Full wwPDB X-ray Structure Validation Report (i)

Feb 20, 2024 – 10:27 AM EST

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

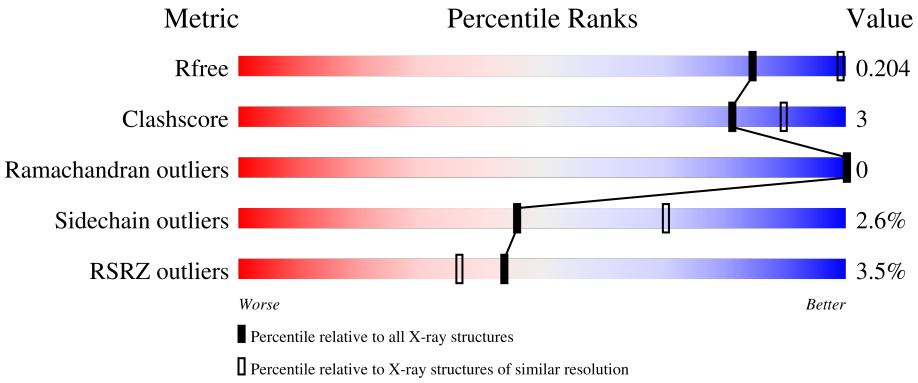
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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

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

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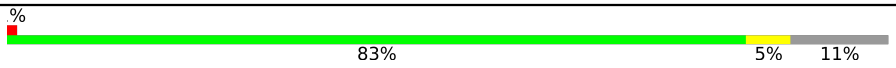
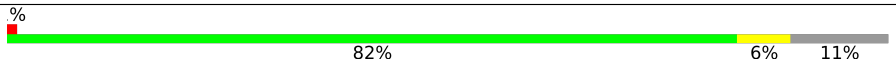
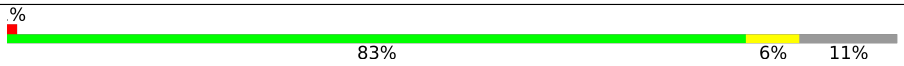
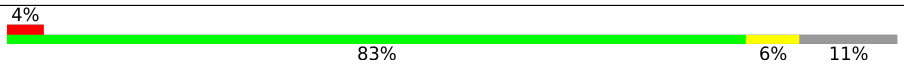
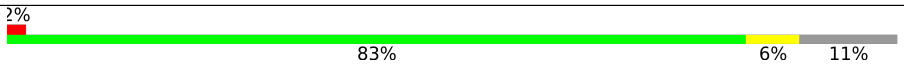
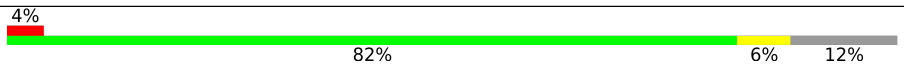
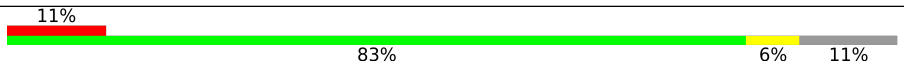
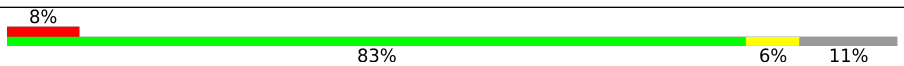
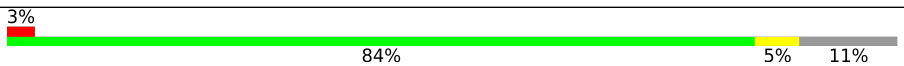
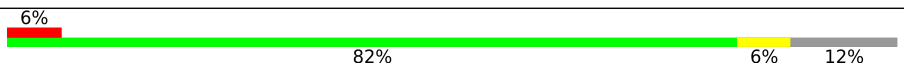
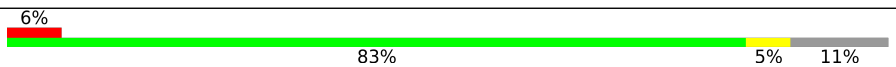
Mol	Chain	Length	Quality of chain
1	F	445	
1	G	445	
1	H	445	
1	I	445	
1	J	445	
1	K	445	
1	L	445	
1	M	445	
1	N	445	
1	O	445	
1	P	445	

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	F	502	-	-	-	X

2 Entry composition (i)

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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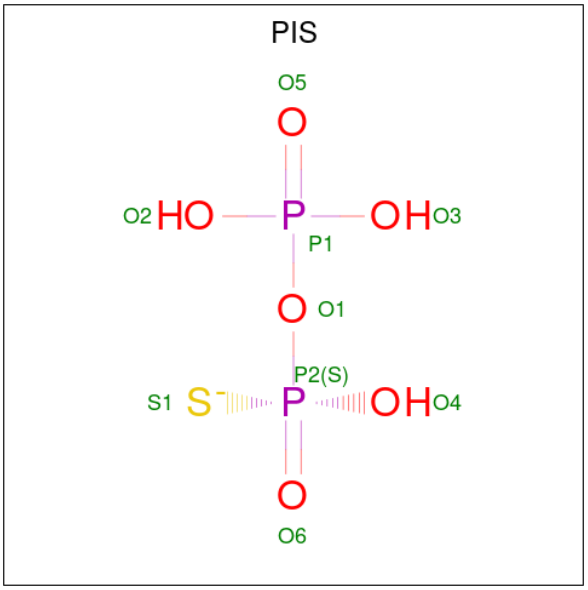
Chain	Residue	Modelled	Actual	Comment	Reference
P	444	HIS	-	expression tag	UNP A1DN10
P	445	HIS	-	expression tag	UNP A1DN10

- Molecule 2 is TRIHYDROGEN THIODIPHOSPHATE (three-letter code: PIS) (formula: $H_3O_6P_2S$).



