



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:29 PM GMT

PDB ID : 4LD7
Title : Crystal structure of AnaPT from Neosartorya fischeri
Authors : Zocher, G.; Stehle, T.
Deposited on : 2013-06-24
Resolution : 2.83 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

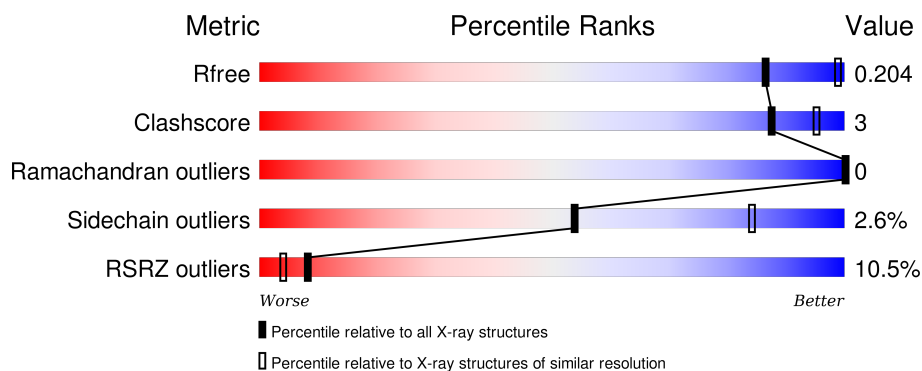
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.83 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3170 (2.88-2.80)
Clashscore	102246	3658 (2.88-2.80)
Ramachandran outliers	100387	3591 (2.88-2.80)
Sidechain outliers	100360	3594 (2.88-2.80)
RSRZ outliers	91569	3184 (2.88-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	445	 2% 83% 6% 11%
1	B	445	 3% 83% 6% 11%
1	C	445	 4% 83% 6% 11%
1	D	445	 3% 82% 7% 11%
1	E	445	 2% 84% 5% 11%

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Mol	Chain	Length	Quality of chain
1	F	445	
1	G	445	
1	H	445	
1	I	445	
1	J	445	
1	K	445	
1	L	445	
1	M	445	
1	N	445	
1	O	445	
1	P	445	

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	NA	D	502	-	-	-	X
3	NA	F	502	-	-	-	X
3	NA	H	502	-	-	-	X
3	NA	J	502	-	-	-	X
3	NA	L	502	-	-	-	X
3	NA	N	502	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 48979 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 Dimethylallyl tryptophan synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3057	1987	502	558	10			
1	B	397	Total	C	N	O	S	0	0	0
			3056	1987	501	558	10			
1	C	397	Total	C	N	O	S	0	0	0
			3058	1987	502	559	10			
1	D	397	Total	C	N	O	S	0	0	0
			3054	1986	499	559	10			
1	E	397	Total	C	N	O	S	0	0	0
			3050	1983	499	558	10			
1	F	397	Total	C	N	O	S	0	0	0
			3056	1985	502	559	10			
1	G	397	Total	C	N	O	S	0	0	0
			3058	1987	502	559	10			
1	H	397	Total	C	N	O	S	0	0	0
			3058	1987	502	559	10			
1	I	397	Total	C	N	O	S	0	0	0
			3056	1987	502	557	10			
1	J	397	Total	C	N	O	S	0	0	0
			3058	1987	502	559	10			
1	K	392	Total	C	N	O	S	0	0	0
			3022	1964	496	552	10			
1	L	397	Total	C	N	O	S	0	0	0
			3058	1987	502	559	10			
1	M	397	Total	C	N	O	S	0	0	0
			3050	1983	498	559	10			
1	N	397	Total	C	N	O	S	0	0	0
			3058	1987	502	559	10			
1	O	391	Total	C	N	O	S	0	0	0
			3012	1957	494	551	10			
1	P	397	Total	C	N	O	S	0	0	0
			3058	1987	502	559	10			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	438	ARG	-	EXPRESSION TAG	UNP A1DN10
A	439	SER	-	EXPRESSION TAG	UNP A1DN10
A	440	HIS	-	EXPRESSION TAG	UNP A1DN10
A	441	HIS	-	EXPRESSION TAG	UNP A1DN10
A	442	HIS	-	EXPRESSION TAG	UNP A1DN10
A	443	HIS	-	EXPRESSION TAG	UNP A1DN10
A	444	HIS	-	EXPRESSION TAG	UNP A1DN10
A	445	HIS	-	EXPRESSION TAG	UNP A1DN10
B	438	ARG	-	EXPRESSION TAG	UNP A1DN10
B	439	SER	-	EXPRESSION TAG	UNP A1DN10
B	440	HIS	-	EXPRESSION TAG	UNP A1DN10
B	441	HIS	-	EXPRESSION TAG	UNP A1DN10
B	442	HIS	-	EXPRESSION TAG	UNP A1DN10
B	443	HIS	-	EXPRESSION TAG	UNP A1DN10
B	444	HIS	-	EXPRESSION TAG	UNP A1DN10
B	445	HIS	-	EXPRESSION TAG	UNP A1DN10
C	438	ARG	-	EXPRESSION TAG	UNP A1DN10
C	439	SER	-	EXPRESSION TAG	UNP A1DN10
C	440	HIS	-	EXPRESSION TAG	UNP A1DN10
C	441	HIS	-	EXPRESSION TAG	UNP A1DN10
C	442	HIS	-	EXPRESSION TAG	UNP A1DN10
C	443	HIS	-	EXPRESSION TAG	UNP A1DN10
C	444	HIS	-	EXPRESSION TAG	UNP A1DN10
C	445	HIS	-	EXPRESSION TAG	UNP A1DN10
D	438	ARG	-	EXPRESSION TAG	UNP A1DN10
D	439	SER	-	EXPRESSION TAG	UNP A1DN10
D	440	HIS	-	EXPRESSION TAG	UNP A1DN10
D	441	HIS	-	EXPRESSION TAG	UNP A1DN10
D	442	HIS	-	EXPRESSION TAG	UNP A1DN10
D	443	HIS	-	EXPRESSION TAG	UNP A1DN10
D	444	HIS	-	EXPRESSION TAG	UNP A1DN10
D	445	HIS	-	EXPRESSION TAG	UNP A1DN10
E	438	ARG	-	EXPRESSION TAG	UNP A1DN10
E	439	SER	-	EXPRESSION TAG	UNP A1DN10
E	440	HIS	-	EXPRESSION TAG	UNP A1DN10
E	441	HIS	-	EXPRESSION TAG	UNP A1DN10
E	442	HIS	-	EXPRESSION TAG	UNP A1DN10
E	443	HIS	-	EXPRESSION TAG	UNP A1DN10
E	444	HIS	-	EXPRESSION TAG	UNP A1DN10
E	445	HIS	-	EXPRESSION TAG	UNP A1DN10
F	438	ARG	-	EXPRESSION TAG	UNP A1DN10
F	439	SER	-	EXPRESSION TAG	UNP A1DN10

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Chain	Residue	Modelled	Actual	Comment	Reference
F	440	HIS	-	EXPRESSION TAG	UNP A1DN10
F	441	HIS	-	EXPRESSION TAG	UNP A1DN10
F	442	HIS	-	EXPRESSION TAG	UNP A1DN10
F	443	HIS	-	EXPRESSION TAG	UNP A1DN10
F	444	HIS	-	EXPRESSION TAG	UNP A1DN10
F	445	HIS	-	EXPRESSION TAG	UNP A1DN10
G	438	ARG	-	EXPRESSION TAG	UNP A1DN10
G	439	SER	-	EXPRESSION TAG	UNP A1DN10
G	440	HIS	-	EXPRESSION TAG	UNP A1DN10
G	441	HIS	-	EXPRESSION TAG	UNP A1DN10
G	442	HIS	-	EXPRESSION TAG	UNP A1DN10
G	443	HIS	-	EXPRESSION TAG	UNP A1DN10
G	444	HIS	-	EXPRESSION TAG	UNP A1DN10
G	445	HIS	-	EXPRESSION TAG	UNP A1DN10
H	438	ARG	-	EXPRESSION TAG	UNP A1DN10
H	439	SER	-	EXPRESSION TAG	UNP A1DN10
H	440	HIS	-	EXPRESSION TAG	UNP A1DN10
H	441	HIS	-	EXPRESSION TAG	UNP A1DN10
H	442	HIS	-	EXPRESSION TAG	UNP A1DN10
H	443	HIS	-	EXPRESSION TAG	UNP A1DN10
H	444	HIS	-	EXPRESSION TAG	UNP A1DN10
H	445	HIS	-	EXPRESSION TAG	UNP A1DN10
I	438	ARG	-	EXPRESSION TAG	UNP A1DN10
I	439	SER	-	EXPRESSION TAG	UNP A1DN10
I	440	HIS	-	EXPRESSION TAG	UNP A1DN10
I	441	HIS	-	EXPRESSION TAG	UNP A1DN10
I	442	HIS	-	EXPRESSION TAG	UNP A1DN10
I	443	HIS	-	EXPRESSION TAG	UNP A1DN10
I	444	HIS	-	EXPRESSION TAG	UNP A1DN10
I	445	HIS	-	EXPRESSION TAG	UNP A1DN10
J	438	ARG	-	EXPRESSION TAG	UNP A1DN10
J	439	SER	-	EXPRESSION TAG	UNP A1DN10
J	440	HIS	-	EXPRESSION TAG	UNP A1DN10
J	441	HIS	-	EXPRESSION TAG	UNP A1DN10
J	442	HIS	-	EXPRESSION TAG	UNP A1DN10
J	443	HIS	-	EXPRESSION TAG	UNP A1DN10
J	444	HIS	-	EXPRESSION TAG	UNP A1DN10
J	445	HIS	-	EXPRESSION TAG	UNP A1DN10
K	438	ARG	-	EXPRESSION TAG	UNP A1DN10
K	439	SER	-	EXPRESSION TAG	UNP A1DN10
K	440	HIS	-	EXPRESSION TAG	UNP A1DN10
K	441	HIS	-	EXPRESSION TAG	UNP A1DN10

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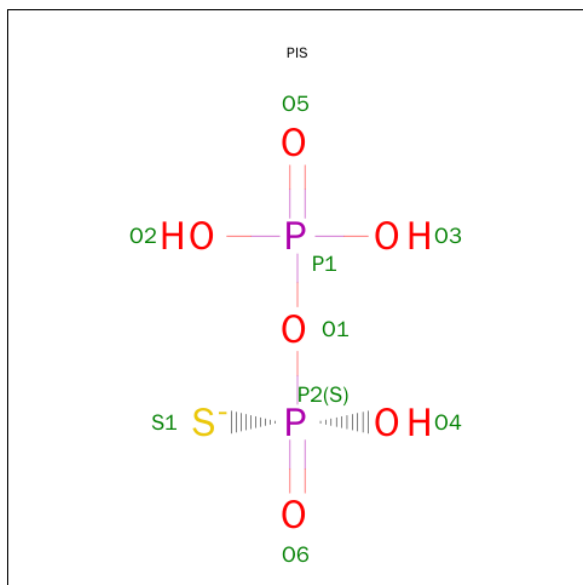
Chain	Residue	Modelled	Actual	Comment	Reference
K	442	HIS	-	EXPRESSION TAG	UNP A1DN10
K	443	HIS	-	EXPRESSION TAG	UNP A1DN10
K	444	HIS	-	EXPRESSION TAG	UNP A1DN10
K	445	HIS	-	EXPRESSION TAG	UNP A1DN10
L	438	ARG	-	EXPRESSION TAG	UNP A1DN10
L	439	SER	-	EXPRESSION TAG	UNP A1DN10
L	440	HIS	-	EXPRESSION TAG	UNP A1DN10
L	441	HIS	-	EXPRESSION TAG	UNP A1DN10
L	442	HIS	-	EXPRESSION TAG	UNP A1DN10
L	443	HIS	-	EXPRESSION TAG	UNP A1DN10
L	444	HIS	-	EXPRESSION TAG	UNP A1DN10
L	445	HIS	-	EXPRESSION TAG	UNP A1DN10
M	438	ARG	-	EXPRESSION TAG	UNP A1DN10
M	439	SER	-	EXPRESSION TAG	UNP A1DN10
M	440	HIS	-	EXPRESSION TAG	UNP A1DN10
M	441	HIS	-	EXPRESSION TAG	UNP A1DN10
M	442	HIS	-	EXPRESSION TAG	UNP A1DN10
M	443	HIS	-	EXPRESSION TAG	UNP A1DN10
M	444	HIS	-	EXPRESSION TAG	UNP A1DN10
M	445	HIS	-	EXPRESSION TAG	UNP A1DN10
N	438	ARG	-	EXPRESSION TAG	UNP A1DN10
N	439	SER	-	EXPRESSION TAG	UNP A1DN10
N	440	HIS	-	EXPRESSION TAG	UNP A1DN10
N	441	HIS	-	EXPRESSION TAG	UNP A1DN10
N	442	HIS	-	EXPRESSION TAG	UNP A1DN10
N	443	HIS	-	EXPRESSION TAG	UNP A1DN10
N	444	HIS	-	EXPRESSION TAG	UNP A1DN10
N	445	HIS	-	EXPRESSION TAG	UNP A1DN10
O	438	ARG	-	EXPRESSION TAG	UNP A1DN10
O	439	SER	-	EXPRESSION TAG	UNP A1DN10
O	440	HIS	-	EXPRESSION TAG	UNP A1DN10
O	441	HIS	-	EXPRESSION TAG	UNP A1DN10
O	442	HIS	-	EXPRESSION TAG	UNP A1DN10
O	443	HIS	-	EXPRESSION TAG	UNP A1DN10
O	444	HIS	-	EXPRESSION TAG	UNP A1DN10
O	445	HIS	-	EXPRESSION TAG	UNP A1DN10
P	438	ARG	-	EXPRESSION TAG	UNP A1DN10
P	439	SER	-	EXPRESSION TAG	UNP A1DN10
P	440	HIS	-	EXPRESSION TAG	UNP A1DN10
P	441	HIS	-	EXPRESSION TAG	UNP A1DN10
P	442	HIS	-	EXPRESSION TAG	UNP A1DN10
P	443	HIS	-	EXPRESSION TAG	UNP A1DN10

