Full wwPDB X-ray Structure Validation Report (i)

Jul 15, 2024 – 01:19 PM EDT

PDB ID	:	8U7J
Title	:	Crystal Structure of Staphylococcus aureus PLP synthase complex
Authors	:	Barra, A.L.C.; Brognaro, H.; Betzel, C.; Nascimento, A.S.
Deposited on	:	2023-09-15
Resolution	:	3.02 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 (i) 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 (1)) were used in the production of this report:

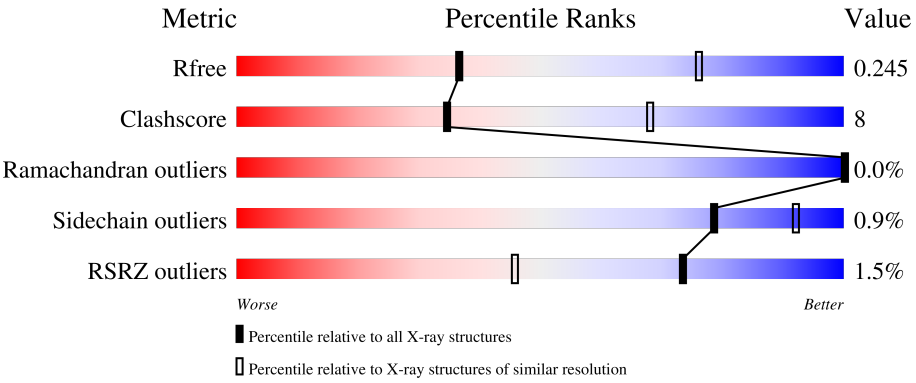
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.02 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}	130704	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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 <=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	297	70% 20% 10%
1	B	297	69% 21% 10%
1	C	297	. 72% 18% 10%
1	D	297	72% 18% 10%
1	E	297	. 73% 17% 10%

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Mol	Chain	Length	Quality of chain
1	F	297	73% 17% 10%
1	G	297	71% 19% 10%
1	H	297	72% 18% 10%
1	I	297	72% 18% 10%
1	J	297	73% 17% 10%
1	K	297	71% 19% 10%
1	L	297	73% 17% 10%
2	M	188	81% 19%
2	N	188	80% 20%
2	O	188	4% 81% 18%
2	P	188	4% 81% 18%
2	Q	188	24% 81% 18%
2	R	188	81% 19%
2	S	188	81% 18%
2	T	188	80% 19%
2	U	188	79% 20%
2	V	188	3% 82% 17%
2	W	188	81% 18%
2	X	188	79% 20%

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
3	PO4	I	301	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 39705 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 Pyridoxal 5'-phosphate synthase subunit PdxS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			1938	1207	343	372	16			
1	G	267	Total	C	N	O	S	0	0	0
			1938	1207	343	372	16			
1	B	267	Total	C	N	O	S	0	0	0
			1938	1207	343	372	16			
1	L	267	Total	C	N	O	S	0	0	0
			1938	1207	343	372	16			
1	K	267	Total	C	N	O	S	0	0	0
			1938	1207	343	372	16			
1	F	267	Total	C	N	O	S	0	0	0
			1938	1207	343	372	16			
1	J	267	Total	C	N	O	S	0	0	0
			1938	1207	343	372	16			
1	C	267	Total	C	N	O	S	0	0	0
			1938	1207	343	372	16			
1	I	267	Total	C	N	O	S	0	0	0
			1938	1207	343	372	16			
1	H	267	Total	C	N	O	S	0	0	0
			1938	1207	343	372	16			
1	D	267	Total	C	N	O	S	0	0	0
			1938	1207	343	372	16			
1	E	267	Total	C	N	O	S	0	0	0
			1938	1207	343	372	16			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A7WYT1
A	0	ALA	-	expression tag	UNP A7WYT1
G	-1	GLY	-	expression tag	UNP A7WYT1
G	0	ALA	-	expression tag	UNP A7WYT1
B	-1	GLY	-	expression tag	UNP A7WYT1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ALA	-	expression tag	UNP A7WYT1
L	-1	GLY	-	expression tag	UNP A7WYT1
L	0	ALA	-	expression tag	UNP A7WYT1
K	-1	GLY	-	expression tag	UNP A7WYT1
K	0	ALA	-	expression tag	UNP A7WYT1
F	-1	GLY	-	expression tag	UNP A7WYT1
F	0	ALA	-	expression tag	UNP A7WYT1
J	-1	GLY	-	expression tag	UNP A7WYT1
J	0	ALA	-	expression tag	UNP A7WYT1
C	-1	GLY	-	expression tag	UNP A7WYT1
C	0	ALA	-	expression tag	UNP A7WYT1
I	-1	GLY	-	expression tag	UNP A7WYT1
I	0	ALA	-	expression tag	UNP A7WYT1
H	-1	GLY	-	expression tag	UNP A7WYT1
H	0	ALA	-	expression tag	UNP A7WYT1
D	-1	GLY	-	expression tag	UNP A7WYT1
D	0	ALA	-	expression tag	UNP A7WYT1
E	-1	GLY	-	expression tag	UNP A7WYT1
E	0	ALA	-	expression tag	UNP A7WYT1

- Molecule 2 is a protein called Pyridoxal 5'-phosphate synthase subunit PdxT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	187	Total	C	N	O	S	0	0	0
			1356	866	234	251	5			
2	N	187	Total	C	N	O	S	0	0	0
			1356	866	234	251	5			
2	S	187	Total	C	N	O	S	0	0	0
			1356	866	234	251	5			
2	X	187	Total	C	N	O	S	0	0	0
			1356	866	234	251	5			
2	R	187	Total	C	N	O	S	0	0	0
			1353	865	233	250	5			
2	W	187	Total	C	N	O	S	0	0	0
			1356	866	234	251	5			
2	O	187	Total	C	N	O	S	0	0	0
			1356	866	234	251	5			
2	M	187	Total	C	N	O	S	0	0	0
			1356	866	234	251	5			
2	V	187	Total	C	N	O	S	0	0	0
			1356	866	234	251	5			
2	U	187	Total	C	N	O	S	0	0	0
			1356	866	234	251	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	187	Total	C	N	O	S	0	0	0
			1356	866	234	251	5			
2	Q	187	Total	C	N	O	S	0	0	0
			1356	866	234	251	5			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	-1	GLY	-	expression tag	UNP A7WYT2
T	0	ALA	-	expression tag	UNP A7WYT2
T	165	ASN	HIS	engineered mutation	UNP A7WYT2
N	-1	GLY	-	expression tag	UNP A7WYT2
N	0	ALA	-	expression tag	UNP A7WYT2
N	165	ASN	HIS	engineered mutation	UNP A7WYT2
S	-1	GLY	-	expression tag	UNP A7WYT2
S	0	ALA	-	expression tag	UNP A7WYT2
S	165	ASN	HIS	engineered mutation	UNP A7WYT2
X	-1	GLY	-	expression tag	UNP A7WYT2
X	0	ALA	-	expression tag	UNP A7WYT2
X	165	ASN	HIS	engineered mutation	UNP A7WYT2
R	-1	GLY	-	expression tag	UNP A7WYT2
R	0	ALA	-	expression tag	UNP A7WYT2
R	165	ASN	HIS	engineered mutation	UNP A7WYT2
W	-1	GLY	-	expression tag	UNP A7WYT2
W	0	ALA	-	expression tag	UNP A7WYT2
W	165	ASN	HIS	engineered mutation	UNP A7WYT2
O	-1	GLY	-	expression tag	UNP A7WYT2
O	0	ALA	-	expression tag	UNP A7WYT2
O	165	ASN	HIS	engineered mutation	UNP A7WYT2
M	-1	GLY	-	expression tag	UNP A7WYT2
M	0	ALA	-	expression tag	UNP A7WYT2
M	165	ASN	HIS	engineered mutation	UNP A7WYT2
V	-1	GLY	-	expression tag	UNP A7WYT2
V	0	ALA	-	expression tag	UNP A7WYT2
V	165	ASN	HIS	engineered mutation	UNP A7WYT2
U	-1	GLY	-	expression tag	UNP A7WYT2
U	0	ALA	-	expression tag	UNP A7WYT2
U	165	ASN	HIS	engineered mutation	UNP A7WYT2
P	-1	GLY	-	expression tag	UNP A7WYT2
P	0	ALA	-	expression tag	UNP A7WYT2
P	165	ASN	HIS	engineered mutation	UNP A7WYT2
Q	-1	GLY	-	expression tag	UNP A7WYT2

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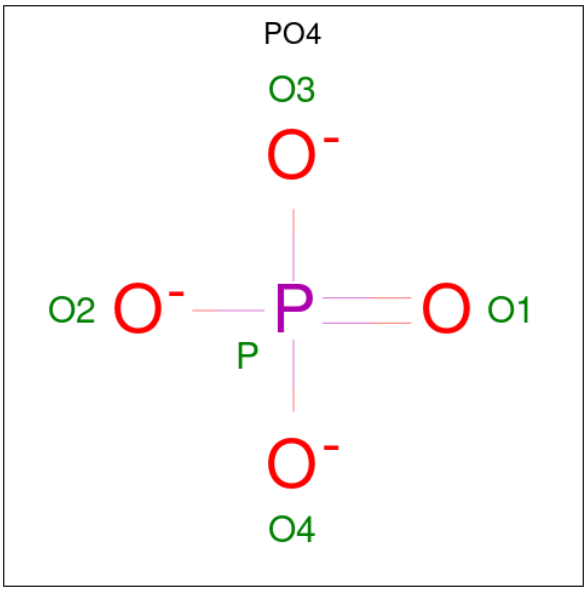
Chain	Residue	Modelled	Actual	Comment	Reference
Q	0	ALA	-	expression tag	UNP A7WYT2
Q	165	ASN	HIS	engineered mutation	UNP A7WYT2

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	G	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	L	1	Total O P 5 4 1	0	0
3	K	1	Total O P 5 4 1	0	0
3	F	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	I	1	Total O P 5 4 1	0	0
3	H	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0

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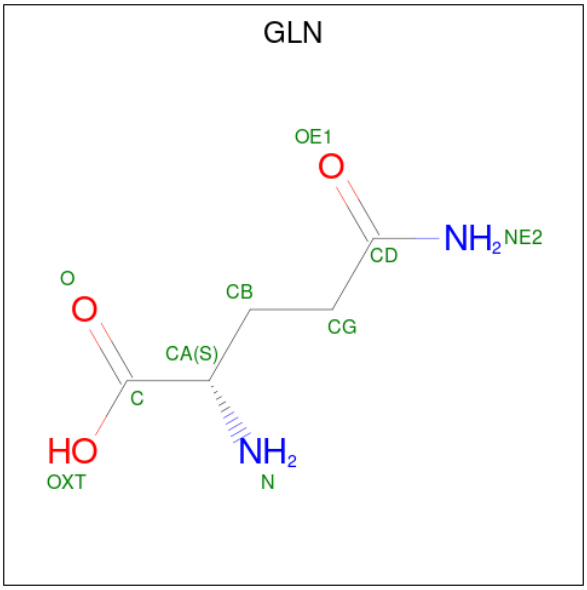
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total O P 5 4 1	0	0

- Molecule 4 is GLUTAMINE (three-letter code: GLN) (formula: $C_5H_{10}N_2O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	T	1	Total C N O 10 5 2 3	0	0
4	N	1	Total C N O 10 5 2 3	0	0
4	S	1	Total C N O 10 5 2 3	0	0
4	X	1	Total C N O 10 5 2 3	0	0
4	R	1	Total C N O 10 5 2 3	0	0
4	W	1	Total C N O 10 5 2 3	0	0
4	O	1	Total C N O 10 5 2 3	0	0
4	M	1	Total C N O 10 5 2 3	0	0
4	V	1	Total C N O 10 5 2 3	0	0
4	U	1	Total C N O 10 5 2 3	0	0

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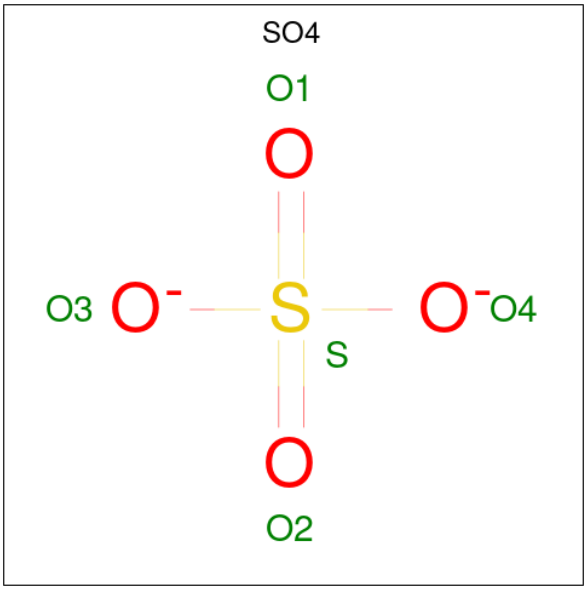
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	P	1	Total C N O 10 5 2 3	0	0
4	Q	1	Total C N O 10 5 2 3	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



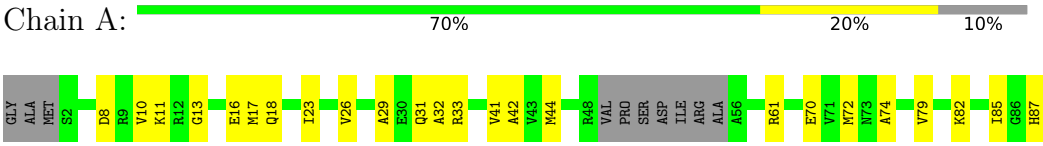
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	J	1	Total O S 5 4 1	0	0

3 Residue-property plots (i)

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.

