



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 8, 2017 – 08:38 PM EST

PDB ID : 4LD7
Title : Crystal structure of AnaPT from Neosartorya fischeri
Authors : Zocher, G.; Stehle, T.
Deposited on : unknown
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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

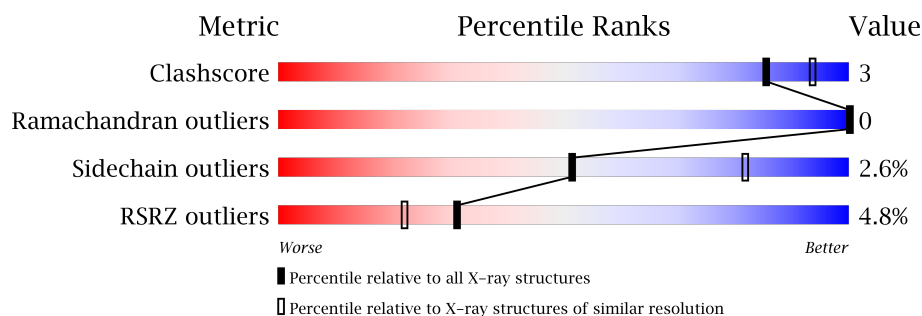
1 Overall quality at a glance

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))
Clashscore	112137	3975 (2.88-2.80)
Ramachandran outliers	110173	3902 (2.88-2.80)
Sidechain outliers	110143	3905 (2.88-2.80)
RSRZ outliers	101464	3501 (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	
1	B	445	
1	C	445	
1	D	445	
1	E	445	
1	F	445	
1	G	445	

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Mol	Chain	Length	Quality of chain
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	F	502	-	-	-	X
3	NA	H	502	-	-	-	X
3	NA	J	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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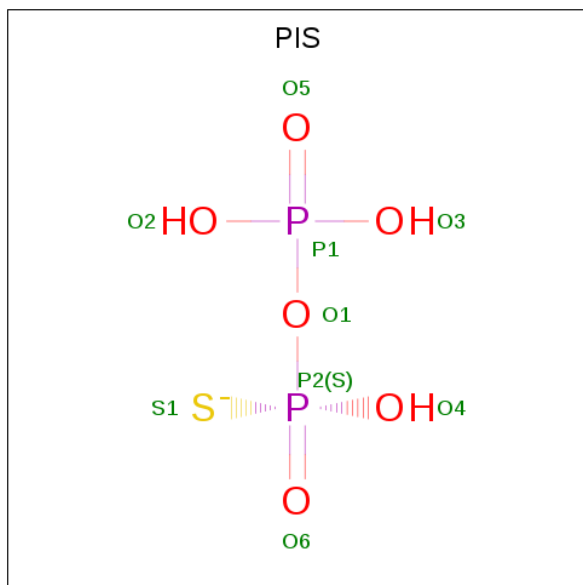
Chain	Residue	Modelled	Actual	Comment	Reference
K	442	HIS	-	EXPRESSION TAG	UNP A1DN10
K	443	HIS	-	EXPRESSION TAG	UNP A1DN10
K	444	HIS	-	EXPRESSION TAG	UNP A1DN10
K	445	HIS	-	EXPRESSION TAG	UNP A1DN10
L	438	ARG	-	EXPRESSION TAG	UNP A1DN10
L	439	SER	-	EXPRESSION TAG	UNP A1DN10
L	440	HIS	-	EXPRESSION TAG	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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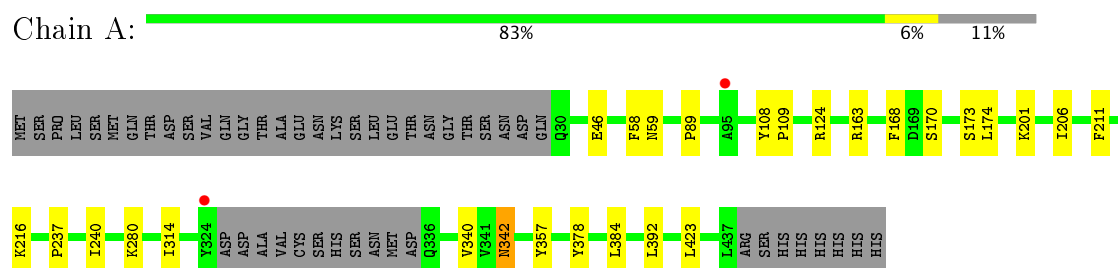
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	1	Total 1	Na 1	0	0
3	F	1	Total 1	Na 1	0	0
3	M	1	Total 1	Na 1	0	0

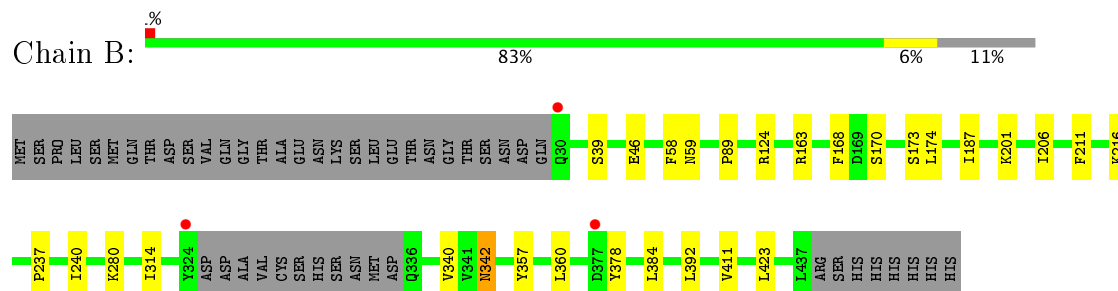
3 Residue-property plots [i](#)

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

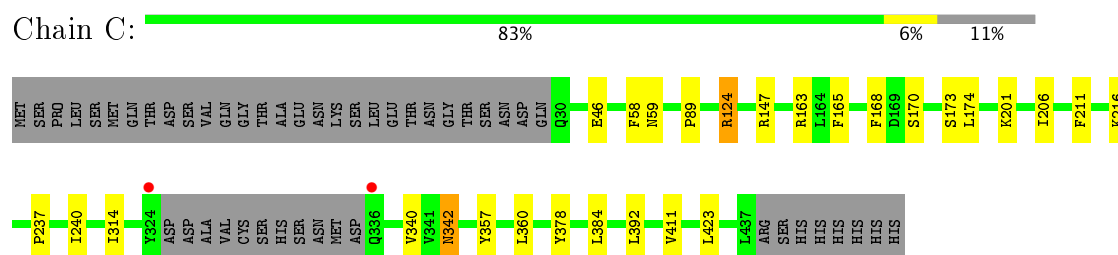
- Molecule 1: Dimethylallyl tryptophan synthase



