	H	24	GLU	CA-C-N	-5.05	113.44	119.05
1	H	24	GLU	C-N-CA	-5.05	113.44	119.05
1	H	3	ILE	CB-CA-C	-5.02	105.13	110.95
1	B	114	THR	CA-C-N	-5.02	114.41	119.83
1	B	114	THR	C-N-CA	-5.02	114.41	119.83

There are no chirality outliers.

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	4146	0	4209	57	0
1	B	4169	0	4212	73	0
1	C	4171	0	4224	97	0
1	D	4153	0	4218	78	0
1	E	4137	0	4193	70	0
1	F	4160	0	4198	73	0
1	G	4156	0	4213	87	0
1	H	4164	0	4221	64	0
2	A	12	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	0	6	0
2	C	9	0	0	4	0
2	D	8	0	0	4	0
2	E	8	0	0	4	0
2	F	10	0	0	4	0
2	G	7	0	0	5	0
2	H	8	0	0	4	0
3	A	7	0	2	0	0
3	C	7	0	2	0	0
3	D	7	0	2	1	0
3	E	7	0	2	0	0
3	H	7	0	2	0	0
4	A	34	0	0	1	0
4	B	26	0	0	1	0
4	C	23	0	0	2	0
4	D	22	0	0	0	0
4	E	26	0	0	2	0
4	F	21	0	0	0	0
4	G	19	0	0	0	0
4	H	29	0	0	0	0
All	All	33563	0	33698	592	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 9.

