



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 07:53 am BST

PDB ID : 3AZ8  
Title : Beta-Hydroxyacyl-Acyl Carrier Protein Dehydratase (FabZ) from Plasmodium falciparum in complex with NAS21  
Authors : Maity, K.; Venkata, B.S.; Kapoor, N.; Surolia, N.; Surolia, A.; Suguna, K.  
Deposited on : 2011-05-20  
Resolution : 3.10 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.11  
buster-report : 1.1.7 (2018)  
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) : 2.11

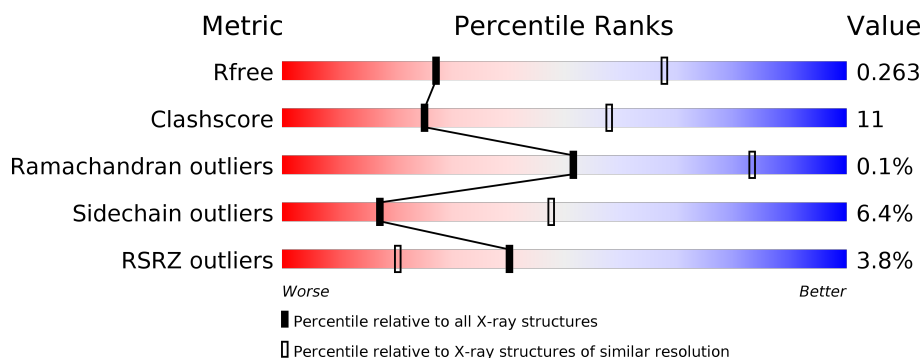
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	154	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>• 6%</div> </div> </div>
1	B	154	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>16%</div> <div>8%</div> </div> </div>
1	C	154	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>• 6%</div> </div> </div>
1	D	154	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>9%</div> </div> </div>
1	E	154	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>18%</div> <div>• 7%</div> </div> </div>
1	F	154	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>19%</div> <div>• 5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	154	
1	H	154	
1	I	154	
1	J	154	
1	K	154	
1	L	154	
1	M	154	
1	N	154	
1	O	154	
1	P	154	
1	Q	154	
1	R	154	
1	S	154	
1	T	154	
1	U	154	
1	V	154	
1	W	154	
1	X	154	