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Chain	Residue	Modelled	Actual	Comment	Reference
P	444	HIS	-	EXPRESSION TAG	UNP A1DN10
P	445	HIS	-	EXPRESSION TAG	UNP A1DN10

- Molecule 2 is TRIHYDROGEN THIODIPHOSPHATE (three-letter code: PIS) (formula: $\text{H}_3\text{O}_6\text{P}_2\text{S}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	O	P	S	0	0
			9	6	2	1		
2	B	1	Total	O	P	S	0	0
			9	6	2	1		
2	C	1	Total	O	P	S	0	0
			9	6	2	1		
2	D	1	Total	O	P	S	0	0
			9	6	2	1		
2	E	1	Total	O	P	S	0	0
			9	6	2	1		
2	F	1	Total	O	P	S	0	0
			9	6	2	1		
2	G	1	Total	O	P	S	0	0
			9	6	2	1		
2	H	1	Total	O	P	S	0	0
			9	6	2	1		
2	I	1	Total	O	P	S	0	0
			9	6	2	1		
2	J	1	Total	O	P	S	0	0
			9	6	2	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	K	1	Total	O	P	S	0	0
			9	6	2	1		
2	L	1	Total	O	P	S	0	0
			9	6	2	1		
2	M	1	Total	O	P	S	0	0
			9	6	2	1		
2	N	1	Total	O	P	S	0	0
			9	6	2	1		
2	O	1	Total	O	P	S	0	0
			9	6	2	1		
2	P	1	Total	O	P	S	0	0
			9	6	2	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total	Na	0	0
			1	1		
3	G	1	Total	Na	0	0
			1	1		
3	J	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		
3	K	1	Total	Na	0	0
			1	1		
3	E	1	Total	Na	0	0
			1	1		
3	H	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		
3	I	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		
3	N	1	Total	Na	0	0
			1	1		
3	O	1	Total	Na	0	0
			1	1		

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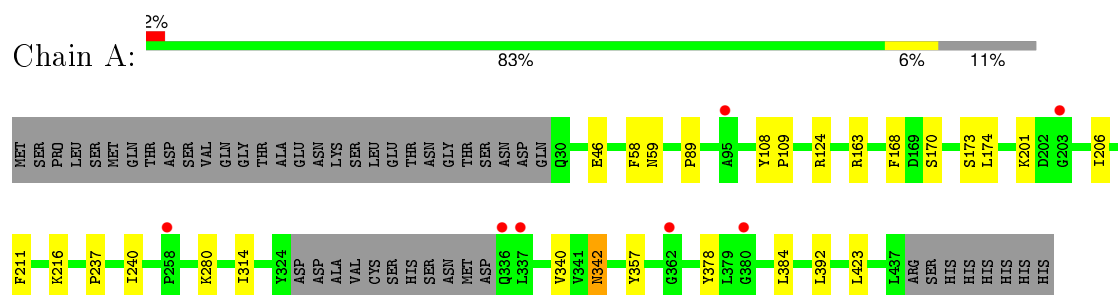
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	1	Total 1	Na 1	0	0
3	F	1	Total 1	Na 1	0	0
3	M	1	Total 1	Na 1	0	0

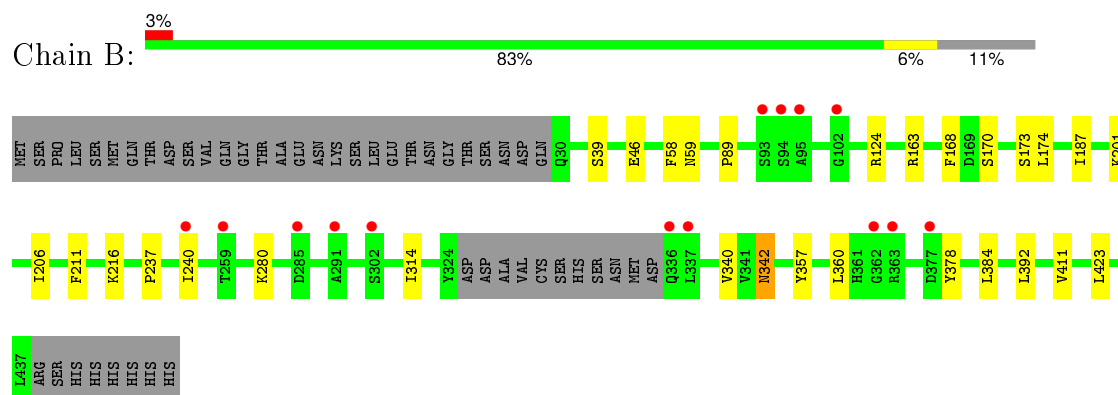
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

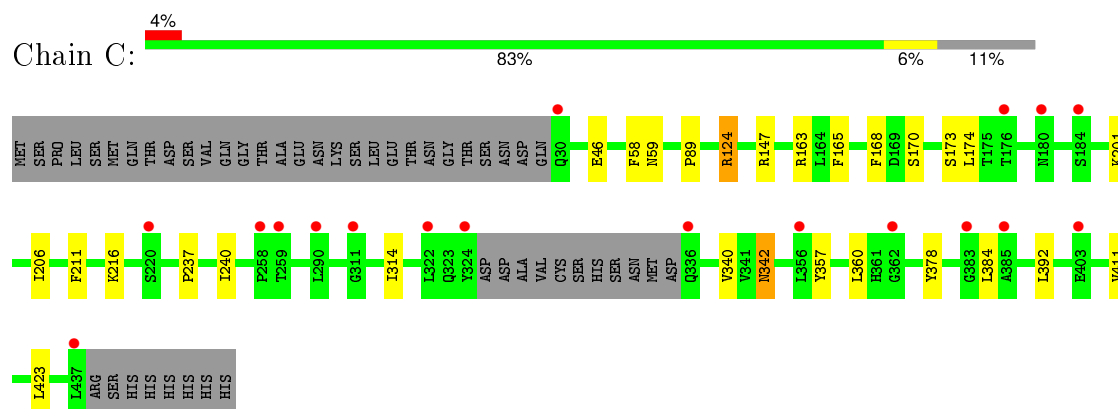
- Molecule 1: Dimethylallyl tryptophan synthase



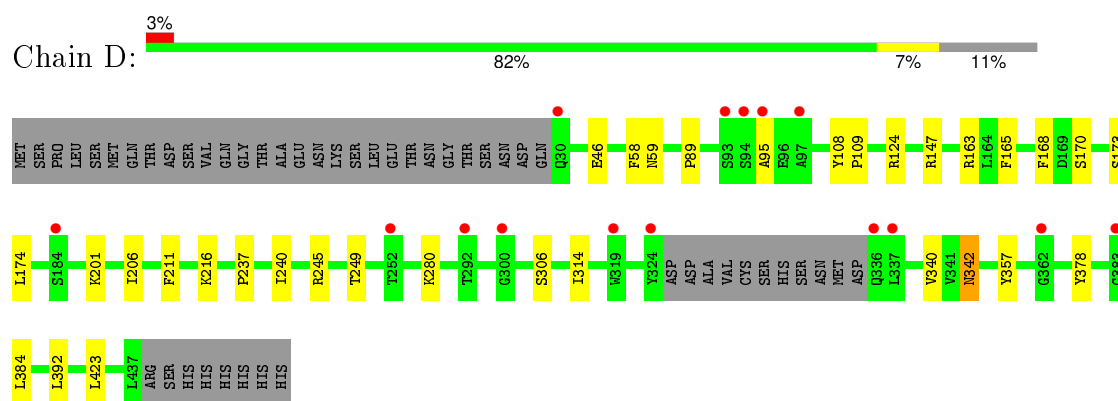
- Molecule 1: Dimethylallyl tryptophan synthase



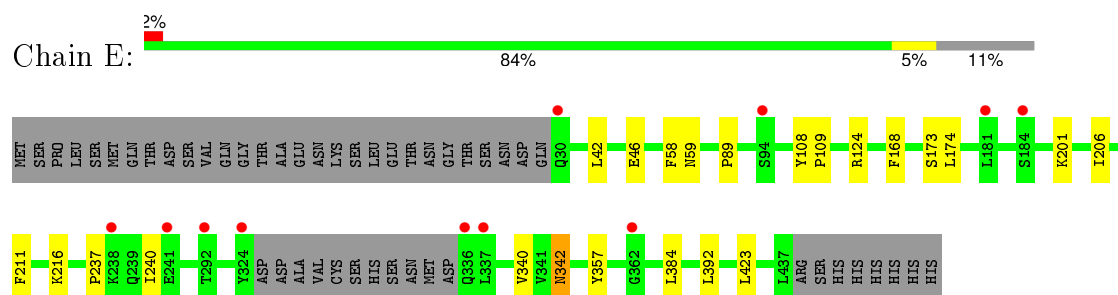
- Molecule 1: Dimethylallyl tryptophan synthase



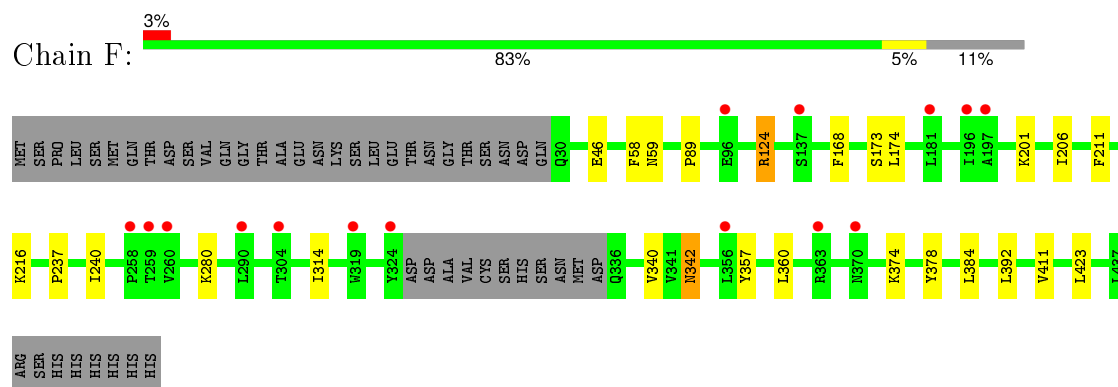
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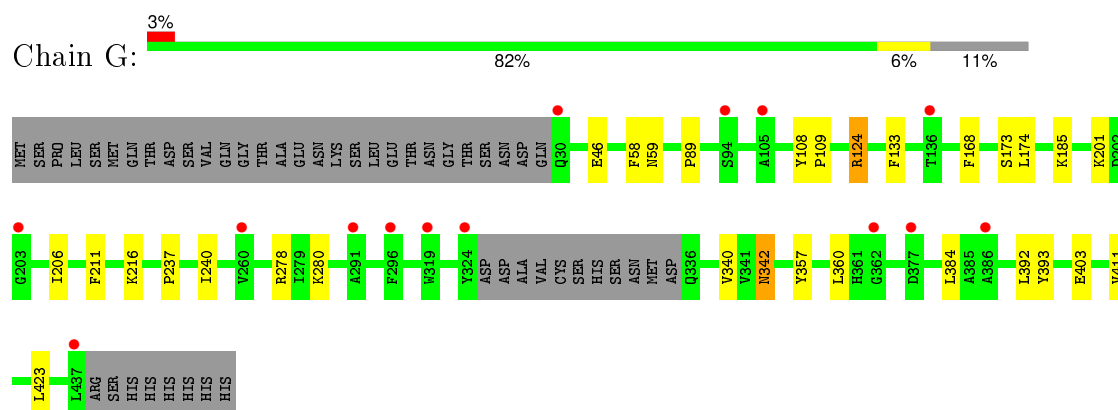
- Molecule 1: Dimethylallyl tryptophan synthase