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 9 6 2 1	0	0
2	L	1	Total O P S 9 6 2 1	0	0
2	M	1	Total O P S 9 6 2 1	0	0
2	N	1	Total O P S 9 6 2 1	0	0
2	O	1	Total O P S 9 6 2 1	0	0
2	P	1	Total O P S 9 6 2 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	B	1	Total Na 1 1	0	0
3	C	1	Total Na 1 1	0	0
3	D	1	Total Na 1 1	0	0
3	E	1	Total Na 1 1	0	0
3	F	1	Total Na 1 1	0	0
3	G	1	Total Na 1 1	0	0
3	H	1	Total Na 1 1	0	0
3	I	1	Total Na 1 1	0	0
3	J	1	Total Na 1 1	0	0
3	K	1	Total Na 1 1	0	0
3	L	1	Total Na 1 1	0	0
3	M	1	Total Na 1 1	0	0

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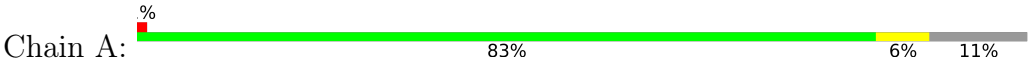
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	N	1	Total Na 1 1	0	0
3	O	1	Total Na 1 1	0	0
3	P	1	Total Na 1 1	0	0

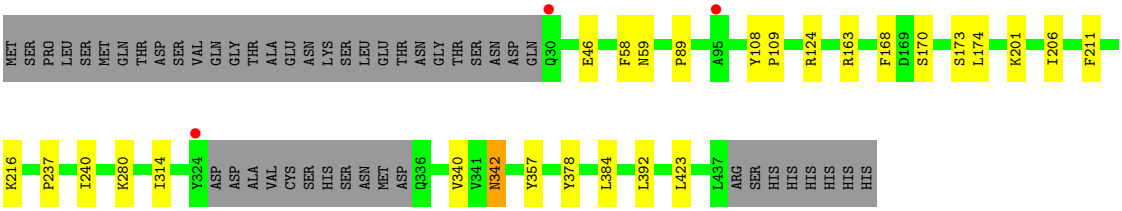
3 Residue-property plots (i)

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

• Molecule 1: Dimethylallyl tryptophan synthase

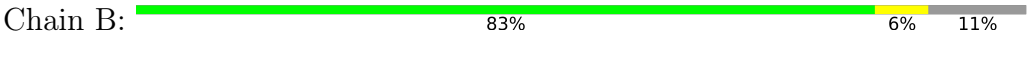
Chain A:

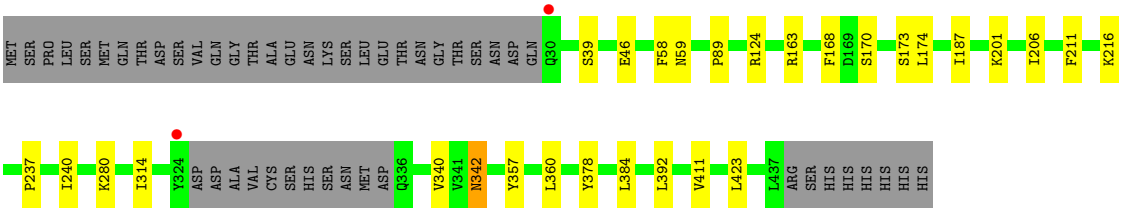




• Molecule 1: Dimethylallyl tryptophan synthase

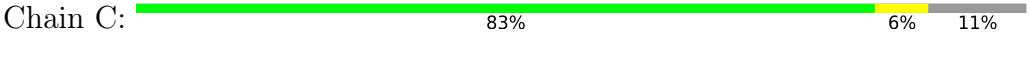
Chain B:

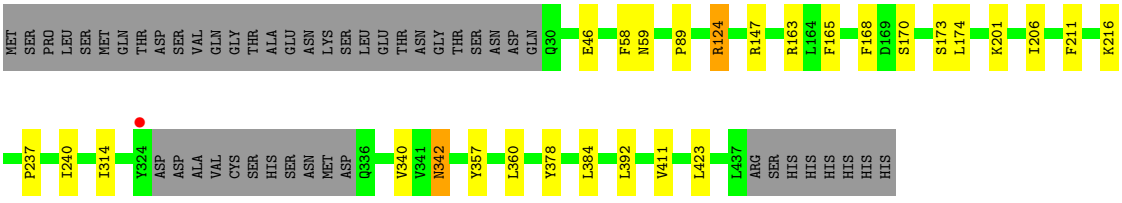




• Molecule 1: Dimethylallyl tryptophan synthase

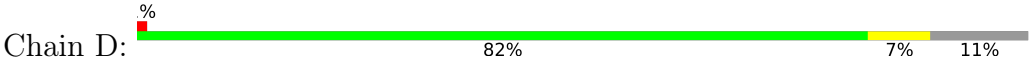
Chain C:

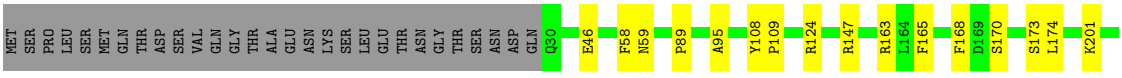


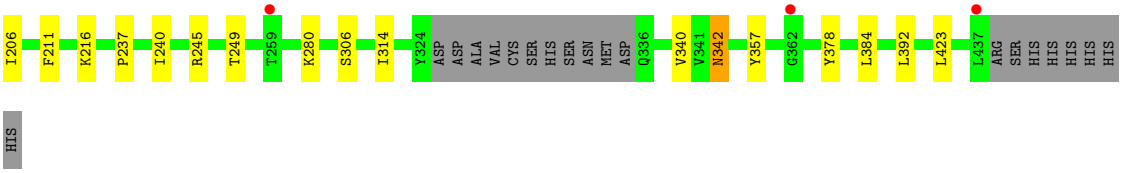


• Molecule 1: Dimethylallyl tryptophan synthase

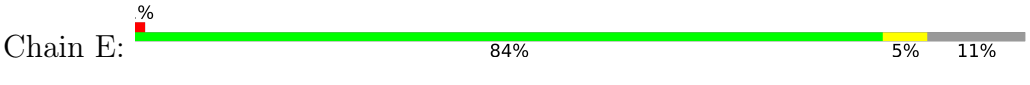
Chain D:

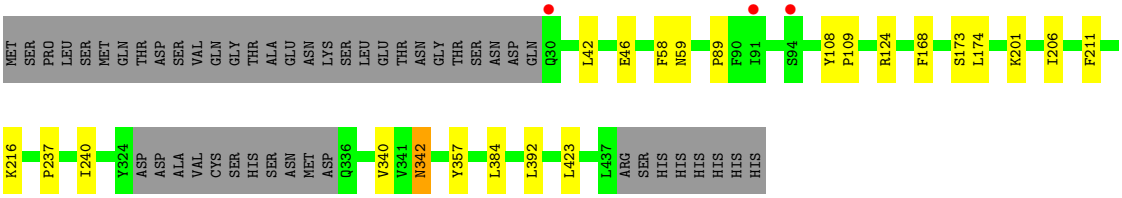




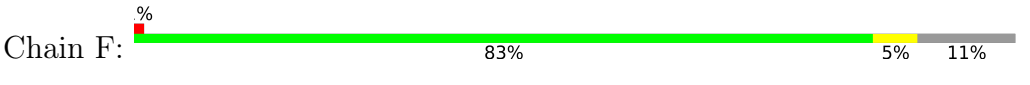


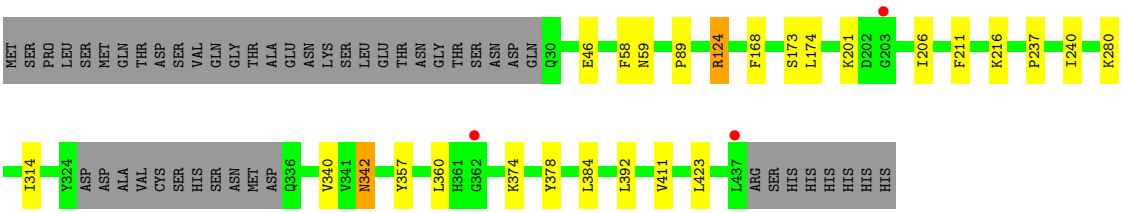
• Molecule 1: Dimethylallyl tryptophan synthase



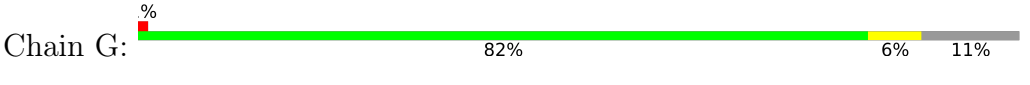


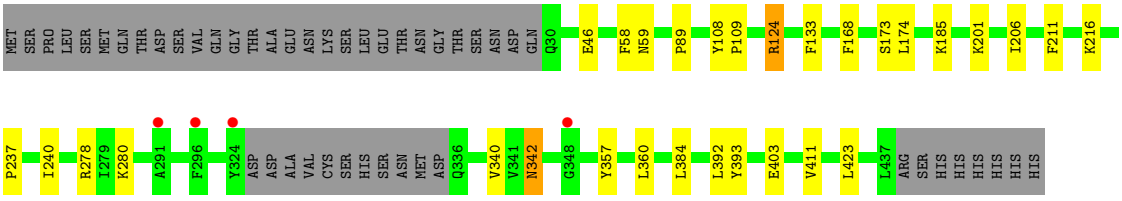
• Molecule 1: Dimethylallyl tryptophan synthase



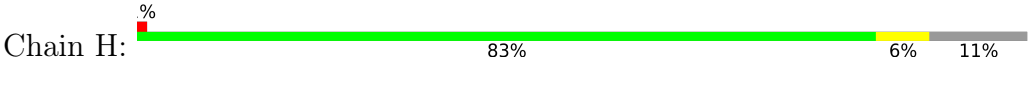


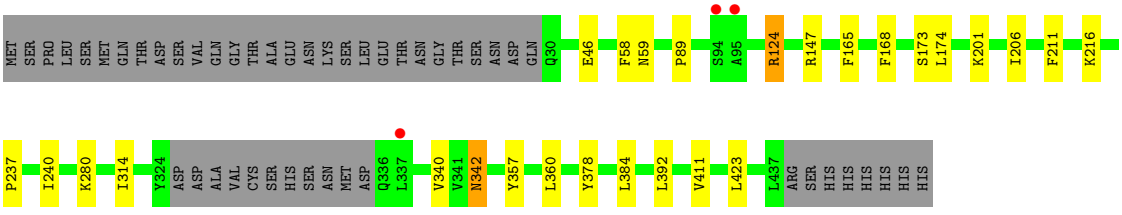
• Molecule 1: Dimethylallyl tryptophan synthase





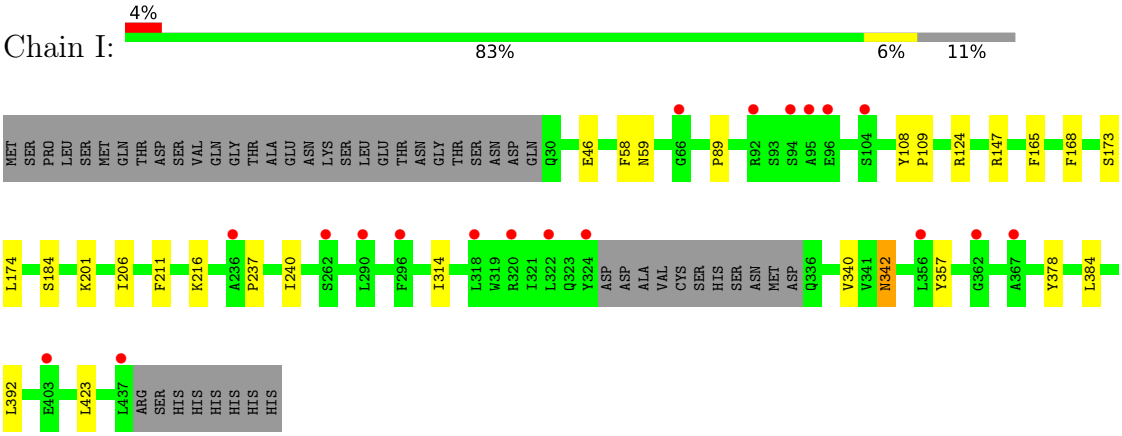
• Molecule 1: Dimethylallyl tryptophan synthase