All (592) 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:E:5:CYS:SG	2:E:605:AUC:AU	1.32	1.56
1:A:5:CYS:SG	2:A:608:AUC:AU	1.54	1.34
1:B:5:CYS:SG	2:B:609:AUC:AU	1.56	1.34
1:C:5:CYS:SG	2:C:601:AUC:AU	1.65	1.24
1:D:5:CYS:SG	2:D:604:AUC:AU	1.64	1.24
2:E:606:AUC:C1	2:E:606:AUC:AU	1.79	1.01
2:A:607:AUC:AU	2:A:607:AUC:C2	1.80	1.00
2:C:602:AUC:AU	2:C:602:AUC:C1	1.80	1.00
2:H:611:AUC:AU	2:H:611:AUC:C2	1.80	0.99
2:C:602:AUC:AU	2:C:602:AUC:C2	1.80	0.99
2:F:614:AUC:AU	2:F:614:AUC:C2	1.81	0.99
2:A:607:AUC:AU	2:A:607:AUC:C1	1.81	0.99
2:E:606:AUC:AU	2:E:606:AUC:C2	1.81	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:615:AUC:AU	2:G:615:AUC:C2	1.80	0.99
2:D:603:AUC:AU	2:D:603:AUC:C2	1.80	0.99
2:D:603:AUC:AU	2:D:603:AUC:C1	1.79	0.98
2:B:610:AUC:AU	2:B:610:AUC:C2	1.80	0.98
2:F:614:AUC:AU	2:F:614:AUC:C1	1.81	0.98
2:H:611:AUC:AU	2:H:611:AUC:C1	1.81	0.98
1:B:163:LEU:HD13	1:B:197:MET:HG2	1.46	0.97
2:G:615:AUC:AU	2:G:615:AUC:C1	1.82	0.97
2:B:610:AUC:AU	2:B:610:AUC:C1	1.81	0.97
1:E:185:LYS:HG3	1:E:190:ILE:HD13	1.49	0.95
1:D:380:ILE:HG23	1:D:381:ASP:H	1.34	0.93
1:B:5:CYS:HG	2:B:609:AUC:AU	1.08	0.92
1:C:5:CYS:HG	2:C:601:AUC:AU	1.06	0.89
1:F:21:ILE:HD11	1:G:21:ILE:HD11	1.54	0.88
1:D:365:ALA:HB2	1:D:377:ILE:HG21	1.54	0.88
1:B:344:ARG:HH12	2:B:610:AUC:C2	1.91	0.84
1:C:244:PRO:HA	1:C:248:HIS:HB2	1.58	0.84
1:G:48:ASP:HB2	2:G:615:AUC:N2	1.94	0.83
1:E:5:CYS:HG	2:E:605:AUC:AU	0.88	0.82
1:D:192:LYS:HA	1:D:192:LYS:HE2	1.62	0.82
1:E:210:ILE:HD12	1:E:410:MET:SD	2.20	0.82
1:D:380:ILE:CG2	1:D:381:ASP:H	1.95	0.80
1:D:380:ILE:HG23	1:D:381:ASP:N	1.97	0.79
1:C:179:GLU:O	1:C:183:ILE:HG13	1.81	0.79
1:D:154:ASP:O	1:D:157:SER:HB3	1.81	0.78
1:C:21:ILE:HD11	1:D:21:ILE:HD11	1.66	0.78
1:E:185:LYS:HG3	1:E:190:ILE:CD1	2.15	0.76
1:E:483:PHE:CZ	1:F:190:ILE:HG12	2.20	0.76
1:D:197:MET:HG3	1:D:237:ILE:HB	1.67	0.76
1:H:496:THR:O	1:H:499:PRO:HD2	1.86	0.75
1:D:525:TRP:HZ2	1:E:525:TRP:CZ2	2.05	0.75
1:D:525:TRP:CZ2	1:E:525:TRP:HZ2	2.06	0.72
1:C:18:TYR:OH	1:C:343:ASP:OD2	2.05	0.72
1:C:384:LYS:HD3	1:C:385:GLU:H	1.54	0.72
1:D:365:ALA:HB2	1:D:377:ILE:CG2	2.20	0.71
1:G:243:LEU:HG	1:G:535:SER:HB2	1.71	0.71
1:D:5:CYS:HG	2:D:604:AUC:AU	0.67	0.71
1:H:60:SER:HB2	1:H:107:GLN:HE22	1.56	0.71
1:C:18:TYR:HA	1:C:341:ASN:HB3	1.72	0.70
1:H:150:LYS:H	1:H:150:LYS:HD2	1.54	0.70
1:D:282:THR:O	1:D:286:VAL:HG23	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:430:LEU:HD21	1:G:437:ARG:HG3	1.75	0.69
1:A:5:CYS:HG	2:A:608:AUC:AU	0.64	0.69
1:H:7:MET:HG3	1:H:44:GLU:HG2	1.74	0.68
1:G:218:MET:HG2	1:G:309:MET:HE2	1.75	0.68
1:F:168:PRO:HG3	1:F:363:ASN:HB2	1.76	0.67
1:F:56:TYR:HB2	1:G:96:MET:HE3	1.76	0.67
1:H:56:TYR:HB2	1:H:96:MET:HE2	1.76	0.67
1:H:379:SER:C	1:H:380:ILE:HG12	2.20	0.66
1:E:163:LEU:HD13	1:E:197:MET:HG2	1.77	0.66
1:G:333:PHE:CE2	1:G:505:MET:HG3	2.31	0.66
1:B:413:ALA:O	1:B:417:ILE:HD12	1.96	0.66
1:F:453:LYS:HE2	1:F:461:ARG:NH2	2.11	0.66
1:E:57:HIS:O	1:E:61:GLN:HG3	1.95	0.66
1:B:411:GLY:HA3	1:B:467:ASP:HA	1.78	0.65
1:G:12:PRO:HG3	1:G:344:ARG:HD2	1.76	0.65
1:C:103:GLU:O	1:C:107:GLN:HG3	1.97	0.65
1:H:428:LYS:O	1:H:432:ILE:HG13	1.97	0.65
1:D:368:VAL:HG23	1:D:374:LYS:HD2	1.78	0.64
1:G:244:PRO:HA	1:G:248:HIS:HB2	1.78	0.64
1:H:433:TYR:CE2	1:H:436:LEU:HD13	2.33	0.64
1:D:209:LEU:O	1:D:213:VAL:HG23	1.97	0.64
1:D:262:SER:HB3	1:D:299:ARG:HG3	1.80	0.63
1:G:5:CYS:SG	1:G:290:LYS:HA	2.38	0.63
1:A:372:VAL:O	1:A:376:GLU:HG2	1.99	0.63
1:D:380:ILE:O	1:D:381:ASP:HB2	1.98	0.63
1:D:237:ILE:HG23	1:D:266:THR:HB	1.80	0.63
1:B:453:LYS:O	1:B:454:LYS:HB2	1.97	0.63
1:B:185:LYS:HG3	1:B:190:ILE:HG12	1.82	0.62
1:G:48:ASP:HB2	2:G:615:AUC:C2	2.28	0.62
1:H:198:ILE:HG21	1:H:216:VAL:HG13	1.82	0.62
1:G:118:SER:O	1:G:158:VAL:HA	1.99	0.62
1:H:150:LYS:H	1:H:150:LYS:CD	2.12	0.62
1:C:433:TYR:HE1	1:C:435:ILE:HG22	1.64	0.62
1:E:483:PHE:HZ	1:F:190:ILE:HG12	1.65	0.62
1:H:33:THR:O	1:H:39:GLY:HA3	2.00	0.62
1:B:48:ASP:OD1	1:B:82:ARG:HD3	2.00	0.61
1:F:498:LYS:HB3	1:F:499:PRO:HD3	1.82	0.61
1:G:411:GLY:HA3	1:G:467:ASP:HA	1.82	0.61
1:F:128:GLY:HA3	1:F:179:GLU:HB3	1.82	0.61
1:H:490:TYR:HA	1:H:493:LEU:HD12	1.82	0.61
1:B:174:ASP:HB2	1:B:226:TRP:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:282:THR:O	1:H:286:VAL:HG23	2.01	0.61
1:A:123:PRO:HA	1:A:163:LEU:HB3	1.82	0.61
1:A:492:THR:HG21	1:C:503:HIS:HB2	1.83	0.61
1:G:109:LYS:HG3	1:G:115:PRO:HD3	1.82	0.61
1:B:170:LEU:HB3	1:B:219:ALA:HB2	1.82	0.61
1:C:101:ILE:HG23	1:C:117:ILE:HD13	1.82	0.61
1:B:244:PRO:HA	1:B:248:HIS:HB2	1.82	0.61
1:E:193:ASP:HA	1:E:232:VAL:HG23	1.83	0.61
1:G:197:MET:HG3	1:G:237:ILE:HB	1.82	0.61
1:C:48:ASP:OD1	1:C:50:GLU:N	2.31	0.60
1:C:335:SER:HB2	1:C:393:SER:HB3	1.82	0.60
1:F:168:PRO:CG	1:F:363:ASN:HB2	2.30	0.60
1:C:21:ILE:HD11	1:D:21:ILE:CD1	2.31	0.60
1:G:83:ILE:HG22	1:G:97:SER:HB2	1.82	0.60
1:G:134:PHE:O	1:G:138:VAL:HG23	2.00	0.60
1:H:243:LEU:HD13	1:H:399:TYR:CE2	2.36	0.60
1:H:498:LYS:HB3	1:H:499:PRO:HD3	1.82	0.60
1:G:371:GLU:O	1:G:375:GLN:HG2	2.01	0.60
1:D:98:ILE:HG22	1:D:141:VAL:HG11	1.83	0.59
1:G:172:ASN:HB3	1:G:175:ARG:HE	1.66	0.59
1:C:451:VAL:O	1:C:498:LYS:HD2	2.01	0.59
1:D:380:ILE:CG2	1:D:381:ASP:N	2.61	0.59
1:F:170:LEU:HD21	1:F:198:ILE:HG23	1.84	0.59
1:D:496:THR:O	1:D:499:PRO:HD2	2.03	0.59
1:G:372:VAL:O	1:G:376:GLU:HG2	2.02	0.59
1:E:330:THR:HG22	1:E:505:MET:HE1	1.85	0.59
1:C:217:LEU:HD21	1:C:260:THR:O	2.03	0.58
1:G:172:ASN:CB	1:G:175:ARG:HE	2.14	0.58
1:D:498:LYS:HE2	1:D:502:MET:HE2	1.85	0.58
1:E:104:THR:HA	1:E:107:GLN:HE21	1.68	0.58
1:C:201:SER:HB3	1:C:246:ARG:HD2	1.85	0.58
1:G:209:LEU:HB3	1:G:410:MET:HG3	1.85	0.58
1:C:488:GLU:HG3	4:C:714:HOH:O	2.02	0.58
1:A:513:ARG:HG2	1:A:513:ARG:HH11	1.69	0.58
1:B:467:ASP:O	1:B:471:VAL:HG23	2.03	0.58
1:C:86:ALA:HB2	1:C:94:GLN:OE1	2.03	0.58
1:C:168:PRO:HG3	1:C:363:ASN:HB2	1.86	0.58
1:E:498:LYS:HB3	1:E:499:PRO:HD3	1.86	0.58
1:D:199:ALA:HB1	3:D:901:MLI:O7	2.05	0.57
1:A:31:GLY:HA2	1:A:40:LEU:HD12	1.86	0.57
1:D:411:GLY:CA	1:D:471:VAL:HG23	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:ARG:O	1:C:357:GLU:HB2	2.04	0.57
1:H:48:ASP:HB2	2:H:611:AUC:C2	2.35	0.57
1:F:370:ASP:HB3	1:F:373:LEU:HD23	1.87	0.56
1:H:48:ASP:HB2	2:H:611:AUC:N2	2.20	0.56
1:D:459:GLU:O	1:D:463:GLU:HG3	2.04	0.56
1:G:370:ASP:OD1	1:G:372:VAL:HG12	2.05	0.56
1:C:476:ASN:HD22	1:C:476:ASN:H	1.53	0.56
1:D:325:LEU:HD22	1:D:384:LYS:HE3	1.86	0.56
1:F:472:ASN:HA	1:F:477:LEU:HD12	1.88	0.56