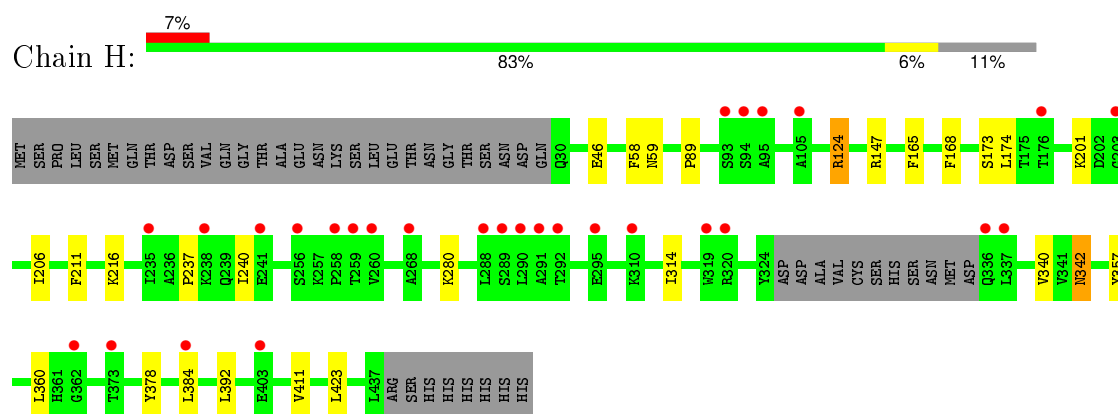
- Molecule 1: Dimethylallyl tryptophan synthase



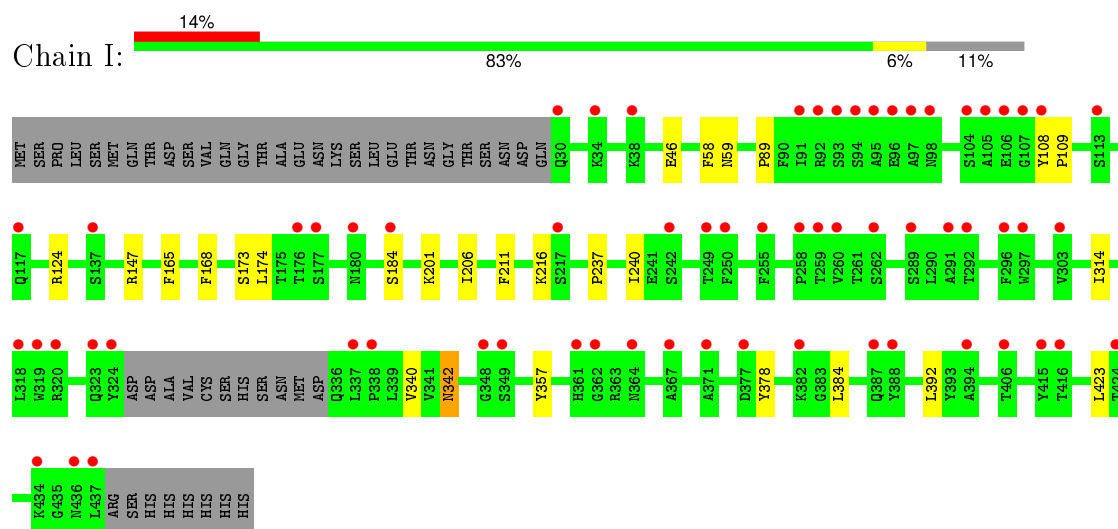
- Molecule 1: Dimethylallyl tryptophan synthase



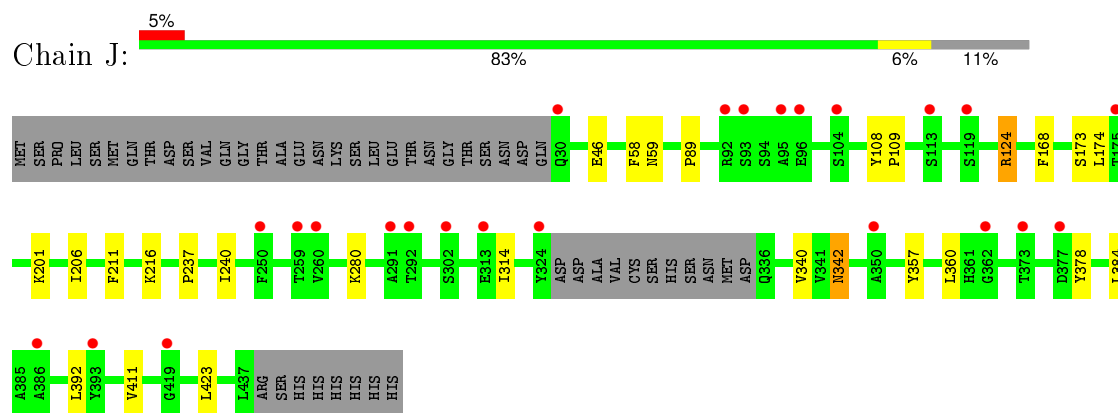
- Molecule 1: Dimethylallyl tryptophan synthase



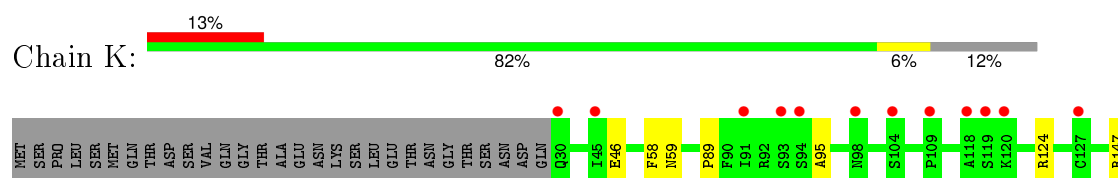
• Molecule 1: Dimethylallyl tryptophan synthase

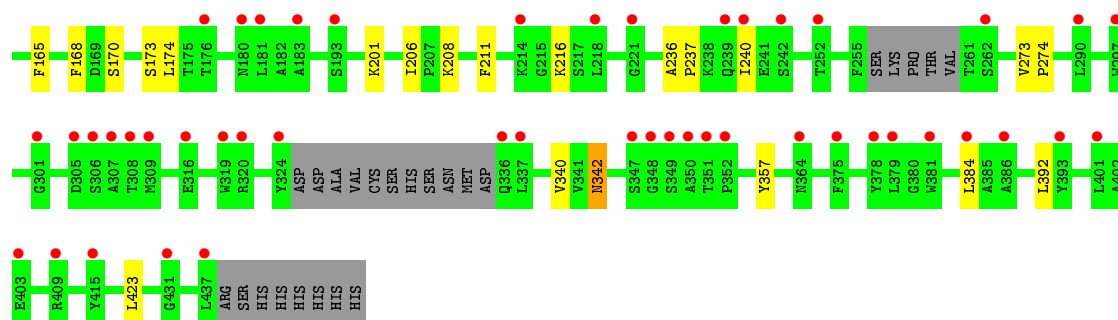


• Molecule 1: Dimethylallyl tryptophan synthase

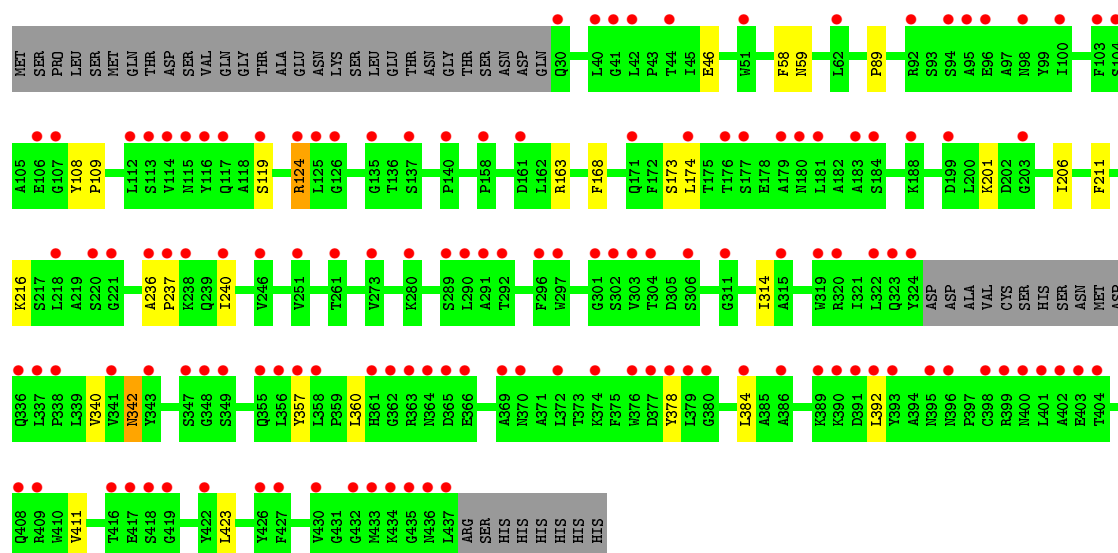
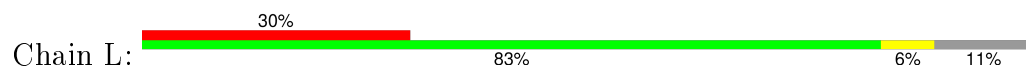


• Molecule 1: Dimethylallyl tryptophan synthase

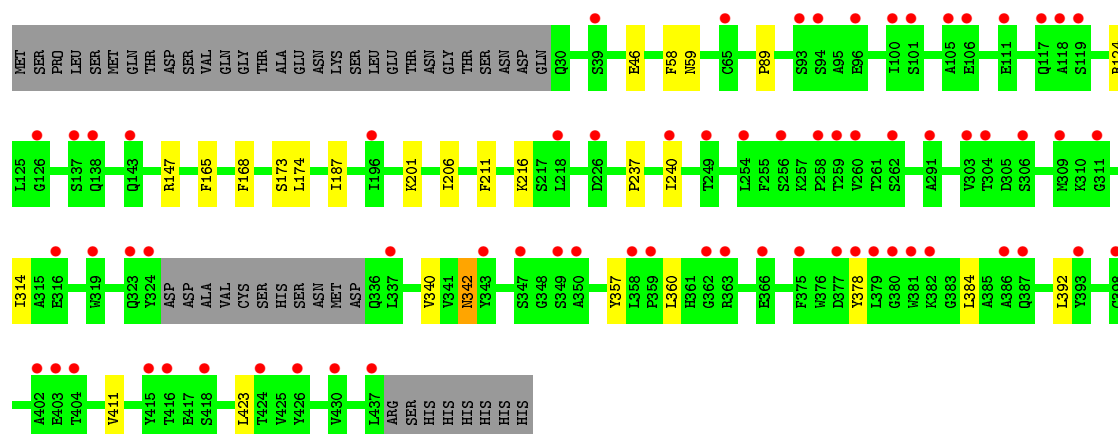
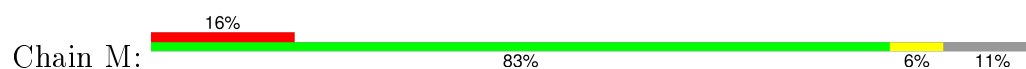




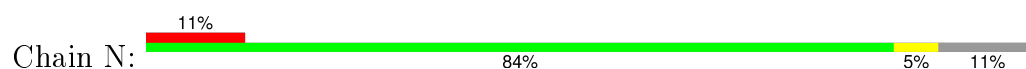
• Molecule 1: Dimethylallyl tryptophan synthase

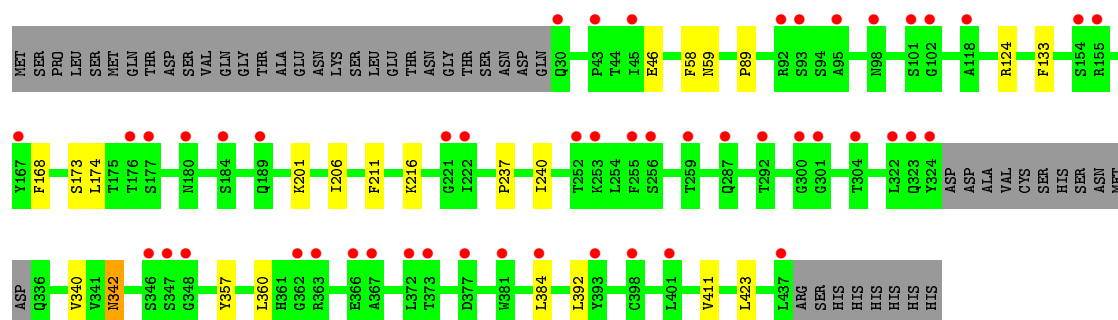


• Molecule 1: Dimethylallyl tryptophan synthase

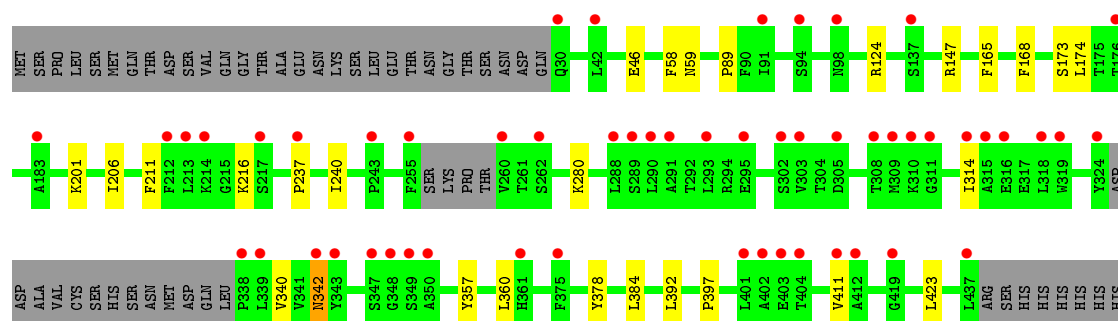
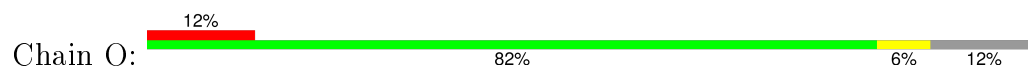