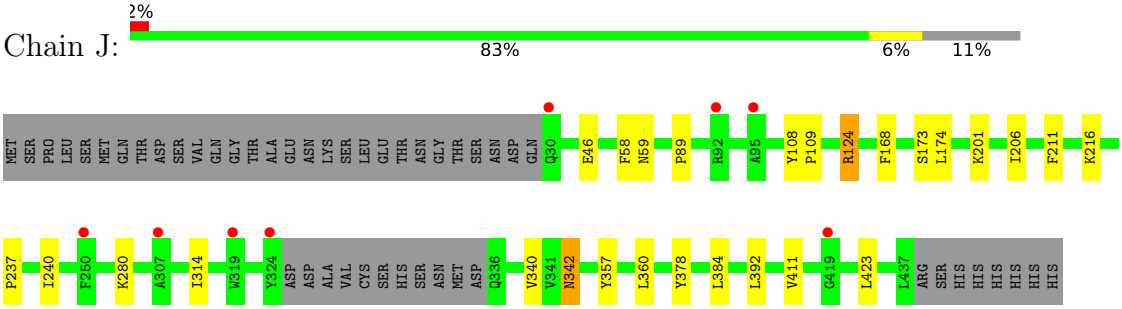
• Molecule 1: Dimethylallyl tryptophan synthase

Chain I:



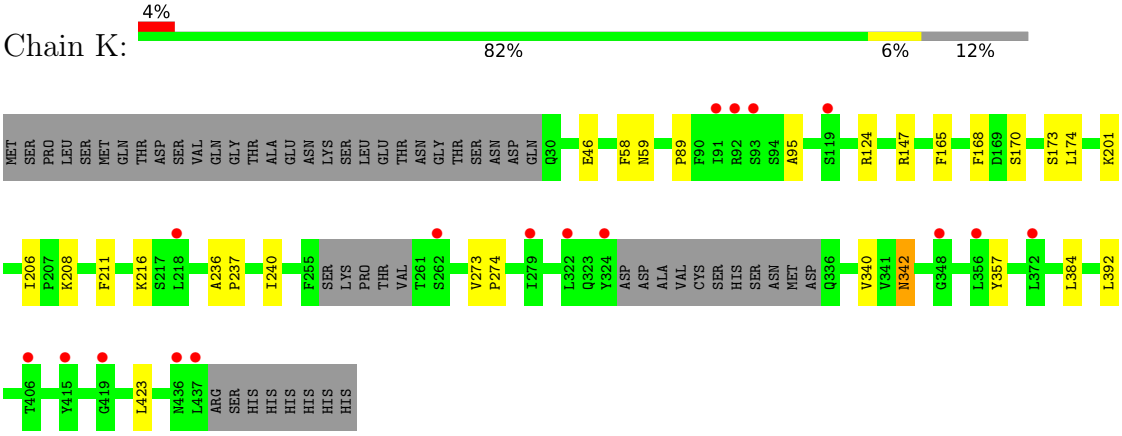
• Molecule 1: Dimethylallyl tryptophan synthase

Chain J:



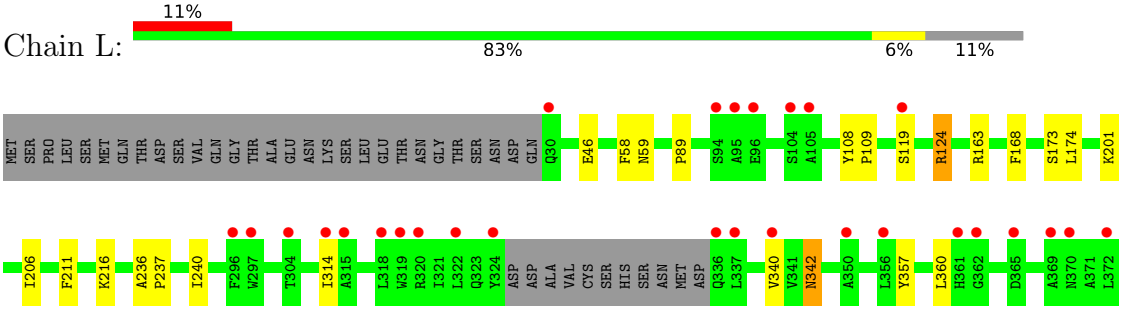
• Molecule 1: Dimethylallyl tryptophan synthase

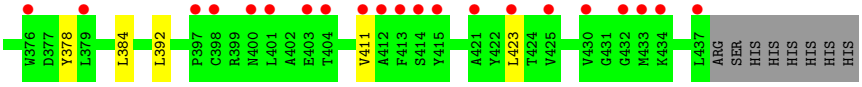
Chain K:



• Molecule 1: Dimethylallyl tryptophan synthase

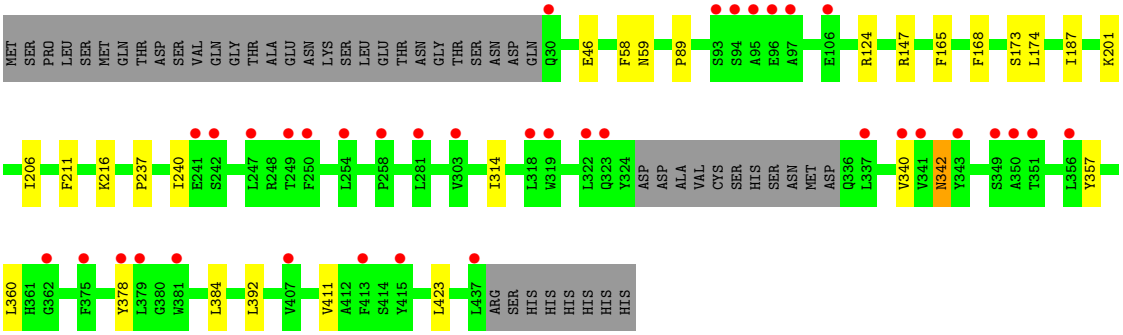
Chain L:





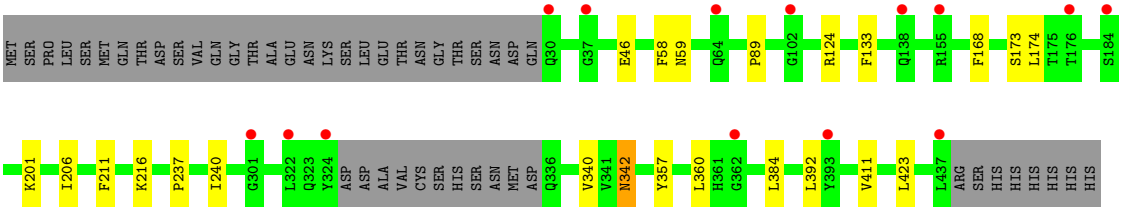
• Molecule 1: Dimethylallyl tryptophan synthase

Chain M:



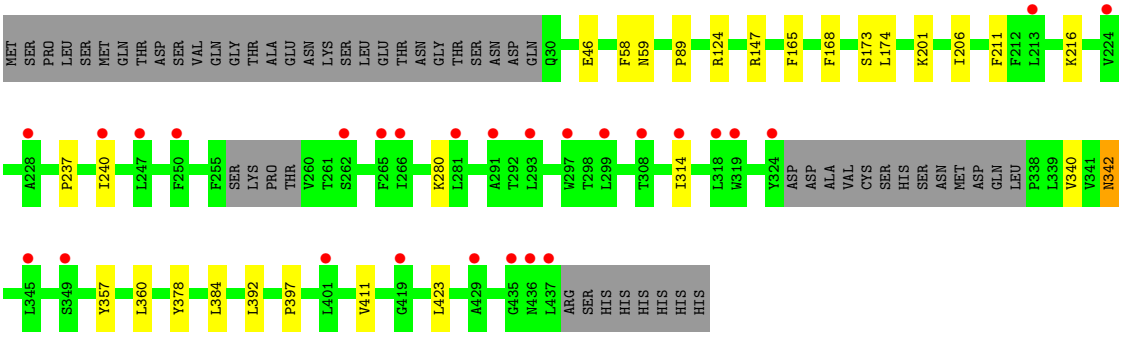
• Molecule 1: Dimethylallyl tryptophan synthase

Chain N:



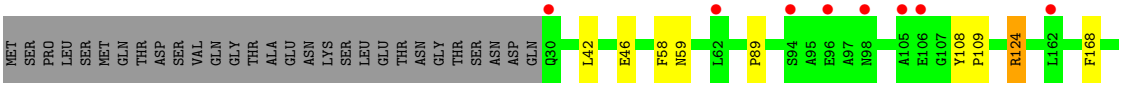
• Molecule 1: Dimethylallyl tryptophan synthase

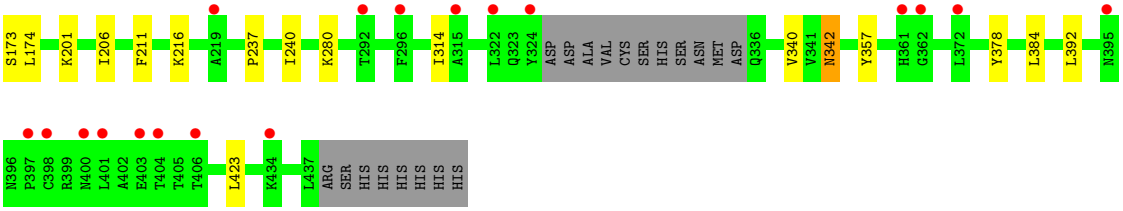
Chain O:



• Molecule 1: Dimethylallyl tryptophan synthase

Chain P:




S173
L174
K201
I206
F211
K216
A219
P237
I240
K280
T292
F296
I314
A315
L322
Q323
Y324
ASP
ASP
ALA
VAL
CYS
SER
HIS
SER
ASN
MET
ASP
Q336
V340
V341
N342
Y357
H361
G362
L372
Y378
L384
L392
N395
M396
P397
C398
R399
N400
L401
A402
E403
T404
T405
T406
L423
K434
L437
ARG
SER
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (2.00%)	wwPDB-VP
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 , 12.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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:46:GLU:HG2	1:K:89:PRO:HA	1.99	0.44
1:K:168:PHE:CB	1:K:211:PHE:HE2	2.30	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: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:G:185:LYS:O	1:M:187:ILE:HG22	2.21	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: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: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: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: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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	307/382 (80%)	299 (97%)	8 (3%)	46	70
1	B	308/382 (81%)	299 (97%)	9 (3%)	42	67
1	C	308/382 (81%)	300 (97%)	8 (3%)	46	70
1	D	308/382 (81%)	300 (97%)	8 (3%)	46	70
1	E	306/382 (80%)	298 (97%)	8 (3%)	46	70
1	F	308/382 (81%)	300 (97%)	8 (3%)	46	70
1	G	308/382 (81%)	300 (97%)	8 (3%)	46	70
1	H	308/382 (81%)	300 (97%)	8 (3%)	46	70
1	I	306/382 (80%)	298 (97%)	8 (3%)	46	70
1	J	308/382 (81%)	300 (97%)	8 (3%)	46	70
1	K	303/382 (79%)	295 (97%)	8 (3%)	46	70
1	L	308/382 (81%)	300 (97%)	8 (3%)	46	70
1	M	306/382 (80%)	298 (97%)	8 (3%)	46	70
1	N	308/382 (81%)	300 (97%)	8 (3%)	46	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	O	302/382 (79%)	294 (97%)	8 (3%)	46 70
1	P	308/382 (81%)	300 (97%)	8 (3%)	46 70
All	All	4910/6112 (80%)	4781 (97%)	129 (3%)	46 70