1:F:163:LEU:HD13	1:F:197:MET:HG2	1.86	0.56
1:F:406:GLU:O	1:F:410:MET:HG3	2.05	0.56
1:A:524:GLU:O	1:A:528:ARG:HG3	2.06	0.56
1:F:21:ILE:HD11	1:G:21:ILE:CD1	2.30	0.56
1:F:212:GLY:O	1:F:216:VAL:HG23	2.04	0.56
1:H:379:SER:O	1:H:380:ILE:HG12	2.06	0.56
1:F:92:PHE:HB3	1:G:56:TYR:OH	2.06	0.56
1:H:333:PHE:CE2	1:H:505:MET:HG2	2.39	0.56
1:A:459:GLU:O	1:A:463:GLU:HG3	2.05	0.55
1:A:52:LYS:HD3	4:A:762:HOH:O	2.06	0.55
1:C:21:ILE:HD12	1:C:55:PRO:HD3	1.89	0.55
1:F:459:GLU:O	1:F:463:GLU:HG3	2.05	0.55
1:E:90:SER:OG	1:E:93:ARG:HD2	2.07	0.55
1:F:360:ASN:HB3	1:F:363:ASN:HD21	1.72	0.55
1:A:167:VAL:HG13	1:A:215:SER:HB3	1.88	0.55
1:A:305:ASP:O	1:A:309:MET:HG3	2.06	0.55
1:D:5:CYS:SG	1:D:293:ILE:HG21	2.47	0.55
1:B:238:LEU:HB2	1:B:264:ILE:HD12	1.89	0.55
1:B:485:ASN:OD1	1:B:495:LYS:HE3	2.07	0.55
1:H:134:PHE:O	1:H:138:VAL:HG23	2.06	0.55
1:E:98:ILE:HA	1:E:101:ILE:HD12	1.87	0.55
1:A:35:GLN:HA	1:A:39:GLY:O	2.07	0.55
1:C:433:TYR:CE2	1:C:436:LEU:HD13	2.43	0.54
1:G:44:GLU:HG3	1:G:78:ARG:HB3	1.88	0.54
1:G:195:ARG:HG3	1:G:235:SER:HB3	1.89	0.54
1:G:244:PRO:HB2	1:G:406:GLU:HG2	1.90	0.54
1:G:273:LEU:O	1:G:277:HIS:HB2	2.07	0.54
1:A:244:PRO:HB2	1:A:406:GLU:HG2	1.90	0.54
1:C:345:LEU:O	1:C:346:THR:C	2.50	0.54
1:D:12:PRO:HG3	1:D:344:ARG:HD2	1.89	0.54
1:E:18:TYR:HE2	1:E:20:SER:HB3	1.73	0.54
1:H:333:PHE:CE2	1:H:505:MET:CG	2.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:162:PRO:HG2	1:F:196:ILE:HG22	1.89	0.54
1:B:172:ASN:HB2	1:B:175:ARG:HG3	1.89	0.54
1:C:433:TYR:CE1	1:C:435:ILE:HG22	2.41	0.54
1:D:102:ILE:HG13	1:D:141:VAL:HG12	1.90	0.54
1:H:515:SER:HB3	1:H:518:GLU:HB2	1.89	0.54
1:C:433:TYR:HE1	1:C:435:ILE:CG2	2.21	0.53
1:H:306:LYS:HA	1:H:309:MET:HE3	1.89	0.53
1:C:345:LEU:HD21	1:D:57:HIS:CD2	2.42	0.53
1:G:29:ILE:HG23	1:G:66:LEU:HD23	1.90	0.53
1:E:524:GLU:OE2	1:E:528:ARG:NH2	2.42	0.53
1:B:496:THR:HG22	1:G:496:THR:O	2.08	0.53
1:D:208:GLY:HA2	1:D:320:TYR:CD1	2.44	0.53
1:A:46:MET:HA	1:A:80:THR:O	2.08	0.52
1:B:6:SER:HB2	1:B:42:ILE:HG23	1.91	0.52
1:G:533:ARG:NH2	1:G:536:ILE:O	2.34	0.52
1:D:411:GLY:HA2	1:D:471:VAL:HG23	1.91	0.52
1:F:319:HIS:CD2	1:F:413:ALA:HA	2.45	0.52
1:H:335:SER:HB2	1:H:393:SER:HB3	1.91	0.52
1:D:525:TRP:CZ2	1:E:525:TRP:CZ2	2.87	0.52
1:F:490:TYR:O	1:F:493:LEU:HB2	2.09	0.52
1:A:411:GLY:HA2	1:A:471:VAL:HG23	1.92	0.52
1:B:53:LEU:HG	1:B:53:LEU:O	2.09	0.52
1:D:42:ILE:HG22	1:D:43:GLU:N	2.25	0.52
1:E:330:THR:HG22	1:E:505:MET:CE	2.39	0.52
1:G:524:GLU:OE1	1:G:528:ARG:NH2	2.43	0.52
1:F:330:THR:HG23	1:F:505:MET:HE1	1.92	0.52
1:A:387:ALA:O	1:A:389:PRO:HD3	2.10	0.52
1:B:206:SER:HB2	1:B:207:TYR:CD2	2.45	0.52
1:C:345:LEU:O	1:C:347:LYS:HG2	2.10	0.52
1:D:185:LYS:HG3	1:D:190:ILE:HG22	1.90	0.52
1:D:201:SER:HB3	1:D:246:ARG:HD2	1.92	0.52
1:G:437:ARG:NH2	1:G:475:LEU:O	2.42	0.52
1:E:328:ILE:O	1:E:332:SER:HB2	2.10	0.51
1:G:1:MET:HG2	1:G:2:LYS:N	2.25	0.51
1:B:31:GLY:HA2	1:B:40:LEU:HG	1.92	0.51
1:C:63:ALA:O	1:C:67:ILE:HG13	2.10	0.51
1:C:451:VAL:HG11	1:C:494:LEU:HB3	1.92	0.51
1:D:335:SER:HB2	1:D:393:SER:HB3	1.91	0.51
1:D:370:ASP:OD1	1:D:372:VAL:HG12	2.11	0.51
1:E:381:ASP:C	1:E:383:SER:H	2.17	0.51
1:F:163:LEU:HA	1:F:197:MET:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:144:MET:O	1:G:148:ASN:ND2	2.44	0.51
1:C:244:PRO:HB2	1:C:406:GLU:HG2	1.92	0.51
1:G:172:ASN:HD21	1:G:367:LEU:HD21	1.75	0.51
1:B:373:LEU:O	1:B:374:LYS:C	2.53	0.51
1:F:244:PRO:HA	1:F:248:HIS:HB2	1.91	0.51
1:F:518:GLU:N	1:F:518:GLU:OE1	2.43	0.51
1:F:48:ASP:HB2	2:F:614:AUC:N1	2.26	0.51
1:F:159:ARG:HH22	1:F:194:LEU:HD13	1.76	0.51
1:G:311:GLU:OE2	1:G:369:LYS:HE2	2.11	0.51
1:H:212:GLY:O	1:H:216:VAL:HG23	2.10	0.51
1:B:46:MET:HA	1:B:80:THR:O	2.11	0.51
1:E:88:LYS:HE3	1:E:88:LYS:HA	1.91	0.51
1:C:461:ARG:O	1:C:465:LYS:HG3	2.11	0.51
1:F:51:GLY:O	1:F:345:LEU:N	2.44	0.51
1:B:143:ASP:O	1:B:147:LYS:HG2	2.11	0.51
1:H:303:GLU:OE1	1:H:303:GLU:HA	2.09	0.51
1:E:143:ASP:O	1:E:147:LYS:HE3	2.10	0.50
1:F:210:ILE:HG13	1:F:410:MET:SD	2.51	0.50
1:G:433:TYR:CE2	1:G:436:LEU:HD13	2.47	0.50
1:B:210:ILE:HD12	1:B:410:MET:SD	2.51	0.50
1:B:496:THR:O	1:G:496:THR:HG22	2.12	0.50
1:C:172:ASN:CG	1:C:172:ASN:O	2.55	0.50
1:C:473:GLU:O	1:C:476:ASN:ND2	2.44	0.50
1:E:508:GLU:HB3	1:E:511:VAL:HG23	1.92	0.50
1:E:244:PRO:HB2	1:E:406:GLU:HG2	1.93	0.50
1:F:16:GLU:OE2	1:F:531:LYS:HE2	2.11	0.50
1:C:411:GLY:HA3	1:C:467:ASP:HA	1.91	0.50
1:B:105:ASN:HB3	1:B:153:LEU:CD2	2.41	0.50
1:C:371:GLU:C	1:C:373:LEU:H	2.17	0.50
1:G:56:TYR:HB2	1:G:96:MET:HE2	1.94	0.50
1:G:200:ARG:HG2	1:G:238:LEU:HD11	1.94	0.50
1:D:360:ASN:HB3	1:D:363:ASN:OD1	2.11	0.50
1:F:137:ARG:O	1:F:140:SER:OG	2.27	0.50
1:G:451:VAL:HG11	1:G:494:LEU:HB3	1.93	0.50
1:B:48:ASP:HB2	2:B:610:AUC:N1	2.27	0.49
1:B:448:ASN:HD22	1:B:491:HIS:HD2	1.60	0.49
1:H:356:ARG:HB3	1:H:388:VAL:HG13	1.93	0.49
1:D:110:GLU:HG2	1:D:151:THR:OG1	2.12	0.49
1:F:209:LEU:O	1:F:213:VAL:HG23	2.12	0.49
1:H:174:ASP:O	1:H:178:ASP:HB2	2.12	0.49
1:B:4:PRO:HB3	1:B:43:GLU:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:448:ASN:ND2	1:C:491:HIS:ND1	2.53	0.49
1:C:382:ASN:N	1:C:382:ASN:HD22	2.08	0.49
1:G:140:SER:O	1:G:143:ASP:HB2	2.13	0.49
1:E:205:MET:HG3	1:E:394:PHE:CD2	2.47	0.49
1:E:403:MET:O	1:E:404:PRO:C	2.53	0.49
1:B:33:THR:HB	1:B:39:GLY:HA3	1.94	0.49
1:F:244:PRO:HB2	1:F:406:GLU:HG2	1.95	0.49
1:H:433:TYR:CD1	1:H:436:LEU:HB2	2.48	0.49
1:B:448:ASN:HD22	1:B:491:HIS:CD2	2.31	0.49
1:D:185:LYS:HG3	1:D:190:ILE:CG2	2.43	0.49
1:G:1:MET:HG2	1:G:2:LYS:H	1.77	0.49
1:G:205:MET:HG3	1:G:394:PHE:CD2	2.48	0.49
1:H:123:PRO:HA	1:H:163:LEU:HB3	1.95	0.49
1:E:195:ARG:HG3	1:E:235:SER:HB3	1.95	0.49
1:H:236:PRO:HB2	1:H:264:ILE:HD13	1.94	0.49
1:A:411:GLY:HA3	1:A:467:ASP:HA	1.95	0.48
1:C:476:ASN:HD22	1:C:476:ASN:N	2.10	0.48
1:B:456:ILE:HG22	1:B:457:ASP:O	2.12	0.48
1:C:214:LEU:HD22	1:C:309:MET:HG2	1.95	0.48
1:E:337:PHE:CE1	1:E:519:LEU:HD22	2.48	0.48
1:B:303:GLU:HA	1:B:303:GLU:OE1	2.13	0.48
1:E:123:PRO:HA	1:E:163:LEU:HB3	1.94	0.48
1:E:52:LYS:C	1:E:54:THR:H	2.22	0.48
1:F:1:MET:HG3	1:F:75:LYS:O	2.13	0.48
1:F:453:LYS:HE2	1:F:461:ARG:HH22	1.77	0.48
1:G:225:LYS:O	1:G:228:GLU:HB2	2.13	0.48
1:E:524:GLU:O	1:E:528:ARG:HG3	2.14	0.48
1:H:200:ARG:HG2	1:H:238:LEU:HD11	1.96	0.48
1:A:122:VAL:HG11	1:A:134:PHE:CD2	2.49	0.48
1:C:244:PRO:HA	1:C:248:HIS:CB	2.36	0.48
1:E:244:PRO:HA	1:E:248:HIS:HB2	1.95	0.48
1:G:106:VAL:O	1:G:110:GLU:HG3	2.13	0.48
1:H:403:MET:O	1:H:404:PRO:C	2.55	0.48
1:A:475:LEU:O	1:A:476:ASN:C	2.57	0.48
1:C:96:MET:HG2	1:D:96:MET:HG2	1.95	0.48