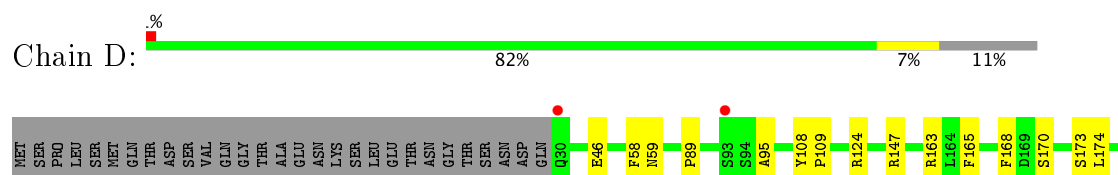
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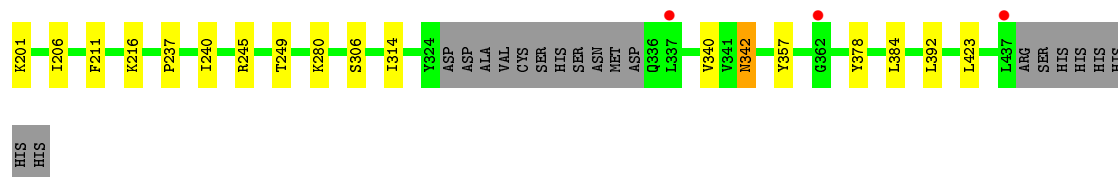


- Molecule 1: Dimethylallyl tryptophan synthase

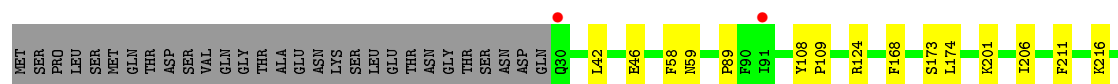
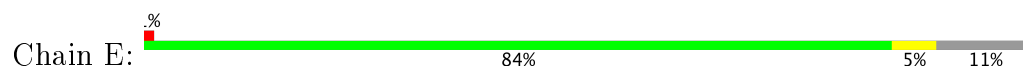


- Molecule 1: Dimethylallyl tryptophan synthase

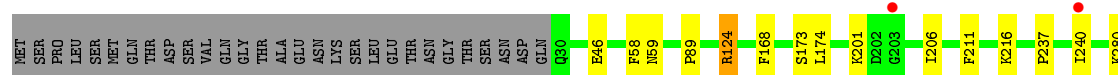
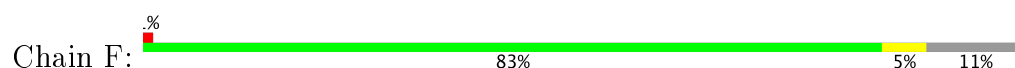




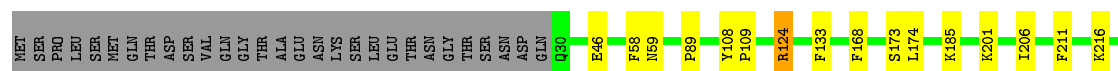
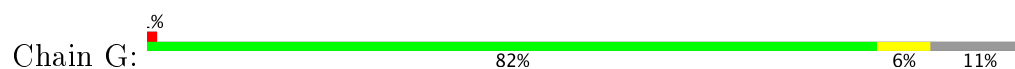
- Molecule 1: Dimethylallyl tryptophan synthase



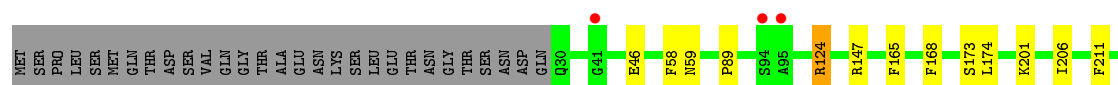
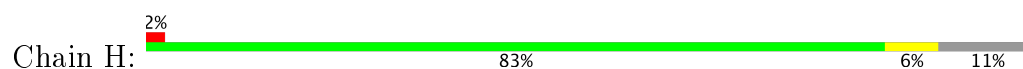
- Molecule 1: Dimethylallyl tryptophan synthase



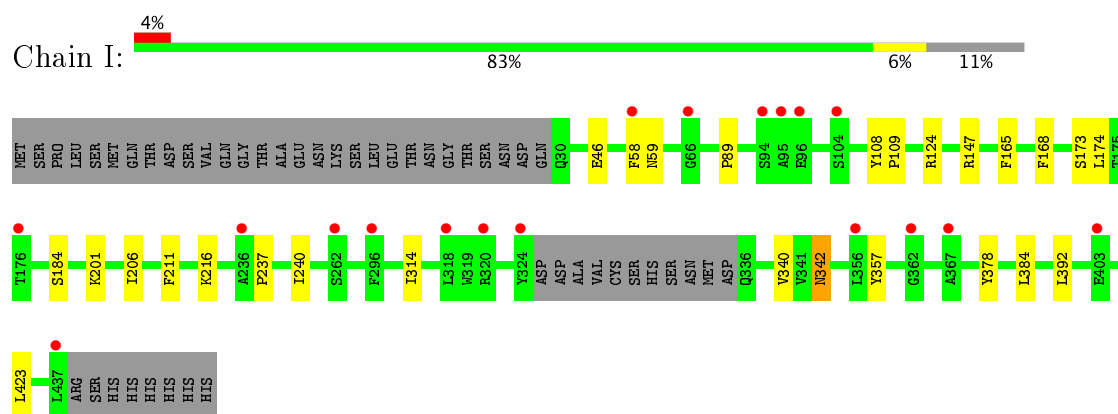
- Molecule 1: Dimethylallyl tryptophan synthase



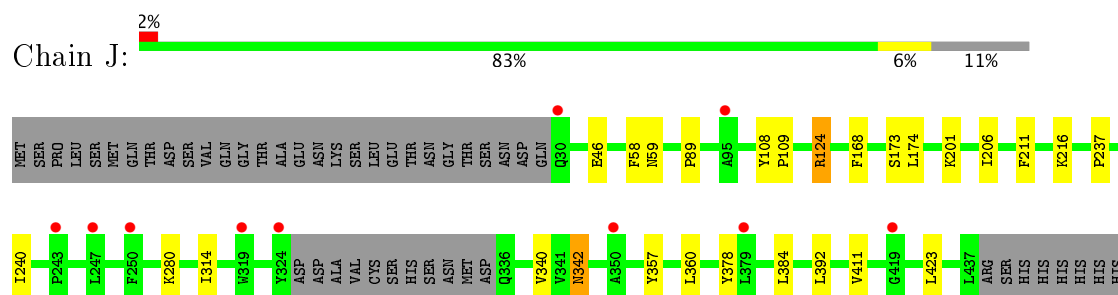
- Molecule 1: Dimethylallyl tryptophan synthase