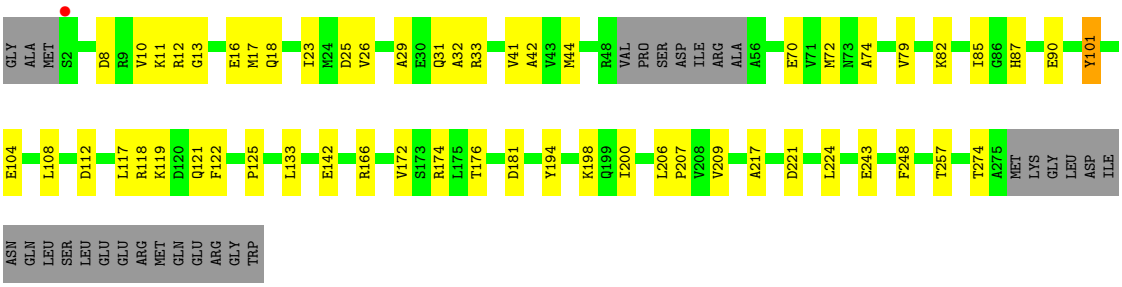
• Molecule 1: Pyridoxal 5'-phosphate synthase subunit PdxS

Chain A:



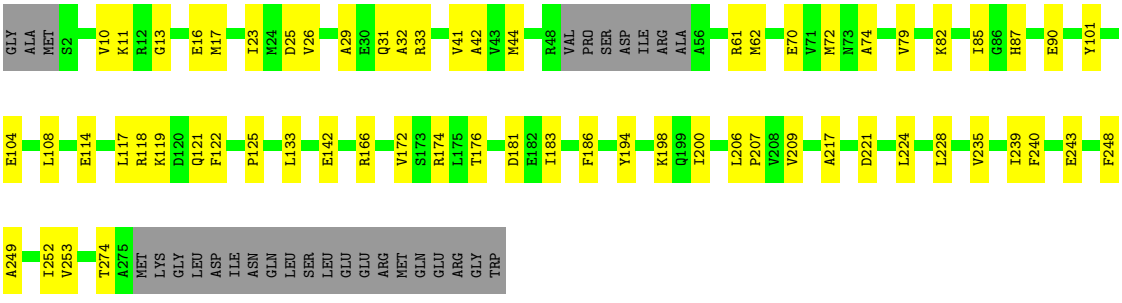
• Molecule 1: Pyridoxal 5'-phosphate synthase subunit PdxS

Chain G:



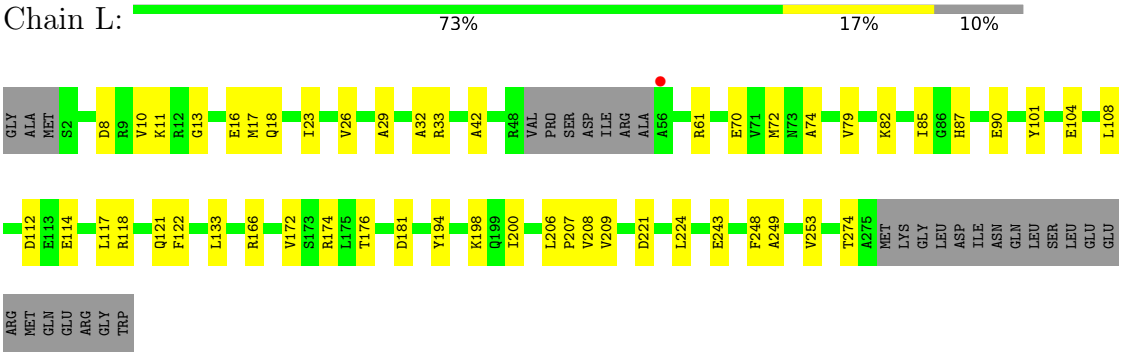
• Molecule 1: Pyridoxal 5'-phosphate synthase subunit PdxS

Chain B:



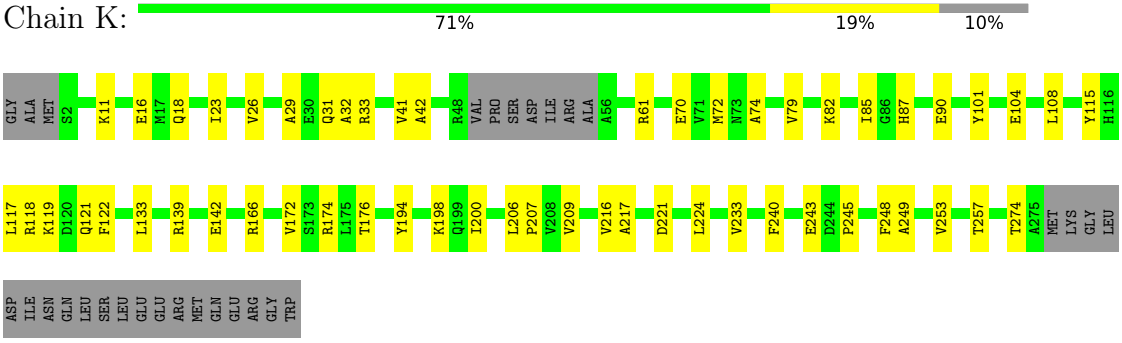
• Molecule 1: Pyridoxal 5'-phosphate synthase subunit PdxS

Chain L:



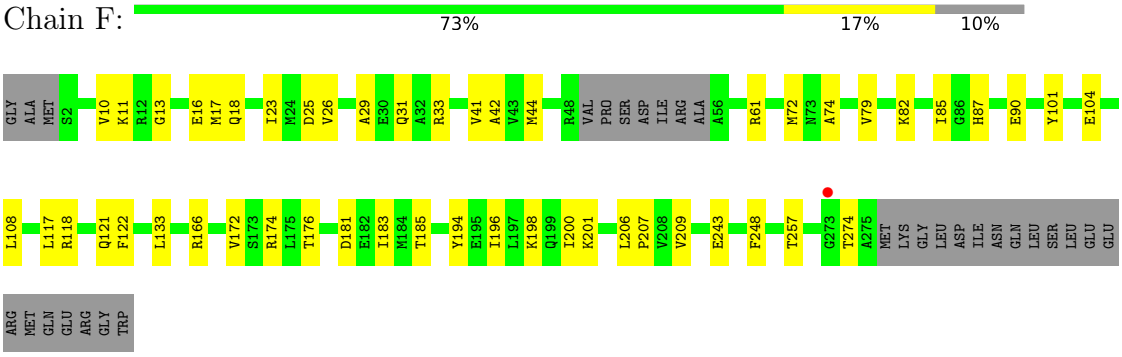
• Molecule 1: Pyridoxal 5'-phosphate synthase subunit PdxS

Chain K:



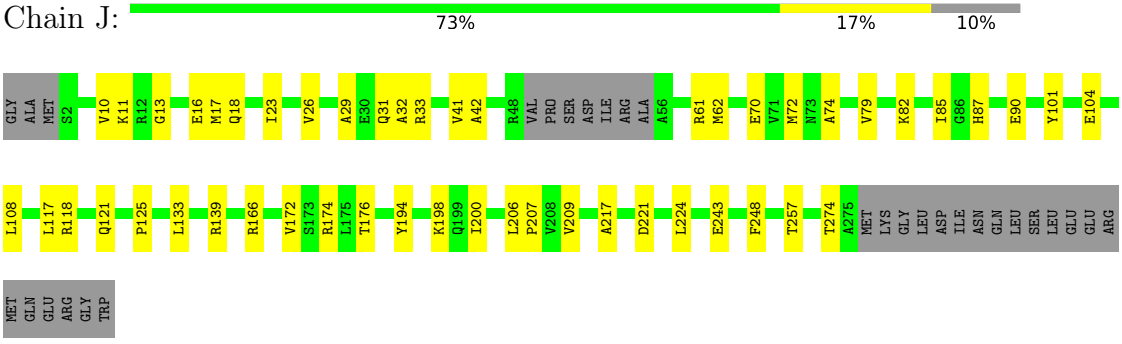
• Molecule 1: Pyridoxal 5'-phosphate synthase subunit PdxS

Chain F:



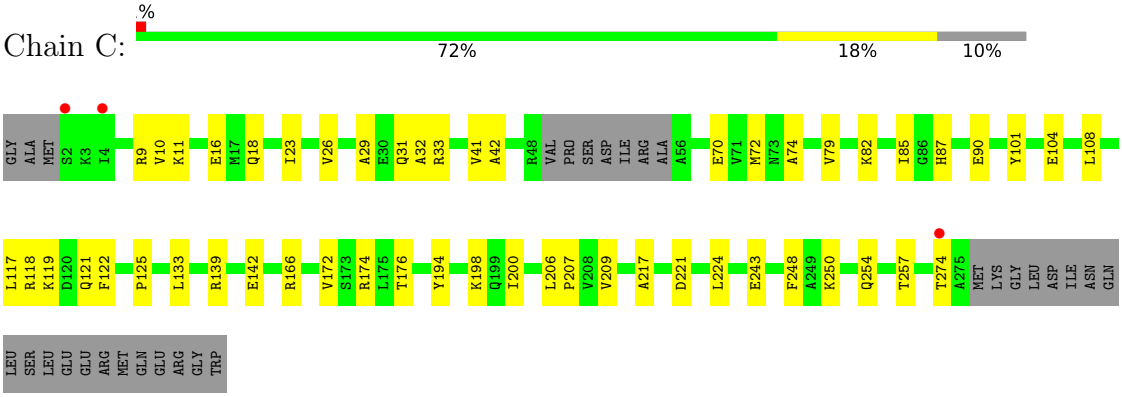
• Molecule 1: Pyridoxal 5'-phosphate synthase subunit PdxS

Chain J:



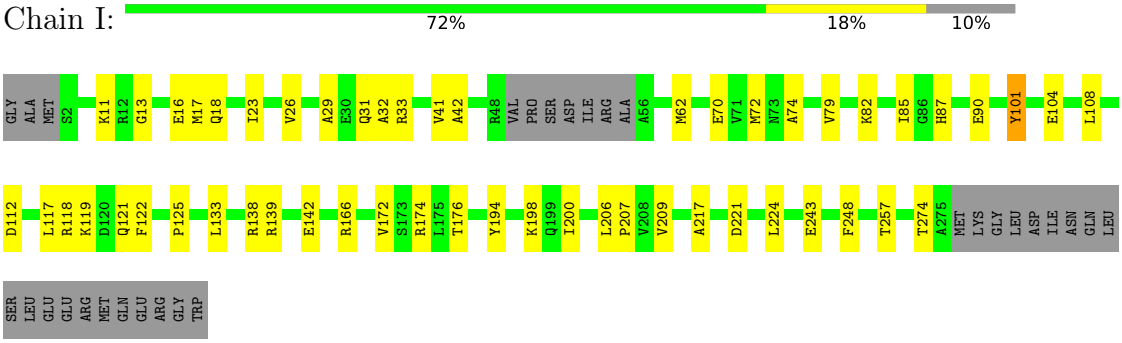
• Molecule 1: Pyridoxal 5'-phosphate synthase subunit PdxS

Chain C:



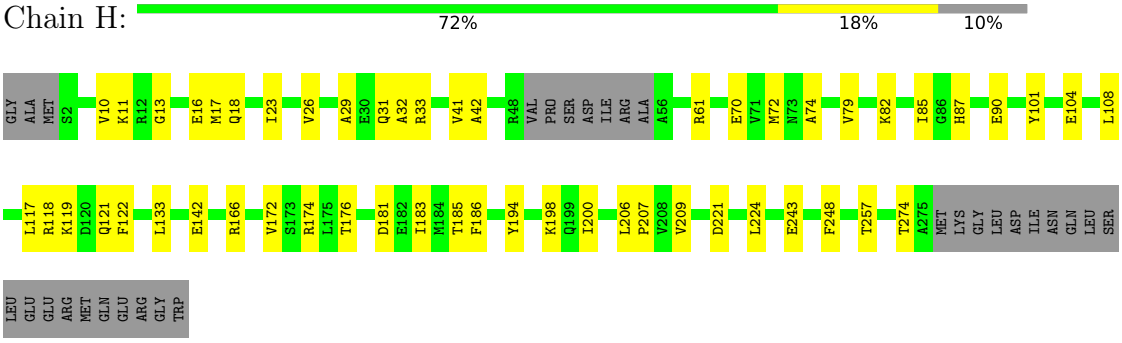
• Molecule 1: Pyridoxal 5'-phosphate synthase subunit PdxS

Chain I:



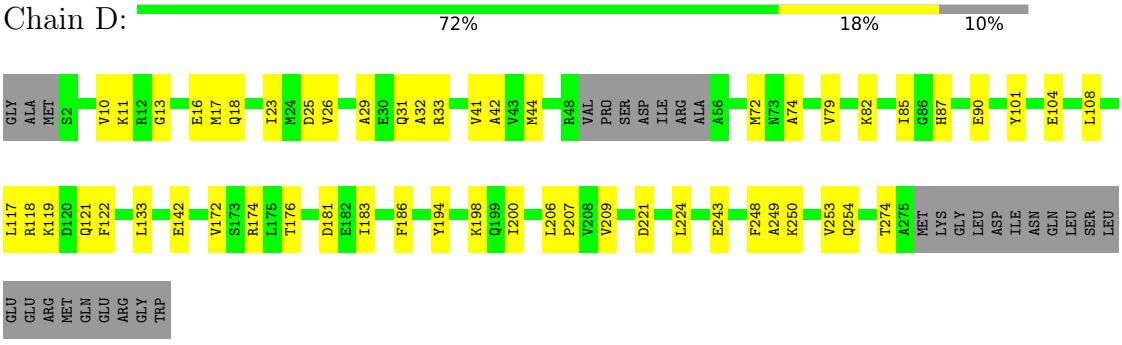
• Molecule 1: Pyridoxal 5'-phosphate synthase subunit PdxS

Chain H:



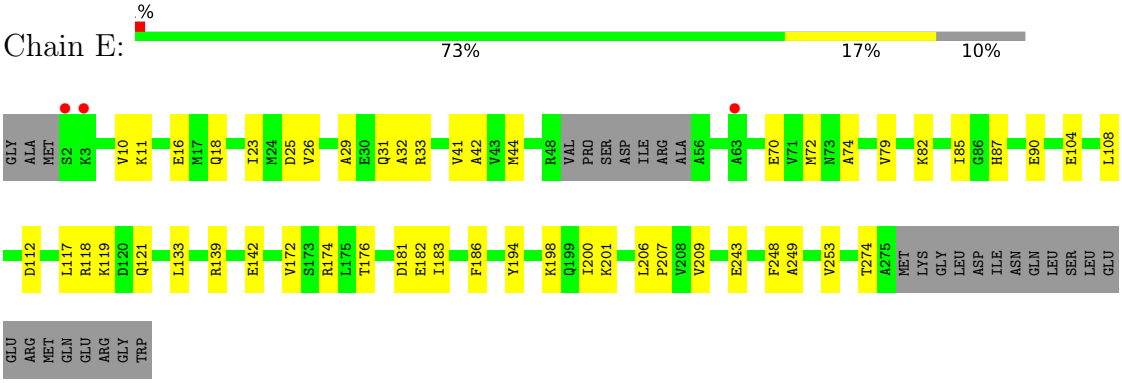
• Molecule 1: Pyridoxal 5'-phosphate synthase subunit PdxS

Chain D:



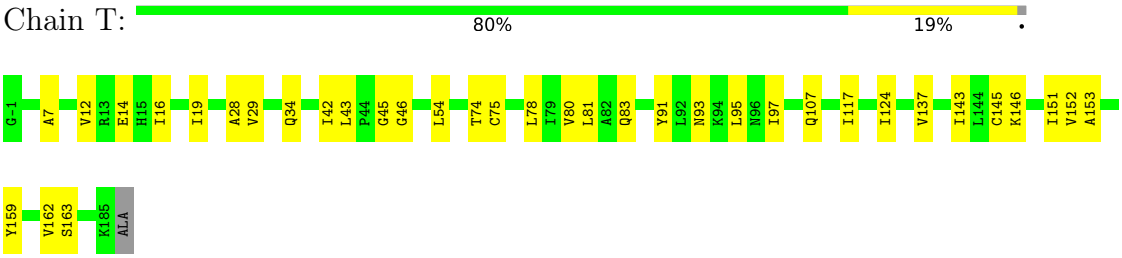
• Molecule 1: Pyridoxal 5'-phosphate synthase subunit PdxS

Chain E:



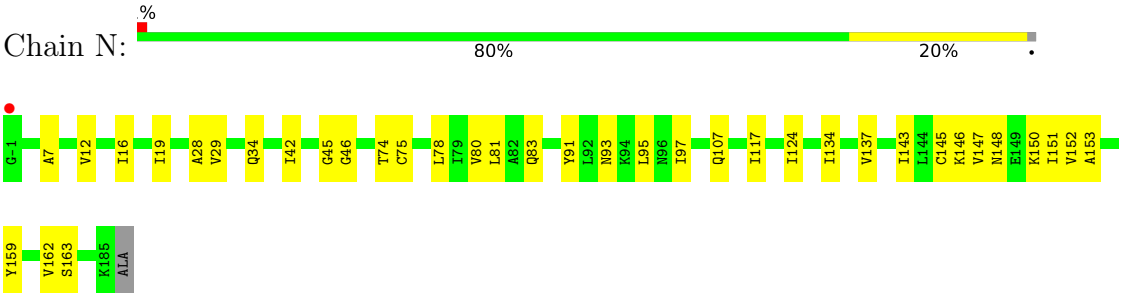
• Molecule 2: Pyridoxal 5'-phosphate synthase subunit PdxT

Chain T:



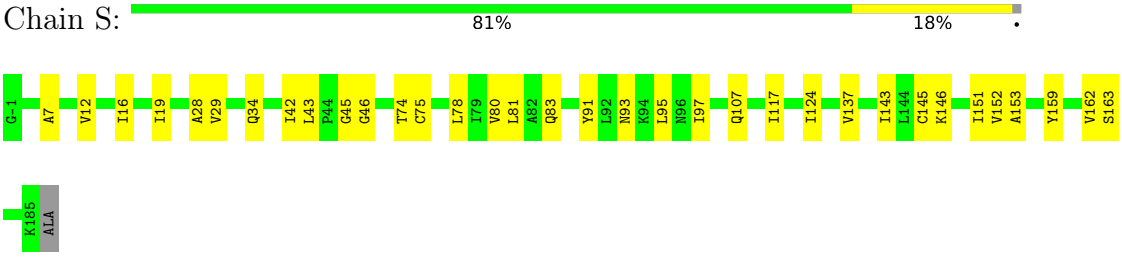
• Molecule 2: Pyridoxal 5'-phosphate synthase subunit PdxT

Chain N:



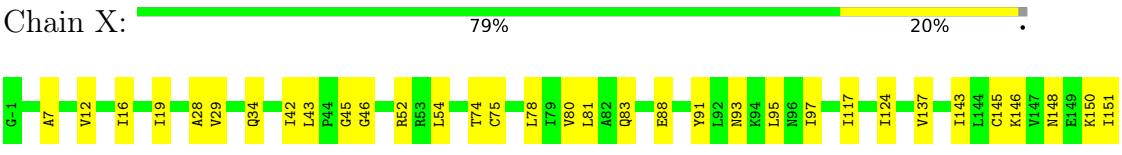
• Molecule 2: Pyridoxal 5'-phosphate synthase subunit PdxT

Chain S:



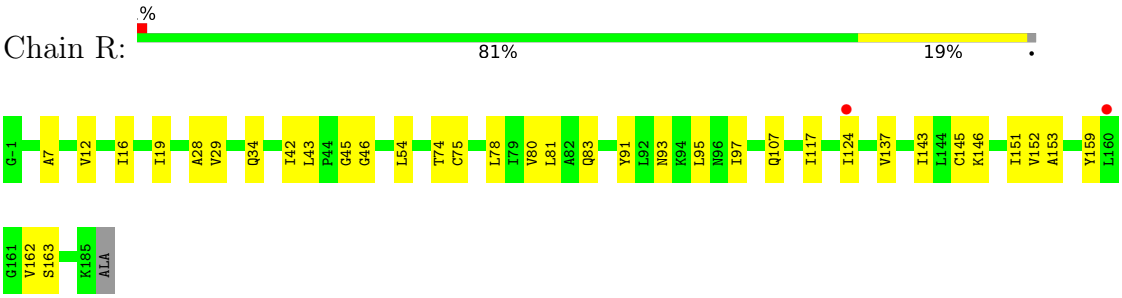
• Molecule 2: Pyridoxal 5'-phosphate synthase subunit PdxT

Chain X:



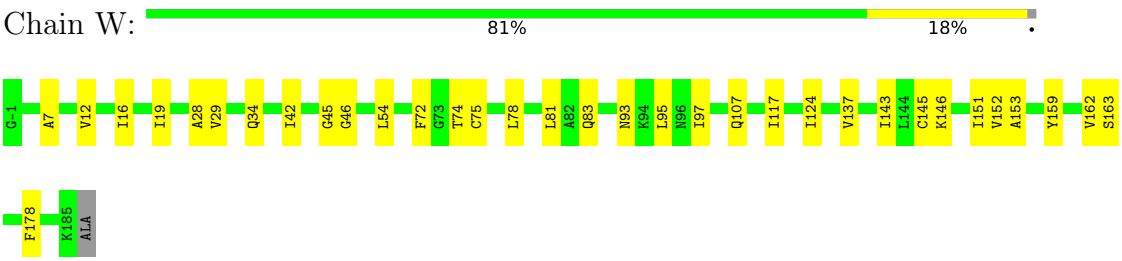
• Molecule 2: Pyridoxal 5'-phosphate synthase subunit PdxT

Chain R:



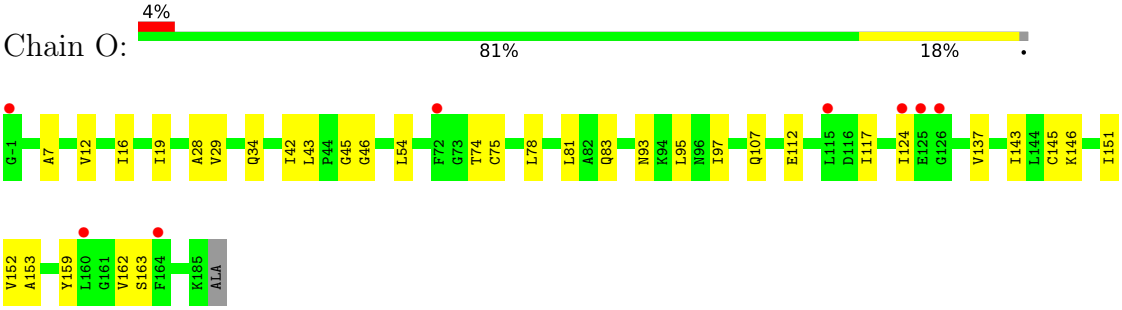
• Molecule 2: Pyridoxal 5'-phosphate synthase subunit PdxT

Chain W:



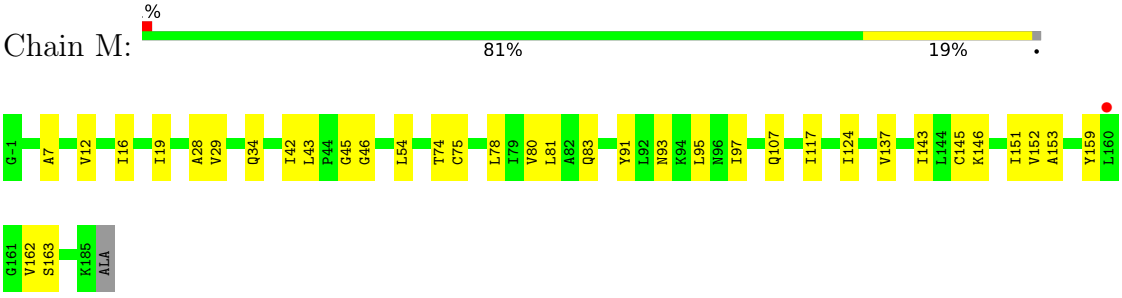
• Molecule 2: Pyridoxal 5'-phosphate synthase subunit PdxT

Chain O:



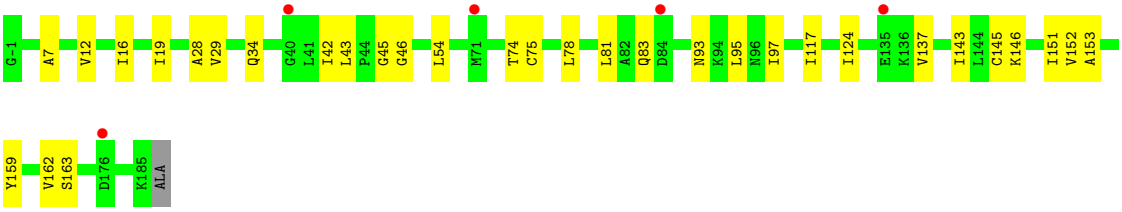
• Molecule 2: Pyridoxal 5'-phosphate synthase subunit PdxT

Chain M:

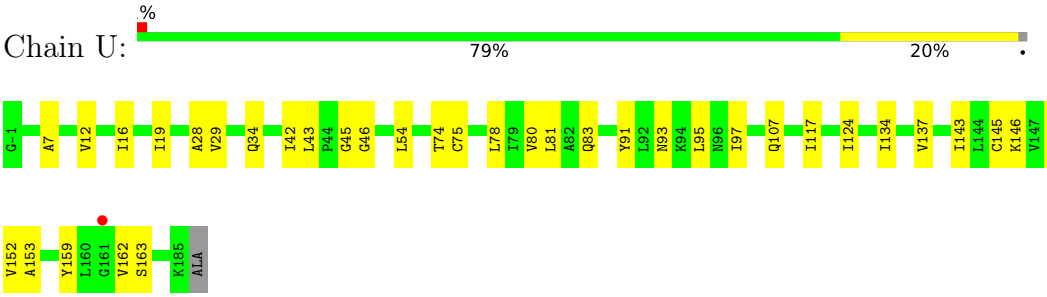


• Molecule 2: Pyridoxal 5'-phosphate synthase subunit PdxT

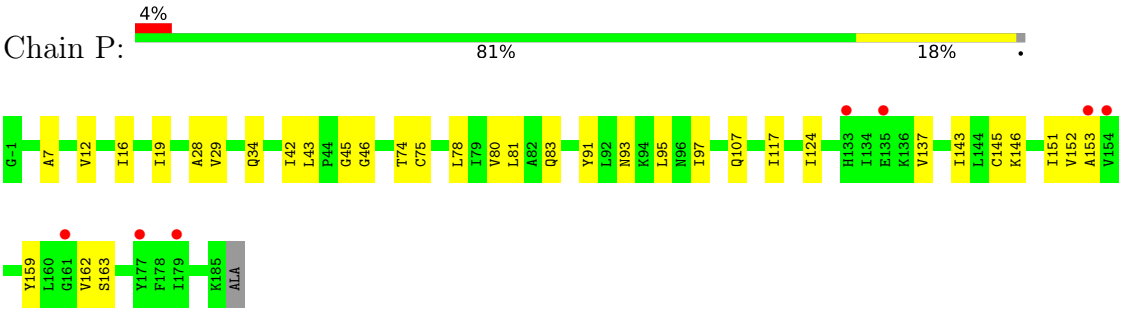
Chain V:



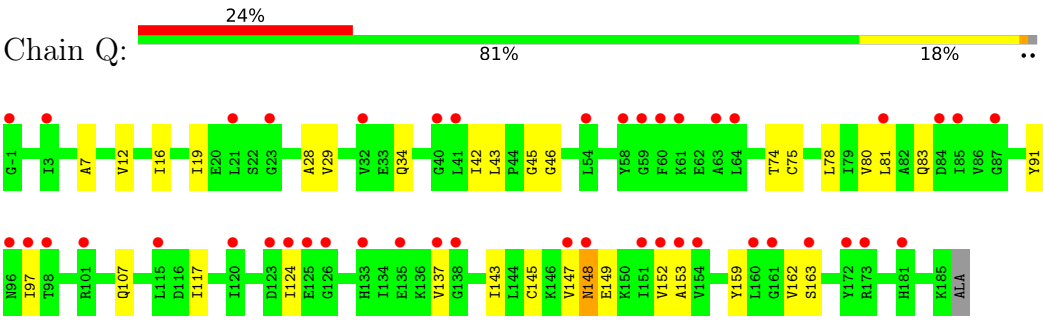
• Molecule 2: Pyridoxal 5'-phosphate synthase subunit PdxT



• Molecule 2: Pyridoxal 5'-phosphate synthase subunit PdxT



• Molecule 2: Pyridoxal 5'-phosphate synthase subunit PdxT



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	101.23Å 132.37Å 142.10Å 106.49° 109.51° 105.56°	Depositor
Resolution (Å)	54.83 – 3.02 54.84 – 3.02	Depositor EDS
% Data completeness (in resolution range)	59.2 (54.83-3.02) 59.2 (54.84-3.02)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 3.01Å)	Xtriage
Refinement program	PHENIX (dev_4788: ???)	Depositor
R, R_{free}	0.200 , 0.247 0.200 , 0.245	Depositor DCC
R_{free} test set	3644 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	69.5	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 21.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	39705	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PO4, 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	0.25	0/1961	0.49	0/2652
1	B	0.25	0/1961	0.50	0/2652
1	C	0.25	0/1961	0.49	0/2652
1	D	0.25	0/1961	0.49	0/2652
1	E	0.25	0/1961	0.49	0/2652
1	F	0.25	0/1961	0.49	0/2652
1	G	0.25	0/1961	0.49	0/2652
1	H	0.25	0/1961	0.49	0/2652
1	I	0.25	0/1961	0.49	0/2652
1	J	0.25	0/1961	0.49	0/2652
1	K	0.25	0/1961	0.49	0/2652
1	L	0.25	0/1961	0.49	0/2652
2	M	0.24	0/1376	0.47	0/1873
2	N	0.25	0/1376	0.48	0/1873
2	O	0.24	0/1376	0.47	0/1873
2	P	0.24	0/1376	0.46	0/1873
2	Q	0.25	0/1376	0.49	0/1873
2	R	0.24	0/1373	0.47	0/1869
2	S	0.24	0/1376	0.47	0/1873
2	T	0.24	0/1376	0.47	0/1873
2	U	0.24	0/1376	0.46	0/1873
2	V	0.24	0/1376	0.47	0/1873
2	W	0.24	0/1376	0.47	0/1873
2	X	0.24	0/1376	0.46	0/1873
All	All	0.25	0/40041	0.48	0/54296

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1938	0	1896	38	0
1	B	1938	0	1896	46	0
1	C	1938	0	1896	34	0
1	D	1938	0	1896	32	0
1	E	1938	0	1896	34	0
1	F	1938	0	1896	35	0
1	G	1938	0	1896	39	0
1	H	1938	0	1896	35	0
1	I	1938	0	1896	36	0
1	J	1938	0	1896	34	0
1	K	1938	0	1896	38	0
1	L	1938	0	1896	35	0
2	M	1356	0	1311	23	0
2	N	1356	0	1311	25	0
2	O	1356	0	1311	23	0
2	P	1356	0	1311	21	0
2	Q	1356	0	1311	22	0
2	R	1353	0	1307	23	0
2	S	1356	0	1311	22	0
2	T	1356	0	1311	24	0
2	U	1356	0	1311	24	0
2	V	1356	0	1311	21	0
2	W	1356	0	1311	21	0
2	X	1356	0	1311	23	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	1	0
3	D	5	0	0	0	0
3	E	5	0	0	1	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
3	I	5	0	0	2	0
3	K	5	0	0	1	0
3	L	5	0	0	0	0
4	M	10	0	7	2	0
4	N	10	0	7	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	O	10	0	7	2	0
4	P	10	0	7	2	0
4	Q	10	0	7	2	0
4	R	10	0	7	2	0
4	S	10	0	7	2	0
4	T	10	0	7	2	0
4	U	10	0	7	2	0
4	V	10	0	7	2	0
4	W	10	0	7	2	0
4	X	10	0	7	2	0
5	J	5	0	0	1	0
All	All	39705	0	38564	647	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 8.