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
5	S21	D	231	-	-	X	-
5	S21	F	231	-	-	X	-
5	S21	P	4	-	-	X	-
5	S21	R	1	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 27454 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 Beta-hydroxyacyl-ACP dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	145	Total	C	N	O	S	0	0	0
			1121	731	184	201	5			
1	B	141	Total	C	N	O	S	0	0	0
			1094	713	180	196	5			
1	C	144	Total	C	N	O	S	0	0	0
			1116	727	184	200	5			
1	D	140	Total	C	N	O	S	0	0	0
			1075	699	176	195	5			
1	E	143	Total	C	N	O	S	0	0	0
			1109	722	182	200	5			
1	F	146	Total	C	N	O	S	0	1	0
			1136	736	188	207	5			
1	G	145	Total	C	N	O	S	0	0	0
			1111	722	183	201	5			
1	H	141	Total	C	N	O	S	0	0	0
			1090	710	179	196	5			
1	I	143	Total	C	N	O	S	0	1	0
			1118	732	183	198	5			
1	J	144	Total	C	N	O	S	0	0	0
			1098	714	180	199	5			
1	K	145	Total	C	N	O	S	0	0	0
			1123	731	184	203	5			
1	L	146	Total	C	N	O	S	0	0	0
			1124	728	186	205	5			
1	M	145	Total	C	N	O	S	0	0	0
			1123	731	184	203	5			
1	N	145	Total	C	N	O	S	0	0	0
			1114	724	184	201	5			
1	O	144	Total	C	N	O	S	0	0	0
			1116	727	184	200	5			
1	P	145	Total	C	N	O	S	0	0	0
			1099	714	181	199	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	142	Total	C	N	O	S	0	0	0
			1103	719	181	198	5			
1	R	146	Total	C	N	O	S	0	0	0
			1127	731	186	205	5			
1	S	146	Total	C	N	O	S	0	1	0
			1133	740	184	204	5			
1	T	142	Total	C	N	O	S	0	0	0
			1098	715	181	197	5			
1	U	144	Total	C	N	O	S	0	0	0
			1116	727	184	200	5			
1	V	144	Total	C	N	O	S	0	0	0
			1098	713	180	200	5			
1	W	142	Total	C	N	O	S	0	0	0
			1103	719	181	198	5			
1	X	145	Total	C	N	O	S	0	0	0
			1119	727	185	202	5			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	GLY	-	EXPRESSION TAG	UNP Q965D7
A	78	SER	-	EXPRESSION TAG	UNP Q965D7
A	79	HIS	-	EXPRESSION TAG	UNP Q965D7
A	80	MET	-	EXPRESSION TAG	UNP Q965D7
B	77	GLY	-	EXPRESSION TAG	UNP Q965D7
B	78	SER	-	EXPRESSION TAG	UNP Q965D7
B	79	HIS	-	EXPRESSION TAG	UNP Q965D7
B	80	MET	-	EXPRESSION TAG	UNP Q965D7
C	77	GLY	-	EXPRESSION TAG	UNP Q965D7
C	78	SER	-	EXPRESSION TAG	UNP Q965D7
C	79	HIS	-	EXPRESSION TAG	UNP Q965D7
C	80	MET	-	EXPRESSION TAG	UNP Q965D7
D	77	GLY	-	EXPRESSION TAG	UNP Q965D7
D	78	SER	-	EXPRESSION TAG	UNP Q965D7
D	79	HIS	-	EXPRESSION TAG	UNP Q965D7
D	80	MET	-	EXPRESSION TAG	UNP Q965D7
E	77	GLY	-	EXPRESSION TAG	UNP Q965D7
E	78	SER	-	EXPRESSION TAG	UNP Q965D7
E	79	HIS	-	EXPRESSION TAG	UNP Q965D7
E	80	MET	-	EXPRESSION TAG	UNP Q965D7
F	77	GLY	-	EXPRESSION TAG	UNP Q965D7
F	78	SER	-	EXPRESSION TAG	UNP Q965D7
F	79	HIS	-	EXPRESSION TAG	UNP Q965D7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	80	MET	-	EXPRESSION TAG	UNP Q965D7
G	77	GLY	-	EXPRESSION TAG	UNP Q965D7
G	78	SER	-	EXPRESSION TAG	UNP Q965D7
G	79	HIS	-	EXPRESSION TAG	UNP Q965D7
G	80	MET	-	EXPRESSION TAG	UNP Q965D7
H	77	GLY	-	EXPRESSION TAG	UNP Q965D7
H	78	SER	-	EXPRESSION TAG	UNP Q965D7
H	79	HIS	-	EXPRESSION TAG	UNP Q965D7
H	80	MET	-	EXPRESSION TAG	UNP Q965D7
I	77	GLY	-	EXPRESSION TAG	UNP Q965D7
I	78	SER	-	EXPRESSION TAG	UNP Q965D7
I	79	HIS	-	EXPRESSION TAG	UNP Q965D7
I	80	MET	-	EXPRESSION TAG	UNP Q965D7
J	77	GLY	-	EXPRESSION TAG	UNP Q965D7
J	78	SER	-	EXPRESSION TAG	UNP Q965D7
J	79	HIS	-	EXPRESSION TAG	UNP Q965D7
J	80	MET	-	EXPRESSION TAG	UNP Q965D7
K	77	GLY	-	EXPRESSION TAG	UNP Q965D7
K	78	SER	-	EXPRESSION TAG	UNP Q965D7
K	79	HIS	-	EXPRESSION TAG	UNP Q965D7
K	80	MET	-	EXPRESSION TAG	UNP Q965D7
L	77	GLY	-	EXPRESSION TAG	UNP Q965D7
L	78	SER	-	EXPRESSION TAG	UNP Q965D7
L	79	HIS	-	EXPRESSION TAG	UNP Q965D7
L	80	MET	-	EXPRESSION TAG	UNP Q965D7
M	77	GLY	-	EXPRESSION TAG	UNP Q965D7
M	78	SER	-	EXPRESSION TAG	UNP Q965D7
M	79	HIS	-	EXPRESSION TAG	UNP Q965D7
M	80	MET	-	EXPRESSION TAG	UNP Q965D7
N	77	GLY	-	EXPRESSION TAG	UNP Q965D7
N	78	SER	-	EXPRESSION TAG	UNP Q965D7
N	79	HIS	-	EXPRESSION TAG	UNP Q965D7
N	80	MET	-	EXPRESSION TAG	UNP Q965D7
O	77	GLY	-	EXPRESSION TAG	UNP Q965D7
O	78	SER	-	EXPRESSION TAG	UNP Q965D7
O	79	HIS	-	EXPRESSION TAG	UNP Q965D7
O	80	MET	-	EXPRESSION TAG	UNP Q965D7
P	77	GLY	-	EXPRESSION TAG	UNP Q965D7
P	78	SER	-	EXPRESSION TAG	UNP Q965D7
P	79	HIS	-	EXPRESSION TAG	UNP Q965D7
P	80	MET	-	EXPRESSION TAG	UNP Q965D7
Q	77	GLY	-	EXPRESSION TAG	UNP Q965D7