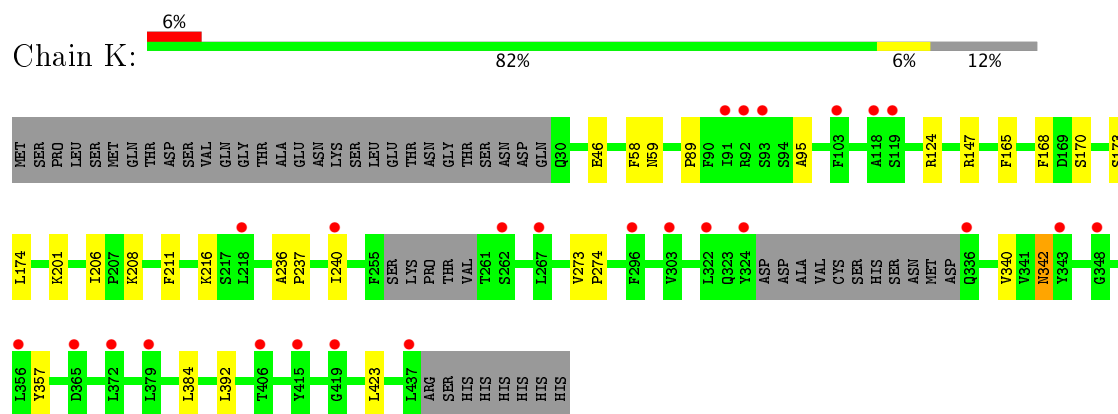
- Molecule 1: Dimethylallyl tryptophan synthase



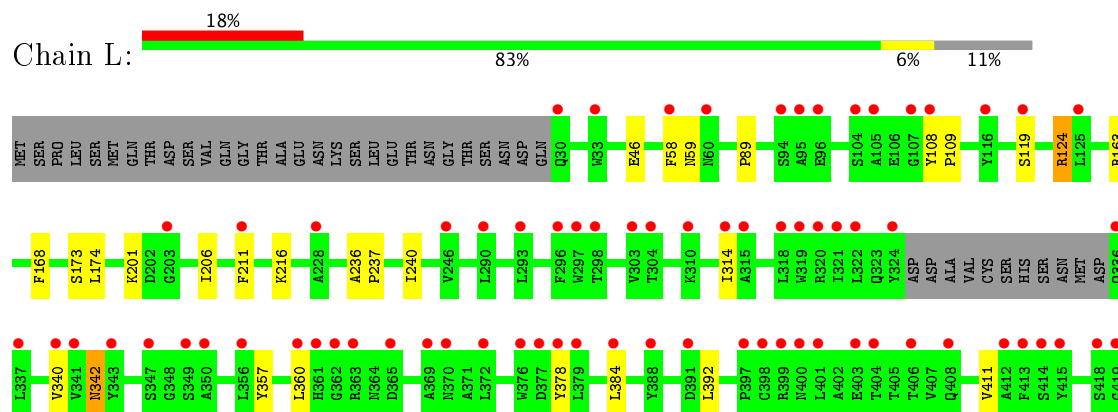
• Molecule 1: Dimethylallyl tryptophan synthase

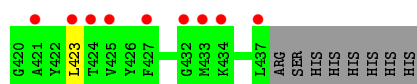


• Molecule 1: Dimethylallyl tryptophan synthase

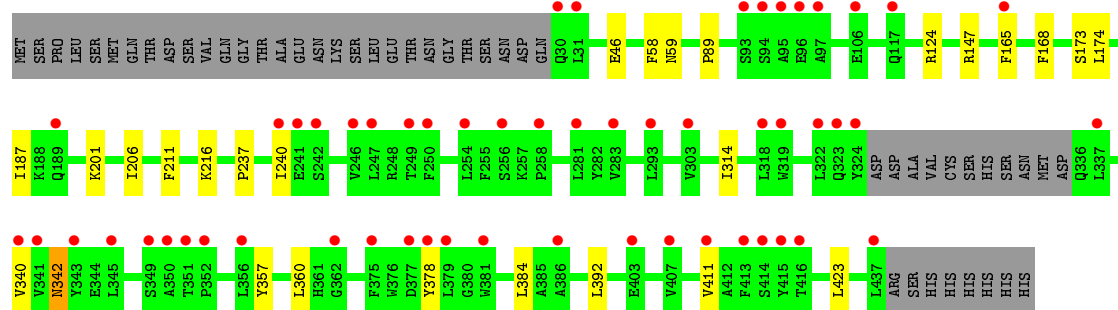
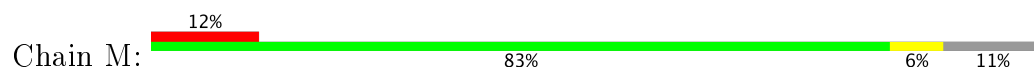


• Molecule 1: Dimethylallyl tryptophan synthase

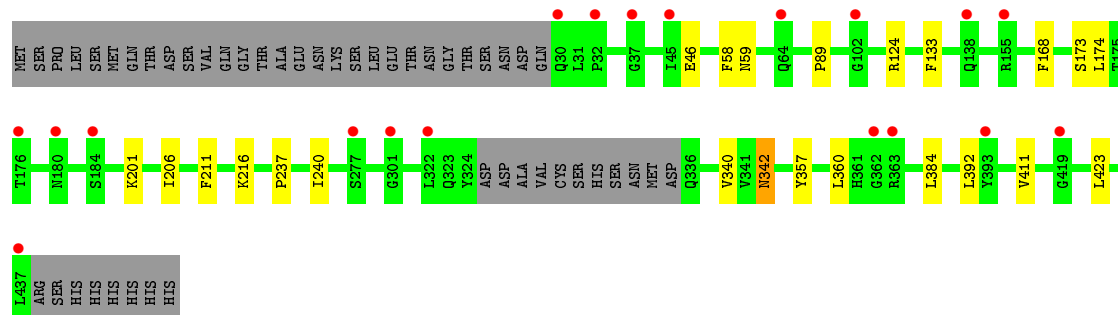
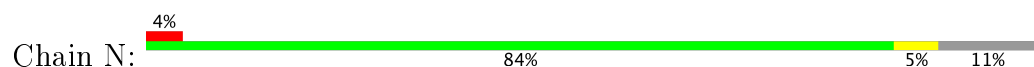