1:E:83:ILE:HG22	1:E:97:SER:HB2	1.96	0.48
1:G:234:ILE:HG22	1:G:236:PRO:HD3	1.96	0.48
1:A:33:THR:HG22	1:A:37:LYS:HB3	1.96	0.48
1:A:498:LYS:HB3	1:A:499:PRO:HD3	1.95	0.48
1:A:166:ASP:HB3	1:A:169:ALA:HB3	1.96	0.47
1:C:282:THR:O	1:C:286:VAL:HG23	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:92:PHE:HE1	1:G:102:ILE:HB	1.78	0.47
1:B:105:ASN:HB3	1:B:153:LEU:HD21	1.97	0.47
1:B:449:GLY:HA3	1:B:465:LYS:HE3	1.95	0.47
1:G:131:ILE:HD13	1:G:162:PRO:HB3	1.94	0.47
1:D:328:ILE:O	1:D:332:SER:HB2	2.14	0.47
1:E:521:ILE:O	1:E:522:LEU:C	2.56	0.47
1:F:480:ASP:HB3	1:F:483:PHE:HB3	1.96	0.47
1:H:12:PRO:HG3	1:H:344:ARG:HD2	1.95	0.47
1:F:33:THR:HB	1:F:39:GLY:HA3	1.95	0.47
1:F:241:GLY:N	1:F:246:ARG:O	2.48	0.47
1:H:411:GLY:HA3	1:H:467:ASP:HA	1.95	0.47
1:H:521:ILE:O	1:H:525:TRP:HD1	1.97	0.47
1:A:173:ILE:HG13	1:A:173:ILE:O	2.13	0.47
1:C:382:ASN:HD22	1:C:382:ASN:H	1.62	0.47
1:C:384:LYS:O	1:C:386:TYR:N	2.41	0.47
1:D:324:PHE:C	1:D:324:PHE:CD2	2.92	0.47
1:D:361:LEU:HD11	1:D:380:ILE:HG22	1.96	0.47
1:F:56:TYR:CB	1:G:96:MET:HE3	2.43	0.47
1:G:403:MET:O	1:G:404:PRO:C	2.58	0.47
1:B:200:ARG:HG2	1:B:238:LEU:HD11	1.96	0.47
1:B:442:PHE:C	1:B:442:PHE:CD2	2.93	0.47
1:C:286:VAL:HG12	1:C:290:LYS:HE3	1.95	0.47
1:C:497:THR:O	1:C:500:ILE:HG22	2.15	0.47
1:F:322:GLN:O	1:F:326:LYS:HE3	2.15	0.47
1:A:244:PRO:HA	1:A:248:HIS:HB2	1.97	0.47
1:B:52:LYS:HG3	1:B:343:ASP:O	2.14	0.47
1:C:345:LEU:O	1:C:347:LYS:N	2.48	0.47
1:C:102:ILE:HG13	1:C:141:VAL:HG12	1.96	0.47
1:C:200:ARG:NH1	1:C:245:PHE:O	2.46	0.47
1:C:518:GLU:OE1	1:C:518:GLU:N	2.48	0.47
1:B:12:PRO:HG3	1:B:344:ARG:HD2	1.97	0.47
1:E:205:MET:HE1	1:E:389:PRO:HD2	1.96	0.47
1:F:121:VAL:HA	1:F:161:ILE:O	2.15	0.47
1:H:326:LYS:NZ	1:H:463:GLU:OE2	2.47	0.47
1:A:323:THR:OG1	1:A:412:ARG:NH2	2.43	0.46
1:A:518:GLU:H	1:A:518:GLU:CD	2.22	0.46
1:F:46:MET:HA	1:F:80:THR:O	2.15	0.46
1:F:398:MET:HB2	1:F:405:PRO:HG3	1.98	0.46
1:G:509:GLU:HG3	1:G:510:ASN:N	2.29	0.46
1:C:442:PHE:C	1:C:442:PHE:CD2	2.94	0.46
1:E:432:ILE:C	1:E:434:PRO:HD3	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:PRO:HG2	1:F:37:LYS:HB2	1.97	0.46
1:G:258:LEU:O	1:G:262:SER:HB2	2.15	0.46
1:G:137:ARG:O	1:G:141:VAL:HG23	2.16	0.46
1:G:167:VAL:HB	1:G:207:TYR:CD2	2.50	0.46
1:H:328:ILE:O	1:H:332:SER:HB2	2.15	0.46
1:A:525:TRP:CZ3	1:A:528:ARG:HD2	2.50	0.46
1:B:84:PRO:HB3	1:B:89:GLU:CD	2.40	0.46
1:C:347:LYS:HE2	1:C:347:LYS:HB3	1.87	0.46
1:E:33:THR:HB	1:E:39:GLY:HA3	1.96	0.46
1:E:282:THR:O	1:E:286:VAL:HG23	2.15	0.46
1:G:163:LEU:HA	1:G:197:MET:O	2.15	0.46
1:H:289:LEU:C	1:H:291:GLU:H	2.23	0.46
1:G:473:GLU:O	1:G:476:ASN:ND2	2.48	0.46
1:C:5:CYS:HA	1:C:265:LYS:O	2.16	0.46
1:D:305:ASP:O	1:D:306:LYS:C	2.59	0.46
1:G:35:GLN:NE2	1:G:40:LEU:O	2.48	0.46
1:A:170:LEU:CD1	1:A:203:THR:HG21	2.46	0.46
1:C:83:ILE:HB	1:C:84:PRO:HD2	1.98	0.46
1:E:252:GLU:HG2	1:E:253:ASN:OD1	2.15	0.46
1:E:381:ASP:HB2	1:E:383:SER:OG	2.16	0.46
1:F:53:LEU:HG	1:F:53:LEU:O	2.15	0.46
1:F:218:MET:HE1	1:F:310:LYS:HE3	1.98	0.46
1:A:411:GLY:CA	1:A:471:VAL:HG23	2.46	0.46
1:E:179:GLU:O	1:E:183:ILE:HG13	2.16	0.46
1:F:125:ILE:HD13	1:F:125:ILE:HA	1.81	0.46
1:F:453:LYS:O	1:F:454:LYS:HB2	2.14	0.46
1:G:193:ASP:HA	1:G:233:THR:H	1.81	0.46
1:A:236:PRO:HB2	1:A:264:ILE:HD13	1.98	0.46
1:C:525:TRP:CZ3	1:C:528:ARG:HD2	2.51	0.46
1:H:201:SER:HB3	1:H:246:ARG:HD2	1.98	0.46
1:B:208:GLY:HA2	1:B:320:TYR:CD1	2.51	0.45
1:F:195:ARG:HG3	1:F:235:SER:O	2.16	0.45
1:E:483:PHE:C	1:E:483:PHE:CD2	2.94	0.45
1:F:21:ILE:HD12	1:F:55:PRO:HD3	1.97	0.45
1:C:346:THR:O	1:C:347:LYS:HE3	2.16	0.45
1:C:384:LYS:HD3	1:C:385:GLU:N	2.29	0.45
1:A:183:ILE:HG22	1:A:187:LYS:HE2	1.98	0.45
1:B:58:GLN:HA	1:B:61:GLN:OE1	2.17	0.45
1:B:490:TYR:HA	1:B:493:LEU:HD12	1.97	0.45
1:H:524:GLU:O	1:H:528:ARG:HG3	2.17	0.45
1:A:201:SER:HB3	1:A:246:ARG:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:PRO:HG3	1:C:344:ARG:HD2	1.99	0.45
1:C:373:LEU:O	1:C:377:ILE:HG13	2.16	0.45
1:A:513:ARG:HG2	1:A:513:ARG:NH1	2.32	0.45
1:C:293:ILE:C	1:C:295:GLN:H	2.25	0.45
1:F:250:SER:HB3	1:F:253:ASN:ND2	2.31	0.45
1:C:173:ILE:O	1:C:177:LEU:HG	2.16	0.45
1:E:172:ASN:HB2	1:E:175:ARG:NH2	2.32	0.45
1:E:310:LYS:HG2	1:E:367:LEU:HD22	1.98	0.45
1:E:342:ARG:HG2	4:E:882:HOH:O	2.16	0.45
1:G:213:VAL:HG21	1:G:433:TYR:OH	2.16	0.45
1:H:345:LEU:O	1:H:346:THR:HG23	2.17	0.45
1:B:305:ASP:O	1:B:309:MET:HG3	2.17	0.45
1:B:86:ALA:HB2	1:B:94:GLN:CD	2.42	0.45
1:D:493:LEU:O	1:D:494:LEU:C	2.60	0.45
1:G:52:LYS:C	1:G:54:THR:H	2.25	0.45
1:B:365:ALA:O	1:B:374:LYS:HE2	2.16	0.44
1:C:363:ASN:O	1:C:367:LEU:CD1	2.66	0.44
1:C:403:MET:O	1:C:404:PRO:C	2.59	0.44
1:D:154:ASP:O	1:D:157:SER:CB	2.59	0.44
1:G:365:ALA:HB1	1:G:374:LYS:HG3	1.99	0.44
1:A:48:ASP:HB3	1:A:52:LYS:HE3	1.98	0.44
1:C:33:THR:HB	1:C:39:GLY:HA3	1.98	0.44
1:C:191:LEU:HG	4:C:749:HOH:O	2.17	0.44
1:C:515:SER:O	1:C:519:LEU:HG	2.18	0.44
1:H:25:PRO:HA	1:H:62:ILE:HG12	1.98	0.44
1:C:363:ASN:O	1:C:367:LEU:HD12	2.17	0.44
1:D:361:LEU:HD21	1:D:380:ILE:HG21	1.99	0.44
1:G:7:MET:HA	1:G:44:GLU:O	2.17	0.44
1:F:83:ILE:HG22	1:F:97:SER:HB2	2.00	0.44
1:A:170:LEU:HB3	1:A:219:ALA:HB2	1.99	0.44
1:B:506:GLY:O	1:B:507:LEU:HD23	2.17	0.44
1:C:365:ALA:HB2	1:C:377:ILE:HG21	1.99	0.44
1:E:461:ARG:HD3	4:E:781:HOH:O	2.17	0.44
1:G:33:THR:O	1:G:39:GLY:HA3	2.17	0.44
1:B:373:LEU:HA	1:B:376:GLU:OE2	2.18	0.44
1:E:103:GLU:O	1:E:107:GLN:HG3	2.18	0.44
1:B:106:VAL:HG13	1:B:151:THR:HB	1.99	0.44
1:C:423:GLN:O	1:C:424:GLU:C	2.60	0.44
1:H:333:PHE:CE2	1:H:505:MET:HG3	2.53	0.44
1:F:57:HIS:ND1	1:F:57:HIS:N	2.66	0.44
1:H:90:SER:OG	1:H:93:ARG:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:ILE:H	1:D:190:ILE:HG13	1.66	0.44
1:H:196:ILE:O	1:H:196:ILE:HG13	2.18	0.44
1:B:201:SER:HB3	1:B:246:ARG:HD2	1.99	0.43
1:C:337:PHE:HE1	1:C:519:LEU:HD22	1.83	0.43
1:D:42:ILE:CG2	1:D:43:GLU:N	2.81	0.43
1:B:204:ALA:HA	1:B:208:GLY:O	2.18	0.43
1:B:360:ASN:OD1	1:B:360:ASN:C	2.61	0.43
1:C:261:TYR:O	1:C:262:SER:C	2.60	0.43
1:G:79:VAL:O	1:G:117:ILE:HG23	2.18	0.43
1:G:229:LYS:HD3	1:G:230:HIS:CE1	2.53	0.43
1:B:1:MET:HG2	1:B:2:LYS:N	2.33	0.43
1:D:98:ILE:HA	1:D:101:ILE:HD12	1.99	0.43
1:F:451:VAL:HA	1:F:498:LYS:HD2	1.99	0.43
1:C:409:GLY:HA2	1:C:412:ARG:NH2	2.33	0.43
1:D:1:MET:O	1:D:78:ARG:NH1	2.50	0.43
1:A:44:GLU:OE2	1:A:80:THR:OG1	2.26	0.43
1:B:413:ALA:C	1:B:417:ILE:HD12	2.43	0.43
1:C:248:HIS:CE1	1:C:253:ASN:HD21	2.35	0.43
1:C:398:MET:HE3	1:C:403:MET:O	2.19	0.43
1:D:95:LEU:O	1:D:96:MET:C	2.61	0.43