• Molecule 1: Dimethylallyl tryptophan synthase

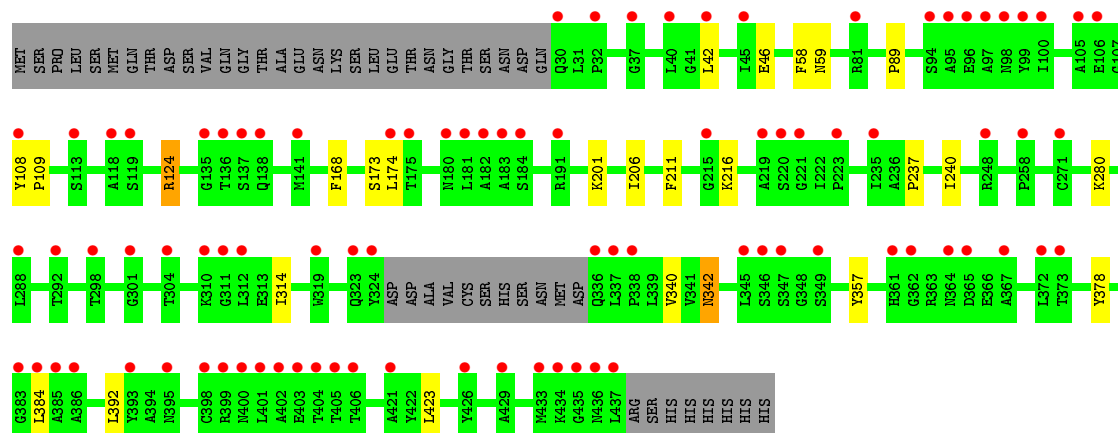
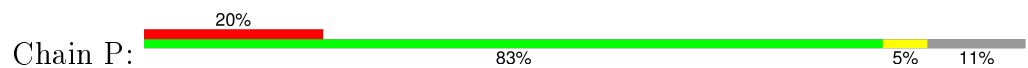




• Molecule 1: Dimethylallyl tryptophan synthase



• Molecule 1: Dimethylallyl tryptophan synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.55Å 242.59Å 145.32Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	39.95 – 2.83 39.95 – 2.83	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.95-2.83) 99.9 (39.95-2.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0044	Depositor
R, R_{free}	0.203 , 0.202 0.202 , 0.204	Depositor DCC
R_{free} test set	3202 reflections (2.04%)	DCC
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 27.6	EDS
Estimated twinning fraction	0.544 for H, K, L 0.456 for -H, -K, L 0.449 for h,-k,-l	Xtriage
Reported twinning fraction	0.544 for H, K, L 0.456 for -H, -K, L	Depositor
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 160059 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	48979	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, PIS

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	0.31	0/3136	0.45	0/4276
1	B	0.32	0/3135	0.45	0/4275
1	C	0.31	0/3137	0.45	0/4277
1	D	0.32	0/3133	0.45	0/4273
1	E	0.31	0/3129	0.45	0/4267
1	F	0.32	0/3135	0.45	0/4275
1	G	0.31	0/3137	0.45	0/4277
1	H	0.32	0/3137	0.45	0/4277
1	I	0.32	0/3135	0.45	0/4275
1	J	0.32	0/3137	0.45	0/4277
1	K	0.32	0/3099	0.45	0/4223
1	L	0.31	0/3137	0.45	0/4277
1	M	0.32	0/3129	0.45	0/4268
1	N	0.32	0/3137	0.45	0/4277
1	O	0.32	0/3089	0.45	0/4210
1	P	0.32	0/3137	0.45	0/4277
All	All	0.32	0/50079	0.45	0/68281

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	3057	0	2943	16	0
1	B	3056	0	2947	17	0
1	C	3058	0	2946	17	0
1	D	3054	0	2942	23	0
1	E	3050	0	2930	13	0
1	F	3056	0	2942	15	0
1	G	3058	0	2946	24	0
1	H	3058	0	2946	15	0
1	I	3056	0	2940	16	0
1	J	3058	0	2946	16	0
1	K	3022	0	2904	20	0
1	L	3058	0	2946	17	0
1	M	3050	0	2928	18	0
1	N	3058	0	2946	12	0
1	O	3012	0	2890	15	0
1	P	3058	0	2946	15	0
2	A	9	0	0	1	0
2	B	9	0	0	1	0
2	C	9	0	0	1	0
2	D	9	0	0	1	0
2	E	9	0	0	0	0
2	F	9	0	0	2	0
2	G	9	0	0	3	0
2	H	9	0	0	2	0
2	I	9	0	0	0	0
2	J	9	0	0	2	0
2	K	9	0	0	1	0
2	L	9	0	0	1	0
2	M	9	0	0	0	0
2	N	9	0	0	0	0
2	O	9	0	0	1	0
2	P	9	0	0	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
All	All	48979	0	46988	247	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 3.