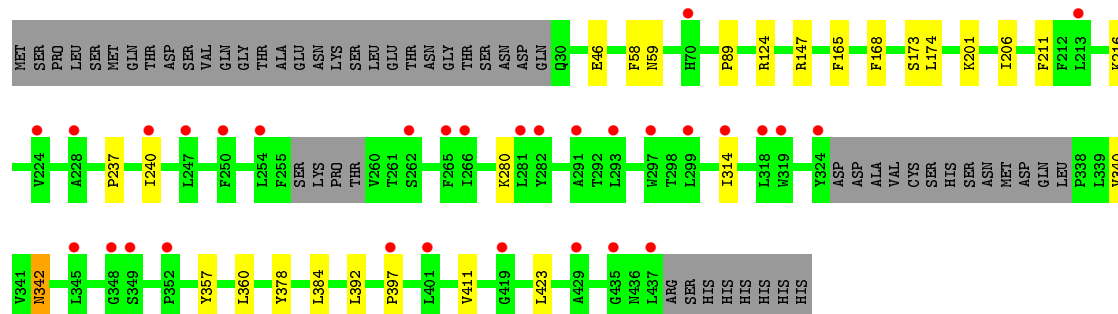
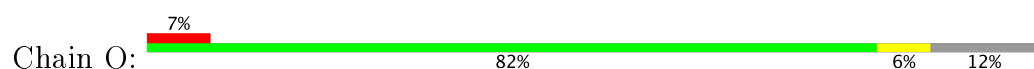
• Molecule 1: Dimethylallyl tryptophan synthase



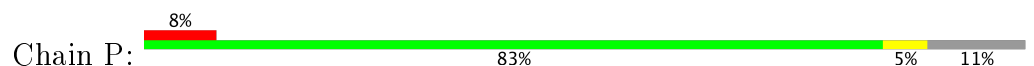
• Molecule 1: Dimethylallyl tryptophan synthase