1:D:328:ILE:HG23	1:D:329:ASP:N	2.34	0.43
1:G:398:MET:HE3	1:G:403:MET:O	2.18	0.43
1:H:1:MET:HG2	1:H:2:LYS:N	2.33	0.43
1:A:433:TYR:CE2	1:A:436:LEU:HD13	2.54	0.43
1:D:166:ASP:CG	1:D:168:PRO:HD2	2.44	0.43
1:A:56:TYR:CD1	1:E:96:MET:HG3	2.53	0.43
1:C:337:PHE:CE1	1:C:519:LEU:HD22	2.53	0.43
1:C:371:GLU:C	1:C:373:LEU:N	2.77	0.43
1:A:315:ILE:HG13	1:A:373:LEU:HD21	1.99	0.43
1:B:200:ARG:HD2	1:B:200:ARG:O	2.18	0.43
1:B:464:TYR:O	1:B:467:ASP:HB2	2.19	0.43
1:D:289:LEU:O	1:D:290:LYS:C	2.62	0.43
1:D:499:PRO:HG2	1:E:496:THR:CG2	2.48	0.43
1:D:48:ASP:OD1	1:D:82:ARG:HD3	2.19	0.43
1:G:319:HIS:HE1	1:G:416:GLU:OE1	2.02	0.43
1:G:463:GLU:O	1:G:466:GLU:HB2	2.19	0.43
1:H:13:ASP:O	1:H:536:ILE:HG22	2.19	0.43
1:A:335:SER:HA	1:A:338:ILE:HG12	2.01	0.42
1:E:380:ILE:H	1:E:380:ILE:HG13	1.68	0.42
1:B:456:ILE:HD13	1:B:456:ILE:HA	1.86	0.42
1:D:440:LEU:HD13	1:D:471:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:237:ILE:HG23	1:G:266:THR:HB	2.00	0.42
1:H:35:GLN:HE21	1:H:35:GLN:HB2	1.56	0.42
1:B:498:LYS:HB3	1:B:499:PRO:HD3	2.01	0.42
1:E:470:TYR:O	1:E:471:VAL:C	2.62	0.42
1:F:198:ILE:HG21	1:F:216:VAL:HG13	2.00	0.42
1:G:178:ASP:O	1:G:182:GLU:HB2	2.18	0.42
1:A:33:THR:HB	1:A:39:GLY:HA3	2.01	0.42
1:A:33:THR:O	1:A:39:GLY:HA3	2.20	0.42
1:B:277:HIS:CD2	1:B:277:HIS:N	2.85	0.42
1:C:197:MET:HG3	1:C:237:ILE:HB	2.01	0.42
1:D:308:LEU:O	1:D:309:MET:C	2.63	0.42
1:H:83:ILE:HB	1:H:84:PRO:HD2	2.01	0.42
1:D:7:MET:HA	1:D:44:GLU:HB3	2.02	0.42
1:D:35:GLN:C	1:D:37:LYS:H	2.28	0.42
1:E:122:VAL:HG11	1:E:134:PHE:CE2	2.54	0.42
1:A:146:ASN:OD1	1:A:152:LYS:HA	2.20	0.42
1:E:436:LEU:O	1:E:437:ARG:C	2.62	0.42
1:C:7:MET:HE3	1:C:44:GLU:CD	2.45	0.42
1:C:365:ALA:HB1	1:C:374:LYS:HG3	2.02	0.42
1:D:209:LEU:HD13	1:D:245:PHE:HA	2.01	0.42
1:D:250:SER:OG	1:D:251:GLU:N	2.52	0.42
1:F:132:SER:HB3	1:F:187:LYS:NZ	2.35	0.42
1:G:201:SER:HB3	1:G:246:ARG:HD2	2.00	0.42
1:G:361:LEU:HD21	1:G:377:ILE:O	2.19	0.42
1:B:237:ILE:HG23	1:B:266:THR:HB	2.02	0.42
1:E:122:VAL:HG11	1:E:134:PHE:CD2	2.54	0.42
1:F:206:SER:HB2	1:F:207:TYR:CD2	2.55	0.42
1:A:177:LEU:O	1:A:178:ASP:C	2.62	0.42
1:A:270:GLN:O	1:A:274:ARG:HG3	2.19	0.42
1:A:361:LEU:HD11	1:A:380:ILE:HB	2.02	0.42
1:C:8:MET:HE1	1:C:27:GLU:HG2	2.00	0.42
1:C:25:PRO:HA	1:C:62:ILE:HG12	2.02	0.42
1:C:448:ASN:HB3	1:C:451:VAL:HG22	2.02	0.42
1:F:101:ILE:HG23	1:F:117:ILE:HD13	2.02	0.42
1:B:56:TYR:N	4:B:768:HOH:O	2.53	0.42
1:C:125:ILE:HD13	1:C:125:ILE:HA	1.80	0.42
1:C:459:GLU:O	1:C:463:GLU:HG3	2.19	0.42
1:E:337:PHE:HE1	1:E:519:LEU:HD22	1.85	0.42
1:G:122:VAL:HA	1:G:123:PRO:HD3	1.76	0.42
1:H:207:TYR:HE1	1:H:364:VAL:CG1	2.32	0.42
1:A:382:ASN:O	1:A:384:LYS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:ARG:HG3	1:B:235:SER:O	2.20	0.41
1:B:497:THR:O	1:B:500:ILE:HG22	2.20	0.41
1:C:98:ILE:O	1:C:99:MET:C	2.63	0.41
1:D:257:ILE:HD13	1:D:257:ILE:HA	1.94	0.41
1:F:307:ASP:O	1:F:311:GLU:HG2	2.21	0.41
1:F:400:THR:C	1:F:402:GLY:H	2.28	0.41
1:F:218:MET:HE1	1:F:310:LYS:CE	2.50	0.41
1:B:357:GLU:HB2	1:B:388:VAL:HG22	2.02	0.41
1:E:205:MET:CE	1:E:389:PRO:HD2	2.51	0.41
1:G:214:LEU:O	1:G:218:MET:HG3	2.21	0.41
1:H:5:CYS:HB3	1:H:293:ILE:HG13	2.01	0.41
1:E:183:ILE:HG22	1:E:187:LYS:HE2	2.02	0.41
1:E:373:LEU:O	1:E:374:LYS:C	2.63	0.41
1:F:44:GLU:HG3	1:F:78:ARG:HB2	2.02	0.41
1:G:205:MET:O	1:G:320:TYR:OH	2.30	0.41
1:H:320:TYR:CE1	1:H:408:MET:HE3	2.56	0.41
1:B:120:VAL:CG2	1:B:160:ILE:HD13	2.50	0.41
1:C:20:SER:OG	1:C:23:GLN:HG3	2.20	0.41
1:D:195:ARG:HG3	1:D:235:SER:HB3	2.02	0.41
1:D:244:PRO:HA	1:D:248:HIS:HB2	2.02	0.41
1:F:456:ILE:HD13	1:F:456:ILE:HA	1.74	0.41
1:G:24:GLU:O	1:G:27:GLU:HB3	2.19	0.41
1:G:83:ILE:HB	1:G:84:PRO:HD2	2.01	0.41
1:A:452:SER:HB3	1:A:456:ILE:HG13	2.02	0.41
1:D:110:GLU:CG	1:D:151:THR:OG1	2.69	0.41
1:E:105:ASN:HB3	1:E:153:LEU:HD21	2.03	0.41
1:E:375:GLN:C	1:E:377:ILE:H	2.29	0.41
1:F:118:SER:C	1:F:119:GLU:HG3	2.45	0.41
1:G:11:HIS:CD2	2:G:615:AUC:C1	3.04	0.41
1:H:433:TYR:CG	1:H:436:LEU:HB2	2.55	0.41
1:B:398:MET:HB3	1:B:403:MET:O	2.21	0.41
1:B:458:GLU:HA	1:B:458:GLU:OE1	2.21	0.41
1:C:245:PHE:HB2	1:C:406:GLU:CD	2.46	0.41
1:D:244:PRO:HB2	1:D:406:GLU:HG2	2.02	0.41
1:E:456:ILE:CG2	1:E:457:ASP:N	2.84	0.41
1:F:525:TRP:CZ2	1:H:525:TRP:CZ2	3.09	0.41
1:G:302:SER:O	1:G:305:ASP:HB2	2.21	0.41
1:A:8:MET:HE3	1:A:8:MET:HB2	1.92	0.41
1:C:208:GLY:HA2	1:C:320:TYR:CE1	2.56	0.41
1:D:52:LYS:C	1:D:54:THR:H	2.29	0.41
1:D:57:HIS:O	1:D:61:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:453:LYS:HD3	1:D:461:ARG:NH2	2.36	0.41
1:E:122:VAL:HA	1:E:123:PRO:HD3	1.85	0.41
1:E:432:ILE:O	1:E:434:PRO:HD3	2.21	0.41
1:E:456:ILE:HG22	1:E:457:ASP:O	2.20	0.41
1:G:238:LEU:HD23	1:G:240:CYS:HB3	2.02	0.41
1:G:251:GLU:CD	1:G:281:ALA:HB1	2.45	0.41
1:A:497:THR:O	1:A:498:LYS:C	2.64	0.41
1:C:122:VAL:HG11	1:C:134:PHE:CE2	2.56	0.41
1:D:411:GLY:HA2	1:D:471:VAL:CG2	2.52	0.41
1:G:138:VAL:O	1:G:142:VAL:HG23	2.20	0.41
1:A:122:VAL:HG11	1:A:134:PHE:CE2	2.55	0.40
1:C:243:LEU:O	1:C:244:PRO:C	2.63	0.40
1:F:106:VAL:HG13	1:F:151:THR:HB	2.03	0.40
1:F:131:ILE:H	1:F:131:ILE:HG13	1.74	0.40
1:H:3:ILE:HD13	1:H:78:ARG:NH2	2.37	0.40
1:A:174:ASP:O	1:A:178:ASP:HB2	2.21	0.40
1:B:470:TYR:O	1:B:471:VAL:C	2.63	0.40
1:C:46:MET:HA	1:C:80:THR:O	2.20	0.40
1:C:508:GLU:HG3	1:C:511:VAL:HB	2.03	0.40
1:D:433:TYR:CD1	1:D:433:TYR:C	2.98	0.40
1:H:229:LYS:HA	1:H:229:LYS:HD3	1.80	0.40
1:H:289:LEU:C	1:H:291:GLU:N	2.77	0.40
1:A:21:ILE:H	1:A:21:ILE:HG12	1.73	0.40
1:A:166:ASP:HB3	1:A:169:ALA:CB	2.50	0.40
1:B:172:ASN:O	1:B:172:ASN:CG	2.64	0.40
1:B:398:MET:HB2	1:B:405:PRO:HD3	2.04	0.40
1:E:311:GLU:O	1:E:315:ILE:HD12	2.21	0.40
1:F:200:ARG:NH1	1:F:245:PHE:O	2.49	0.40
1:F:243:LEU:O	1:F:244:PRO:C	2.64	0.40
1:H:5:CYS:SG	1:H:290:LYS:HA	2.61	0.40
1:H:7:MET:HA	1:H:44:GLU:HB3	2.03	0.40
1:A:447:ALA:HB1	1:A:468:MET:SD	2.61	0.40
1:B:21:ILE:HD11	1:H:21:ILE:CD1	2.52	0.40
1:B:499:PRO:HB2	1:G:496:THR:HG23	2.03	0.40
1:C:5:CYS:HB3	1:C:293:ILE:HG12	2.03	0.40
1:C:159:ARG:HH21	1:C:194:LEU:HD12	1.87	0.40
1:E:73:PRO:HA	1:E:77:VAL:O	2.21	0.40
1:E:381:ASP:C	1:E:383:SER:N	2.79	0.40
1:F:48:ASP:HB2	2:F:614:AUC:C1	2.52	0.40
1:F:253:ASN:O	1:F:254:ILE:C	2.65	0.40
1:H:56:TYR:CB	1:H:96:MET:HE2	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:138:VAL:HG21	1:H:160:ILE:HD11	2.04	0.40
1:A:415:ASN:O	1:A:419:THR:HG23	2.21	0.40
1:D:150:LYS:HD3	1:D:150:LYS:HA	1.83	0.40
1:G:33:THR:HA	1:G:34:PRO:HD2	1.85	0.40
1:H:333:PHE:HE2	1:H:505:MET:HG3	1.87	0.40