All (247) 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:F:374:LYS:CB	1:L:119:SER:HB3	2.16	0.75
1:D:245:ARG:O	1:D:249:THR:HG23	1.87	0.75
1:G:185:LYS:HB3	1:M:187:ILE:HG21	1.70	0.74
1:D:95:ALA:CB	1:K:95:ALA:HB2	2.18	0.72
1:D:95:ALA:HB2	1:K:95:ALA:HB2	1.71	0.72
1:O:280:LYS:NZ	2:O:501:PIS:O4	2.28	0.66
1:P:124:ARG:NH2	2:P:501:PIS:S1	2.68	0.66
1:G:280:LYS:NZ	2:G:501:PIS:O4	2.29	0.65
1:F:124:ARG:NH2	2:F:501:PIS:S1	2.71	0.64
1:F:168:PHE:HB2	1:F:211:PHE:HE2	1.64	0.63
1:P:168:PHE:HB2	1:P:211:PHE:HE2	1.65	0.62
1:K:168:PHE:HB2	1:K:211:PHE:HE2	1.65	0.62
1:N:168:PHE:HB2	1:N:211:PHE:HE2	1.65	0.62
1:L:168:PHE:HB2	1:L:211:PHE:HE2	1.64	0.62
1:D:168:PHE:HB2	1:D:211:PHE:HE2	1.64	0.62
1:C:168:PHE:HB2	1:C:211:PHE:HE2	1.65	0.62
1:B:168:PHE:HB2	1:B:211:PHE:HE2	1.64	0.62
1:H:168:PHE:HB2	1:H:211:PHE:HE2	1.65	0.61
1:C:163:ARG:O	1:D:170:SER:HB2	2.01	0.61
1:E:168:PHE:HB2	1:E:211:PHE:HE2	1.65	0.61
1:M:168:PHE:HB2	1:M:211:PHE:HE2	1.64	0.61
1:O:168:PHE:HB2	1:O:211:PHE:HE2	1.65	0.60
1:G:168:PHE:HB2	1:G:211:PHE:HE2	1.64	0.60
1:J:168:PHE:HB2	1:J:211:PHE:HE2	1.65	0.60
1:G:403:GLU:OE2	1:O:397:PRO:HB2	2.02	0.60
1:J:124:ARG:NH2	2:J:501:PIS:S1	2.75	0.60
1:I:168:PHE:HB2	1:I:211:PHE:HE2	1.65	0.59
1:A:168:PHE:HB2	1:A:211:PHE:HE2	1.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:ALA:CB	1:K:95:ALA:CB	2.80	0.59
1:D:306:SER:HA	1:G:393:TYR:CE2	2.39	0.57
1:G:185:LYS:HB3	1:M:187:ILE:CG2	2.34	0.56
1:P:342:ASN:HB3	1:P:357:TYR:HE1	1.70	0.56
1:J:342:ASN:HB3	1:J:357:TYR:HE1	1.71	0.56
1:G:342:ASN:HB3	1:G:357:TYR:HE1	1.71	0.56
1:C:124:ARG:NH2	2:C:501:PIS:S1	2.79	0.56
1:A:342:ASN:HB3	1:A:357:TYR:HE1	1.71	0.56
1:O:342:ASN:HB3	1:O:357:TYR:HE1	1.71	0.56
1:K:342:ASN:HB3	1:K:357:TYR:HE1	1.71	0.56
1:E:342:ASN:HB3	1:E:357:TYR:HE1	1.71	0.55
1:F:342:ASN:HB3	1:F:357:TYR:HE1	1.71	0.55
1:A:170:SER:HB2	1:B:163:ARG:O	2.07	0.55
1:C:342:ASN:HB3	1:C:357:TYR:HE1	1.70	0.55
1:F:280:LYS:NZ	2:F:501:PIS:O6	2.40	0.55
1:L:342:ASN:HB3	1:L:357:TYR:HE1	1.70	0.55
1:M:342:ASN:HB3	1:M:357:TYR:HE1	1.71	0.55
1:H:342:ASN:HB3	1:H:357:TYR:HE1	1.71	0.55
1:B:342:ASN:HB3	1:B:357:TYR:HE1	1.72	0.55
1:I:342:ASN:HB3	1:I:357:TYR:HE1	1.71	0.54
1:N:342:ASN:HB3	1:N:357:TYR:HE1	1.71	0.54
1:D:342:ASN:HB3	1:D:357:TYR:HE1	1.72	0.53
1:D:95:ALA:HB2	1:K:95:ALA:CB	2.38	0.53
1:E:168:PHE:HB2	1:E:211:PHE:CE2	2.44	0.53
1:N:168:PHE:HB2	1:N:211:PHE:CE2	2.45	0.52
1:K:201:LYS:HD3	1:K:206:ILE:HD12	1.91	0.52
1:E:201:LYS:HD3	1:E:206:ILE:HD12	1.92	0.52
1:K:168:PHE:HB2	1:K:211:PHE:CE2	2.45	0.52
1:I:201:LYS:HD3	1:I:206:ILE:HD12	1.92	0.52
1:N:201:LYS:HD3	1:N:206:ILE:HD12	1.92	0.52
1:M:168:PHE:HB2	1:M:211:PHE:CE2	2.45	0.52
1:P:201:LYS:HD3	1:P:206:ILE:HD12	1.92	0.52
1:D:168:PHE:HB2	1:D:211:PHE:CE2	2.44	0.52
1:M:201:LYS:HD3	1:M:206:ILE:HD12	1.92	0.52
1:A:201:LYS:HD3	1:A:206:ILE:HD12	1.92	0.52
1:F:201:LYS:HD3	1:F:206:ILE:HD12	1.92	0.51
1:J:201:LYS:HD3	1:J:206:ILE:HD12	1.92	0.51
1:L:168:PHE:HB2	1:L:211:PHE:CE2	2.45	0.51
1:F:168:PHE:HB2	1:F:211:PHE:CE2	2.45	0.51
1:C:168:PHE:HB2	1:C:211:PHE:CE2	2.44	0.51
1:H:201:LYS:HD3	1:H:206:ILE:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:201:LYS:HD3	1:O:206:ILE:HD12	1.92	0.51
1:B:168:PHE:HB2	1:B:211:PHE:CE2	2.44	0.51
1:G:201:LYS:HD3	1:G:206:ILE:HD12	1.91	0.51
1:H:168:PHE:HB2	1:H:211:PHE:CE2	2.45	0.51
1:C:201:LYS:HD3	1:C:206:ILE:HD12	1.93	0.51
1:D:201:LYS:HD3	1:D:206:ILE:HD12	1.92	0.50
1:L:201:LYS:HD3	1:L:206:ILE:HD12	1.92	0.50
1:J:168:PHE:HB2	1:J:211:PHE:CE2	2.45	0.50
1:H:280:LYS:NZ	2:H:501:PIS:O6	2.45	0.50
1:O:168:PHE:HB2	1:O:211:PHE:CE2	2.45	0.50
1:G:168:PHE:HB2	1:G:211:PHE:CE2	2.44	0.50
1:I:237:PRO:HD2	1:I:240:ILE:HG12	1.94	0.50
1:M:237:PRO:HD2	1:M:240:ILE:HG12	1.94	0.50
1:B:201:LYS:HD3	1:B:206:ILE:HD12	1.92	0.50
1:D:280:LYS:NZ	2:D:501:PIS:O6	2.45	0.50
1:H:237:PRO:HD2	1:H:240:ILE:HG12	1.94	0.50
1:C:237:PRO:HD2	1:C:240:ILE:HG12	1.94	0.49
1:F:237:PRO:HD2	1:F:240:ILE:HG12	1.93	0.49
1:P:168:PHE:HB2	1:P:211:PHE:CE2	2.45	0.49
1:L:237:PRO:HD2	1:L:240:ILE:HG12	1.94	0.49
1:J:237:PRO:HD2	1:J:240:ILE:HG12	1.94	0.49
1:N:237:PRO:HD2	1:N:240:ILE:HG12	1.94	0.49
1:B:187:ILE:HG21	1:I:184:SER:O	2.12	0.49
1:A:280:LYS:NZ	2:A:501:PIS:O6	2.45	0.49
1:P:237:PRO:HD2	1:P:240:ILE:HG12	1.94	0.49
1:O:237:PRO:HD2	1:O:240:ILE:HG12	1.94	0.49
1:I:168:PHE:HB2	1:I:211:PHE:CE2	2.45	0.49
1:L:124:ARG:NH2	2:L:501:PIS:S1	2.85	0.49
1:G:185:LYS:CB	1:M:187:ILE:HG21	2.40	0.49
1:A:168:PHE:HB2	1:A:211:PHE:CE2	2.45	0.48
1:D:237:PRO:HD2	1:D:240:ILE:HG12	1.95	0.48
1:E:237:PRO:HD2	1:E:240:ILE:HG12	1.95	0.48
1:K:237:PRO:HD2	1:K:240:ILE:HG12	1.94	0.48
1:G:237:PRO:HD2	1:G:240:ILE:HG12	1.94	0.48
1:B:237:PRO:HD2	1:B:240:ILE:HG12	1.94	0.48
1:E:42:LEU:O	1:G:133:PHE:CZ	2.66	0.48
1:G:124:ARG:NH2	2:G:501:PIS:S1	2.86	0.48
1:A:237:PRO:HD2	1:A:240:ILE:HG12	1.95	0.47
1:D:174:LEU:HD21	1:D:216:LYS:HA	1.97	0.47
1:E:174:LEU:HD21	1:E:216:LYS:HA	1.97	0.47
1:M:174:LEU:HD21	1:M:216:LYS:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:174:LEU:HD21	1:I:216:LYS:HA	1.97	0.47
1:K:174:LEU:HD21	1:K:216:LYS:HA	1.97	0.46
1:L:174:LEU:HD21	1:L:216:LYS:HA	1.97	0.46
1:C:174:LEU:HD21	1:C:216:LYS:HA	1.96	0.46
1:B:280:LYS:NZ	2:B:501:PIS:O4	2.49	0.46
1:O:174:LEU:HD21	1:O:216:LYS:HA	1.97	0.46
1:J:174:LEU:HD21	1:J:216:LYS:HA	1.97	0.46
1:H:174:LEU:HD21	1:H:216:LYS:HA	1.96	0.46
1:G:174:LEU:HD21	1:G:216:LYS:HA	1.98	0.46
1:B:174:LEU:HD21	1:B:216:LYS:HA	1.97	0.46
1:E:42:LEU:O	1:G:133:PHE:CE1	2.69	0.45
1:H:46:GLU:HG2	1:H:89:PRO:HA	1.98	0.45
1:A:46:GLU:HG2	1:A:89:PRO:HA	1.99	0.45
1:N:46:GLU:HG2	1:N:89:PRO:HA	1.99	0.45
1:P:174:LEU:HD21	1:P:216:LYS:HA	1.97	0.45
1:J:46:GLU:HG2	1:J:89:PRO:HA	1.99	0.45
1:A:174:LEU:HD21	1:A:216:LYS:HA	1.97	0.45
1:F:340:VAL:HB	1:F:357:TYR:HB2	1.99	0.45
1:N:168:PHE:CB	1:N:211:PHE:HE2	2.30	0.45
1:N:174:LEU:HD21	1:N:216:LYS:HA	1.97	0.45
1:P:46:GLU:HG2	1:P:89:PRO:HA	1.99	0.45
1:I:46:GLU:HG2	1:I:89:PRO:HA	1.99	0.45
1:A:168:PHE:CB	1:A:211:PHE:HE2	2.30	0.45
1:L:340:VAL:HB	1:L:357:TYR:HB2	1.99	0.45
1:B:187:ILE:HD13	1:I:184:SER:O	2.16	0.45
1:M:340:VAL:HB	1:M:357:TYR:HB2	1.99	0.45
1:F:174:LEU:HD21	1:F:216:LYS:HA	1.97	0.45
1:F:46:GLU:HG2	1:F:89:PRO:HA	1.99	0.45
1:O:340:VAL:HB	1:O:357:TYR:HB2	1.99	0.44
1:M:46:GLU:HG2	1:M:89:PRO:HA	1.99	0.44
1:A:340:VAL:HB	1:A:357:TYR:HB2	1.99	0.44
1:D:340:VAL:HB	1:D:357:TYR:HB2	2.00	0.44
1:G:108:TYR:HA	1:G:109:PRO:HD3	1.85	0.44
1:K:168:PHE:CB	1:K:211:PHE:HE2	2.30	0.44
1:K:46:GLU:HG2	1:K:89:PRO:HA	1.99	0.44
1:D:108:TYR:HA	1:D:109:PRO:HD3	1.85	0.44
1:G:46:GLU:HG2	1:G:89:PRO:HA	1.99	0.44
1:O:46:GLU:HG2	1:O:89:PRO:HA	1.99	0.44
1:B:340:VAL:HB	1:B:357:TYR:HB2	2.00	0.44
1:E:46:GLU:HG2	1:E:89:PRO:HA	1.98	0.44
1:C:46:GLU:HG2	1:C:89:PRO:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:PHE:CB	1:C:211:PHE:HE2	2.29	0.44
1:B:46:GLU:HG2	1:B:89:PRO:HA	1.99	0.44
1:L:46:GLU:HG2	1:L:89:PRO:HA	1.99	0.44
1:B:168:PHE:CB	1:B:211:PHE:HE2	2.30	0.44
1:G:340:VAL:HB	1:G:357:TYR:HB2	1.99	0.44
1:E:340:VAL:HB	1:E:357:TYR:HB2	2.00	0.44
1:P:168:PHE:CB	1:P:211:PHE:HE2	2.30	0.43
1:G:168:PHE:CB	1:G:211:PHE:HE2	2.29	0.43
1:J:340:VAL:HB	1:J:357:TYR:HB2	1.99	0.43
1:D:46:GLU:HG2	1:D:89:PRO:HA	1.99	0.43
1:K:208:LYS:NZ	2:K:501:PIS:O2	2.51	0.43
1:H:340:VAL:HB	1:H:357:TYR:HB2	2.00	0.43
1:N:340:VAL:HB	1:N:357:TYR:HB2	1.99	0.43
1:I:168:PHE:CB	1:I:211:PHE:HE2	2.30	0.43
1:P:340:VAL:HB	1:P:357:TYR:HB2	1.99	0.43
1:I:340:VAL:HB	1:I:357:TYR:HB2	1.99	0.43
1:I:108:TYR:HA	1:I:109:PRO:HD3	1.85	0.43
1:J:108:TYR:HA	1:J:109:PRO:HD3	1.85	0.43
1:G:168:PHE:CB	1:G:211:PHE:CE2	3.02	0.43
1:K:340:VAL:HB	1:K:357:TYR:HB2	1.99	0.43
1:C:168:PHE:CB	1:C:211:PHE:CE2	3.02	0.43
1:E:168:PHE:CB	1:E:211:PHE:CE2	3.02	0.43
1:C:340:VAL:HB	1:C:357:TYR:HB2	1.99	0.43
1:L:108:TYR:HA	1:L:109:PRO:HD3	1.85	0.43
1:K:168:PHE:CB	1:K:211:PHE:CE2	3.02	0.42
1:B:168:PHE:CB	1:B:211:PHE:CE2	3.02	0.42
1:M:168:PHE:CB	1:M:211:PHE:HE2	2.29	0.42
1:E:168:PHE:CB	1:E:211:PHE:HE2	2.30	0.42
1:M:168:PHE:CB	1:M:211:PHE:CE2	3.02	0.42
1:L:168:PHE:CB	1:L:211:PHE:CE2	3.02	0.42
1:A:108:TYR:HA	1:A:109:PRO:HD3	1.85	0.42
1:E:108:TYR:HA	1:E:109:PRO:HD3	1.85	0.42
1:A:168:PHE:CB	1:A:211:PHE:CE2	3.02	0.42
1:D:168:PHE:CB	1:D:211:PHE:HE2	2.30	0.42
1:H:168:PHE:CB	1:H:211:PHE:HE2	2.30	0.42
1:H:168:PHE:CB	1:H:211:PHE:CE2	3.03	0.42
1:F:168:PHE:CB	1:F:211:PHE:CE2	3.02	0.42
1:J:168:PHE:CB	1:J:211:PHE:CE2	3.03	0.42
1:O:168:PHE:CB	1:O:211:PHE:HE2	2.30	0.42
1:C:170:SER:HB2	1:D:163:ARG:O	2.19	0.42
1:P:314:ILE:HG23	1:P:378:TYR:HE2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:168:PHE:CB	1:P:211:PHE:CE2	3.02	0.42
1:I:168:PHE:CB	1:I:211:PHE:CE2	3.03	0.42
1:J:342:ASN:HB3	1:J:357:TYR:CE1	2.54	0.42
1:G:342:ASN:HB3	1:G:357:TYR:CE1	2.54	0.42
1:K:273:VAL:HA	1:K:274:PRO:HD3	1.96	0.41
1:L:168:PHE:CB	1:L:211:PHE:HE2	2.30	0.41
1:M:342:ASN:HB3	1:M:357:TYR:CE1	2.54	0.41
1:O:360:LEU:HD11	1:O:411:VAL:HG13	2.03	0.41
1:D:95:ALA:HB3	1:K:95:ALA:CB	2.50	0.41
1:G:278:ARG:NH2	2:G:501:PIS:O3	2.53	0.41
1:A:314:ILE:HG23	1:A:378:TYR:HE2	1.86	0.41
1:G:185:LYS:O	1:M:187:ILE:HG22	2.21	0.41
1:O:168:PHE:CB	1:O:211:PHE:CE2	3.03	0.41
1:J:168:PHE:CB	1:J:211:PHE:HE2	2.30	0.41
1:I:342:ASN:HB3	1:I:357:TYR:CE1	2.54	0.41
1:H:314:ILE:HG23	1:H:378:TYR:HE2	1.86	0.41
1:L:314:ILE:HG23	1:L:378:TYR:HE2	1.86	0.41
1:F:314:ILE:HG23	1:F:378:TYR:HE2	1.86	0.41
1:K:170:SER:HB2	1:L:163:ARG:O	2.21	0.41
1:M:147:ARG:HD3	1:M:165:PHE:CE1	2.56	0.41
1:C:314:ILE:HG23	1:C:378:TYR:HE2	1.86	0.41
1:M:314:ILE:HG23	1:M:378:TYR:HE2	1.86	0.41
1:L:360:LEU:HD11	1:L:411:VAL:HG13	2.03	0.41
1:D:314:ILE:HG23	1:D:378:TYR:HE2	1.86	0.41
1:J:360:LEU:HD11	1:J:411:VAL:HG13	2.03	0.41
1:N:168:PHE:CB	1:N:211:PHE:CE2	3.02	0.41
1:D:168:PHE:CB	1:D:211:PHE:CE2	3.02	0.41
1:A:342:ASN:HB3	1:A:357:TYR:CE1	2.54	0.41
1:C:342:ASN:HB3	1:C:357:TYR:CE1	2.53	0.41
1:K:236:ALA:HA	1:K:237:PRO:HD3	1.96	0.41
1:K:147:ARG:HD3	1:K:165:PHE:CE1	2.56	0.41
1:O:314:ILE:HG23	1:O:378:TYR:HE2	1.86	0.41
1:N:133:PHE:CZ	1:P:42:LEU:O	2.74	0.41
1:P:108:TYR:HA	1:P:109:PRO:HD3	1.85	0.41
1:A:163:ARG:O	1:B:170:SER:HB2	2.21	0.41
1:P:280:LYS:NZ	2:P:501:PIS:O6	2.54	0.40
1:L:236:ALA:HA	1:L:237:PRO:HD3	1.96	0.40
1:I:147:ARG:HD3	1:I:165:PHE:CE1	2.57	0.40
1:M:360:LEU:HD11	1:M:411:VAL:HG13	2.03	0.40
1:H:147:ARG:HD3	1:H:165:PHE:CE1	2.56	0.40
1:F:360:LEU:HD11	1:F:411:VAL:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:168:PHE:CB	1:F:211:PHE:HE2	2.30	0.40
1:J:280:LYS:NZ	2:J:501:PIS:O4	2.54	0.40
1:H:360:LEU:HD11	1:H:411:VAL:HG13	2.03	0.40
1:G:360:LEU:HD11	1:G:411:VAL:HG13	2.03	0.40
1:H:124:ARG:NH2	2:H:501:PIS:S1	2.94	0.40
1:B:314:ILE:HG23	1:B:378:TYR:HE2	1.86	0.40
1:B:360:LEU:HD11	1:B:411:VAL:HG13	2.04	0.40
1:O:147:ARG:HD3	1:O:165:PHE:CE1	2.57	0.40
1:J:314:ILE:HG23	1:J:378:TYR:HE2	1.86	0.40
1:I:314:ILE:HG23	1:I:378:TYR:HE2	1.86	0.40
1:N:360:LEU:HD11	1:N:411:VAL:HG13	2.03	0.40
1:D:147:ARG:HD3	1:D:165:PHE:CE1	2.57	0.40
1:C:147:ARG:HD3	1:C:165:PHE:CE1	2.57	0.40
1:C:360:LEU:HD11	1:C:411:VAL:HG13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	393/445 (88%)	387 (98%)	6 (2%)	0	100	100
1	B	393/445 (88%)	387 (98%)	6 (2%)	0	100	100
1	C	393/445 (88%)	387 (98%)	6 (2%)	0	100	100
1	D	393/445 (88%)	387 (98%)	6 (2%)	0	100	100
1	E	393/445 (88%)	387 (98%)	6 (2%)	0	100	100
1	F	393/445 (88%)	386 (98%)	7 (2%)	0	100	100
1	G	393/445 (88%)	387 (98%)	6 (2%)	0	100	100
1	H	393/445 (88%)	387 (98%)	6 (2%)	0	100	100
1	I	393/445 (88%)	387 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	393/445 (88%)	387 (98%)	6 (2%)	0	100	100
1	K	386/445 (87%)	380 (98%)	6 (2%)	0	100	100
1	L	393/445 (88%)	387 (98%)	6 (2%)	0	100	100
1	M	393/445 (88%)	386 (98%)	7 (2%)	0	100	100
1	N	393/445 (88%)	387 (98%)	6 (2%)	0	100	100
1	O	385/445 (86%)	379 (98%)	6 (2%)	0	100	100
1	P	393/445 (88%)	387 (98%)	6 (2%)	0	100	100
All	All	6273/7120 (88%)	6175 (98%)	98 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	307/382 (80%)	299 (97%)	8 (3%)	54	84
1	B	308/382 (81%)	299 (97%)	9 (3%)	50	81
1	C	308/382 (81%)	300 (97%)	8 (3%)	54	84
1	D	308/382 (81%)	300 (97%)	8 (3%)	54	84
1	E	306/382 (80%)	298 (97%)	8 (3%)	54	84
1	F	308/382 (81%)	300 (97%)	8 (3%)	54	84
1	G	308/382 (81%)	300 (97%)	8 (3%)	54	84
1	H	308/382 (81%)	300 (97%)	8 (3%)	54	84
1	I	306/382 (80%)	298 (97%)	8 (3%)	54	84
1	J	308/382 (81%)	300 (97%)	8 (3%)	54	84
1	K	303/382 (79%)	295 (97%)	8 (3%)	54	84
1	L	308/382 (81%)	300 (97%)	8 (3%)	54	84
1	M	306/382 (80%)	298 (97%)	8 (3%)	54	84
1	N	308/382 (81%)	300 (97%)	8 (3%)	54	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	302/382 (79%)	294 (97%)	8 (3%)	54	84
1	P	308/382 (81%)	300 (97%)	8 (3%)	54	84
All	All	4910/6112 (80%)	4781 (97%)	129 (3%)	54	84