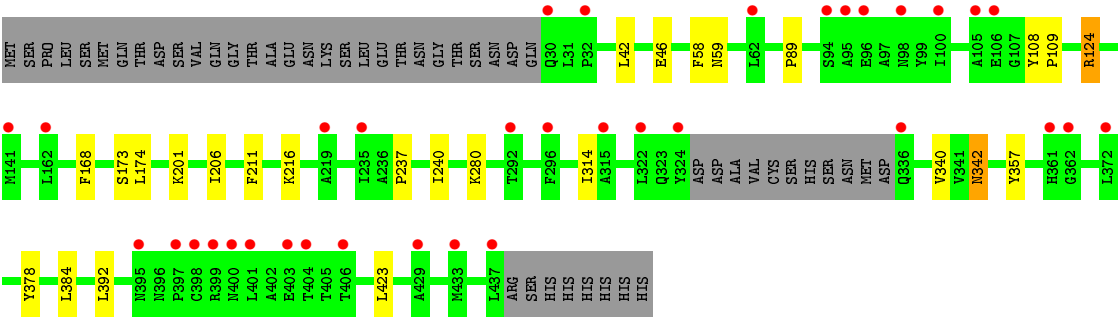


• Molecule 1: Dimethylallyl tryptophan synthase



• 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) 99.8 (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 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.449 for h,-k,-l	Xtriage
Reported twinning fraction	0.544 for H, K, L 0.456 for -h,-k,l	Depositor
Outliers	0 of 160059 reflections	Xtriage
F_o, F_c correlation	0.92	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [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:D:168:PHE:HB2	1:D:211:PHE:HE2	1.64	0.62
1:L:168:PHE:HB2	1:L: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:G:168:PHE:HB2	1:G:211:PHE:HE2	1.64	0.60
1:O:168:PHE:HB2	1:O:211:PHE:HE2	1.65	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:A:168:PHE:HB2	1:A:211:PHE:HE2	1.65	0.59
1:I:168:PHE:HB2	1:I: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:G:342:ASN:HB3	1:G:357:TYR:HE1	1.71	0.56
1:J:342:ASN:HB3	1:J:357:TYR:HE1	1.71	0.56
1:P:342:ASN:HB3	1:P:357:TYR:HE1	1.70	0.56
1:A:342:ASN:HB3	1:A:357:TYR:HE1	1.71	0.56
1:C:124:ARG:NH2	2:C:501:PIS:S1	2.79	0.56
1:K:342:ASN:HB3	1:K:357:TYR:HE1	1.71	0.56
1:O:342:ASN:HB3	1:O:357:TYR:HE1	1.71	0.56
1:E:342:ASN:HB3	1:E:357:TYR:HE1	1.71	0.55
1:A:170:SER:HB2	1:B:163:ARG:O	2.07	0.55
1:F:342:ASN:HB3	1:F:357:TYR:HE1	1.71	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:I:201:LYS:HD3	1:I:206:ILE:HD12	1.92	0.52
1:K:168:PHE:HB2	1:K:211:PHE:CE2	2.45	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:C:168:PHE:HB2	1:C:211:PHE:CE2	2.44	0.51
1:F:168:PHE:HB2	1:F:211:PHE:CE2	2.45	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:C:201:LYS:HD3	1:C:206:ILE:HD12	1.93	0.51
1:H:168:PHE:HB2	1:H:211:PHE:CE2	2.45	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: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:O:168:PHE:HB2	1:O:211:PHE:CE2	2.45	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:L:237:PRO:HD2	1:L:240:ILE:HG12	1.94	0.49
1:P:168:PHE:HB2	1:P:211:PHE:CE2	2.45	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:O:237:PRO:HD2	1:O:240:ILE:HG12	1.94	0.49
1:P:237:PRO:HD2	1:P: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:B:237:PRO:HD2	1:B:240:ILE:HG12	1.94	0.48
1:G:237:PRO:HD2	1:G:240:ILE:HG12	1.94	0.48
1:K:237:PRO:HD2	1:K: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:C:174:LEU:HD21	1:C:216:LYS:HA	1.96	0.46
1:L:174:LEU:HD21	1:L:216:LYS:HA	1.97	0.46
1:B:280:LYS:NZ	2:B:501:PIS:O4	2.49	0.46
1:G:174:LEU:HD21	1:G:216:LYS:HA	1.98	0.46
1:H:174:LEU:HD21	1:H:216:LYS:HA	1.96	0.46
1:J:174:LEU:HD21	1:J:216:LYS:HA	1.97	0.46
1:O:174:LEU:HD21	1:O:216:LYS:HA	1.97	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:A:174:LEU:HD21	1:A:216:LYS:HA	1.97	0.45
1:J:46:GLU:HG2	1:J:89:PRO:HA	1.99	0.45
1:P:174:LEU:HD21	1:P:216:LYS:HA	1.97	0.45
1:F:340:VAL:HB	1:F:357:TYR:HB2	1.99	0.45
1:I:46:GLU:HG2	1:I:89:PRO:HA	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:A:168:PHE:CB	1:A:211:PHE:HE2	2.30	0.45
1:B:187:ILE:HD13	1:I:184:SER:O	2.16	0.45
1:L:340:VAL:HB	1:L:357:TYR:HB2	1.99	0.45
1:F:174:LEU:HD21	1:F:216:LYS:HA	1.97	0.45
1:M:340:VAL:HB	1:M:357:TYR:HB2	1.99	0.45
1:F:46:GLU:HG2	1:F:89:PRO:HA	1.99	0.45
1:M:46:GLU:HG2	1:M:89:PRO:HA	1.99	0.44
1:O:340:VAL:HB	1:O:357:TYR:HB2	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:D:108:TYR:HA	1:D: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: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:C:46:GLU:HG2	1:C:89:PRO:HA	1.98	0.44
1:E:46:GLU:HG2	1:E:89:PRO:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:GLU:HG2	1:B:89:PRO:HA	1.99	0.44
1:C:168:PHE:CB	1:C:211:PHE:HE2	2.29	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:E:340:VAL:HB	1:E:357:TYR:HB2	2.00	0.44
1:G:340:VAL:HB	1:G:357:TYR:HB2	1.99	0.44
1:D:46:GLU:HG2	1:D:89:PRO:HA	1.99	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:P:168:PHE:CB	1:P:211:PHE:HE2	2.30	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:108:TYR:HA	1:I:109:PRO:HD3	1.85	0.43
1:I:168:PHE:CB	1:I:211:PHE:HE2	2.30	0.43
1:I:340:VAL:HB	1:I:357:TYR:HB2	1.99	0.43
1:P:340:VAL:HB	1:P:357:TYR:HB2	1.99	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:C:340:VAL:HB	1:C:357:TYR:HB2	1.99	0.43
1:E:168:PHE:CB	1:E:211:PHE:CE2	3.02	0.43
1:L:108:TYR:HA	1:L:109:PRO:HD3	1.85	0.43
1:B:168:PHE:CB	1:B:211:PHE:CE2	3.02	0.42
1:K:168:PHE:CB	1:K: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: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:L:168:PHE:CB	1:L:211:PHE:CE2	3.02	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:C:170:SER:HB2	1:D:163:ARG:O	2.19	0.42
1:O:168:PHE:CB	1:O:211:PHE:HE2	2.30	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:G:342:ASN:HB3	1:G:357:TYR:CE1	2.54	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:P:168:PHE:CB	1:P:211:PHE:CE2	3.02	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:A:314:ILE:HG23	1:A:378:TYR:HE2	1.86	0.41
1:G:278:ARG:NH2	2:G:501:PIS:O3	2.53	0.41
1:D:95:ALA:HB3	1:K:95:ALA:CB	2.50	0.41
1:I:342:ASN:HB3	1:I:357:TYR:CE1	2.54	0.41
1:J:168:PHE:CB	1:J:211:PHE:HE2	2.30	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:F:314:ILE:HG23	1:F:378:TYR:HE2	1.86	0.41
1:H:314:ILE:HG23	1:H:378:TYR:HE2	1.86	0.41
1:K:170:SER:HB2	1:L:163:ARG:O	2.21	0.41
1:L:314:ILE:HG23	1:L:378:TYR:HE2	1.86	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:L:360:LEU:HD11	1:L:411:VAL:HG13	2.03	0.41
1:M:314:ILE:HG23	1:M:378:TYR:HE2	1.86	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:A:163:ARG:O	1:B:170:SER:HB2	2.21	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:D:168:PHE:CB	1:D:211:PHE:CE2	3.02	0.41
1:K:147:ARG:HD3	1:K:165:PHE:CE1	2.56	0.41
1:K:236:ALA:HA	1:K:237:PRO:HD3	1.96	0.41
1:N:133:PHE:CZ	1:P:42:LEU:O	2.74	0.41
1:N:168:PHE:CB	1:N:211:PHE:CE2	3.02	0.41
1:O:314:ILE:HG23	1:O:378:TYR:HE2	1.86	0.41
1:P:108:TYR:HA	1:P:109:PRO:HD3	1.85	0.41
1:F:360:LEU:HD11	1:F:411:VAL:HG13	2.03	0.40
1:H:147:ARG:HD3	1:H:165:PHE:CE1	2.56	0.40
1:I:147:ARG:HD3	1:I:165:PHE:CE1	2.57	0.40
1:L:236:ALA:HA	1:L:237:PRO:HD3	1.96	0.40
1:M:360:LEU:HD11	1:M:411:VAL:HG13	2.03	0.40
1:P:280:LYS:NZ	2:P:501:PIS:O6	2.54	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:G:360:LEU:HD11	1:G:411:VAL:HG13	2.03	0.40
1:H:360:LEU:HD11	1:H:411:VAL:HG13	2.03	0.40
1:J:280:LYS:NZ	2:J:501:PIS:O4	2.54	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:H:124:ARG:NH2	2:H:501:PIS:S1	2.94	0.40
1:J:314:ILE:HG23	1:J:378:TYR:HE2	1.86	0.40
1:O:147:ARG:HD3	1:O:165:PHE:CE1	2.57	0.40
1:I:314:ILE:HG23	1:I:378:TYR:HE2	1.86	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
1:D:147:ARG:HD3	1:D:165:PHE:CE1	2.57	0.40
1:N:360:LEU:HD11	1:N: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%)	51	82
1	B	308/382 (81%)	299 (97%)	9 (3%)	48	79
1	C	308/382 (81%)	300 (97%)	8 (3%)	51	82
1	D	308/382 (81%)	300 (97%)	8 (3%)	51	82
1	E	306/382 (80%)	298 (97%)	8 (3%)	51	82
1	F	308/382 (81%)	300 (97%)	8 (3%)	51	82
1	G	308/382 (81%)	300 (97%)	8 (3%)	51	82
1	H	308/382 (81%)	300 (97%)	8 (3%)	51	82
1	I	306/382 (80%)	298 (97%)	8 (3%)	51	82
1	J	308/382 (81%)	300 (97%)	8 (3%)	51	82
1	K	303/382 (79%)	295 (97%)	8 (3%)	51	82
1	L	308/382 (81%)	300 (97%)	8 (3%)	51	82
1	M	306/382 (80%)	298 (97%)	8 (3%)	51	82
1	N	308/382 (81%)	300 (97%)	8 (3%)	51	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	302/382 (79%)	294 (97%)	8 (3%)	51	82
1	P	308/382 (81%)	300 (97%)	8 (3%)	51	82
All	All	4910/6112 (80%)	4781 (97%)	129 (3%)	51	82