All (647) 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:10:VAL:HG12	2:Q:107:GLN:HE22	1.53	0.74
1:J:174:ARG:HD2	1:E:174:ARG:HD2	1.69	0.74
2:N:146:LYS:HA	2:N:151:ILE:HA	1.68	0.73
2:N:75:CYS:SG	4:N:201:GLN:NE2	2.62	0.72
2:S:75:CYS:SG	4:S:201:GLN:NE2	2.63	0.72
2:U:75:CYS:SG	4:U:201:GLN:NE2	2.63	0.71
2:M:75:CYS:SG	4:M:201:GLN:NE2	2.62	0.71
2:R:75:CYS:SG	4:R:201:GLN:NE2	2.63	0.71
2:W:75:CYS:SG	4:W:201:GLN:NE2	2.63	0.70
2:O:75:CYS:SG	4:O:201:GLN:NE2	2.64	0.70
2:X:75:CYS:SG	4:X:201:GLN:NE2	2.65	0.70
2:V:75:CYS:SG	4:V:201:GLN:NE2	2.65	0.69
2:Q:75:CYS:SG	4:Q:201:GLN:NE2	2.65	0.69
1:C:174:ARG:HD2	1:H:174:ARG:HD2	1.73	0.69
1:G:174:ARG:HD2	1:B:174:ARG:HD2	1.73	0.68
1:L:194:TYR:OH	1:F:118:ARG:NH1	2.27	0.68
2:T:75:CYS:SG	4:T:201:GLN:NE2	2.66	0.68
1:G:29:ALA:HB2	1:G:70:GLU:HG2	1.77	0.67
2:P:75:CYS:SG	4:P:201:GLN:NE2	2.67	0.67
1:I:23:ILE:HG12	1:I:42:ALA:HB3	1.76	0.67
1:F:23:ILE:HG12	1:F:42:ALA:HB3	1.77	0.67
1:A:174:ARG:HD2	1:L:174:ARG:HD2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:23:ILE:HG12	1:J:42:ALA:HB3	1.78	0.66
1:D:23:ILE:HG12	1:D:42:ALA:HB3	1.78	0.66
1:E:23:ILE:HG12	1:E:42:ALA:HB3	1.78	0.66
1:K:23:ILE:HG12	1:K:42:ALA:HB3	1.78	0.65
2:U:81:LEU:HB3	2:U:95:LEU:HD13	1.79	0.65
1:K:174:ARG:HD2	1:F:174:ARG:HD2	1.78	0.65
1:A:23:ILE:HG12	1:A:42:ALA:HB3	1.78	0.65
2:V:29:VAL:HG23	2:V:34:GLN:HB2	1.78	0.65
2:O:29:VAL:HG23	2:O:34:GLN:HB2	1.79	0.64
1:C:23:ILE:HG12	1:C:42:ALA:HB3	1.79	0.64
2:W:81:LEU:HB3	2:W:95:LEU:HD13	1.80	0.64
2:U:29:VAL:HG23	2:U:34:GLN:HB2	1.80	0.64
2:O:81:LEU:HB3	2:O:95:LEU:HD13	1.80	0.64
1:B:235:VAL:HG11	1:B:239:ILE:HG12	1.79	0.64
1:L:118:ARG:NH1	1:F:194:TYR:OH	2.30	0.64
1:I:174:ARG:HD2	1:D:174:ARG:HD2	1.78	0.64
2:M:81:LEU:HB3	2:M:95:LEU:HD13	1.79	0.64
1:A:194:TYR:OH	1:G:118:ARG:NH1	2.30	0.64
2:V:81:LEU:HB3	2:V:95:LEU:HD13	1.78	0.64
2:Q:29:VAL:HG23	2:Q:34:GLN:HB2	1.80	0.64
2:W:29:VAL:HG23	2:W:34:GLN:HB2	1.80	0.64
2:N:29:VAL:HG23	2:N:34:GLN:HB2	1.79	0.64
2:P:81:LEU:HB3	2:P:95:LEU:HD13	1.80	0.64
1:H:23:ILE:HG12	1:H:42:ALA:HB3	1.79	0.63
2:S:81:LEU:HB3	2:S:95:LEU:HD13	1.80	0.63
1:B:23:ILE:HG12	1:B:42:ALA:HB3	1.80	0.63
2:M:29:VAL:HG23	2:M:34:GLN:HB2	1.80	0.63
2:Q:81:LEU:HB3	2:Q:95:LEU:HD13	1.78	0.63
2:T:81:LEU:HB3	2:T:95:LEU:HD13	1.80	0.63
2:S:29:VAL:HG23	2:S:34:GLN:HB2	1.79	0.63
2:X:81:LEU:HB3	2:X:95:LEU:HD13	1.80	0.63
1:G:23:ILE:HG12	1:G:42:ALA:HB3	1.79	0.63
2:P:29:VAL:HG23	2:P:34:GLN:HB2	1.80	0.63
1:E:16:GLU:HA	1:E:209:VAL:HG21	1.81	0.63
2:X:29:VAL:HG23	2:X:34:GLN:HB2	1.81	0.62
2:R:29:VAL:HG23	2:R:34:GLN:HB2	1.80	0.62
2:T:29:VAL:HG23	2:T:34:GLN:HB2	1.80	0.62
2:N:81:LEU:HB3	2:N:95:LEU:HD13	1.80	0.62
1:I:200:ILE:HG12	1:I:207:PRO:HD3	1.82	0.62
2:R:81:LEU:HB3	2:R:95:LEU:HD13	1.80	0.62
1:A:200:ILE:HG12	1:A:207:PRO:HD3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:ILE:HG12	1:E:207:PRO:HD3	1.82	0.61
1:G:200:ILE:HG12	1:G:207:PRO:HD3	1.82	0.61
1:L:23:ILE:HG12	1:L:42:ALA:HB3	1.81	0.61
1:K:16:GLU:HA	1:K:209:VAL:HG21	1.83	0.60
1:K:139:ARG:NH2	3:K:301:PO4:O3	2.34	0.60
1:L:16:GLU:HA	1:L:209:VAL:HG21	1.84	0.60
1:F:16:GLU:HA	1:F:209:VAL:HG21	1.84	0.60
1:K:194:TYR:OH	1:E:118:ARG:NH1	2.34	0.59
2:Q:147:VAL:O	2:Q:148:ASN:HB2	2.02	0.59
1:F:85:ILE:HD13	1:F:104:GLU:HG2	1.84	0.59
2:Q:145:CYS:HB3	2:Q:153:ALA:HB3	1.83	0.59
1:I:16:GLU:HA	1:I:209:VAL:HG21	1.84	0.59
1:C:243:GLU:H	1:C:274:THR:HG21	1.67	0.59
1:C:16:GLU:HA	1:C:209:VAL:HG21	1.85	0.59
1:H:16:GLU:HA	1:H:209:VAL:HG21	1.85	0.59
1:B:61:ARG:HH12	1:C:217:ALA:HB3	1.67	0.58
1:D:200:ILE:HG12	1:D:207:PRO:HD3	1.85	0.58
1:F:200:ILE:HG12	1:F:207:PRO:HD3	1.85	0.58
1:D:16:GLU:HA	1:D:209:VAL:HG21	1.85	0.58
1:L:200:ILE:HG12	1:L:207:PRO:HD3	1.84	0.58
1:D:82:LYS:HB3	1:D:108:LEU:HD11	1.86	0.58
2:S:19:ILE:HD11	2:S:42:ILE:HD12	1.85	0.58
1:K:72:MET:HG3	1:K:79:VAL:HG11	1.86	0.58
1:K:200:ILE:HG12	1:K:207:PRO:HD3	1.84	0.58
1:C:85:ILE:HD13	1:C:104:GLU:HG2	1.84	0.58
2:W:146:LYS:HA	2:W:151:ILE:HA	1.86	0.58
1:A:72:MET:HG3	1:A:79:VAL:HG11	1.86	0.57
1:H:243:GLU:H	1:H:274:THR:HG21	1.68	0.57
1:B:16:GLU:HA	1:B:209:VAL:HG21	1.86	0.57
1:A:82:LYS:HB3	1:A:108:LEU:HD11	1.86	0.57
2:S:146:LYS:HA	2:S:151:ILE:HA	1.85	0.57
2:O:146:LYS:HA	2:O:151:ILE:HA	1.87	0.57
1:K:85:ILE:HD13	1:K:104:GLU:HG2	1.87	0.57
1:J:72:MET:HG3	1:J:79:VAL:HG11	1.85	0.57
1:I:139:ARG:NH2	3:I:301:PO4:O2	2.37	0.57
1:A:16:GLU:HA	1:A:209:VAL:HG21	1.87	0.57
1:D:118:ARG:HG3	1:D:121:GLN:HG2	1.87	0.57
1:C:200:ILE:HG12	1:C:207:PRO:HD3	1.85	0.56
1:I:72:MET:HG3	1:I:79:VAL:HG11	1.87	0.56
2:R:146:LYS:HA	2:R:151:ILE:HA	1.87	0.56
2:P:146:LYS:HA	2:P:151:ILE:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:118:ARG:HG3	1:G:121:GLN:HG2	1.87	0.56
1:J:243:GLU:H	1:J:274:THR:HG21	1.69	0.56
2:T:146:LYS:HA	2:T:151:ILE:HA	1.87	0.56
1:D:243:GLU:H	1:D:274:THR:HG21	1.70	0.56
2:N:19:ILE:HD11	2:N:42:ILE:HD12	1.87	0.56
2:U:146:LYS:HA	2:U:151:ILE:HA	1.88	0.56
1:L:72:MET:HG3	1:L:79:VAL:HG11	1.87	0.56
1:H:200:ILE:HG12	1:H:207:PRO:HD3	1.87	0.56
2:N:145:CYS:HB3	2:N:153:ALA:HB3	1.87	0.56
2:X:46:GLY:O	4:X:201:GLN:NE2	2.38	0.56
2:X:146:LYS:HA	2:X:151:ILE:HA	1.87	0.56
2:R:46:GLY:O	4:R:201:GLN:NE2	2.39	0.56
2:M:146:LYS:HA	2:M:151:ILE:HA	1.87	0.56
2:V:19:ILE:HD11	2:V:42:ILE:HD12	1.88	0.56
1:B:239:ILE:HD11	1:B:252:ILE:HG13	1.88	0.56
2:U:46:GLY:O	4:U:201:GLN:NE2	2.38	0.56
1:H:118:ARG:HG3	1:H:121:GLN:HG2	1.86	0.56
2:U:19:ILE:HD11	2:U:42:ILE:HD12	1.88	0.56
1:G:82:LYS:HB3	1:G:108:LEU:HD11	1.88	0.56
1:B:200:ILE:HG12	1:B:207:PRO:HD3	1.87	0.56
1:C:118:ARG:HG3	1:C:121:GLN:HG2	1.87	0.56
2:N:152:VAL:HB	2:N:163:SER:HB2	1.88	0.56
2:U:152:VAL:HB	2:U:163:SER:HB2	1.87	0.55
2:P:19:ILE:HD11	2:P:42:ILE:HD12	1.88	0.55
2:Q:46:GLY:O	4:Q:201:GLN:NE2	2.39	0.55
1:K:257:THR:HG21	2:X:54:LEU:HD11	1.88	0.55
1:I:82:LYS:HB3	1:I:108:LEU:HD11	1.88	0.55
1:E:118:ARG:HG3	1:E:121:GLN:HG2	1.88	0.55
2:S:46:GLY:O	4:S:201:GLN:NE2	2.39	0.55
2:X:19:ILE:HD11	2:X:42:ILE:HD12	1.89	0.55
2:W:46:GLY:O	4:W:201:GLN:NE2	2.39	0.55
2:V:46:GLY:O	4:V:201:GLN:NE2	2.39	0.55
2:T:19:ILE:HD11	2:T:42:ILE:HD12	1.89	0.55
2:T:46:GLY:O	4:T:201:GLN:NE2	2.39	0.55
2:T:97:ILE:HG22	2:T:137:VAL:HA	1.89	0.55
1:F:243:GLU:H	1:F:274:THR:HG21	1.69	0.55
2:O:19:ILE:HD11	2:O:42:ILE:HD12	1.88	0.55
2:M:46:GLY:O	4:M:201:GLN:NE2	2.39	0.55
2:P:46:GLY:O	4:P:201:GLN:NE2	2.39	0.55
1:L:118:ARG:HG3	1:L:121:GLN:HG2	1.87	0.55
1:A:118:ARG:HG3	1:A:121:GLN:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:146:LYS:HA	2:V:151:ILE:HA	1.87	0.55
1:B:82:LYS:HB3	1:B:108:LEU:HD11	1.88	0.55
1:F:118:ARG:HG3	1:F:121:GLN:HG2	1.87	0.55
2:T:74:THR:O	2:T:78:LEU:N	2.35	0.55
1:G:72:MET:HG3	1:G:79:VAL:HG11	1.88	0.55
1:J:16:GLU:HA	1:J:209:VAL:HG21	1.88	0.55
1:J:118:ARG:HG3	1:J:121:GLN:HG2	1.89	0.55
2:O:46:GLY:O	4:O:201:GLN:NE2	2.40	0.55
2:Q:19:ILE:HD11	2:Q:42:ILE:HD12	1.88	0.54
2:P:97:ILE:HG22	2:P:137:VAL:HA	1.87	0.54
2:P:117:ILE:HD12	2:P:124:ILE:HG13	1.89	0.54
1:B:72:MET:HG3	1:B:79:VAL:HG11	1.89	0.54
2:W:19:ILE:HD11	2:W:42:ILE:HD12	1.89	0.54
2:U:145:CYS:HB3	2:U:153:ALA:HB3	1.88	0.54
2:R:19:ILE:HD11	2:R:42:ILE:HD12	1.90	0.54
2:U:97:ILE:HG22	2:U:137:VAL:HA	1.90	0.54
1:A:217:ALA:HB3	1:F:61:ARG:HH12	1.73	0.54
1:H:85:ILE:HD13	1:H:104:GLU:HG2	1.89	0.54
1:F:10:VAL:HG12	2:R:107:GLN:HE22	1.73	0.54
1:E:243:GLU:H	1:E:274:THR:HG21	1.73	0.54
2:N:117:ILE:HD12	2:N:124:ILE:HG13	1.89	0.54
1:A:85:ILE:HD13	1:A:104:GLU:HG2	1.89	0.54
2:V:145:CYS:HB3	2:V:153:ALA:HB3	1.90	0.54
2:X:152:VAL:HB	2:X:163:SER:HB2	1.90	0.53
1:I:85:ILE:HD13	1:I:104:GLU:HG2	1.90	0.53
2:X:145:CYS:HB3	2:X:153:ALA:HB3	1.89	0.53
1:D:85:ILE:HD13	1:D:104:GLU:HG2	1.90	0.53
2:S:97:ILE:HG22	2:S:137:VAL:HA	1.91	0.53
2:W:97:ILE:HG22	2:W:137:VAL:HA	1.90	0.53
2:R:97:ILE:HG22	2:R:137:VAL:HA	1.91	0.53
1:K:118:ARG:HG3	1:K:121:GLN:HG2	1.90	0.53
1:K:243:GLU:H	1:K:274:THR:HG21	1.74	0.53
1:J:200:ILE:HG12	1:J:207:PRO:HD3	1.90	0.53
2:V:97:ILE:HG22	2:V:137:VAL:HA	1.90	0.53
1:L:10:VAL:HG12	2:S:107:GLN:HE22	1.73	0.53
1:A:243:GLU:H	1:A:274:THR:HG21	1.73	0.53
1:B:85:ILE:HD13	1:B:104:GLU:HG2	1.91	0.53
2:M:19:ILE:HD11	2:M:42:ILE:HD12	1.90	0.53
2:P:145:CYS:HB3	2:P:153:ALA:HB3	1.91	0.53
1:A:104:GLU:HG3	1:A:117:LEU:HD12	1.91	0.53
2:R:137:VAL:HG21	2:R:143:ILE:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:TYR:OH	1:I:118:ARG:NH1	2.41	0.52
1:C:257:THR:HG21	2:O:54:LEU:HD11	1.90	0.52
2:N:97:ILE:HG22	2:N:137:VAL:HA	1.91	0.52
1:E:139:ARG:NH2	3:E:301:PO4:O3	2.40	0.52
2:X:117:ILE:HD12	2:X:124:ILE:HG13	1.91	0.52
2:Q:7:ALA:HA	2:Q:12:VAL:HG21	1.91	0.52
1:G:16:GLU:HA	1:G:209:VAL:HG21	1.90	0.52
1:B:118:ARG:HG3	1:B:121:GLN:HG2	1.92	0.52
1:J:61:ARG:HH12	1:I:217:ALA:HB3	1.72	0.52
1:H:33:ARG:HE	1:H:74:ALA:HB1	1.74	0.52
1:A:118:ARG:NH1	1:G:194:TYR:OH	2.43	0.52
1:L:82:LYS:HB3	1:L:108:LEU:HD11	1.90	0.52
1:L:85:ILE:HD13	1:L:104:GLU:HG2	1.90	0.52
1:I:118:ARG:HG3	1:I:121:GLN:HG2	1.90	0.52
1:E:72:MET:HG3	1:E:79:VAL:HG11	1.91	0.52
1:F:82:LYS:HB3	1:F:108:LEU:HD11	1.91	0.52
2:W:145:CYS:HB3	2:W:153:ALA:HB3	1.92	0.52
2:M:97:ILE:HG22	2:M:137:VAL:HA	1.90	0.52
2:V:117:ILE:HD12	2:V:124:ILE:HG13	1.91	0.52
1:C:104:GLU:HG3	1:C:117:LEU:HD12	1.91	0.52
1:I:243:GLU:H	1:I:274:THR:HG21	1.74	0.52
2:R:7:ALA:HA	2:R:12:VAL:HG21	1.92	0.52
2:O:137:VAL:HG21	2:O:143:ILE:HD11	1.92	0.52
2:N:46:GLY:O	4:N:201:GLN:NE2	2.43	0.52
2:S:117:ILE:HD12	2:S:124:ILE:HG13	1.91	0.52
2:P:137:VAL:HG21	2:P:143:ILE:HD11	1.92	0.52
1:A:11:LYS:NZ	1:A:122:PHE:O	2.42	0.52
1:G:87:HIS:CE1	1:G:90:GLU:HG3	2.45	0.52
1:F:104:GLU:HG3	1:F:117:LEU:HD12	1.91	0.52
1:G:85:ILE:HD13	1:G:104:GLU:HG2	1.92	0.52
1:H:82:LYS:HB3	1:H:108:LEU:HD11	1.92	0.52
2:R:145:CYS:HB3	2:R:153:ALA:HB3	1.92	0.52
2:T:117:ILE:HD12	2:T:124:ILE:HG13	1.92	0.51
2:O:97:ILE:HG22	2:O:137:VAL:HA	1.91	0.51
2:U:117:ILE:HD12	2:U:124:ILE:HG13	1.91	0.51
2:Q:97:ILE:HG22	2:Q:137:VAL:HA	1.92	0.51
1:E:104:GLU:HG3	1:E:117:LEU:HD12	1.93	0.51