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	521/560 (93%)	496 (95%)	24 (5%)	1 (0%)	43	66
1	B	525/560 (94%)	486 (93%)	38 (7%)	1 (0%)	43	66
1	C	526/560 (94%)	483 (92%)	31 (6%)	12 (2%)	5	14
1	D	522/560 (93%)	484 (93%)	34 (6%)	4 (1%)	16	37
1	E	520/560 (93%)	484 (93%)	28 (5%)	8 (2%)	8	23
1	F	525/560 (94%)	486 (93%)	35 (7%)	4 (1%)	16	37
1	G	523/560 (93%)	478 (91%)	42 (8%)	3 (1%)	21	45
1	H	521/560 (93%)	496 (95%)	23 (4%)	2 (0%)	30	53
All	All	4183/4480 (93%)	3893 (93%)	255 (6%)	35 (1%)	16	37

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	346	THR
1	C	347	LYS
1	C	357	GLU
1	D	384	LYS
1	C	385	GLU

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Mol	Chain	Res	Type
1	D	381	ASP
1	E	89	GLU
1	E	370	ASP
1	F	294	ALA
1	F	343	ASP
1	G	209	LEU
1	G	358	VAL
1	H	356	ARG
1	C	2	LYS
1	C	89	GLU
1	C	294	ALA
1	C	424	GLU
1	E	53	LEU
1	E	374	LYS
1	F	124	MET
1	A	383	SER
1	B	89	GLU
1	E	361	LEU
1	E	471	VAL
1	F	89	GLU
1	C	130	GLU
1	D	382	ASN
1	E	535	SER
1	G	53	LEU
1	H	290	LYS
1	C	476	ASN
1	C	471	VAL
1	D	236	PRO
1	E	168	PRO
1	C	377	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	462/493 (94%)	433 (94%)	29 (6%)	16 38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	462/493 (94%)	427 (92%)	35 (8%)	12	31
1	C	463/493 (94%)	426 (92%)	37 (8%)	11	28
1	D	463/493 (94%)	432 (93%)	31 (7%)	15	36
1	E	461/493 (94%)	430 (93%)	31 (7%)	15	36
1	F	461/493 (94%)	416 (90%)	45 (10%)	7	21
1	G	462/493 (94%)	427 (92%)	35 (8%)	12	31
1	H	462/493 (94%)	432 (94%)	30 (6%)	15	37
All	All	3696/3944 (94%)	3423 (93%)	273 (7%)	13	32