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	-	5,8,8	1.20	1 (20%)	6,13,13	2.20	2 (33%)
2	PIS	B	501	-	5,8,8	0.97	0	6,13,13	2.42	2 (33%)
2	PIS	C	501	-	5,8,8	1.09	0	6,13,13	2.20	2 (33%)
2	PIS	D	501	-	5,8,8	1.19	1 (20%)	6,13,13	2.36	2 (33%)
2	PIS	E	501	-	5,8,8	1.22	1 (20%)	6,13,13	2.01	2 (33%)
2	PIS	F	501	-	5,8,8	1.18	1 (20%)	6,13,13	2.33	2 (33%)
2	PIS	G	501	-	5,8,8	1.03	0	6,13,13	2.39	2 (33%)
2	PIS	H	501	-	5,8,8	1.20	1 (20%)	6,13,13	2.22	2 (33%)
2	PIS	I	501	-	5,8,8	1.14	1 (20%)	6,13,13	2.24	2 (33%)
2	PIS	J	501	-	5,8,8	1.03	0	6,13,13	2.34	2 (33%)
2	PIS	K	501	-	5,8,8	1.06	0	6,13,13	2.15	2 (33%)
2	PIS	L	501	-	5,8,8	1.19	1 (20%)	6,13,13	2.19	2 (33%)
2	PIS	M	501	-	5,8,8	1.13	1 (20%)	6,13,13	2.37	2 (33%)
2	PIS	N	501	-	5,8,8	1.13	0	6,13,13	2.25	2 (33%)
2	PIS	O	501	-	5,8,8	1.00	0	6,13,13	2.31	2 (33%)
2	PIS	P	501	-	5,8,8	1.15	0	6,13,13	2.21	2 (33%)

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	-	-	0/4/6/6	0/0/0/0
2	PIS	B	501	-	-	0/4/6/6	0/0/0/0
2	PIS	C	501	-	-	0/4/6/6	0/0/0/0
2	PIS	D	501	-	-	0/4/6/6	0/0/0/0
2	PIS	E	501	-	-	0/4/6/6	0/0/0/0
2	PIS	F	501	-	-	0/4/6/6	0/0/0/0
2	PIS	G	501	-	-	0/4/6/6	0/0/0/0
2	PIS	H	501	-	-	0/4/6/6	0/0/0/0
2	PIS	I	501	-	-	0/4/6/6	0/0/0/0
2	PIS	J	501	-	-	0/4/6/6	0/0/0/0
2	PIS	K	501	-	-	0/4/6/6	0/0/0/0
2	PIS	L	501	-	-	0/4/6/6	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PIS	M	501	-	-	0/4/6/6	0/0/0/0
2	PIS	N	501	-	-	0/4/6/6	0/0/0/0
2	PIS	O	501	-	-	0/4/6/6	0/0/0/0
2	PIS	P	501	-	-	0/4/6/6	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	PIS	P2-O4	-2.12	1.51	1.56
2	H	501	PIS	P2-O4	-2.12	1.51	1.56
2	A	501	PIS	P2-O4	-2.10	1.51	1.56
2	E	501	PIS	P2-O4	-2.09	1.51	1.56
2	M	501	PIS	P2-O4	-2.07	1.51	1.56
2	F	501	PIS	P2-O4	-2.06	1.51	1.56
2	L	501	PIS	P2-O4	-2.05	1.51	1.56
2	I	501	PIS	P2-O4	-2.04	1.51	1.56

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	501	PIS	P1-O1-P2	-3.45	120.91	132.29
2	B	501	PIS	P1-O1-P2	-3.24	121.58	132.29
2	G	501	PIS	P1-O1-P2	-3.20	121.75	132.29
2	D	501	PIS	P1-O1-P2	-3.14	121.93	132.29
2	I	501	PIS	P1-O1-P2	-3.13	121.97	132.29
2	A	501	PIS	P1-O1-P2	-3.06	122.19	132.29
2	K	501	PIS	P1-O1-P2	-3.05	122.22	132.29
2	J	501	PIS	P1-O1-P2	-3.03	122.29	132.29
2	F	501	PIS	P1-O1-P2	-3.00	122.39	132.29
2	O	501	PIS	P1-O1-P2	-2.98	122.47	132.29
2	L	501	PIS	P1-O1-P2	-2.95	122.55	132.29
2	N	501	PIS	P1-O1-P2	-2.93	122.63	132.29
2	P	501	PIS	P1-O1-P2	-2.78	123.12	132.29
2	C	501	PIS	P1-O1-P2	-2.73	123.28	132.29
2	H	501	PIS	P1-O1-P2	-2.72	123.33	132.29
2	E	501	PIS	P1-O1-P2	-2.70	123.38	132.29
2	E	501	PIS	O4-P2-O6	3.40	117.08	109.87
2	K	501	PIS	O4-P2-O6	3.54	117.37	109.87
2	A	501	PIS	O4-P2-O6	3.78	117.88	109.87
2	L	501	PIS	O4-P2-O6	3.78	117.88	109.87
2	I	501	PIS	O4-P2-O6	3.82	117.97	109.87
2	N	501	PIS	O4-P2-O6	3.95	118.24	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	501	PIS	O4-P2-O6	3.95	118.25	109.87
2	C	501	PIS	O4-P2-O6	3.96	118.26	109.87
2	M	501	PIS	O4-P2-O6	3.99	118.33	109.87
2	O	501	PIS	O4-P2-O6	4.07	118.51	109.87
2	H	501	PIS	O4-P2-O6	4.08	118.52	109.87
2	F	501	PIS	O4-P2-O6	4.11	118.59	109.87
2	G	501	PIS	O4-P2-O6	4.16	118.69	109.87
2	J	501	PIS	O4-P2-O6	4.17	118.72	109.87
2	D	501	PIS	O4-P2-O6	4.19	118.75	109.87
2	B	501	PIS	O4-P2-O6	4.20	118.78	109.87

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%)	-0.20	2 (0%) 90 88	28, 43, 66, 77	0
1	B	397/445 (89%)	-0.17	3 (0%) 86 82	29, 48, 73, 86	0
1	C	397/445 (89%)	-0.17	2 (0%) 90 88	28, 46, 70, 84	0
1	D	397/445 (89%)	-0.12	5 (1%) 77 72	31, 46, 72, 88	0
1	E	397/445 (89%)	-0.09	3 (0%) 86 82	31, 50, 69, 83	0
1	F	397/445 (89%)	-0.04	4 (1%) 82 78	32, 54, 89, 100	0
1	G	397/445 (89%)	-0.13	3 (0%) 86 82	30, 50, 72, 85	0
1	H	397/445 (89%)	-0.11	8 (2%) 65 57	31, 49, 78, 97	0
1	I	397/445 (89%)	0.51	18 (4%) 34 25	50, 78, 110, 121	0
1	J	397/445 (89%)	0.01	10 (2%) 58 49	37, 55, 81, 92	0
1	K	392/445 (88%)	0.50	25 (6%) 20 13	53, 76, 106, 117	0
1	L	397/445 (89%)	1.25	82 (20%) 1 1	59, 92, 133, 148	0
1	M	397/445 (89%)	0.84	55 (13%) 3 2	58, 80, 110, 119	0
1	N	397/445 (89%)	0.28	19 (4%) 31 22	47, 62, 76, 88	0
1	O	391/445 (87%)	0.57	31 (7%) 13 8	57, 78, 103, 113	0
1	P	397/445 (89%)	0.58	35 (8%) 11 6	57, 75, 98, 119	0
All	All	6341/7120 (89%)	0.22	305 (4%) 31 22	28, 62, 103, 148	0