1:H:72:MET:HG3	1:H:79:VAL:HG11	1.92	0.51
2:Q:117:ILE:HD12	2:Q:124:ILE:HG13	1.91	0.51
1:J:85:ILE:HD13	1:J:104:GLU:HG2	1.92	0.51
1:C:9:ARG:NH2	2:O:112:GLU:OE1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:MET:HG3	1:D:79:VAL:HG11	1.92	0.51
1:A:29:ALA:HB2	1:A:70:GLU:HG2	1.93	0.51
2:N:74:THR:O	2:N:78:LEU:N	2.36	0.51
2:O:145:CYS:HB3	2:O:153:ALA:HB3	1.93	0.51
2:T:145:CYS:HB3	2:T:153:ALA:HB3	1.92	0.51
2:T:7:ALA:HA	2:T:12:VAL:HG21	1.92	0.51
1:K:82:LYS:HB3	1:K:108:LEU:HD11	1.93	0.51
1:J:133:LEU:HD13	1:J:172:VAL:HG12	1.93	0.51
1:A:61:ARG:HH12	1:B:217:ALA:HB3	1.75	0.51
2:T:137:VAL:HG21	2:T:143:ILE:HD11	1.93	0.51
2:U:7:ALA:HA	2:U:12:VAL:HG21	1.92	0.51
1:L:29:ALA:HB2	1:L:70:GLU:HG2	1.93	0.50
1:C:29:ALA:HB2	1:C:70:GLU:HG2	1.92	0.50
1:E:194:TYR:CZ	1:E:198:LYS:HD2	2.47	0.50
2:S:145:CYS:HB3	2:S:153:ALA:HB3	1.92	0.50
2:X:97:ILE:HG22	2:X:137:VAL:HA	1.93	0.50
2:W:7:ALA:HA	2:W:12:VAL:HG21	1.93	0.50
2:W:117:ILE:HD12	2:W:124:ILE:HG13	1.93	0.50
2:V:74:THR:O	2:V:78:LEU:N	2.35	0.50
1:J:82:LYS:HB3	1:J:108:LEU:HD11	1.93	0.50
1:L:104:GLU:HG3	1:L:117:LEU:HD12	1.93	0.50
1:C:72:MET:HG3	1:C:79:VAL:HG11	1.93	0.50
2:R:16:ILE:HD11	2:R:28:ALA:HB2	1.93	0.50
2:Q:16:ILE:HD11	2:Q:28:ALA:HB2	1.94	0.50
1:A:133:LEU:HD13	1:A:172:VAL:HG12	1.94	0.50
1:G:243:GLU:H	1:G:274:THR:HG21	1.76	0.50
1:B:118:ARG:NH1	1:H:194:TYR:OH	2.44	0.50
2:O:7:ALA:HA	2:O:12:VAL:HG21	1.93	0.50
2:O:117:ILE:HD12	2:O:124:ILE:HG13	1.94	0.50
1:B:133:LEU:HD13	1:B:172:VAL:HG12	1.94	0.50
1:C:82:LYS:HB3	1:C:108:LEU:HD11	1.94	0.50
1:H:29:ALA:HB2	1:H:70:GLU:HG2	1.93	0.50
1:E:29:ALA:HB2	1:E:70:GLU:HG2	1.92	0.50
2:S:137:VAL:HG21	2:S:143:ILE:HD11	1.93	0.50
1:G:194:TYR:CZ	1:G:198:LYS:HD2	2.47	0.50
2:R:117:ILE:HD12	2:R:124:ILE:HG13	1.94	0.50
2:M:145:CYS:HB3	2:M:153:ALA:HB3	1.92	0.50
1:G:119:LYS:NZ	1:G:142:GLU:OE1	2.45	0.49
2:N:134:ILE:HB	2:N:151:ILE:HG13	1.93	0.49
2:X:7:ALA:HA	2:X:12:VAL:HG21	1.92	0.49
2:M:7:ALA:HA	2:M:12:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:7:ALA:HA	2:V:12:VAL:HG21	1.93	0.49
2:V:137:VAL:HG21	2:V:143:ILE:HD11	1.93	0.49
2:V:152:VAL:HB	2:V:163:SER:HB2	1.94	0.49
1:A:33:ARG:HE	1:A:74:ALA:HB1	1.77	0.49
2:W:137:VAL:HG21	2:W:143:ILE:HD11	1.95	0.49
1:L:87:HIS:CE1	1:L:90:GLU:HG3	2.48	0.49
1:C:10:VAL:HG12	2:O:107:GLN:HE22	1.76	0.49
1:J:194:TYR:OH	1:D:118:ARG:NH1	2.46	0.49
1:I:23:ILE:HG13	1:I:41:VAL:HG23	1.94	0.49
2:X:16:ILE:HD11	2:X:28:ALA:HB2	1.95	0.49
1:K:29:ALA:HB2	1:K:70:GLU:HG2	1.95	0.49
1:H:104:GLU:HG3	1:H:117:LEU:HD12	1.95	0.49
1:A:166:ARG:HH12	1:L:181:ASP:HB2	1.78	0.49
1:J:104:GLU:HG3	1:J:117:LEU:HD12	1.93	0.49
2:M:16:ILE:HD11	2:M:28:ALA:HB2	1.95	0.49
2:U:16:ILE:HD11	2:U:28:ALA:HB2	1.94	0.49
1:H:257:THR:HG21	2:U:54:LEU:HD11	1.94	0.49
2:W:152:VAL:HB	2:W:163:SER:HB2	1.94	0.49
2:M:117:ILE:HD12	2:M:124:ILE:HG13	1.93	0.49
2:M:137:VAL:HG21	2:M:143:ILE:HD11	1.94	0.49
1:C:139:ARG:NH2	3:C:301:PO4:O1	2.38	0.49
2:V:16:ILE:HD11	2:V:28:ALA:HB2	1.94	0.49
1:A:10:VAL:HG12	2:M:107:GLN:HE22	1.78	0.48
1:K:23:ILE:HG13	1:K:41:VAL:HG23	1.95	0.48
1:C:33:ARG:HE	1:C:74:ALA:HB1	1.77	0.48
1:C:119:LYS:NZ	1:C:142:GLU:OE1	2.46	0.48
1:H:23:ILE:HG13	1:H:41:VAL:HG23	1.95	0.48
1:E:133:LEU:HD13	1:E:172:VAL:HG12	1.94	0.48
1:L:33:ARG:HE	1:L:74:ALA:HB1	1.78	0.48
2:R:152:VAL:HB	2:R:163:SER:HB2	1.93	0.48
1:G:26:VAL:HG23	1:G:31:GLN:HB2	1.96	0.48
1:I:87:HIS:CE1	1:I:90:GLU:HG3	2.48	0.48
1:B:194:TYR:OH	1:H:118:ARG:NH1	2.46	0.48
1:D:104:GLU:HG3	1:D:117:LEU:HD12	1.94	0.48
1:K:133:LEU:HD13	1:K:172:VAL:HG12	1.96	0.48
1:K:166:ARG:HH12	1:F:181:ASP:HB2	1.78	0.48
1:I:104:GLU:HG3	1:I:117:LEU:HD12	1.95	0.48
2:S:7:ALA:HA	2:S:12:VAL:HG21	1.95	0.48
1:B:29:ALA:HB2	1:B:70:GLU:HG2	1.94	0.48
1:C:118:ARG:NH1	1:I:194:TYR:OH	2.46	0.48
2:U:137:VAL:HG21	2:U:143:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:74:THR:O	2:P:78:LEU:N	2.37	0.48
1:H:133:LEU:HD13	1:H:172:VAL:HG12	1.96	0.48
1:H:194:TYR:CZ	1:H:198:LYS:HD2	2.49	0.48
2:X:137:VAL:HG21	2:X:143:ILE:HD11	1.95	0.48
1:B:104:GLU:HG3	1:B:117:LEU:HD12	1.96	0.48
1:K:172:VAL:HG11	1:K:206:LEU:HD13	1.96	0.48
2:S:74:THR:O	2:S:78:LEU:N	2.35	0.48
2:S:152:VAL:HB	2:S:163:SER:HB2	1.96	0.48
1:A:194:TYR:CZ	1:A:198:LYS:HD2	2.48	0.48
1:I:172:VAL:HG11	1:I:206:LEU:HD13	1.94	0.48
1:H:10:VAL:HG12	2:U:107:GLN:HE22	1.78	0.48
2:R:74:THR:O	2:R:78:LEU:N	2.36	0.48
2:P:7:ALA:HA	2:P:12:VAL:HG21	1.94	0.48
1:G:11:LYS:NZ	1:G:122:PHE:O	2.47	0.47
1:G:133:LEU:HD13	1:G:172:VAL:HG12	1.96	0.47
1:I:166:ARG:HH12	1:D:181:ASP:HB2	1.79	0.47
2:N:16:ILE:HD11	2:N:28:ALA:HB2	1.95	0.47
1:A:172:VAL:HG11	1:A:206:LEU:HD13	1.96	0.47
1:L:243:GLU:H	1:L:274:THR:HG21	1.79	0.47
1:I:194:TYR:CZ	1:I:198:LYS:HD2	2.49	0.47
1:K:104:GLU:HG3	1:K:117:LEU:HD12	1.95	0.47
2:S:16:ILE:HD11	2:S:28:ALA:HB2	1.95	0.47
2:X:74:THR:O	2:X:78:LEU:N	2.37	0.47
2:W:16:ILE:HD11	2:W:28:ALA:HB2	1.96	0.47
1:B:172:VAL:HG11	1:B:206:LEU:HD13	1.96	0.47
1:K:118:ARG:NH1	1:E:194:TYR:OH	2.47	0.47
1:J:87:HIS:CE1	1:J:90:GLU:HG3	2.50	0.47
2:T:16:ILE:HD11	2:T:28:ALA:HB2	1.95	0.47
1:L:172:VAL:HG11	1:L:206:LEU:HD13	1.97	0.47
1:F:166:ARG:NE	1:E:112:ASP:OD2	2.47	0.47
2:O:16:ILE:HD11	2:O:28:ALA:HB2	1.95	0.47
1:G:172:VAL:HG11	1:G:206:LEU:HD13	1.97	0.47
1:E:85:ILE:HD13	1:E:104:GLU:HG2	1.94	0.47
2:M:152:VAL:HB	2:M:163:SER:HB2	1.97	0.47
1:K:194:TYR:CZ	1:K:198:LYS:HD2	2.49	0.47
1:J:166:ARG:HH12	1:E:181:ASP:HB2	1.79	0.47
2:N:7:ALA:HA	2:N:12:VAL:HG21	1.95	0.47
2:X:148:ASN:C	2:X:150:LYS:H	2.18	0.47
2:M:74:THR:O	2:M:78:LEU:N	2.36	0.47
2:U:74:THR:O	2:U:78:LEU:N	2.37	0.47
1:F:257:THR:HG21	2:R:54:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:29:ALA:HB2	1:I:70:GLU:HG2	1.96	0.47
2:P:16:ILE:HD11	2:P:28:ALA:HB2	1.97	0.47
1:B:119:LYS:NZ	1:B:142:GLU:OE1	2.47	0.47
1:B:172:VAL:O	1:B:176:THR:HG23	2.15	0.46
1:L:133:LEU:HD13	1:L:172:VAL:HG12	1.97	0.46
1:E:172:VAL:O	1:E:176:THR:HG23	2.15	0.46
2:Q:74:THR:O	2:Q:78:LEU:N	2.36	0.46
1:L:208:VAL:HG22	1:L:209:VAL:H	1.81	0.46
1:F:133:LEU:HD13	1:F:172:VAL:HG12	1.96	0.46
1:I:257:THR:HG21	2:V:54:LEU:HD11	1.98	0.46
1:D:23:ILE:HG13	1:D:41:VAL:HG23	1.97	0.46
1:D:172:VAL:O	1:D:176:THR:HG23	2.15	0.46
2:N:137:VAL:HG21	2:N:143:ILE:HD11	1.97	0.46
1:G:29:ALA:HB1	1:G:74:ALA:HB2	1.98	0.46
1:G:172:VAL:O	1:G:176:THR:HG23	2.16	0.46
1:B:62:MET:HE3	1:B:90:GLU:HG2	1.98	0.46
1:H:172:VAL:HG11	1:H:206:LEU:HD13	1.97	0.46
2:P:152:VAL:HB	2:P:163:SER:HB2	1.97	0.46
1:D:87:HIS:CE1	1:D:90:GLU:HG3	2.51	0.46
2:N:147:VAL:O	2:N:147:VAL:HG13	2.16	0.46
1:L:61:ARG:HH12	1:K:217:ALA:HB3	1.80	0.46
2:R:74:THR:HA	2:R:162:VAL:HG23	1.98	0.46
1:G:33:ARG:HE	1:G:74:ALA:HB1	1.80	0.46
1:I:119:LYS:NZ	1:I:142:GLU:OE1	2.49	0.46
1:A:87:HIS:CE1	1:A:90:GLU:HG3	2.51	0.46
1:B:44:MET:HE2	1:B:82:LYS:HG3	1.98	0.46
1:L:172:VAL:O	1:L:176:THR:HG23	2.15	0.46
1:H:119:LYS:NZ	1:H:142:GLU:OE1	2.49	0.46
2:O:152:VAL:HB	2:O:163:SER:HB2	1.97	0.46
1:D:133:LEU:HD13	1:D:172:VAL:HG12	1.97	0.46
1:E:26:VAL:HG21	1:E:32:ALA:HB2	1.98	0.46
2:Q:152:VAL:HB	2:Q:163:SER:HB2	1.98	0.46
1:J:23:ILE:HG13	1:J:41:VAL:HG23	1.97	0.46
1:C:194:TYR:CZ	1:C:198:LYS:HD2	2.51	0.46
1:A:172:VAL:O	1:A:176:THR:HG23	2.16	0.45
1:B:87:HIS:CE1	1:B:90:GLU:HG3	2.51	0.45
1:K:26:VAL:HG23	1:K:31:GLN:HB2	1.98	0.45
1:F:194:TYR:CZ	1:F:198:LYS:HD2	2.50	0.45
1:K:29:ALA:O	1:K:33:ARG:HG2	2.16	0.45
1:J:194:TYR:CZ	1:J:198:LYS:HD2	2.51	0.45
1:D:11:LYS:NZ	1:D:122:PHE:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:74:THR:HA	2:O:162:VAL:HG23	1.99	0.45
2:T:107:GLN:HE22	1:G:10:VAL:HG12	1.82	0.45
1:J:172:VAL:O	1:J:176:THR:HG23	2.17	0.45
1:D:10:VAL:HG12	2:P:107:GLN:HE22	1.82	0.45
1:E:172:VAL:HG11	1:E:206:LEU:HD13	1.97	0.45
1:G:104:GLU:HG3	1:G:117:LEU:HD12	1.99	0.45
1:I:133:LEU:HD13	1:I:172:VAL:HG12	1.98	0.45
1:K:33:ARG:HE	1:K:74:ALA:HB1	1.81	0.45
1:J:139:ARG:NH2	5:J:301:SO4:O2	2.50	0.45
2:P:74:THR:HA	2:P:162:VAL:HG23	1.98	0.45
2:Q:137:VAL:HG21	2:Q:143:ILE:HD11	1.97	0.45
2:T:83:GLN:HA	2:T:93:ASN:HA	1.99	0.45
1:K:172:VAL:O	1:K:176:THR:HG23	2.16	0.45
1:F:172:VAL:O	1:F:176:THR:HG23	2.17	0.45
1:E:82:LYS:HB3	1:E:108:LEU:HD11	1.98	0.45
2:U:74:THR:HA	2:U:162:VAL:HG23	1.98	0.45
1:B:194:TYR:CZ	1:B:198:LYS:HD2	2.51	0.45
1:F:87:HIS:CE1	1:F:90:GLU:HG3	2.52	0.45
1:J:33:ARG:HE	1:J:74:ALA:HB1	1.81	0.45
1:A:221:ASP:HA	1:A:224:LEU:HB3	1.99	0.45
1:G:23:ILE:HG13	1:G:41:VAL:HG23	1.98	0.45
1:K:61:ARG:HH12	1:J:217:ALA:HB3	1.81	0.45
1:C:26:VAL:HG21	1:C:32:ALA:HB2	1.99	0.45
1:C:172:VAL:O	1:C:176:THR:HG23	2.17	0.45
1:I:11:LYS:NZ	1:I:122:PHE:O	2.50	0.45
1:I:138:ARG:NE	3:I:301:PO4:O1	2.47	0.45
2:N:74:THR:HA	2:N:162:VAL:HG23	1.99	0.45
1:B:33:ARG:HE	1:B:74:ALA:HB1	1.82	0.45
1:L:221:ASP:HA	1:L:224:LEU:HB3	1.99	0.44
1:C:23:ILE:HG13	1:C:41:VAL:HG23	1.99	0.44
2:M:74:THR:HA	2:M:162:VAL:HG23	1.99	0.44
1:B:26:VAL:HG23	1:B:31:GLN:HB2	1.99	0.44
1:G:112:ASP:OD2	1:L:166:ARG:NE	2.50	0.44
1:B:29:ALA:O	1:B:33:ARG:HG2	2.18	0.44
1:E:119:LYS:NZ	1:E:142:GLU:OE1	2.50	0.44
1:A:13:GLY:O	1:A:17:MET:HG2	2.17	0.44
1:B:10:VAL:HG12	2:N:107:GLN:HE22	1.82	0.44
1:J:118:ARG:NH1	1:D:194:TYR:OH	2.50	0.44
1:I:172:VAL:O	1:I:176:THR:HG23	2.16	0.44
2:N:95:LEU:HD11	2:N:159:TYR:HB3	2.00	0.44
1:F:72:MET:HG3	1:F:79:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:172:VAL:HG11	1:F:206:LEU:HD13	1.99	0.44
1:D:194:TYR:CZ	1:D:198:LYS:HD2	2.53	0.44
2:W:74:THR:O	2:W:78:LEU:N	2.35	0.44
1:B:26:VAL:HG21	1:B:32:ALA:HB2	2.00	0.44
1:B:243:GLU:CB	1:B:274:THR:HG21	2.47	0.44
1:C:11:LYS:NZ	1:C:122:PHE:O	2.50	0.44
1:I:221:ASP:HA	1:I:224:LEU:HB3	2.00	0.44
1:D:29:ALA:O	1:D:33:ARG:HG2	2.17	0.44
1:J:257:THR:HG21	2:W:54:LEU:HD11	1.99	0.44
2:N:83:GLN:HA	2:N:93:ASN:HA	1.99	0.44
2:W:74:THR:HA	2:W:162:VAL:HG23	1.99	0.44
2:T:152:VAL:HB	2:T:163:SER:HB2	1.98	0.44
2:R:83:GLN:HA	2:R:93:ASN:HA	2.00	0.44
2:Q:74:THR:HA	2:Q:162:VAL:HG23	1.99	0.44
2:T:74:THR:HA	2:T:162:VAL:HG23	2.00	0.43
1:L:11:LYS:NZ	1:L:122:PHE:O	2.51	0.43