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

Sometimes 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

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	I	501	-	4,8,8	1.20	1 (25%)	8,13,13	1.61	1 (12%)
2	PIS	H	501	-	4,8,8	1.26	1 (25%)	8,13,13	1.68	1 (12%)
2	PIS	J	501	-	4,8,8	1.08	0	8,13,13	1.78	1 (12%)
2	PIS	O	501	-	4,8,8	1.02	0	8,13,13	1.73	1 (12%)
2	PIS	M	501	-	4,8,8	1.23	1 (25%)	8,13,13	1.67	1 (12%)
2	PIS	F	501	-	4,8,8	1.22	1 (25%)	8,13,13	1.76	2 (25%)
2	PIS	G	501	-	4,8,8	1.01	0	8,13,13	1.75	1 (12%)
2	PIS	D	501	-	4,8,8	1.26	1 (25%)	8,13,13	1.75	1 (12%)
2	PIS	P	501	-	4,8,8	1.20	1 (25%)	8,13,13	1.66	1 (12%)
2	PIS	K	501	-	4,8,8	1.06	0	8,13,13	1.55	1 (12%)
2	PIS	E	501	-	4,8,8	1.22	1 (25%)	8,13,13	1.49	1 (12%)
2	PIS	N	501	-	4,8,8	1.08	0	8,13,13	1.67	1 (12%)
2	PIS	B	501	-	4,8,8	1.03	0	8,13,13	1.81	2 (25%)
2	PIS	C	501	-	4,8,8	1.05	0	8,13,13	1.67	1 (12%)
2	PIS	L	501	-	4,8,8	1.22	1 (25%)	8,13,13	1.60	1 (12%)
2	PIS	A	501	-	4,8,8	1.24	1 (25%)	8,13,13	1.60	1 (12%)

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	I	501	-	-	0/4/6/6	-
2	PIS	H	501	-	-	0/4/6/6	-
2	PIS	J	501	-	-	0/4/6/6	-
2	PIS	O	501	-	-	1/4/6/6	-
2	PIS	M	501	-	-	0/4/6/6	-
2	PIS	F	501	-	-	0/4/6/6	-
2	PIS	G	501	-	-	0/4/6/6	-
2	PIS	D	501	-	-	1/4/6/6	-
2	PIS	P	501	-	-	0/4/6/6	-
2	PIS	K	501	-	-	0/4/6/6	-
2	PIS	E	501	-	-	0/4/6/6	-
2	PIS	N	501	-	-	0/4/6/6	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PIS	B	501	-	-	1/4/6/6	-
2	PIS	C	501	-	-	3/4/6/6	-
2	PIS	L	501	-	-	0/4/6/6	-
2	PIS	A	501	-	-	0/4/6/6	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	PIS	P2-O4	-2.17	1.51	1.56
2	H	501	PIS	P2-O4	-2.16	1.51	1.56
2	A	501	PIS	P2-O4	-2.14	1.51	1.56
2	E	501	PIS	P2-O4	-2.13	1.51	1.56
2	M	501	PIS	P2-O4	-2.11	1.51	1.56
2	F	501	PIS	P2-O4	-2.10	1.51	1.56
2	L	501	PIS	P2-O4	-2.10	1.51	1.56
2	I	501	PIS	P2-O4	-2.08	1.51	1.56
2	P	501	PIS	P2-O4	-2.03	1.51	1.56

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	PIS	O4-P2-O6	4.15	118.78	109.91
2	D	501	PIS	O4-P2-O6	4.14	118.75	109.91
2	J	501	PIS	O4-P2-O6	4.12	118.72	109.91
2	G	501	PIS	O4-P2-O6	4.11	118.69	109.91
2	F	501	PIS	O4-P2-O6	4.06	118.59	109.91
2	H	501	PIS	O4-P2-O6	4.03	118.52	109.91
2	O	501	PIS	O4-P2-O6	4.02	118.51	109.91
2	M	501	PIS	O4-P2-O6	3.94	118.33	109.91
2	C	501	PIS	O4-P2-O6	3.91	118.26	109.91
2	P	501	PIS	O4-P2-O6	3.90	118.25	109.91
2	N	501	PIS	O4-P2-O6	3.90	118.24	109.91
2	I	501	PIS	O4-P2-O6	3.77	117.97	109.91
2	L	501	PIS	O4-P2-O6	3.73	117.88	109.91
2	A	501	PIS	O4-P2-O6	3.73	117.88	109.91
2	K	501	PIS	O4-P2-O6	3.49	117.37	109.91
2	E	501	PIS	O4-P2-O6	3.36	117.08	109.91
2	F	501	PIS	O3-P1-O2	2.02	115.34	107.64
2	B	501	PIS	O3-P1-O2	2.01	115.31	107.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	PIS	P1-O1-P2-O4
2	C	501	PIS	P2-O1-P1-O2
2	D	501	PIS	P1-O1-P2-O4
2	O	501	PIS	P1-O1-P2-O4
2	C	501	PIS	P2-O1-P1-O5
2	C	501	PIS	P2-O1-P1-O3

There are no ring outliers.