All (305) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	324	TYR	10.2
1	L	322	LEU	9.9
1	L	324	TYR	9.0
1	L	336	GLN	8.7
1	P	401	LEU	8.4

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Mol	Chain	Res	Type	RSRZ
1	L	372	LEU	6.8
1	K	262	SER	5.9
1	L	337	LEU	5.8
1	L	362	GLY	5.5
1	L	433	MET	5.5
1	L	104	SER	5.1
1	L	397	PRO	5.0
1	P	98	ASN	5.0
1	I	96	GLU	5.0
1	M	378	TYR	4.9
1	L	361	HIS	4.9
1	O	324	TYR	4.8
1	M	337	LEU	4.8
1	G	324	TYR	4.6
1	L	376	TRP	4.5
1	L	96	GLU	4.4
1	M	95	ALA	4.4
1	P	398	CYS	4.4
1	L	401	LEU	4.4
1	M	97	ALA	4.3
1	L	437	LEU	4.2
1	P	397	PRO	4.2
1	P	324	TYR	4.2
1	O	349	SER	4.2
1	P	362	GLY	4.2
1	L	95	ALA	4.1
1	L	365	ASP	4.1
1	M	415	TYR	4.1
1	M	437	LEU	4.1
1	P	372	LEU	4.0
1	L	318	LEU	4.0
1	P	219	ALA	4.0
1	J	324	TYR	4.0
1	L	404	THR	3.9
1	M	350	ALA	3.9
1	I	320	ARG	3.8
1	E	30	GLN	3.8
1	P	400	ASN	3.8
1	M	93	SER	3.8
1	C	324	TYR	3.8
1	L	403	GLU	3.8
1	M	30	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	I	236	ALA	3.7
1	I	403	GLU	3.7
1	P	406	THR	3.6
1	P	96	GLU	3.6
1	O	299	LEU	3.6
1	P	106	GLU	3.6
1	N	362	GLY	3.6
1	I	362	GLY	3.6
1	L	370	ASN	3.6
1	M	250	PHE	3.6
1	M	303	VAL	3.6
1	L	412	ALA	3.5
1	I	95	ALA	3.5
1	L	369	ALA	3.5
1	N	301	GLY	3.4
1	L	296	PHE	3.4
1	M	413	PHE	3.4
1	L	415	TYR	3.4
1	I	318	LEU	3.4
1	F	203	GLY	3.3
1	L	414	SER	3.3
1	J	419	GLY	3.3
1	N	437	LEU	3.3
1	M	323	GLN	3.3
1	I	262	SER	3.2
1	K	92	ARG	3.2
1	N	102	GLY	3.2
1	L	423	LEU	3.2
1	M	343	TYR	3.2
1	O	224	VAL	3.2
1	N	30	GLN	3.2
1	I	437	LEU	3.2
1	M	340	VAL	3.2
1	M	379	LEU	3.2
1	O	250	PHE	3.2
1	M	356	LEU	3.1
1	O	293	LEU	3.1
1	P	361	HIS	3.1
1	M	322	LEU	3.1
1	K	91	ILE	3.1
1	I	66	GLY	3.1
1	L	434	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	K	348	GLY	3.1
1	L	321	ILE	3.1
1	O	228	ALA	3.0
1	I	296	PHE	3.0
1	J	319	TRP	3.0
1	E	324	TYR	3.0
1	L	340	VAL	3.0
1	N	138	GLN	3.0
1	L	304	THR	3.0
1	O	262	SER	3.0
1	L	388	TYR	3.0
1	P	395	ASN	3.0
1	H	310	LYS	3.0
1	L	297	TRP	3.0
1	O	318	LEU	3.0
1	K	93	SER	3.0
1	L	107	GLY	3.0
1	K	336	GLN	2.9
1	L	119	SER	2.9
1	L	398	CYS	2.9
1	L	421	ALA	2.9
1	I	104	SER	2.9
1	L	347	SER	2.9
1	N	37	GLY	2.9
1	L	105	ALA	2.9
1	L	356	LEU	2.9
1	M	351	THR	2.9
1	M	318	LEU	2.9
1	O	401	LEU	2.9
1	L	341	VAL	2.9
1	O	314	ILE	2.8
1	M	407	VAL	2.8
1	M	241	GLU	2.8
1	M	345	LEU	2.8
1	N	155	ARG	2.8
1	I	324	TYR	2.8
1	J	350	ALA	2.8
1	M	381	TRP	2.8
1	M	362	GLY	2.8
1	O	266	ILE	2.8
1	M	249	THR	2.8
1	N	176	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	L	319	TRP	2.7
1	O	297	TRP	2.7
1	H	95	ALA	2.7
1	K	379	LEU	2.7
1	H	94	SER	2.7
1	O	345	LEU	2.7
1	L	432	GLY	2.7
1	M	256	SER	2.7
1	K	218	LEU	2.7
1	M	96	GLU	2.7
1	M	349	SER	2.7
1	L	379	LEU	2.7
1	L	350	ALA	2.7
1	O	240	ILE	2.6
1	L	108	TYR	2.6
1	L	293	LEU	2.6
1	K	240	ILE	2.6
1	M	319	TRP	2.6
1	O	319	TRP	2.6
1	I	367	ALA	2.6
1	P	403	GLU	2.6
1	I	356	LEU	2.6
1	O	419	GLY	2.6
1	L	33	TRP	2.6
1	L	228	ALA	2.6
1	P	296	PHE	2.6
1	K	322	LEU	2.6
1	N	393	TYR	2.6
1	K	406	THR	2.6
1	L	377	ASP	2.6
1	P	94	SER	2.6
1	G	296	PHE	2.6
1	K	118	ALA	2.6
1	O	265	PHE	2.6
1	L	314	ILE	2.5
1	H	337	LEU	2.5
1	I	176	THR	2.5
1	L	384	LEU	2.5
1	L	406	THR	2.5
1	P	404	THR	2.5
1	M	375	PHE	2.5
1	B	30	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	250	PHE	2.5
1	K	415	TYR	2.5
1	J	30	GLN	2.5
1	M	117	GLN	2.5
1	P	30	GLN	2.5
1	P	399	ARG	2.5
1	L	303	VAL	2.5
1	L	320	ARG	2.5
1	F	362	GLY	2.5
1	M	242	SER	2.5
1	O	435	GLY	2.5
1	E	91	ILE	2.5
1	O	281	LEU	2.5
1	P	62	LEU	2.5
1	P	95	ALA	2.5
1	H	324	TYR	2.5
1	M	94	SER	2.4
1	J	95	ALA	2.4
1	A	95	ALA	2.4
1	I	94	SER	2.4
1	D	437	LEU	2.4
1	K	372	LEU	2.4
1	B	324	TYR	2.4
1	M	31	LEU	2.4
1	K	343	TYR	2.4
1	M	416	THR	2.4
1	P	433	MET	2.4
1	A	324	TYR	2.4