1:C:87:HIS:CE1	1:C:90:GLU:HG3	2.52	0.43
2:N:148:ASN:C	2:N:150:LYS:H	2.21	0.43
1:C:11:LYS:HB3	1:C:125:PRO:HB3	1.99	0.43
2:O:83:GLN:HA	2:O:93:ASN:HA	2.00	0.43
2:V:83:GLN:HA	2:V:93:ASN:HA	2.00	0.43
1:A:23:ILE:HG13	1:A:41:VAL:HG23	2.00	0.43
1:K:11:LYS:NZ	1:K:122:PHE:O	2.52	0.43
1:C:221:ASP:HA	1:C:224:LEU:HB3	1.99	0.43
1:I:11:LYS:H	1:I:11:LYS:HG2	1.62	0.43
1:G:11:LYS:H	1:G:11:LYS:HG2	1.62	0.43
1:H:26:VAL:HG21	1:H:32:ALA:HB2	2.00	0.43
2:S:74:THR:HA	2:S:162:VAL:HG23	2.00	0.43
1:H:13:GLY:O	1:H:17:MET:HG2	2.19	0.43
1:D:221:ASP:HA	1:D:224:LEU:HB3	2.00	0.43
2:V:74:THR:HA	2:V:162:VAL:HG23	1.99	0.43
2:P:83:GLN:HA	2:P:93:ASN:HA	2.00	0.43
1:E:33:ARG:HE	1:E:74:ALA:HB1	1.83	0.43
2:X:95:LEU:HD11	2:X:159:TYR:HB3	1.99	0.43
1:A:257:THR:HG21	2:M:54:LEU:HD11	2.00	0.43
1:G:217:ALA:HB3	1:H:61:ARG:HH12	1.84	0.43
1:B:11:LYS:NZ	1:B:122:PHE:O	2.51	0.43
1:B:25:ASP:HA	1:B:44:MET:HB3	2.01	0.43
2:N:80:VAL:HG13	2:N:91:TYR:HD2	1.83	0.43
2:W:83:GLN:HA	2:W:93:ASN:HA	2.00	0.43
1:B:23:ILE:HG13	1:B:41:VAL:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:23:ILE:HG13	1:F:41:VAL:HG23	2.00	0.43
2:Q:83:GLN:HA	2:Q:93:ASN:HA	2.00	0.43
1:L:118:ARG:HH22	1:F:198:LYS:HE3	1.82	0.43
1:L:198:LYS:HE3	1:F:118:ARG:HH22	1.83	0.43
1:I:112:ASP:OD2	1:H:166:ARG:NE	2.52	0.43
1:H:11:LYS:NZ	1:H:122:PHE:O	2.51	0.43
1:E:11:LYS:H	1:E:11:LYS:HG2	1.66	0.43
2:O:74:THR:O	2:O:78:LEU:N	2.36	0.43
2:U:43:LEU:HD12	2:U:81:LEU:HG	2.00	0.43
1:J:29:ALA:HB2	1:J:70:GLU:HG2	2.01	0.43
1:J:62:MET:HE3	1:J:90:GLU:HG2	2.01	0.43
1:H:87:HIS:CE1	1:H:90:GLU:HG3	2.54	0.43
1:H:172:VAL:O	1:H:176:THR:HG23	2.18	0.43
2:S:83:GLN:HA	2:S:93:ASN:HA	2.00	0.42
2:M:45:GLY:HA2	2:M:75:CYS:O	2.19	0.42
2:P:43:LEU:HD12	2:P:81:LEU:HG	2.01	0.42
1:G:221:ASP:HA	1:G:224:LEU:HB3	2.01	0.42
2:X:74:THR:HA	2:X:162:VAL:HG23	2.01	0.42
2:W:95:LEU:HD11	2:W:159:TYR:HB3	2.00	0.42
2:M:95:LEU:HD11	2:M:159:TYR:HB3	2.01	0.42
2:V:95:LEU:HD11	2:V:159:TYR:HB3	2.01	0.42
2:U:95:LEU:HD11	2:U:159:TYR:HB3	2.01	0.42
2:T:45:GLY:HA2	2:T:75:CYS:O	2.19	0.42
1:B:221:ASP:HA	1:B:224:LEU:HB3	2.00	0.42
1:J:13:GLY:O	1:J:17:MET:HG2	2.18	0.42
1:D:26:VAL:HG23	1:D:31:GLN:HB2	2.02	0.42
2:X:83:GLN:HA	2:X:93:ASN:HA	2.00	0.42
1:A:26:VAL:HG23	1:A:31:GLN:HB2	2.00	0.42
1:G:26:VAL:HG21	1:G:32:ALA:HB2	2.01	0.42
1:L:13:GLY:O	1:L:17:MET:HG2	2.19	0.42
1:L:26:VAL:HG21	1:L:32:ALA:HB2	2.01	0.42
1:F:26:VAL:HG23	1:F:31:GLN:HB2	2.01	0.42
1:F:29:ALA:O	1:F:33:ARG:HG2	2.19	0.42
1:J:172:VAL:HG11	1:J:206:LEU:HD13	2.01	0.42
1:E:87:HIS:CE1	1:E:90:GLU:HG3	2.53	0.42
2:S:95:LEU:HD11	2:S:159:TYR:HB3	2.01	0.42
2:X:43:LEU:HD12	2:X:81:LEU:HG	2.02	0.42
1:G:166:ARG:HH12	1:B:181:ASP:HB2	1.85	0.42
1:B:13:GLY:O	1:B:17:MET:HG2	2.19	0.42
1:L:112:ASP:OD2	1:K:166:ARG:NE	2.52	0.42
1:C:26:VAL:HG23	1:C:31:GLN:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:83:GLN:HA	2:U:93:ASN:HA	2.00	0.42
1:K:87:HIS:CE1	1:K:90:GLU:HG3	2.55	0.42
1:F:33:ARG:HE	1:F:74:ALA:HB1	1.85	0.42
1:J:10:VAL:HG12	2:W:107:GLN:HE22	1.84	0.42
1:J:221:ASP:HA	1:J:224:LEU:HB3	2.01	0.42
1:H:11:LYS:H	1:H:11:LYS:HG2	1.62	0.42
1:H:183:ILE:O	1:H:186:PHE:HB3	2.20	0.42
2:S:80:VAL:HG13	2:S:91:TYR:HD2	1.85	0.42
2:R:95:LEU:HD11	2:R:159:TYR:HB3	2.02	0.42
2:R:95:LEU:HB3	2:R:97:ILE:HG12	2.02	0.42
2:M:83:GLN:HA	2:M:93:ASN:HA	2.01	0.42
2:V:45:GLY:HA2	2:V:75:CYS:O	2.19	0.42
2:U:45:GLY:HA2	2:U:75:CYS:O	2.20	0.42
2:U:80:VAL:HG13	2:U:91:TYR:HD2	1.84	0.42
2:T:95:LEU:HD11	2:T:159:TYR:HB3	2.02	0.42
1:G:181:ASP:HB2	1:B:166:ARG:HH12	1.84	0.42
1:K:87:HIS:HB3	1:K:90:GLU:HB2	2.01	0.42
1:C:166:ARG:HH12	1:H:181:ASP:HB2	1.84	0.42
1:D:183:ILE:O	1:D:186:PHE:HB3	2.20	0.42
2:S:43:LEU:HD12	2:S:81:LEU:HG	2.01	0.42
2:S:45:GLY:HA2	2:S:75:CYS:O	2.20	0.42
1:A:183:ILE:O	1:A:186:PHE:HB3	2.19	0.42
2:T:43:LEU:HD12	2:T:81:LEU:HG	2.01	0.42
1:B:11:LYS:HB3	1:B:125:PRO:HB3	2.02	0.42
1:B:87:HIS:NE2	1:C:221:ASP:HB3	2.35	0.42
1:J:26:VAL:HG21	1:J:32:ALA:HB2	2.02	0.42
2:R:80:VAL:HG13	2:R:91:TYR:HD2	1.85	0.42
1:F:11:LYS:NZ	1:F:122:PHE:O	2.52	0.42
1:C:133:LEU:HD13	1:C:172:VAL:HG12	2.01	0.42
1:L:194:TYR:CZ	1:L:198:LYS:HD2	2.55	0.42
1:J:11:LYS:H	1:J:11:LYS:HG2	1.63	0.42
1:J:26:VAL:HG23	1:J:31:GLN:HB2	2.02	0.42
1:C:172:VAL:HG11	1:C:206:LEU:HD13	2.01	0.42
1:D:26:VAL:HG21	1:D:32:ALA:HB2	2.02	0.42
1:E:23:ILE:HG13	1:E:41:VAL:HG23	2.00	0.42
1:A:44:MET:HE2	1:A:82:LYS:HG3	2.01	0.41
1:K:11:LYS:H	1:K:11:LYS:HG2	1.63	0.41
1:C:250:LYS:O	1:C:254:GLN:HG2	2.20	0.41
1:H:26:VAL:HG23	1:H:31:GLN:HB2	2.02	0.41
1:H:29:ALA:O	1:H:33:ARG:HG2	2.20	0.41
2:X:52:ARG:NH1	2:X:88:GLU:OE1	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:80:VAL:HG13	2:M:91:TYR:HD2	1.85	0.41
2:T:80:VAL:HG13	2:T:91:TYR:HD2	1.85	0.41
1:F:13:GLY:O	1:F:17:MET:HG2	2.20	0.41
1:J:11:LYS:HB3	1:J:125:PRO:HB3	2.02	0.41
1:I:26:VAL:HG23	1:I:31:GLN:HB2	2.02	0.41
1:I:33:ARG:HE	1:I:74:ALA:HB1	1.84	0.41
2:N:134:ILE:HB	2:N:151:ILE:CG1	2.50	0.41
2:W:45:GLY:HA2	2:W:75:CYS:O	2.20	0.41
2:P:45:GLY:HA2	2:P:75:CYS:O	2.20	0.41
2:Q:95:LEU:HD11	2:Q:159:TYR:HB3	2.02	0.41
1:A:26:VAL:HG21	1:A:32:ALA:HB2	2.02	0.41
1:K:119:LYS:NZ	1:K:142:GLU:OE1	2.53	0.41
1:K:221:ASP:HA	1:K:224:LEU:HB3	2.02	0.41
1:E:29:ALA:O	1:E:33:ARG:HG2	2.20	0.41
2:N:45:GLY:HA2	2:N:75:CYS:O	2.19	0.41
1:B:11:LYS:H	1:B:11:LYS:HG2	1.64	0.41
1:B:249:ALA:O	1:B:253:VAL:HG23	2.20	0.41
1:F:196:ILE:O	1:F:200:ILE:HG13	2.21	0.41
1:J:29:ALA:O	1:J:33:ARG:HG2	2.20	0.41
1:H:221:ASP:HA	1:H:224:LEU:HB3	2.02	0.41
1:D:33:ARG:HE	1:D:74:ALA:HB1	1.85	0.41
1:A:249:ALA:O	1:A:253:VAL:HG23	2.21	0.41
1:L:249:ALA:O	1:L:253:VAL:HG23	2.21	0.41
2:M:95:LEU:HB3	2:M:97:ILE:HG12	2.03	0.41
2:Q:80:VAL:HG13	2:Q:91:TYR:HD2	1.85	0.41
2:T:54:LEU:HD11	1:G:257:THR:HG21	2.01	0.41
1:G:25:ASP:HA	1:G:44:MET:HB3	2.02	0.41
1:B:114:GLU:O	1:H:185:THR:HG21	2.19	0.41
1:K:115:TYR:CZ	1:E:182:GLU:HG2	2.56	0.41
1:K:249:ALA:O	1:K:253:VAL:HG23	2.21	0.41
2:R:43:LEU:HD12	2:R:81:LEU:HG	2.02	0.41
2:O:95:LEU:HD11	2:O:159:TYR:HB3	2.02	0.41
2:U:134:ILE:HB	2:U:151:ILE:HG13	2.03	0.41
2:U:148:ASN:C	2:U:150:LYS:H	2.24	0.41
1:A:131:ARG:NH2	1:A:135:GLU:OE2	2.53	0.41
1:G:13:GLY:O	1:G:17:MET:HG2	2.20	0.41
1:K:26:VAL:HG21	1:K:32:ALA:HB2	2.02	0.41
1:E:249:ALA:O	1:E:253:VAL:HG23	2.21	0.41
2:M:43:LEU:HD12	2:M:81:LEU:HG	2.02	0.41
2:P:95:LEU:HD11	2:P:159:TYR:HB3	2.01	0.41
1:A:29:ALA:O	1:A:33:ARG:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LYS:NZ	1:A:142:GLU:OE1	2.54	0.41
1:I:26:VAL:HG21	1:I:32:ALA:HB2	2.03	0.41
1:D:119:LYS:NZ	1:D:142:GLU:OE1	2.54	0.41
1:E:26:VAL:HG23	1:E:31:GLN:HB2	2.03	0.41
2:O:45:GLY:HA2	2:O:75:CYS:O	2.21	0.41
2:Q:45:GLY:HA2	2:Q:75:CYS:O	2.20	0.41
1:G:44:MET:HE2	1:G:82:LYS:HG3	2.02	0.41
1:B:87:HIS:HB3	1:B:90:GLU:HB2	2.03	0.41
1:L:114:GLU:O	1:F:185:THR:HG21	2.21	0.41
1:I:13:GLY:O	1:I:17:MET:HG2	2.20	0.41
1:D:25:ASP:HA	1:D:44:MET:HB3	2.02	0.41
1:D:249:ALA:O	1:D:253:VAL:HG23	2.21	0.41
1:D:250:LYS:O	1:D:254:GLN:HG2	2.20	0.41
1:E:183:ILE:O	1:E:186:PHE:HB3	2.21	0.41
2:N:95:LEU:HB3	2:N:97:ILE:HG12	2.02	0.41
2:S:95:LEU:HB3	2:S:97:ILE:HG12	2.03	0.41
2:X:45:GLY:HA2	2:X:75:CYS:O	2.20	0.41
2:P:80:VAL:HG13	2:P:91:TYR:HD2	1.86	0.41
2:Q:43:LEU:HD12	2:Q:81:LEU:HG	2.02	0.41
1:A:8:ASP:HA	1:A:11:LYS:HG3	2.03	0.41
2:T:95:LEU:HB3	2:T:97:ILE:HG12	2.03	0.41
1:G:8:ASP:HA	1:G:11:LYS:HG3	2.03	0.41
1:B:183:ILE:O	1:B:186:PHE:HB3	2.21	0.41
1:L:8:ASP:HA	1:L:11:LYS:HG3	2.03	0.41
1:D:172:VAL:HG11	1:D:206:LEU:HD13	2.02	0.41
2:X:80:VAL:HG13	2:X:91:TYR:HD2	1.86	0.41
2:O:95:LEU:HB3	2:O:97:ILE:HG12	2.03	0.41
2:T:14:GLU:OE1	2:T:14:GLU:N	2.52	0.40
1:G:101:TYR:CZ	1:G:125:PRO:HB2	2.57	0.40
1:K:240:PHE:HA	1:K:245:PRO:HB3	2.02	0.40
1:D:13:GLY:O	1:D:17:MET:HG2	2.21	0.40
1:E:25:ASP:HA	1:E:44:MET:HB3	2.03	0.40
1:K:216:VAL:HG21	1:K:233:VAL:HG13	2.03	0.40
1:F:25:ASP:HA	1:F:44:MET:HB3	2.03	0.40
1:I:101:TYR:CZ	1:I:125:PRO:HB2	2.56	0.40
2:Q:95:LEU:HB3	2:Q:97:ILE:HG12	2.03	0.40
1:A:228:LEU:HD23	1:A:228:LEU:HA	1.93	0.40
1:L:29:ALA:O	1:L:33:ARG:HG2	2.21	0.40
1:F:87:HIS:HB3	1:F:90:GLU:HB2	2.03	0.40
1:I:62:MET:HE3	1:I:90:GLU:HG2	2.02	0.40
1:E:183:ILE:HD11	1:E:201:LYS:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:45:GLY:HA2	2:R:75:CYS:O	2.20	0.40
2:V:43:LEU:HD12	2:V:81:LEU:HG	2.03	0.40
2:V:95:LEU:HB3	2:V:97:ILE:HG12	2.03	0.40
1:G:8:ASP:O	1:G:12:ARG:HG2	2.21	0.40
1:B:228:LEU:HD23	1:B:228:LEU:HA	1.89	0.40
1:F:183:ILE:HD11	1:F:201:LYS:HD2	2.03	0.40
1:I:29:ALA:O	1:I:33:ARG:HG2	2.22	0.40
2:W:72:PHE:HB2	2:W:178:PHE:CE1	2.56	0.40
2:O:43:LEU:HD12	2:O:81:LEU:HG	2.02	0.40
1:B:31:GLN:HB3	1:B:240:PHE:CZ	2.57	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	263/297 (89%)	253 (96%)	10 (4%)	0	100	100
1	B	263/297 (89%)	252 (96%)	11 (4%)	0	100	100
1	C	263/297 (89%)	253 (96%)	10 (4%)	0	100	100
1	D	263/297 (89%)	253 (96%)	10 (4%)	0	100	100
1	E	263/297 (89%)	253 (96%)	10 (4%)	0	100	100
1	F	263/297 (89%)	253 (96%)	10 (4%)	0	100	100
1	G	263/297 (89%)	253 (96%)	10 (4%)	0	100	100
1	H	263/297 (89%)	253 (96%)	10 (4%)	0	100	100
1	I	263/297 (89%)	253 (96%)	10 (4%)	0	100	100
1	J	263/297 (89%)	253 (96%)	10 (4%)	0	100	100
1	K	263/297 (89%)	253 (96%)	10 (4%)	0	100	100
1	L	263/297 (89%)	253 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	185/188 (98%)	169 (91%)	16 (9%)	0	100	100
2	N	185/188 (98%)	169 (91%)	16 (9%)	0	100	100
2	O	185/188 (98%)	169 (91%)	16 (9%)	0	100	100
2	P	185/188 (98%)	169 (91%)	16 (9%)	0	100	100
2	Q	185/188 (98%)	167 (90%)	16 (9%)	2 (1%)	14	48
2	R	185/188 (98%)	169 (91%)	16 (9%)	0	100	100
2	S	185/188 (98%)	168 (91%)	17 (9%)	0	100	100
2	T	185/188 (98%)	169 (91%)	16 (9%)	0	100	100
2	U	185/188 (98%)	168 (91%)	17 (9%)	0	100	100
2	V	185/188 (98%)	169 (91%)	16 (9%)	0	100	100
2	W	185/188 (98%)	169 (91%)	16 (9%)	0	100	100
2	X	185/188 (98%)	169 (91%)	16 (9%)	0	100	100
All	All	5376/5820 (92%)	5059 (94%)	315 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Q	148	ASN
2	Q	149	GLU