All (273) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	CYS
1	A	16	GLU
1	A	21	ILE
1	A	69	ASN
1	A	78	ARG
1	A	91	VAL
1	A	126	GLU
1	A	147	LYS
1	A	164	VAL
1	A	182	GLU
1	A	211	SER
1	A	265	LYS
1	A	299	ARG
1	A	300	ASN
1	A	302	SER
1	A	330	THR
1	A	344	ARG
1	A	368	VAL
1	A	372	VAL
1	A	376	GLU
1	A	388	VAL
1	A	452	SER
1	A	469	LYS
1	A	471	VAL
1	A	486	GLU
1	A	492	THR
1	A	495	LYS
1	A	510	ASN

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Mol	Chain	Res	Type
1	A	516	THR
1	B	2	LYS
1	B	5	CYS
1	B	6	SER
1	B	75	LYS
1	B	91	VAL
1	B	93	ARG
1	B	120	VAL
1	B	153	LEU
1	B	166	ASP
1	B	172	ASN
1	B	173	ILE
1	B	174	ASP
1	B	200	ARG
1	B	201	SER
1	B	202	ASP
1	B	203	THR
1	B	211	SER
1	B	225	LYS
1	B	344	ARG
1	B	346	THR
1	B	361	LEU
1	B	372	VAL
1	B	375	GLN
1	B	383	SER
1	B	384	LYS
1	B	385	GLU
1	B	390	ARG
1	B	420	LYS
1	B	438	LYS
1	B	454	LYS
1	B	469	LYS
1	B	508	GLU
1	B	509	GLU
1	B	510	ASN
1	B	516	THR
1	C	5	CYS
1	C	16	GLU
1	C	25	PRO
1	C	60	SER
1	C	88	LYS
1	C	97	SER

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Mol	Chain	Res	Type
1	C	147	LYS
1	C	155	LEU
1	C	167	VAL
1	C	172	ASN
1	C	175	ARG
1	C	200	ARG
1	C	201	SER
1	C	206	SER
1	C	211	SER
1	C	235	SER
1	C	262	SER
1	C	280	GLU
1	C	295	GLN
1	C	300	ASN
1	C	304	GLU
1	C	325	LEU
1	C	332	SER
1	C	340	LYS
1	C	364	VAL
1	C	369	LYS
1	C	382	ASN
1	C	384	LYS
1	C	388	VAL
1	C	452	SER
1	C	466	GLU
1	C	469	LYS
1	C	476	ASN
1	C	502	MET
1	C	508	GLU
1	C	511	VAL
1	C	520	LYS
1	D	68	SER
1	D	150	LYS
1	D	157	SER
1	D	167	VAL
1	D	173	ILE
1	D	185	LYS
1	D	190	ILE
1	D	200	ARG
1	D	201	SER
1	D	211	SER
1	D	229	LYS

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Mol	Chain	Res	Type
1	D	237	ILE
1	D	262	SER
1	D	282	THR
1	D	293	ILE
1	D	297	LYS
1	D	332	SER
1	D	358	VAL
1	D	364	VAL
1	D	371	GLU
1	D	372	VAL
1	D	374	LYS
1	D	380	ILE
1	D	384	LYS
1	D	388	VAL
1	D	452	SER
1	D	453	LYS
1	D	456	ILE
1	D	469	LYS
1	D	486	GLU
1	D	509	GLU
1	E	5	CYS
1	E	88	LYS
1	E	91	VAL
1	E	97	SER
1	E	144	MET
1	E	147	LYS
1	E	153	LEU
1	E	172	ASN
1	E	200	ARG
1	E	211	SER
1	E	232	VAL
1	E	235	SER
1	E	262	SER
1	E	265	LYS
1	E	304	GLU
1	E	330	THR
1	E	332	SER
1	E	361	LEU
1	E	364	VAL
1	E	368	VAL
1	E	380	ILE
1	E	419	THR

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Mol	Chain	Res	Type
1	E	452	SER
1	E	454	LYS
1	E	469	LYS
1	E	473	GLU
1	E	505	MET
1	E	509	GLU
1	E	516	THR
1	E	531	LYS
1	E	535	SER
1	F	2	LYS
1	F	3	ILE
1	F	30	LYS
1	F	35	GLN
1	F	52	LYS
1	F	82	ARG
1	F	89	GLU
1	F	91	VAL
1	F	97	SER
1	F	119	GLU
1	F	124	MET
1	F	125	ILE
1	F	126	GLU
1	F	155	LEU
1	F	159	ARG
1	F	173	ILE
1	F	174	ASP
1	F	190	ILE
1	F	200	ARG
1	F	201	SER
1	F	202	ASP
1	F	206	SER
1	F	211	SER
1	F	262	SER
1	F	280	GLU
1	F	332	SER
1	F	340	LYS
1	F	344	ARG
1	F	361	LEU
1	F	367	LEU
1	F	368	VAL
1	F	380	ILE
1	F	385	GLU

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Mol	Chain	Res	Type
1	F	393	SER
1	F	418	LYS
1	F	419	THR
1	F	426	ILE
1	F	452	SER
1	F	456	ILE
1	F	475	LEU
1	F	515	SER
1	F	516	THR
1	F	523	ASN
1	F	531	LYS
1	F	535	SER
1	G	35	GLN
1	G	58	GLN
1	G	72	ILE
1	G	91	VAL
1	G	97	SER
1	G	111	LEU
1	G	129	LYS
1	G	147	LYS
1	G	150	LYS
1	G	154	ASP
1	G	192	LYS
1	G	200	ARG
1	G	201	SER
1	G	202	ASP
1	G	211	SER
1	G	280	GLU
1	G	291	GLU
1	G	302	SER
1	G	304	GLU
1	G	364	VAL
1	G	371	GLU
1	G	376	GLU
1	G	378	LEU
1	G	381	ASP
1	G	383	SER
1	G	384	LYS
1	G	388	VAL
1	G	424	GLU
1	G	430	LEU
1	G	437	ARG

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Mol	Chain	Res	Type
1	G	454	LYS
1	G	469	LYS
1	G	505	MET
1	G	509	GLU
1	G	531	LYS
1	H	2	LYS
1	H	35	GLN
1	H	59	THR
1	H	60	SER
1	H	118	SER
1	H	150	LYS
1	H	173	ILE
1	H	190	ILE
1	H	200	ARG
1	H	202	ASP
1	H	211	SER
1	H	229	LYS
1	H	291	GLU
1	H	293	ILE
1	H	297	LYS
1	H	303	GLU
1	H	322	GLN
1	H	332	SER
1	H	354	TYR
1	H	358	VAL
1	H	368	VAL
1	H	376	GLU
1	H	380	ILE
1	H	475	LEU
1	H	486	GLU
1	H	502	MET
1	H	508	GLU
1	H	509	GLU
1	H	511	VAL
1	H	531	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	69	ASN
1	A	107	GLN

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Mol	Chain	Res	Type
1	A	230	HIS
1	A	253	ASN
1	A	487	ASN
1	A	503	HIS
1	B	23	GLN
1	B	300	ASN
1	B	448	ASN
1	B	487	ASN
1	C	69	ASN
1	C	107	GLN
1	C	172	ASN
1	C	253	ASN
1	C	341	ASN
1	C	363	ASN
1	C	382	ASN
1	C	448	ASN
1	C	476	ASN
1	C	487	ASN
1	C	503	HIS
1	D	341	ASN
1	D	487	ASN
1	D	503	HIS
1	E	87	ASN
1	E	107	GLN
1	E	156	ASN
1	E	415	ASN
1	E	476	ASN
1	E	503	HIS
1	F	23	GLN
1	F	87	ASN
1	F	148	ASN
1	F	230	HIS
1	F	253	ASN
1	F	360	ASN
1	F	363	ASN
1	F	487	ASN
1	F	503	HIS
1	G	14	ASN
1	G	107	GLN
1	G	148	ASN
1	G	230	HIS
1	G	277	HIS

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Mol	Chain	Res	Type
1	G	375	GLN
1	G	487	ASN
1	H	23	GLN
1	H	58	GLN
1	H	69	ASN
1	H	107	GLN
1	H	341	ASN
1	H	375	GLN
1	H	487	ASN
1	H	503	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 ⓘ