1	M	403	GLU	2.4
1	M	247	LEU	2.4
1	O	254	LEU	2.4
1	C	336	GLN	2.4
1	L	343	TYR	2.4
1	M	341	VAL	2.4
1	M	414	SER	2.4
1	O	348	GLY	2.3
1	K	296	PHE	2.3
1	L	203	GLY	2.3
1	N	180	ASN	2.3
1	L	427	PHE	2.3
1	P	32	PRO	2.3
1	L	310	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	M	254	LEU	2.3
1	J	243	PRO	2.3
1	L	290	LEU	2.3
1	O	213	LEU	2.3
1	L	378	TYR	2.3
1	N	322	LEU	2.3
1	D	362	GLY	2.3
1	L	211	PHE	2.3
1	P	336	GLN	2.3
1	K	356	LEU	2.3
1	L	315	ALA	2.3
1	H	319	TRP	2.3
1	O	397	PRO	2.3
1	P	322	LEU	2.2
1	L	391	ASP	2.2
1	L	246	VAL	2.2
1	N	277	SER	2.2
1	F	240	ILE	2.2
1	M	386	ALA	2.2
1	P	235	ILE	2.2
1	G	291	ALA	2.2
1	K	267	LEU	2.2
1	N	32	PRO	2.2
1	O	291	ALA	2.2
1	K	119	SER	2.2
1	L	418	SER	2.2
1	P	292	THR	2.2
1	P	437	LEU	2.2
1	M	283	VAL	2.2
1	P	162	LEU	2.2
1	D	93	SER	2.2
1	L	424	THR	2.2
1	N	45	ILE	2.2
1	N	184	SER	2.2
1	O	70	HIS	2.2
1	M	377	ASP	2.2
1	M	189	GLN	2.2
1	L	116	TYR	2.2
1	L	425	VAL	2.2
1	L	363	ARG	2.2
1	P	429	ALA	2.2
1	M	258	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	58	PHE	2.1
1	M	281	LEU	2.1
1	P	315	ALA	2.1
1	O	247	LEU	2.1
1	M	106	GLU	2.1
1	P	141	MET	2.1
1	L	419	GLY	2.1
1	N	419	GLY	2.1
1	O	437	LEU	2.1
1	H	348	GLY	2.1
1	L	298	THR	2.1
1	F	437	LEU	2.1
1	M	165	PHE	2.1
1	L	408	GLN	2.1
1	K	419	GLY	2.1
1	O	352	PRO	2.1
1	D	337	LEU	2.1
1	L	360	LEU	2.1
1	L	400	ASN	2.1
1	L	58	PHE	2.1
1	M	293	LEU	2.1
1	B	377	ASP	2.1
1	M	240	ILE	2.1
1	J	247	LEU	2.1
1	K	437	LEU	2.1
1	L	349	SER	2.1
1	M	324	TYR	2.1
1	O	429	ALA	2.1
1	J	379	LEU	2.1
1	L	125	LEU	2.1
1	L	413	PHE	2.1
1	O	282	TYR	2.1
1	P	100	ILE	2.1
1	K	303	VAL	2.1
1	L	60	ASN	2.1
1	L	399	ARG	2.0
1	K	103	PHE	2.0
1	L	30	GLN	2.0
1	K	365	ASP	2.0
1	L	94	SER	2.0
1	P	105	ALA	2.0
1	N	64	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	M	411	VAL	2.0
1	D	30	GLN	2.0
1	M	352	PRO	2.0
1	H	41	GLY	2.0
1	M	246	VAL	2.0
1	N	363	ARG	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 carbohydrates 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. 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	J	502	1/1	0.92	1.39	29.58	104,104,104,104	0
3	NA	F	502	1/1	0.82	0.34	4.98	92,92,92,92	0
3	NA	H	502	1/1	0.62	0.28	2.29	60,60,60,60	0
3	NA	O	502	1/1	0.83	0.31	1.83	59,59,59,59	0
3	NA	I	502	1/1	0.88	0.30	1.80	121,121,121,121	0
3	NA	A	502	1/1	0.76	0.24	0.84	51,51,51,51	0
3	NA	D	502	1/1	0.98	0.18	-0.11	43,43,43,43	0
2	PIS	N	501	9/9	0.91	0.18	-0.23	38,40,41,41	0
3	NA	G	502	1/1	0.96	0.16	-0.55	39,39,39,39	0
3	NA	K	502	1/1	0.91	0.19	-0.97	70,70,70,70	0
3	NA	N	502	1/1	0.84	0.12	-1.30	60,60,60,60	0
2	PIS	E	501	9/9	0.96	0.12	-1.31	33,34,37,42	0
2	PIS	P	501	9/9	0.94	0.15	-1.58	42,47,49,50	0
3	NA	B	502	1/1	0.91	0.12	-1.79	60,60,60,60	0
3	NA	M	502	1/1	0.87	0.09	-1.87	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	PIS	H	501	9/9	0.98	0.10	-1.91	34,35,36,38	0
2	PIS	C	501	9/9	0.96	0.12	-1.96	32,33,36,39	0
2	PIS	A	501	9/9	0.96	0.10	-2.02	32,34,35,36	0
3	NA	L	502	1/1	0.74	0.16	-2.14	89,89,89,89	0
2	PIS	I	501	9/9	0.96	0.13	-2.23	44,46,48,48	0
2	PIS	F	501	9/9	0.97	0.11	-2.43	37,38,40,42	0
3	NA	P	502	1/1	0.96	0.08	-2.56	58,58,58,58	0
2	PIS	G	501	9/9	0.96	0.11	-2.58	32,35,37,37	0
2	PIS	D	501	9/9	0.98	0.09	-2.67	30,31,34,37	0
2	PIS	O	501	9/9	0.95	0.13	-2.70	47,50,52,55	0
2	PIS	M	501	9/9	0.98	0.11	-2.76	45,47,48,50	0
3	NA	C	502	1/1	0.92	0.13	-2.77	49,49,49,49	0
2	PIS	L	501	9/9	0.97	0.13	-3.04	49,51,54,55	0
2	PIS	J	501	9/9	0.97	0.08	-3.04	30,31,32,35	0
2	PIS	K	501	9/9	0.95	0.15	-3.24	45,49,52,56	0
2	PIS	B	501	9/9	0.98	0.09	-4.00	29,31,32,34	0
3	NA	E	502	1/1	0.93	0.09	-4.65	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.