12 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	501	PIS	2	0
2	J	501	PIS	2	0
2	O	501	PIS	1	0
2	F	501	PIS	2	0
2	G	501	PIS	3	0
2	D	501	PIS	1	0
2	P	501	PIS	2	0
2	K	501	PIS	1	0
2	B	501	PIS	1	0
2	C	501	PIS	1	0
2	L	501	PIS	1	0
2	A	501	PIS	1	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	397/445 (89%)	-0.13	3 (0%) 86 85	28, 43, 66, 77	0
1	B	397/445 (89%)	-0.10	2 (0%) 91 89	29, 48, 73, 86	0
1	C	397/445 (89%)	-0.13	1 (0%) 94 93	28, 46, 70, 84	0
1	D	397/445 (89%)	-0.08	3 (0%) 86 85	31, 46, 72, 88	0
1	E	397/445 (89%)	-0.05	3 (0%) 86 85	31, 50, 69, 83	0
1	F	397/445 (89%)	-0.02	3 (0%) 86 85	32, 54, 89, 100	0
1	G	397/445 (89%)	-0.08	4 (1%) 82 79	30, 50, 72, 85	0
1	H	397/445 (89%)	-0.09	3 (0%) 86 85	31, 49, 78, 97	0
1	I	397/445 (89%)	0.34	19 (4%) 30 23	50, 78, 110, 121	0
1	J	397/445 (89%)	-0.03	8 (2%) 65 60	37, 55, 81, 92	0
1	K	392/445 (88%)	0.31	17 (4%) 35 27	53, 76, 106, 116	0
1	L	397/445 (89%)	0.84	49 (12%) 4 2	59, 92, 133, 148	0
1	M	397/445 (89%)	0.59	37 (9%) 8 4	58, 80, 110, 119	0
1	N	397/445 (89%)	0.20	14 (3%) 44 36	47, 62, 76, 88	0
1	O	391/445 (87%)	0.34	27 (6%) 16 11	57, 78, 103, 113	0
1	P	397/445 (89%)	0.41	26 (6%) 18 13	57, 75, 98, 119	0
All	All	6341/7120 (89%)	0.15	219 (3%) 44 36	28, 62, 103, 148	0

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	322	LEU	10.1
1	K	324	TYR	8.3
1	L	324	TYR	7.5
1	L	372	LEU	5.8
1	L	362	GLY	5.7