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	PHE
1	A	59	ASN
1	A	124	ARG
1	A	173	SER
1	A	342	ASN
1	A	384	LEU
1	A	392	LEU
1	A	423	LEU
1	B	39	SER
1	B	58	PHE
1	B	59	ASN
1	B	124	ARG
1	B	173	SER
1	B	342	ASN
1	B	384	LEU
1	B	392	LEU
1	B	423	LEU
1	C	58	PHE
1	C	59	ASN
1	C	124	ARG
1	C	173	SER
1	C	342	ASN
1	C	384	LEU
1	C	392	LEU
1	C	423	LEU
1	D	58	PHE
1	D	59	ASN
1	D	124	ARG
1	D	173	SER
1	D	342	ASN
1	D	384	LEU
1	D	392	LEU
1	D	423	LEU
1	E	58	PHE

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Mol	Chain	Res	Type
1	E	59	ASN
1	E	124	ARG
1	E	173	SER
1	E	342	ASN
1	E	384	LEU
1	E	392	LEU
1	E	423	LEU
1	F	58	PHE
1	F	59	ASN
1	F	124	ARG
1	F	173	SER
1	F	342	ASN
1	F	384	LEU
1	F	392	LEU
1	F	423	LEU
1	G	58	PHE
1	G	59	ASN
1	G	124	ARG
1	G	173	SER
1	G	342	ASN
1	G	384	LEU
1	G	392	LEU
1	G	423	LEU
1	H	58	PHE
1	H	59	ASN
1	H	124	ARG
1	H	173	SER
1	H	342	ASN
1	H	384	LEU
1	H	392	LEU
1	H	423	LEU
1	I	58	PHE
1	I	59	ASN
1	I	124	ARG
1	I	173	SER
1	I	342	ASN
1	I	384	LEU
1	I	392	LEU
1	I	423	LEU
1	J	58	PHE
1	J	59	ASN
1	J	124	ARG

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Mol	Chain	Res	Type
1	J	173	SER
1	J	342	ASN
1	J	384	LEU
1	J	392	LEU
1	J	423	LEU
1	K	58	PHE
1	K	59	ASN
1	K	124	ARG
1	K	173	SER
1	K	342	ASN
1	K	384	LEU
1	K	392	LEU
1	K	423	LEU
1	L	58	PHE
1	L	59	ASN
1	L	124	ARG
1	L	173	SER
1	L	342	ASN
1	L	384	LEU
1	L	392	LEU
1	L	423	LEU
1	M	58	PHE
1	M	59	ASN
1	M	124	ARG
1	M	173	SER
1	M	342	ASN
1	M	384	LEU
1	M	392	LEU
1	M	423	LEU
1	N	58	PHE
1	N	59	ASN
1	N	124	ARG
1	N	173	SER
1	N	342	ASN
1	N	384	LEU
1	N	392	LEU
1	N	423	LEU
1	O	58	PHE
1	O	59	ASN
1	O	124	ARG
1	O	173	SER
1	O	342	ASN

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Mol	Chain	Res	Type
1	O	384	LEU
1	O	392	LEU
1	O	423	LEU
1	P	58	PHE
1	P	59	ASN
1	P	124	ARG
1	P	173	SER
1	P	342	ASN
1	P	384	LEU
1	P	392	LEU
1	P	423	LEU

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

Mol	Chain	Res	Type
1	E	355	GLN
1	G	98	ASN
1	N	98	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 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	PIS	A	501	-	4,8,8	0.75	0	9,13,13	1.54	2 (22%)
2	PIS	B	501	-	4,8,8	0.75	0	9,13,13	1.69	3 (33%)
2	PIS	C	501	-	4,8,8	0.85	0	9,13,13	1.47	2 (22%)
2	PIS	D	501	-	4,8,8	0.86	0	9,13,13	1.62	2 (22%)
2	PIS	E	501	-	4,8,8	0.64	0	9,13,13	1.38	2 (22%)
2	PIS	F	501	-	4,8,8	0.78	0	9,13,13	1.59	3 (33%)
2	PIS	G	501	-	4,8,8	0.73	0	9,13,13	1.62	2 (22%)
2	PIS	H	501	-	4,8,8	0.77	0	9,13,13	1.51	2 (22%)
2	PIS	I	501	-	4,8,8	0.72	0	9,13,13	1.55	2 (22%)
2	PIS	J	501	-	4,8,8	0.81	0	9,13,13	1.61	3 (33%)
2	PIS	K	501	-	4,8,8	0.69	0	9,13,13	1.50	2 (22%)
2	PIS	L	501	-	4,8,8	0.72	0	9,13,13	1.50	2 (22%)
2	PIS	M	501	-	4,8,8	0.67	0	9,13,13	1.67	2 (22%)
2	PIS	N	501	-	4,8,8	0.73	0	9,13,13	1.52	2 (22%)
2	PIS	O	501	-	4,8,8	0.67	0	9,13,13	1.57	2 (22%)
2	PIS	P	501	-	4,8,8	0.78	0	9,13,13	1.51	2 (22%)

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
2	PIS	A	501	-	-	0/5/6/6	0/0/0/0
2	PIS	B	501	-	-	0/5/6/6	0/0/0/0
2	PIS	C	501	-	-	0/5/6/6	0/0/0/0
2	PIS	D	501	-	-	0/5/6/6	0/0/0/0
2	PIS	E	501	-	-	0/5/6/6	0/0/0/0
2	PIS	F	501	-	-	0/5/6/6	0/0/0/0
2	PIS	G	501	-	-	0/5/6/6	0/0/0/0
2	PIS	H	501	-	-	0/5/6/6	0/0/0/0
2	PIS	I	501	-	-	0/5/6/6	0/0/0/0
2	PIS	J	501	-	-	0/5/6/6	0/0/0/0
2	PIS	K	501	-	-	0/5/6/6	0/0/0/0
2	PIS	L	501	-	-	0/5/6/6	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PIS	M	501	-	-	0/5/6/6	0/0/0/0
2	PIS	N	501	-	-	0/5/6/6	0/0/0/0
2	PIS	O	501	-	-	0/5/6/6	0/0/0/0
2	PIS	P	501	-	-	0/5/6/6	0/0/0/0

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	501	PIS	P1-O1-P2	-3.51	120.91	132.67
2	B	501	PIS	P1-O1-P2	-3.31	121.58	132.67
2	G	501	PIS	P1-O1-P2	-3.26	121.75	132.67
2	D	501	PIS	P1-O1-P2	-3.20	121.93	132.67
2	I	501	PIS	P1-O1-P2	-3.19	121.97	132.67
2	A	501	PIS	P1-O1-P2	-3.13	122.19	132.67
2	K	501	PIS	P1-O1-P2	-3.12	122.22	132.67
2	J	501	PIS	P1-O1-P2	-3.10	122.29	132.67
2	F	501	PIS	P1-O1-P2	-3.06	122.39	132.67
2	O	501	PIS	P1-O1-P2	-3.04	122.47	132.67
2	L	501	PIS	P1-O1-P2	-3.02	122.55	132.67
2	N	501	PIS	P1-O1-P2	-2.99	122.63	132.67
2	P	501	PIS	P1-O1-P2	-2.85	123.12	132.67
2	C	501	PIS	P1-O1-P2	-2.80	123.28	132.67
2	H	501	PIS	P1-O1-P2	-2.78	123.33	132.67
2	E	501	PIS	P1-O1-P2	-2.77	123.38	132.67
2	E	501	PIS	O4-P2-O6	2.00	117.08	111.37
2	J	501	PIS	O3-P1-O2	2.04	115.13	107.38
2	B	501	PIS	O3-P1-O2	2.08	115.31	107.38
2	F	501	PIS	O3-P1-O2	2.09	115.34	107.38
2	K	501	PIS	O4-P2-O6	2.10	117.37	111.37
2	A	501	PIS	O4-P2-O6	2.28	117.88	111.37
2	L	501	PIS	O4-P2-O6	2.28	117.88	111.37
2	I	501	PIS	O4-P2-O6	2.31	117.97	111.37
2	N	501	PIS	O4-P2-O6	2.41	118.24	111.37
2	P	501	PIS	O4-P2-O6	2.41	118.25	111.37
2	C	501	PIS	O4-P2-O6	2.42	118.26	111.37
2	M	501	PIS	O4-P2-O6	2.44	118.33	111.37
2	O	501	PIS	O4-P2-O6	2.50	118.51	111.37
2	H	501	PIS	O4-P2-O6	2.51	118.52	111.37
2	F	501	PIS	O4-P2-O6	2.53	118.59	111.37
2	G	501	PIS	O4-P2-O6	2.56	118.69	111.37
2	J	501	PIS	O4-P2-O6	2.57	118.72	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	PIS	O4-P2-O6	2.59	118.75	111.37
2	B	501	PIS	O4-P2-O6	2.60	118.78	111.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	PIS	1	0
2	B	501	PIS	1	0
2	C	501	PIS	1	0
2	D	501	PIS	1	0
2	F	501	PIS	2	0
2	G	501	PIS	3	0
2	H	501	PIS	2	0
2	J	501	PIS	2	0
2	K	501	PIS	1	0
2	L	501	PIS	1	0
2	O	501	PIS	1	0
2	P	501	PIS	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	397/445 (89%)	0.34	7 (1%) 71 63	28, 43, 66, 77	0
1	B	397/445 (89%)	0.30	14 (3%) 48 37	29, 48, 73, 86	0
1	C	397/445 (89%)	0.27	18 (4%) 37 27	28, 46, 70, 84	0
1	D	397/445 (89%)	0.29	15 (3%) 44 33	31, 46, 72, 88	0
1	E	397/445 (89%)	0.40	11 (2%) 56 46	31, 50, 69, 83	0
1	F	397/445 (89%)	0.44	15 (3%) 44 33	32, 54, 89, 100	0
1	G	397/445 (89%)	0.30	14 (3%) 48 37	30, 50, 72, 85	0
1	H	397/445 (89%)	0.43	29 (7%) 18 10	31, 49, 78, 97	0
1	I	397/445 (89%)	1.00	64 (16%) 3 1	50, 78, 110, 121	0
1	J	397/445 (89%)	0.54	24 (6%) 25 16	37, 55, 81, 92	0
1	K	392/445 (88%)	0.93	59 (15%) 3 2	53, 76, 106, 117	0
1	L	397/445 (89%)	1.66	133 (33%) 0 0	59, 92, 133, 148	0
1	M	397/445 (89%)	1.09	69 (17%) 2 1	58, 80, 110, 119	0
1	N	397/445 (89%)	0.75	49 (12%) 5 3	47, 62, 76, 88	0
1	O	391/445 (87%)	0.85	54 (13%) 4 2	57, 78, 103, 113	0
1	P	397/445 (89%)	1.23	90 (22%) 1 1	57, 75, 98, 119	0
All	All	6341/7120 (89%)	0.68	665 (10%) 8 4	28, 62, 103, 148	0