Of 41 ligands modelled in this entry, 27 are modelled with single atom - leaving 14 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
2	AUC	A	631	-	4,4,4	1.65	2 (50%)	-		
2	AUC	B	610	-	4,4,4	1.61	2 (50%)	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MLI	D	901	-	6,6,6	1.20	0	7,7,7	1.08	1 (14%)
3	MLI	E	901	-	6,6,6	1.20	0	7,7,7	1.48	1 (14%)
3	MLI	H	901	-	6,6,6	1.10	0	7,7,7	1.04	0
2	AUC	A	607	-	4,4,4	1.64	2 (50%)	-		
2	AUC	H	611	-	4,4,4	1.62	2 (50%)	-		
2	AUC	D	603	-	4,4,4	1.67	2 (50%)	-		
3	MLI	C	901	-	6,6,6	1.09	0	7,7,7	1.20	1 (14%)
3	MLI	A	901	-	6,6,6	1.16	0	7,7,7	1.35	0
2	AUC	C	602	-	4,4,4	1.64	2 (50%)	-		
2	AUC	E	606	-	4,4,4	1.68	2 (50%)	-		
2	AUC	G	615	1	4,4,4	1.57	2 (50%)	-		
2	AUC	F	614	-	4,4,4	1.59	2 (50%)	-		

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	MLI	D	901	-	-	2/4/4/4	-
3	MLI	E	901	-	-	2/4/4/4	-
3	MLI	H	901	-	-	2/4/4/4	-
3	MLI	C	901	-	-	4/4/4/4	-
3	MLI	A	901	-	-	2/4/4/4	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	606	AUC	AU-C1	-2.47	1.79	1.97
2	D	603	AUC	AU-C1	-2.39	1.79	1.97
2	A	607	AUC	AU-C2	-2.36	1.80	1.97
2	H	611	AUC	AU-C2	-2.36	1.80	1.97
2	A	631	AUC	AU-C2	-2.36	1.80	1.97
2	C	602	AUC	AU-C2	-2.34	1.80	1.97
2	B	610	AUC	AU-C2	-2.29	1.80	1.97
2	A	631	AUC	AU-C1	-2.27	1.80	1.97
2	C	602	AUC	AU-C1	-2.27	1.80	1.97
2	D	603	AUC	AU-C2	-2.27	1.80	1.97
2	G	615	AUC	AU-C2	-2.26	1.80	1.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	614	AUC	AU-C1	-2.22	1.81	1.97
2	E	606	AUC	AU-C2	-2.22	1.81	1.97
2	F	614	AUC	AU-C2	-2.21	1.81	1.97
2	A	607	AUC	AU-C1	-2.21	1.81	1.97
2	B	610	AUC	AU-C1	-2.19	1.81	1.97
2	H	611	AUC	AU-C1	-2.15	1.81	1.97
2	G	615	AUC	AU-C1	-2.08	1.82	1.97

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	901	MLI	O8-C3-C1	-2.69	114.46	122.11
3	D	901	MLI	C3-C1-C2	-2.11	105.49	112.95
3	C	901	MLI	C3-C1-C2	-2.06	105.69	112.95

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	901	MLI	C3-C1-C2-O6
3	E	901	MLI	C3-C1-C2-O7
3	C	901	MLI	C2-C1-C3-O9
3	A	901	MLI	C2-C1-C3-O8
3	A	901	MLI	C2-C1-C3-O9
3	C	901	MLI	C3-C1-C2-O7
3	C	901	MLI	C2-C1-C3-O8
3	C	901	MLI	C3-C1-C2-O6
3	D	901	MLI	C2-C1-C3-O9
3	H	901	MLI	C2-C1-C3-O8
3	H	901	MLI	C2-C1-C3-O9
3	D	901	MLI	C2-C1-C3-O8

There are no ring outliers.

9 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	610	AUC	4	0
3	D	901	MLI	1	0
2	A	607	AUC	2	0
2	H	611	AUC	4	0
2	D	603	AUC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	602	AUC	2	0
2	E	606	AUC	2	0
2	G	615	AUC	5	0
2	F	614	AUC	4	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	525/560 (93%)	-0.66	0 100 100	37, 55, 74, 101	1 (0%)
1	B	529/560 (94%)	-0.50	1 (0%) 91 90	44, 67, 99, 110	0
1	C	530/560 (94%)	-0.49	4 (0%) 82 78	42, 64, 116, 128	1 (0%)
1	D	526/560 (93%)	-0.51	1 (0%) 91 90	40, 59, 95, 122	0
1	E	524/560 (93%)	-0.49	5 (0%) 79 74	37, 58, 101, 169	1 (0%)
1	F	529/560 (94%)	-0.44	1 (0%) 91 90	51, 69, 110, 118	2 (0%)
1	G	527/560 (94%)	-0.29	6 (1%) 78 73	57, 75, 103, 123	1 (0%)
1	H	527/560 (94%)	-0.52	3 (0%) 85 82	42, 62, 82, 125	4 (0%)
All	All	4217/4480 (94%)	-0.49	21 (0%) 87 83	37, 64, 98, 169	10 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	393	SER	6.5
1	C	348	ALA	4.7
1	E	391	ALA	4.2
1	E	390	ARG	3.8
1	E	392	ILE	3.8
1	G	359	ALA	3.5
1	G	357	GLU	2.9
1	H	380	ILE	2.7
1	G	124	MET	2.6
1	C	389	PRO	2.4
1	E	316	CYS	2.4
1	C	388	VAL	2.4
1	F	355	ASN	2.3
1	D	358	VAL	2.3
1	G	512	MET	2.2
1	C	358	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	358	VAL	2.2
1	B	355	ASN	2.2
1	H	512	MET	2.2
1	G	387	ALA	2.0
1	H	384	LYS	2.0

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(Å ²)	Q<0.9
2	AUC	D	640	1/5	0.76	0.29	99,99,99,99	1
2	AUC	F	637	1/5	0.76	0.17	85,85,85,85	1
3	MLI	H	901	7/7	0.79	0.25	58,59,61,61	7
3	MLI	D	901	7/7	0.84	0.18	52,54,55,55	7
2	AUC	C	634	1/5	0.84	0.23	82,82,82,82	1
2	AUC	A	631	5/5	0.85	0.51	57,58,58,59	5
2	AUC	B	630	1/5	0.87	0.17	107,107,107,107	1
2	AUC	B	638	1/5	0.88	0.24	86,86,86,86	1
2	AUC	F	627	1/5	0.88	0.20	85,85,85,85	1
2	AUC	F	641	1/5	0.88	0.17	108,108,108,108	1
2	AUC	H	629	1/5	0.88	0.16	85,85,85,85	1
3	MLI	C	901	7/7	0.88	0.17	47,48,49,50	7
2	AUC	B	640	1/5	0.88	0.11	93,93,93,93	1
2	AUC	E	628	1/5	0.88	0.24	80,80,80,80	1
2	AUC	C	635	1/5	0.89	0.21	76,76,76,76	1
3	MLI	E	901	7/7	0.90	0.16	41,43,43,44	7
3	MLI	A	901	7/7	0.90	0.12	40,41,43,43	7
2	AUC	E	619	1/5	0.91	0.13	68,68,68,68	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AUC	C	621	1/5	0.92	0.09	70,70,70,70	1
2	AUC	H	617	1/5	0.93	0.07	74,74,74,74	1
2	AUC	A	624	1/5	0.94	0.10	71,71,71,71	1
2	AUC	F	620	1/5	0.95	0.12	69,69,69,69	1
2	AUC	B	622	1/5	0.95	0.10	69,69,69,69	1
2	AUC	G	626	1/5	0.96	0.08	76,76,76,76	1
2	AUC	D	618	1/5	0.97	0.08	82,82,82,82	1
2	AUC	B	610	5/5	0.97	0.14	82,83,84,86	5
2	AUC	F	613	1/5	0.98	0.04	80,80,80,80	0
2	AUC	G	616	1/5	0.98	0.04	86,86,86,86	0
2	AUC	A	608	1/5	0.99	0.02	74,74,74,74	0
2	AUC	D	604	1/5	0.99	0.03	85,85,85,85	0
2	AUC	C	601	1/5	0.99	0.02	75,75,75,75	0
2	AUC	G	615	5/5	0.99	0.06	69,70,70,73	1
2	AUC	B	609	1/5	0.99	0.02	79,79,79,79	0
2	AUC	F	614	5/5	0.99	0.08	80,82,83,83	5
2	AUC	H	612	1/5	0.99	0.03	80,80,80,80	0
2	AUC	E	605	1/5	1.00	0.02	72,72,72,72	0
2	AUC	E	606	5/5	1.00	0.04	72,73,74,74	0
2	AUC	A	607	5/5	1.00	0.03	65,65,66,67	0
2	AUC	H	611	5/5	1.00	0.04	73,75,75,76	0
2	AUC	C	602	5/5	1.00	0.04	73,74,77,78	0
2	AUC	D	603	5/5	1.00	0.04	75,76,77,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.