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Mol	Chain	Res	Type	RSRZ
1	K	262	SER	5.3
1	P	401	LEU	5.2
1	L	336	GLN	5.1
1	P	96	GLU	4.6
1	L	337	LEU	4.6
1	P	397	PRO	4.5
1	L	433	MET	4.5
1	L	403	GLU	4.3
1	G	324	TYR	4.3
1	O	349	SER	4.3
1	J	324	TYR	4.3
1	L	397	PRO	4.2
1	M	95	ALA	4.1
1	O	324	TYR	4.1
1	P	398	CYS	4.1
1	L	318	LEU	4.1
1	I	96	GLU	4.1
1	P	362	GLY	4.0
1	M	97	ALA	4.0
1	L	361	HIS	4.0
1	E	30	GLN	4.0
1	P	98	ASN	4.0
1	M	378	TYR	4.0
1	L	104	SER	4.0
1	L	95	ALA	4.0
1	L	404	THR	4.0
1	M	30	GLN	4.0
1	I	95	ALA	4.0
1	M	337	LEU	3.9
1	L	96	GLU	3.8
1	P	324	TYR	3.8
1	M	415	TYR	3.7
1	M	350	ALA	3.7
1	I	318	LEU	3.7
1	P	400	ASN	3.6
1	I	320	ARG	3.6
1	N	301	GLY	3.6
1	L	437	LEU	3.5
1	M	303	VAL	3.5
1	M	437	LEU	3.5
1	L	376	TRP	3.5
1	O	262	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	M	323	GLN	3.4
1	L	365	ASP	3.4
1	I	262	SER	3.4
1	M	93	SER	3.3
1	L	356	LEU	3.3
1	P	219	ALA	3.3
1	L	401	LEU	3.3
1	L	434	LYS	3.3
1	O	293	LEU	3.3
1	P	372	LEU	3.3
1	I	236	ALA	3.2
1	O	429	ALA	3.2
1	P	106	GLU	3.2
1	L	423	LEU	3.2
1	I	324	TYR	3.2
1	M	250	PHE	3.2
1	J	319	TRP	3.1
1	O	224	VAL	3.1
1	L	369	ALA	3.0
1	I	296	PHE	3.0
1	I	437	LEU	3.0
1	N	30	GLN	3.0
1	J	419	GLY	3.0
1	L	412	ALA	2.9
1	O	228	ALA	2.9
1	M	96	GLU	2.9
1	P	94	SER	2.9
1	M	249	THR	2.9
1	K	91	ILE	2.9
1	L	296	PHE	2.9
1	K	93	SER	2.8
1	P	406	THR	2.8
1	C	324	TYR	2.8
1	L	415	TYR	2.8
1	L	319	TRP	2.8
1	L	340	VAL	2.8
1	O	437	LEU	2.8
1	N	362	GLY	2.7
1	I	403	GLU	2.7
1	K	92	ARG	2.7
1	N	437	LEU	2.7
1	L	315	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	203	GLY	2.7
1	F	362	GLY	2.7
1	L	370	ASN	2.7
1	J	92	ARG	2.7
1	L	350	ALA	2.7
1	I	356	LEU	2.7
1	O	299	LEU	2.7
1	O	314	ILE	2.7
1	K	437	LEU	2.6
1	P	395	ASN	2.6
1	E	91	ILE	2.6
1	B	30	GLN	2.6
1	M	413	PHE	2.6
1	P	361	HIS	2.6
1	M	322	LEU	2.6
1	L	304	THR	2.6
1	O	419	GLY	2.6
1	M	241	GLU	2.6
1	L	297	TRP	2.6
1	M	356	LEU	2.6
1	L	414	SER	2.6
1	J	95	ALA	2.6
1	L	105	ALA	2.6
1	M	362	GLY	2.5
1	K	419	GLY	2.5
1	K	415	TYR	2.5
1	M	242	SER	2.5
1	K	218	LEU	2.5
1	N	184	SER	2.5
1	M	351	THR	2.5
1	M	106	GLU	2.4
1	M	340	VAL	2.4
1	M	375	PHE	2.4
1	L	430	VAL	2.4
1	P	296	PHE	2.4
1	I	290	LEU	2.4
1	O	318	LEU	2.4
1	I	92	ARG	2.4
1	M	379	LEU	2.4
1	B	324	TYR	2.4
1	M	258	PRO	2.4
1	M	319	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	K	119	SER	2.4
1	L	119	SER	2.4
1	P	403	GLU	2.4
1	O	308	THR	2.4
1	I	367	ALA	2.4
1	N	138	GLN	2.4
1	O	291	ALA	2.4
1	M	318	LEU	2.4
1	P	322	LEU	2.4
1	N	102	GLY	2.3
1	D	437	LEU	2.3
1	P	30	GLN	2.3
1	H	94	SER	2.3
1	O	345	LEU	2.3
1	K	348	GLY	2.3
1	O	265	PHE	2.3
1	O	281	LEU	2.3
1	H	337	LEU	2.3
1	G	296	PHE	2.3
1	O	435	GLY	2.3
1	O	266	ILE	2.3
1	I	94	SER	2.3
1	O	247	LEU	2.3
1	O	401	LEU	2.3
1	N	393	TYR	2.3
1	O	240	ILE	2.3
1	L	30	GLN	2.3
1	O	319	TRP	2.2
1	M	407	VAL	2.2
1	K	322	LEU	2.2
1	P	315	ALA	2.2
1	J	30	GLN	2.2
1	P	404	THR	2.2
1	I	362	GLY	2.2
1	N	155	ARG	2.2
1	M	341	VAL	2.2
1	L	400	ASN	2.2
1	L	413	PHE	2.2
1	L	421	ALA	2.2
1	I	322	LEU	2.2
1	G	291	ALA	2.2
1	O	250	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	O	436	ASN	2.2
1	P	434	LYS	2.2
1	A	324	TYR	2.2
1	N	324	TYR	2.2
1	J	307	ALA	2.2
1	M	94	SER	2.2
1	I	66	GLY	2.2
1	M	281	LEU	2.2
1	A	95	ALA	2.2
1	H	95	ALA	2.2
1	K	406	THR	2.1
1	L	379	LEU	2.1
1	E	94	SER	2.1
1	M	349	SER	2.1
1	O	213	LEU	2.1
1	L	320	ARG	2.1
1	M	381	TRP	2.1
1	O	297	TRP	2.1
1	G	348	GLY	2.1
1	M	247	LEU	2.1
1	N	322	LEU	2.1
1	L	94	SER	2.1
1	K	279	ILE	2.1
1	I	104	SER	2.1
1	K	356	LEU	2.1
1	P	62	LEU	2.1
1	D	259	THR	2.1
1	M	343	TYR	2.1
1	L	411	VAL	2.1
1	K	372	LEU	2.1
1	N	176	THR	2.1
1	K	436	ASN	2.1
1	M	254	LEU	2.0
1	D	362	GLY	2.0
1	L	398	CYS	2.0
1	N	37	GLY	2.0
1	P	292	THR	2.0
1	L	425	VAL	2.0
1	N	64	GLN	2.0
1	P	105	ALA	2.0
1	L	314	ILE	2.0
1	L	432	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	J	250	PHE	2.0
1	A	30	GLN	2.0
1	F	437	LEU	2.0
1	P	162	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NA	A	502	1/1	0.66	0.24	51,51,51,51	0
3	NA	H	502	1/1	0.71	0.31	60,60,60,60	0
3	NA	L	502	1/1	0.71	0.21	89,89,89,89	0
3	NA	F	502	1/1	0.74	0.41	92,92,92,92	0
3	NA	B	502	1/1	0.78	0.20	60,60,60,60	0
3	NA	O	502	1/1	0.79	0.29	59,59,59,59	0
3	NA	N	502	1/1	0.82	0.15	60,60,60,60	0
3	NA	J	502	1/1	0.87	1.35	104,104,104,104	0
3	NA	M	502	1/1	0.87	0.08	49,49,49,49	0
3	NA	C	502	1/1	0.88	0.20	49,49,49,49	0
3	NA	K	502	1/1	0.88	0.12	70,70,70,70	0
2	PIS	N	501	9/9	0.91	0.16	38,40,41,41	0
3	NA	E	502	1/1	0.91	0.13	51,51,51,51	0
3	NA	I	502	1/1	0.91	0.20	121,121,121,121	0
2	PIS	K	501	9/9	0.93	0.13	45,49,52,56	0
2	PIS	P	501	9/9	0.94	0.11	42,47,49,50	0
3	NA	G	502	1/1	0.95	0.17	39,39,39,39	0
2	PIS	E	501	9/9	0.95	0.15	33,34,37,42	0
2	PIS	O	501	9/9	0.95	0.11	47,50,52,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NA	D	502	1/1	0.96	0.19	43,43,43,43	0
2	PIS	I	501	9/9	0.96	0.12	44,46,48,48	0
2	PIS	C	501	9/9	0.96	0.14	32,33,36,39	0
2	PIS	L	501	9/9	0.96	0.09	49,51,54,55	0
2	PIS	A	501	9/9	0.97	0.14	32,34,35,36	0
2	PIS	F	501	9/9	0.97	0.10	37,38,40,42	0
2	PIS	G	501	9/9	0.97	0.13	32,35,37,37	0
2	PIS	D	501	9/9	0.97	0.13	30,31,34,37	0
2	PIS	J	501	9/9	0.97	0.10	30,31,32,35	0
3	NA	P	502	1/1	0.97	0.11	58,58,58,58	0
2	PIS	H	501	9/9	0.98	0.11	34,35,36,38	0
2	PIS	M	501	9/9	0.98	0.07	45,47,48,50	0
2	PIS	B	501	9/9	0.98	0.13	29,31,32,34	0

6.5 Other polymers (i)

There are no such residues in this entry.