5.3.2 Protein sidechains (i)

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	189/231 (82%)	186 (98%)	3 (2%)	62	86
1	B	189/231 (82%)	187 (99%)	2 (1%)	73	90
1	C	189/231 (82%)	186 (98%)	3 (2%)	62	86
1	D	189/231 (82%)	186 (98%)	3 (2%)	62	86
1	E	189/231 (82%)	187 (99%)	2 (1%)	73	90
1	F	189/231 (82%)	186 (98%)	3 (2%)	62	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	189/231 (82%)	186 (98%)	3 (2%)	62	86
1	H	189/231 (82%)	186 (98%)	3 (2%)	62	86
1	I	189/231 (82%)	186 (98%)	3 (2%)	62	86
1	J	189/231 (82%)	186 (98%)	3 (2%)	62	86
1	K	189/231 (82%)	186 (98%)	3 (2%)	62	86
1	L	189/231 (82%)	186 (98%)	3 (2%)	62	86
2	M	133/157 (85%)	133 (100%)	0	100	100
2	N	133/157 (85%)	133 (100%)	0	100	100
2	O	133/157 (85%)	133 (100%)	0	100	100
2	P	133/157 (85%)	133 (100%)	0	100	100
2	Q	133/157 (85%)	133 (100%)	0	100	100
2	R	132/157 (84%)	132 (100%)	0	100	100
2	S	133/157 (85%)	133 (100%)	0	100	100
2	T	133/157 (85%)	133 (100%)	0	100	100
2	U	133/157 (85%)	133 (100%)	0	100	100
2	V	133/157 (85%)	133 (100%)	0	100	100
2	W	133/157 (85%)	133 (100%)	0	100	100
2	X	133/157 (85%)	133 (100%)	0	100	100
All	All	3863/4656 (83%)	3829 (99%)	34 (1%)	78	92

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	101	TYR
1	A	248	PHE
1	G	18	GLN
1	G	101	TYR
1	G	248	PHE
1	B	101	TYR
1	B	248	PHE
1	L	18	GLN
1	L	101	TYR
1	L	248	PHE
1	K	18	GLN
1	K	101	TYR

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Mol	Chain	Res	Type
1	K	248	PHE
1	F	18	GLN
1	F	101	TYR
1	F	248	PHE
1	J	18	GLN
1	J	101	TYR
1	J	248	PHE
1	C	18	GLN
1	C	101	TYR
1	C	248	PHE
1	I	18	GLN
1	I	101	TYR
1	I	248	PHE
1	H	18	GLN
1	H	101	TYR
1	H	248	PHE
1	D	18	GLN
1	D	101	TYR
1	D	248	PHE
1	E	18	GLN
1	E	248	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	X	165	ASN
2	W	165	ASN
2	Q	107	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