All (665) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	336	GLN	8.4
1	P	436	ASN	8.3
1	K	324	TYR	8.1
1	P	434	LYS	8.1
1	P	403	GLU	8.0

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Mol	Chain	Res	Type	RSRZ
1	L	403	GLU	7.4
1	P	404	THR	7.4
1	L	349	SER	7.1
1	M	306	SER	7.1
1	F	259	THR	7.0
1	L	361	HIS	6.7
1	I	362	GLY	6.7
1	M	379	LEU	6.6
1	L	324	TYR	6.5
1	L	322	LEU	6.5
1	L	104	SER	6.5
1	L	362	GLY	6.3
1	J	95	ALA	6.3
1	L	203	GLY	6.1
1	M	380	GLY	6.1
1	B	94	SER	6.0
1	L	98	ASN	6.0
1	I	437	LEU	5.9
1	P	365	ASP	5.9
1	N	30	GLN	5.8
1	L	336	GLN	5.8
1	L	376	TRP	5.8
1	J	324	TYR	5.8
1	I	96	GLU	5.7
1	P	324	TYR	5.7
1	P	362	GLY	5.6
1	L	400	ASN	5.5
1	M	316	GLU	5.5
1	K	437	LEU	5.5
1	P	106	GLU	5.4
1	L	396	ASN	5.4
1	H	337	LEU	5.3
1	P	94	SER	5.3
1	P	100	ILE	5.3
1	P	136	THR	5.2
1	G	324	TYR	5.2
1	D	184	SER	5.1
1	L	221	GLY	5.1
1	P	361	HIS	5.0
1	L	292	THR	5.0
1	I	30	GLN	5.0
1	M	93	SER	4.9