24 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	$\#\|Z\| > 2$
4	GLN	U	201	-	8,9,9	0.82	1 (12%)	10,11,11	1.11	2 (20%)
4	GLN	M	201	-	8,9,9	0.81	1 (12%)	10,11,11	1.10	2 (20%)
3	PO4	A	301	-	4,4,4	1.53	1 (25%)	6,6,6	0.46	0
4	GLN	R	201	-	8,9,9	0.81	1 (12%)	10,11,11	1.12	2 (20%)
3	PO4	L	301	-	4,4,4	1.54	1 (25%)	6,6,6	0.46	0
3	PO4	K	301	-	4,4,4	1.53	1 (25%)	6,6,6	0.45	0
3	PO4	E	301	-	4,4,4	1.54	1 (25%)	6,6,6	0.44	0
3	PO4	I	301	-	4,4,4	1.55	1 (25%)	6,6,6	0.44	0
4	GLN	S	201	-	8,9,9	0.80	1 (12%)	10,11,11	1.11	2 (20%)
4	GLN	P	201	-	8,9,9	0.81	1 (12%)	10,11,11	1.11	2 (20%)
3	PO4	F	301	-	4,4,4	1.55	1 (25%)	6,6,6	0.45	0
3	PO4	C	301	-	4,4,4	1.51	1 (25%)	6,6,6	0.46	0
3	PO4	D	301	-	4,4,4	1.51	1 (25%)	6,6,6	0.46	0
4	GLN	V	201	-	8,9,9	0.81	1 (12%)	10,11,11	1.11	2 (20%)
3	PO4	B	301	-	4,4,4	1.53	1 (25%)	6,6,6	0.46	0
4	GLN	O	201	-	8,9,9	0.81	1 (12%)	10,11,11	1.07	2 (20%)
4	GLN	W	201	-	8,9,9	0.80	1 (12%)	10,11,11	1.10	2 (20%)
3	PO4	H	301	-	4,4,4	1.52	1 (25%)	6,6,6	0.45	0
4	GLN	T	201	-	8,9,9	0.81	1 (12%)	10,11,11	1.09	2 (20%)
4	GLN	N	201	-	8,9,9	0.81	1 (12%)	10,11,11	1.09	2 (20%)
4	GLN	Q	201	-	8,9,9	0.81	1 (12%)	10,11,11	1.10	2 (20%)
5	SO4	J	301	-	4,4,4	0.60	0	6,6,6	0.04	0
4	GLN	X	201	-	8,9,9	0.82	1 (12%)	10,11,11	1.09	2 (20%)
3	PO4	G	301	-	4,4,4	1.56	1 (25%)	6,6,6	0.46	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
4	GLN	P	201	-	-	2/9/9/9	-
4	GLN	U	201	-	-	2/9/9/9	-
4	GLN	V	201	-	-	2/9/9/9	-
4	GLN	M	201	-	-	4/9/9/9	-
4	GLN	O	201	-	-	4/9/9/9	-
4	GLN	W	201	-	-	4/9/9/9	-
4	GLN	T	201	-	-	2/9/9/9	-
4	GLN	R	201	-	-	2/9/9/9	-
4	GLN	N	201	-	-	4/9/9/9	-
4	GLN	Q	201	-	-	2/9/9/9	-
4	GLN	X	201	-	-	4/9/9/9	-
4	GLN	S	201	-	-	4/9/9/9	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	301	PO4	P-O1	2.73	1.57	1.50
3	G	301	PO4	P-O1	2.72	1.57	1.50
3	I	301	PO4	P-O1	2.70	1.57	1.50
3	E	301	PO4	P-O1	2.69	1.57	1.50
3	L	301	PO4	P-O1	2.67	1.57	1.50
3	K	301	PO4	P-O1	2.65	1.57	1.50
3	H	301	PO4	P-O1	2.63	1.57	1.50
3	B	301	PO4	P-O1	2.63	1.57	1.50
3	A	301	PO4	P-O1	2.63	1.57	1.50
3	D	301	PO4	P-O1	2.60	1.56	1.50
3	C	301	PO4	P-O1	2.59	1.56	1.50
4	X	201	GLN	OXT-C	-2.18	1.23	1.30
4	U	201	GLN	OXT-C	-2.16	1.23	1.30
4	P	201	GLN	OXT-C	-2.16	1.23	1.30
4	V	201	GLN	OXT-C	-2.15	1.23	1.30
4	Q	201	GLN	OXT-C	-2.15	1.23	1.30
4	R	201	GLN	OXT-C	-2.15	1.23	1.30
4	O	201	GLN	OXT-C	-2.14	1.23	1.30
4	T	201	GLN	OXT-C	-2.14	1.23	1.30
4	N	201	GLN	OXT-C	-2.13	1.23	1.30
4	M	201	GLN	OXT-C	-2.13	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	201	GLN	OXT-C	-2.13	1.23	1.30
4	W	201	GLN	OXT-C	-2.11	1.23	1.30

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	S	201	GLN	OXT-C-O	-2.69	117.97	124.09
4	R	201	GLN	OXT-C-O	-2.68	118.00	124.09
4	W	201	GLN	OXT-C-O	-2.68	118.00	124.09
4	M	201	GLN	OXT-C-O	-2.68	118.00	124.09
4	V	201	GLN	OXT-C-O	-2.66	118.06	124.09
4	P	201	GLN	OXT-C-O	-2.65	118.07	124.09
4	X	201	GLN	OXT-C-O	-2.65	118.08	124.09
4	Q	201	GLN	OXT-C-O	-2.63	118.11	124.09
4	U	201	GLN	OXT-C-O	-2.63	118.12	124.09
4	N	201	GLN	OXT-C-O	-2.63	118.12	124.09
4	O	201	GLN	OXT-C-O	-2.60	118.18	124.09
4	T	201	GLN	OXT-C-O	-2.58	118.22	124.09
4	V	201	GLN	OXT-C-CA	2.27	121.12	113.38
4	P	201	GLN	OXT-C-CA	2.27	121.11	113.38
4	R	201	GLN	OXT-C-CA	2.26	121.09	113.38
4	U	201	GLN	OXT-C-CA	2.26	121.08	113.38
4	T	201	GLN	OXT-C-CA	2.26	121.08	113.38
4	Q	201	GLN	OXT-C-CA	2.23	120.98	113.38
4	S	201	GLN	OXT-C-CA	2.21	120.91	113.38
4	W	201	GLN	OXT-C-CA	2.19	120.84	113.38
4	M	201	GLN	OXT-C-CA	2.19	120.84	113.38
4	N	201	GLN	OXT-C-CA	2.18	120.81	113.38
4	X	201	GLN	OXT-C-CA	2.17	120.79	113.38
4	O	201	GLN	OXT-C-CA	2.14	120.69	113.38

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	T	201	GLN	O-C-CA-N
4	R	201	GLN	O-C-CA-N
4	V	201	GLN	O-C-CA-N
4	U	201	GLN	O-C-CA-N
4	P	201	GLN	O-C-CA-N
4	Q	201	GLN	O-C-CA-N
4	N	201	GLN	OXT-C-CA-N

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Mol	Chain	Res	Type	Atoms
4	S	201	GLN	OXT-C-CA-N
4	X	201	GLN	OXT-C-CA-N
4	W	201	GLN	OXT-C-CA-N
4	O	201	GLN	OXT-C-CA-N
4	M	201	GLN	OXT-C-CA-N
4	T	201	GLN	OXT-C-CA-N
4	R	201	GLN	OXT-C-CA-N
4	V	201	GLN	OXT-C-CA-N
4	U	201	GLN	OXT-C-CA-N
4	P	201	GLN	OXT-C-CA-N
4	Q	201	GLN	OXT-C-CA-N
4	N	201	GLN	O-C-CA-N
4	S	201	GLN	O-C-CA-N
4	X	201	GLN	O-C-CA-N
4	W	201	GLN	O-C-CA-N
4	O	201	GLN	O-C-CA-N
4	M	201	GLN	O-C-CA-N
4	X	201	GLN	OXT-C-CA-CB
4	N	201	GLN	OXT-C-CA-CB
4	S	201	GLN	OXT-C-CA-CB
4	W	201	GLN	OXT-C-CA-CB
4	O	201	GLN	OXT-C-CA-CB
4	M	201	GLN	OXT-C-CA-CB
4	N	201	GLN	O-C-CA-CB
4	S	201	GLN	O-C-CA-CB
4	X	201	GLN	O-C-CA-CB
4	W	201	GLN	O-C-CA-CB
4	O	201	GLN	O-C-CA-CB
4	M	201	GLN	O-C-CA-CB

There are no ring outliers.

17 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	U	201	GLN	2	0
4	M	201	GLN	2	0
4	R	201	GLN	2	0
3	K	301	PO4	1	0
3	E	301	PO4	1	0
3	I	301	PO4	2	0
4	S	201	GLN	2	0
4	P	201	GLN	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	PO4	1	0
4	V	201	GLN	2	0
4	O	201	GLN	2	0
4	W	201	GLN	2	0
4	T	201	GLN	2	0
4	N	201	GLN	2	0
4	Q	201	GLN	2	0
5	J	301	SO4	1	0
4	X	201	GLN	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	267/297 (89%)	-0.65	0 100 100	27, 42, 81, 126	0
1	B	267/297 (89%)	-0.63	0 100 100	27, 44, 78, 127	0
1	C	267/297 (89%)	-0.55	3 (1%) 80 55	33, 51, 95, 155	0
1	D	267/297 (89%)	-0.60	0 100 100	36, 56, 96, 155	0
1	E	267/297 (89%)	-0.49	3 (1%) 80 55	36, 61, 115, 159	0
1	F	267/297 (89%)	-0.57	1 (0%) 92 78	29, 51, 88, 139	0
1	G	267/297 (89%)	-0.64	1 (0%) 92 78	23, 38, 81, 131	0
1	H	267/297 (89%)	-0.64	0 100 100	28, 48, 90, 134	0
1	I	267/297 (89%)	-0.59	0 100 100	31, 51, 92, 130	0
1	J	267/297 (89%)	-0.73	0 100 100	30, 50, 84, 121	0
1	K	267/297 (89%)	-0.62	0 100 100	30, 49, 85, 123	0
1	L	267/297 (89%)	-0.66	1 (0%) 92 78	27, 42, 91, 145	0
2	M	187/188 (99%)	-0.48	1 (0%) 91 75	45, 73, 100, 123	0
2	N	187/188 (99%)	-0.53	1 (0%) 91 75	46, 73, 109, 148	0
2	O	187/188 (99%)	-0.17	8 (4%) 35 13	56, 89, 124, 141	0
2	P	187/188 (99%)	-0.17	7 (3%) 41 17	59, 93, 119, 142	0
2	Q	187/188 (99%)	1.12	46 (24%) 0 0	90, 164, 205, 227	0
2	R	187/188 (99%)	-0.35	2 (1%) 80 55	60, 85, 109, 136	0
2	S	187/188 (99%)	-0.50	0 100 100	39, 72, 105, 143	0
2	T	187/188 (99%)	-0.64	0 100 100	36, 63, 88, 103	0
2	U	187/188 (99%)	-0.49	1 (0%) 91 75	56, 84, 114, 139	0
2	V	187/188 (99%)	-0.31	5 (2%) 54 26	58, 87, 113, 134	0
2	W	187/188 (99%)	-0.47	0 100 100	49, 79, 103, 126	0
2	X	187/188 (99%)	-0.52	0 100 100	41, 63, 90, 118	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	5448/5820 (93%)	-0.48	80 (1%)	73	46	23, 61, 119, 227	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Q	135	GLU	9.6
2	Q	160	LEU	6.0
2	Q	96	ASN	5.7
2	Q	85	ILE	5.5
2	Q	154	VAL	5.3
2	Q	64	LEU	5.1
2	Q	161	GLY	5.1
2	Q	59	GLY	4.8
2	Q	84	ASP	4.6
1	C	2	SER	4.4
1	E	3	LYS	4.4
2	O	-1	GLY	4.3
2	Q	60	PHE	4.2
2	O	160	LEU	4.0
2	O	124	ILE	4.0
2	Q	125	GLU	3.8
2	Q	181	HIS	3.7
2	Q	148	ASN	3.6
2	Q	173	ARG	3.5
1	C	4	ILE	3.4
2	Q	-1	GLY	3.4
2	Q	172	TYR	3.3
2	O	115	LEU	3.3
2	Q	123	ASP	3.3
2	Q	115	LEU	3.2
2	P	135	GLU	3.2
2	Q	23	GLY	3.2
2	Q	21	LEU	3.1
1	F	273	GLY	3.1
2	V	40	GLY	3.1
2	Q	58	TYR	3.1
2	Q	120	ILE	3.1
2	Q	152	VAL	3.0
2	Q	147	VAL	3.0
2	Q	151	ILE	2.9
2	Q	153	ALA	2.9
1	C	274	THR	2.9

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Mol	Chain	Res	Type	RSRZ
2	Q	138	GLY	2.9
2	P	153	ALA	2.9
2	V	84	ASP	2.8
2	Q	54	LEU	2.8
2	U	161	GLY	2.8
2	Q	81	LEU	2.8
2	R	124	ILE	2.7
2	Q	87	GLY	2.7
2	P	179	ILE	2.6
2	Q	124	ILE	2.6
2	O	125	GLU	2.6
2	Q	95	LEU	2.6
2	V	71	MET	2.6
2	Q	137	VAL	2.6
2	Q	40	GLY	2.5
2	Q	163	SER	2.5
1	L	56	ALA	2.5
2	P	154	VAL	2.5
2	P	161	GLY	2.4
2	V	176	ASP	2.4
2	Q	94	LYS	2.4
1	E	2	SER	2.4
2	O	72	PHE	2.4
2	O	164	PHE	2.4
2	Q	61	LYS	2.3
2	Q	126	GLY	2.3
2	Q	41	LEU	2.3
2	P	133	HIS	2.3
2	Q	97	ILE	2.3
2	N	-1	GLY	2.2
2	R	160	LEU	2.2
2	O	126	GLY	2.2
2	Q	98	THR	2.2
2	Q	133	HIS	2.2
2	Q	101	ARG	2.2
2	P	177	TYR	2.1
2	Q	32	VAL	2.1
2	Q	63	ALA	2.1
2	M	160	LEU	2.1
1	E	63	ALA	2.1
2	Q	3	ILE	2.1
2	V	135	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	2	SER	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 monosaccharides 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, 95^{th} 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
4	GLN	S	201	10/10	0.82	0.23	68,75,114,120	0
4	GLN	U	201	10/10	0.83	0.28	74,107,119,120	0
4	GLN	R	201	10/10	0.85	0.21	84,94,126,142	0
4	GLN	M	201	10/10	0.87	0.17	57,68,96,99	0
4	GLN	W	201	10/10	0.88	0.15	77,89,103,123	0
4	GLN	V	201	10/10	0.89	0.23	71,99,106,111	0
4	GLN	Q	201	10/10	0.89	0.25	139,151,160,170	0
4	GLN	P	201	10/10	0.90	0.13	75,99,104,117	0
4	GLN	O	201	10/10	0.90	0.24	61,82,107,115	0
4	GLN	N	201	10/10	0.94	0.14	56,69,87,112	0
4	GLN	T	201	10/10	0.94	0.15	40,56,77,78	0
4	GLN	X	201	10/10	0.95	0.16	39,69,75,75	0
3	PO4	L	301	5/5	0.96	0.11	37,45,61,64	0
3	PO4	D	301	5/5	0.96	0.09	47,48,66,89	0
3	PO4	E	301	5/5	0.96	0.14	53,53,69,72	0
3	PO4	I	301	5/5	0.98	0.10	24,34,59,71	0
3	PO4	H	301	5/5	0.98	0.10	32,49,61,74	0
3	PO4	G	301	5/5	0.98	0.12	25,30,58,58	0
3	PO4	B	301	5/5	0.98	0.10	36,37,59,59	0
3	PO4	A	301	5/5	0.98	0.09	32,39,53,59	0
3	PO4	K	301	5/5	0.98	0.11	43,53,62,85	0
3	PO4	F	301	5/5	0.98	0.10	29,40,64,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PO4	C	301	5/5	0.98	0.09	43,45,53,55	0
5	SO4	J	301	5/5	0.99	0.09	42,55,64,85	0

6.5 Other polymers (i)

There are no such residues in this entry.