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Mol	Chain	Res	Type	RSRZ
1	E	30	GLN	4.9
1	P	30	GLN	4.8
1	M	106	GLU	4.8
1	M	262	SER	4.8
1	M	402	ALA	4.8
1	I	260	VAL	4.8
1	G	203	GLY	4.8
1	I	415	TYR	4.8
1	K	309	MET	4.8
1	M	94	SER	4.7
1	L	404	THR	4.7
1	L	315	ALA	4.7
1	L	402	ALA	4.7
1	L	401	LEU	4.7
1	B	291	ALA	4.7
1	C	30	GLN	4.7
1	H	93	SER	4.7
1	I	262	SER	4.7
1	K	118	ALA	4.7
1	E	324	TYR	4.6
1	I	377	ASP	4.6
1	L	348	GLY	4.6
1	L	107	GLY	4.6
1	L	96	GLU	4.5
1	P	347	SER	4.5
1	P	337	LEU	4.5
1	A	95	ALA	4.5
1	I	93	SER	4.4
1	N	176	THR	4.4
1	M	363	ARG	4.4
1	H	259	THR	4.4
1	I	367	ALA	4.4
1	L	183	ALA	4.4
1	P	437	LEU	4.4
1	P	182	ALA	4.4
1	O	255	PHE	4.4
1	L	384	LEU	4.3
1	L	436	ASN	4.3
1	M	347	SER	4.3
1	P	215	GLY	4.3
1	N	347	SER	4.3
1	P	336	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
1	L	304	THR	4.2
1	L	437	LEU	4.2
1	N	362	GLY	4.2
1	L	220	SER	4.2
1	L	41	GLY	4.2
1	L	42	LEU	4.2
1	K	262	SER	4.1
1	I	92	ARG	4.1
1	O	94	SER	4.1
1	J	259	THR	4.1
1	K	91	ILE	4.1
1	M	437	LEU	4.1
1	K	306	SER	4.1
1	L	372	LEU	4.1
1	M	386	ALA	4.1
1	F	304	THR	4.1
1	L	311	GLY	4.1
1	P	223	PRO	4.1
1	H	95	ALA	4.1
1	N	93	SER	4.1
1	M	362	GLY	4.0
1	K	379	LEU	4.0
1	P	119	SER	4.0
1	O	324	TYR	4.0
1	E	184	SER	4.0
1	M	304	THR	4.0
1	K	347	SER	4.0
1	P	292	THR	4.0
1	I	98	ASN	4.0
1	L	296	PHE	4.0
1	M	259	THR	4.0
1	L	323	GLN	3.9
1	O	262	SER	3.9
1	M	323	GLN	3.9
1	J	93	SER	3.9
1	P	393	TYR	3.9
1	N	184	SER	3.9
1	L	356	LEU	3.9
1	L	297	TRP	3.9
1	L	391	ASP	3.9
1	I	176	THR	3.9
1	E	94	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	M	416	THR	3.8
1	G	386	ALA	3.8
1	N	98	ASN	3.8
1	K	181	LEU	3.8
1	D	95	ALA	3.8
1	L	365	ASP	3.8
1	P	219	ALA	3.8
1	L	369	ALA	3.8
1	L	113	SER	3.8
1	K	305	ASP	3.7
1	O	213	LEU	3.7
1	I	348	GLY	3.7
1	L	399	ARG	3.7
1	K	381	TRP	3.7
1	M	311	GLY	3.7
1	C	259	THR	3.7
1	I	337	LEU	3.7
1	G	30	GLN	3.7
1	N	377	ASP	3.7
1	L	417	GLU	3.7
1	N	348	GLY	3.7
1	L	289	SER	3.6
1	L	306	SER	3.6
1	L	398	CYS	3.6
1	I	113	SER	3.6
1	M	309	MET	3.6
1	B	362	GLY	3.6
1	L	377	ASP	3.6
1	M	350	ALA	3.6
1	L	126	GLY	3.6
1	A	337	LEU	3.6
1	A	380	GLY	3.6
1	K	30	GLN	3.6
1	L	393	TYR	3.6
1	K	316	GLU	3.5
1	L	337	LEU	3.5
1	I	291	ALA	3.5
1	O	217	SER	3.5
1	P	401	LEU	3.5
1	D	30	GLN	3.5
1	L	357	TYR	3.5
1	L	378	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	P	386	ALA	3.5
1	H	288	LEU	3.5
1	I	387	GLN	3.5
1	K	119	SER	3.5
1	J	302	SER	3.5
1	O	419	GLY	3.4
1	P	435	GLY	3.4
1	P	105	ALA	3.4
1	P	183	ALA	3.4
1	C	324	TYR	3.4
1	M	398	CYS	3.4
1	P	398	CYS	3.4
1	D	93	SER	3.4
1	O	309	MET	3.4
1	N	393	TYR	3.4
1	L	408	GLN	3.4
1	M	343	TYR	3.3
1	K	308	THR	3.3
1	L	435	GLY	3.3
1	H	292	THR	3.3
1	I	318	LEU	3.3
1	N	437	LEU	3.3
1	E	336	GLN	3.3
1	E	362	GLY	3.3
1	D	292	THR	3.3
1	L	366	GLU	3.3
1	L	273	VAL	3.3
1	K	364	ASN	3.3
1	L	303	VAL	3.3
1	K	378	TYR	3.3
1	L	236	ALA	3.2
1	P	37	GLY	3.2
1	B	93	SER	3.2
1	B	336	GLN	3.2
1	I	416	THR	3.2
1	I	242	SER	3.2
1	C	383	GLY	3.2
1	O	291	ALA	3.2
1	P	402	ALA	3.2
1	J	92	ARG	3.2
1	K	120	LYS	3.2
1	L	237	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	P	323	GLN	3.2
1	N	322	LEU	3.2
1	P	400	ASN	3.2
1	L	426	TYR	3.2
1	M	426	TYR	3.2
1	I	292	THR	3.1
1	K	349	SER	3.1
1	I	180	ASN	3.1
1	L	158	PRO	3.1
1	P	373	THR	3.1
1	I	258	PRO	3.1
1	M	249	THR	3.1
1	I	104	SER	3.1
1	M	418	SER	3.1
1	M	378	TYR	3.1
1	H	260	VAL	3.1
1	P	220	SER	3.1
1	N	180	ASN	3.1
1	N	384	LEU	3.1
1	M	117	GLN	3.1
1	B	95	ALA	3.0
1	K	183	ALA	3.0
1	E	181	LEU	3.0
1	M	366	GLU	3.0
1	O	176	THR	3.0
1	L	395	ASN	3.0
1	I	105	ALA	3.0
1	O	319	TRP	3.0
1	N	372	LEU	3.0
1	M	143	GLN	3.0
1	I	424	THR	3.0
1	J	250	PHE	3.0
1	H	291	ALA	3.0
1	J	377	ASP	3.0
1	L	386	ALA	3.0
1	J	30	GLN	3.0
1	L	389	LYS	3.0
1	O	260	VAL	3.0
1	F	181	LEU	3.0
1	H	94	SER	3.0
1	I	137	SER	3.0
1	P	406	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	L	30	GLN	3.0
1	P	372	LEU	3.0
1	P	96	GLU	2.9
1	O	314	ILE	2.9
1	L	174	LEU	2.9
1	M	387	GLN	2.9
1	M	101	SER	2.9
1	N	221	GLY	2.9
1	O	350	ALA	2.9
1	P	95	ALA	2.9
1	O	310	LYS	2.9
1	O	348	GLY	2.9
1	K	393	TYR	2.9
1	O	411	VAL	2.9
1	L	419	GLY	2.9
1	F	319	TRP	2.9
1	H	289	SER	2.9
1	M	254	LEU	2.9
1	O	30	GLN	2.9
1	L	347	SER	2.9
1	P	301	GLY	2.9
1	G	377	ASP	2.9
1	I	297	TRP	2.9
1	M	256	SER	2.9
1	H	258	PRO	2.9
1	O	290	LEU	2.9
1	K	252	THR	2.9
1	O	361	HIS	2.9
1	P	364	ASN	2.9
1	P	383	GLY	2.8
1	O	316	GLU	2.8
1	P	135	GLY	2.8
1	I	319	TRP	2.8
1	K	307	ALA	2.8
1	M	377	ASP	2.8
1	I	289	SER	2.8
1	I	320	ARG	2.8
1	I	249	THR	2.8
1	K	351	THR	2.8
1	O	91	ILE	2.8
1	F	96	GLU	2.8
1	M	39	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	N	154	SER	2.8
1	F	260	VAL	2.8
1	L	319	TRP	2.8
1	M	303	VAL	2.8
1	N	381	TRP	2.8
1	C	356	LEU	2.8
1	P	108	TYR	2.8
1	J	386	ALA	2.8
1	M	105	ALA	2.8
1	I	323	GLN	2.8
1	M	319	TRP	2.8
1	L	392	LEU	2.8
1	N	92	ARG	2.8
1	D	362	GLY	2.8
1	M	337	LEU	2.8
1	M	415	TYR	2.8
1	P	138	GLN	2.8
1	L	124	ARG	2.8
1	K	384	LEU	2.8
1	O	308	THR	2.8
1	M	96	GLU	2.7
1	L	176	THR	2.7
1	K	239	GLN	2.7
1	O	315	ALA	2.7
1	L	301	GLY	2.7
1	B	363	ARG	2.7
1	L	280	LYS	2.7
1	G	105	ALA	2.7
1	K	319	TRP	2.7
1	L	94	SER	2.7
1	M	240	ILE	2.7
1	I	388	TYR	2.7
1	E	292	THR	2.7
1	O	289	SER	2.7
1	P	113	SER	2.7
1	I	97	ALA	2.7
1	L	95	ALA	2.7
1	H	403	GLU	2.7
1	P	367	ALA	2.7
1	F	258	PRO	2.7
1	L	338	PRO	2.7
1	M	324	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	292	THR	2.7
1	O	237	PRO	2.7
1	M	430	VAL	2.7
1	B	337	LEU	2.7
1	K	109	PRO	2.7
1	L	114	VAL	2.7
1	L	343	TYR	2.6
1	O	293	LEU	2.6
1	D	252	THR	2.6
1	B	102	GLY	2.6
1	L	418	SER	2.6
1	L	40	LEU	2.6
1	I	406	THR	2.6
1	P	421	ALA	2.6
1	P	181	LEU	2.6
1	L	355	GLN	2.6
1	L	246	VAL	2.6
1	M	260	VAL	2.6
1	N	373	THR	2.6
1	I	250	PHE	2.6
1	M	137	SER	2.6
1	H	384	LEU	2.6
1	O	401	LEU	2.6
1	I	436	ASN	2.6
1	K	337	LEU	2.6
1	L	290	LEU	2.6
1	P	319	TRP	2.6
1	J	362	GLY	2.6
1	P	311	GLY	2.6
1	N	323	GLN	2.6
1	K	352	PRO	2.6
1	C	403	GLU	2.5
1	M	118	ALA	2.5
1	K	180	ASN	2.5
1	I	324	TYR	2.5
1	C	437	LEU	2.5
1	K	127	CYS	2.5
1	N	301	GLY	2.5
1	D	336	GLN	2.5
1	J	175	THR	2.5
1	N	292	THR	2.5
1	P	395	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	116	TYR	2.5
1	L	103	PHE	2.5
1	O	375	PHE	2.5
1	C	176	THR	2.5
1	P	97	ALA	2.5
1	I	177	SER	2.5
1	L	433	MET	2.5
1	P	98	ASN	2.5
1	O	437	LEU	2.5
1	H	373	THR	2.5
1	K	94	SER	2.5
1	P	137	SER	2.5
1	P	433	MET	2.5
1	M	65	CYS	2.5
1	D	337	LEU	2.5
1	P	174	LEU	2.5
1	P	405	THR	2.5
1	O	303	VAL	2.5
1	P	191	ARG	2.5
1	J	393	TYR	2.5
1	P	312	LEU	2.5
1	G	291	ALA	2.5
1	K	240	ILE	2.5
1	K	297	TRP	2.5
1	M	196	ILE	2.5
1	I	106	GLU	2.5
1	A	362	GLY	2.5
1	E	238	LYS	2.5
1	C	385	ALA	2.5
1	I	394	ALA	2.5
1	B	377	ASP	2.5
1	K	93	SER	2.5
1	C	290	LEU	2.5
1	I	91	ILE	2.5
1	I	382	LYS	2.5
1	C	362	GLY	2.5
1	K	348	GLY	2.5
1	E	337	LEU	2.4
1	I	259	THR	2.4
1	N	346	SER	2.4
1	M	258	PRO	2.4
1	O	404	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	P	384	LEU	2.4
1	L	363	ARG	2.4
1	F	137	SER	2.4
1	O	42	LEU	2.4
1	L	370	ASN	2.4
1	H	238	LYS	2.4
1	L	62	LEU	2.4
1	H	290	LEU	2.4
1	L	51	TRP	2.4
1	K	350	ALA	2.4
1	I	364	ASN	2.4
1	L	364	ASN	2.4
1	N	259	THR	2.4
1	P	221	GLY	2.4
1	B	302	SER	2.4
1	K	98	ASN	2.4
1	F	197	ALA	2.4
1	L	179	ALA	2.4
1	N	118	ALA	2.4
1	D	94	SER	2.4
1	D	383	GLY	2.4
1	J	104	SER	2.4
1	L	291	ALA	2.4
1	C	311	GLY	2.4
1	H	241	GLU	2.4
1	I	217	SER	2.4
1	M	226	ASP	2.4
1	L	112	LEU	2.4
1	P	310	LYS	2.4
1	P	385	ALA	2.4
1	D	319	TRP	2.4
1	L	137	SER	2.4
1	L	374	LYS	2.4
1	L	422	TYR	2.4
1	L	434	LYS	2.4
1	L	44	THR	2.4
1	N	304	THR	2.4
1	N	155	ARG	2.3
1	K	214	LYS	2.3
1	O	243	PRO	2.3
1	I	303	VAL	2.3
1	L	119	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	437	LEU	2.3
1	D	300	GLY	2.3
1	I	296	PHE	2.3
1	L	115	ASN	2.3
1	K	290	LEU	2.3
1	K	401	LEU	2.3
1	L	409	ARG	2.3
1	M	393	TYR	2.3
1	P	304	THR	2.3
1	G	260	VAL	2.3
1	N	324	TYR	2.3
1	P	184	SER	2.3
1	P	346	SER	2.3
1	L	261	THR	2.3
1	L	380	GLY	2.3
1	M	424	THR	2.3
1	M	403	GLU	2.3
1	L	125	LEU	2.3
1	L	161	ASP	2.3
1	L	379	LEU	2.3
1	F	324	TYR	2.3
1	I	107	GLY	2.3
1	I	371	ALA	2.3
1	K	176	THR	2.3
1	L	240	ILE	2.3
1	P	399	ARG	2.3
1	H	310	LYS	2.3
1	C	336	GLN	2.3
1	K	336	GLN	2.3
1	L	117	GLN	2.3
1	K	415	TYR	2.3
1	B	259	THR	2.3
1	N	255	PHE	2.3
1	P	175	THR	2.3
1	H	295	GLU	2.3
1	L	135	GLY	2.3
1	L	320	ARG	2.3
1	J	291	ALA	2.3
1	H	319	TRP	2.3
1	A	336	GLN	2.3
1	B	285	ASP	2.3
1	C	258	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	218	LEU	2.3
1	O	183	ALA	2.3
1	O	402	ALA	2.3
1	I	361	HIS	2.3
1	K	242	SER	2.3
1	N	45	ILE	2.3
1	L	251	VAL	2.3
1	I	38	LYS	2.3
1	N	300	GLY	2.3
1	H	105	ALA	2.2
1	G	94	SER	2.2
1	K	320	ARG	2.2
1	L	430	VAL	2.2
1	F	290	LEU	2.2
1	H	203	GLY	2.2
1	L	181	LEU	2.2
1	M	138	GLN	2.2
1	M	381	TRP	2.2
1	C	180	ASN	2.2
1	F	196	ILE	2.2
1	C	220	SER	2.2
1	L	180	ASN	2.2
1	G	136	THR	2.2
1	O	288	LEU	2.2
1	L	184	SER	2.2
1	L	302	SER	2.2
1	P	349	SER	2.2
1	L	432	GLY	2.2
1	J	96	GLU	2.2
1	L	106	GLU	2.2
1	L	188	LYS	2.2
1	M	375	PHE	2.2
1	B	240	ILE	2.2
1	L	177	SER	2.2
1	J	260	VAL	2.2
1	J	419	GLY	2.2
1	I	338	PRO	2.2
1	K	431	GLY	2.2
1	P	141	MET	2.2
1	I	117	GLN	2.2
1	N	95	ALA	2.2
1	P	338	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	P	248	ARG	2.2
1	P	99	TYR	2.2
1	I	184	SER	2.2
1	O	302	SER	2.2
1	L	199	ASP	2.2
1	L	238	LYS	2.2
1	L	416	THR	2.2
1	M	404	THR	2.2
1	I	108	TYR	2.2
1	M	358	LEU	2.2
1	N	363	ARG	2.2
1	O	349	SER	2.2
1	N	222	ILE	2.2
1	P	258	PRO	2.2
1	J	313	GLU	2.2
1	K	403	GLU	2.2
1	L	218	LEU	2.2
1	D	97	ALA	2.2
1	J	113	SER	2.1
1	P	429	ALA	2.2
1	P	45	ILE	2.1
1	K	409	ARG	2.1
1	O	339	LEU	2.1
1	G	319	TRP	2.1
1	M	382	LYS	2.1
1	P	118	ALA	2.1
1	P	426	TYR	2.1
1	O	305	ASP	2.1
1	I	434	LYS	2.1
1	N	287	GLN	2.1
1	N	398	CYS	2.1
1	P	40	LEU	2.1
1	C	184	SER	2.1
1	K	301	GLY	2.1
1	M	126	GLY	2.1
1	L	390	LYS	2.1
1	P	42	LEU	2.1
1	O	98	ASN	2.1
1	I	94	SER	2.1
1	O	311	GLY	2.1
1	K	45	ILE	2.1
1	O	338	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	341	VAL	2.1
1	O	318	LEU	2.1
1	K	104	SER	2.1
1	M	119	SER	2.1
1	O	347	SER	2.1
1	M	111	GLU	2.1
1	M	218	LEU	2.1
1	K	375	PHE	2.1
1	G	362	GLY	2.1
1	H	362	GLY	2.1
1	M	349	SER	2.1
1	N	101	SER	2.1
1	L	140	PRO	2.1
1	O	403	GLU	2.1
1	L	358	LEU	2.1
1	G	296	PHE	2.1
1	N	167	TYR	2.1
1	O	343	TYR	2.1
1	K	193	SER	2.1
1	O	214	LYS	2.1
1	J	350	ALA	2.1
1	N	367	ALA	2.1
1	L	427	PHE	2.1
1	H	235	ILE	2.1
1	M	100	ILE	2.1
1	P	298	THR	2.1
1	H	256	SER	2.1
1	J	119	SER	2.1
1	F	363	ARG	2.1
1	M	291	ALA	2.1
1	A	203	GLY	2.0
1	K	221	GLY	2.0
1	N	102	GLY	2.0
1	L	100	ILE	2.0
1	O	295	GLU	2.0
1	P	271	CYS	2.0
1	N	189	GLN	2.0
1	O	342	ASN	2.0
1	F	356	LEU	2.0
1	O	137	SER	2.0
1	P	81	ARG	2.0
1	P	288	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	268	ALA	2.0
1	M	359	PRO	2.0
1	P	235	ILE	2.0
1	H	176	THR	2.0
1	C	322	LEU	2.0
1	P	345	LEU	2.0
1	I	95	ALA	2.0
1	E	241	GLU	2.0
1	L	171	GLN	2.0
1	N	401	LEU	2.0
1	K	386	ALA	2.0
1	A	258	PRO	2.0
1	N	43	PRO	2.0
1	N	256	SER	2.0
1	H	320	ARG	2.0
1	L	92	ARG	2.0
1	I	34	LYS	2.0
1	N	253	LYS	2.0
1	D	324	TYR	2.0
1	F	370	ASN	2.0
1	J	373	THR	2.0
1	N	252	THR	2.0
1	O	412	ALA	2.0
1	P	180	ASN	2.0
1	I	255	PHE	2.0
1	N	366	GLU	2.0
1	O	212	PHE	2.0
1	I	349	SER	2.0
1	N	177	SER	2.0
1	P	32	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NA	F	502	1/1	0.70	0.95	9.77	92,92,92,92	0
3	NA	J	502	1/1	0.85	0.71	7.63	104,104,104,104	0
3	NA	D	502	1/1	0.89	0.40	3.61	43,43,43,43	0
3	NA	N	502	1/1	0.27	0.47	2.95	60,60,60,60	0
3	NA	H	502	1/1	0.63	0.36	2.02	60,60,60,60	0
3	NA	K	502	1/1	0.66	0.39	1.19	70,70,70,70	0
3	NA	M	502	1/1	0.78	0.38	0.56	49,49,49,49	0
3	NA	I	502	1/1	0.63	0.33	0.42	121,121,121,121	0
3	NA	L	502	1/1	0.33	0.40	0.36	89,89,89,89	0
3	NA	B	502	1/1	0.73	0.23	-0.09	60,60,60,60	0
3	NA	A	502	1/1	0.66	0.22	-0.19	51,51,51,51	0
3	NA	G	502	1/1	0.91	0.17	-0.78	39,39,39,39	0
3	NA	O	502	1/1	0.74	0.19	-0.82	59,59,59,59	0
2	PIS	D	501	9/9	0.93	0.19	-0.90	30,31,34,37	0
3	NA	P	502	1/1	0.75	0.25	-1.00	58,58,58,58	0
3	NA	C	502	1/1	0.64	0.17	-1.17	49,49,49,49	0
2	PIS	C	501	9/9	0.94	0.19	-1.53	32,33,36,39	0
3	NA	E	502	1/1	0.82	0.16	-1.56	51,51,51,51	0
2	PIS	B	501	9/9	0.97	0.16	-1.59	29,31,32,34	0
2	PIS	E	501	9/9	0.96	0.17	-1.69	33,34,37,42	0
2	PIS	G	501	9/9	0.96	0.18	-1.92	32,35,37,37	0
2	PIS	I	501	9/9	0.92	0.19	-2.00	44,46,48,48	0
2	PIS	A	501	9/9	0.96	0.19	-2.04	32,34,35,36	0
2	PIS	O	501	9/9	0.89	0.19	-2.09	47,50,52,55	0
2	PIS	F	501	9/9	0.96	0.17	-2.14	37,38,40,42	0
2	PIS	N	501	9/9	0.92	0.17	-2.34	38,40,41,41	0
2	PIS	M	501	9/9	0.91	0.17	-2.63	45,47,48,50	0
2	PIS	P	501	9/9	0.90	0.16	-2.73	42,47,49,50	0
2	PIS	L	501	9/9	0.92	0.15	-3.00	49,51,54,55	0
2	PIS	H	501	9/9	0.98	0.11	-3.30	34,35,36,38	0
2	PIS	K	501	9/9	0.93	0.16	-3.34	45,49,52,56	0
2	PIS	J	501	9/9	0.96	0.12	-4.72	30,31,32,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.