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	78	SER	-	EXPRESSION TAG	UNP Q965D7
Q	79	HIS	-	EXPRESSION TAG	UNP Q965D7
Q	80	MET	-	EXPRESSION TAG	UNP Q965D7
R	77	GLY	-	EXPRESSION TAG	UNP Q965D7
R	78	SER	-	EXPRESSION TAG	UNP Q965D7
R	79	HIS	-	EXPRESSION TAG	UNP Q965D7
R	80	MET	-	EXPRESSION TAG	UNP Q965D7
S	77	GLY	-	EXPRESSION TAG	UNP Q965D7
S	78	SER	-	EXPRESSION TAG	UNP Q965D7
S	79	HIS	-	EXPRESSION TAG	UNP Q965D7
S	80	MET	-	EXPRESSION TAG	UNP Q965D7
T	77	GLY	-	EXPRESSION TAG	UNP Q965D7
T	78	SER	-	EXPRESSION TAG	UNP Q965D7
T	79	HIS	-	EXPRESSION TAG	UNP Q965D7
T	80	MET	-	EXPRESSION TAG	UNP Q965D7
U	77	GLY	-	EXPRESSION TAG	UNP Q965D7
U	78	SER	-	EXPRESSION TAG	UNP Q965D7
U	79	HIS	-	EXPRESSION TAG	UNP Q965D7
U	80	MET	-	EXPRESSION TAG	UNP Q965D7
V	77	GLY	-	EXPRESSION TAG	UNP Q965D7
V	78	SER	-	EXPRESSION TAG	UNP Q965D7
V	79	HIS	-	EXPRESSION TAG	UNP Q965D7
V	80	MET	-	EXPRESSION TAG	UNP Q965D7
W	77	GLY	-	EXPRESSION TAG	UNP Q965D7
W	78	SER	-	EXPRESSION TAG	UNP Q965D7
W	79	HIS	-	EXPRESSION TAG	UNP Q965D7
W	80	MET	-	EXPRESSION TAG	UNP Q965D7
X	77	GLY	-	EXPRESSION TAG	UNP Q965D7
X	78	SER	-	EXPRESSION TAG	UNP Q965D7
X	79	HIS	-	EXPRESSION TAG	UNP Q965D7
X	80	MET	-	EXPRESSION TAG	UNP Q965D7

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	L	1	Total	C	O	0	0
			6	3	3		
2	M	1	Total	C	O	0	0
			6	3	3		
2	O	1	Total	C	O	0	0
			6	3	3		
2	P	1	Total	C	O	0	0
			6	3	3		
2	R	1	Total	C	O	0	0
			6	3	3		
2	S	1	Total	C	O	0	0
			6	3	3		
2	U	1	Total	C	O	0	0
			6	3	3		
2	W	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	E	1	Total	C	O	0	0
			7	4	3		
3	F	1	Total	C	O	0	0
			7	4	3		
3	F	1	Total	C	O	0	0
			7	4	3		
3	F	1	Total	C	O	0	0
			7	4	3		
3	G	1	Total	C	O	0	0
			7	4	3		
3	H	1	Total	C	O	0	0
			7	4	3		
3	I	1	Total	C	O	0	0
			7	4	3		
3	I	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	N	1	Total C O 7 4 3	0	0
3	O	1	Total C O 7 4 3	0	0
3	O	1	Total C O 7 4 3	0	0
3	O	1	Total C O 7 4 3	0	0
3	O	1	Total C O 7 4 3	0	0
3	Q	1	Total C O 7 4 3	0	0
3	Q	1	Total C O 7 4 3	0	0
3	Q	1	Total C O 7 4 3	0	0
3	R	1	Total C O 7 4 3	0	0
3	R	1	Total C O 7 4 3	0	0
3	S	1	Total C O 7 4 3	0	0
3	S	1	Total C O 7 4 3	0	0
3	S	1	Total C O 7 4 3	0	0
3	S	1	Total C O 7 4 3	0	0
3	U	1	Total C O 7 4 3	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

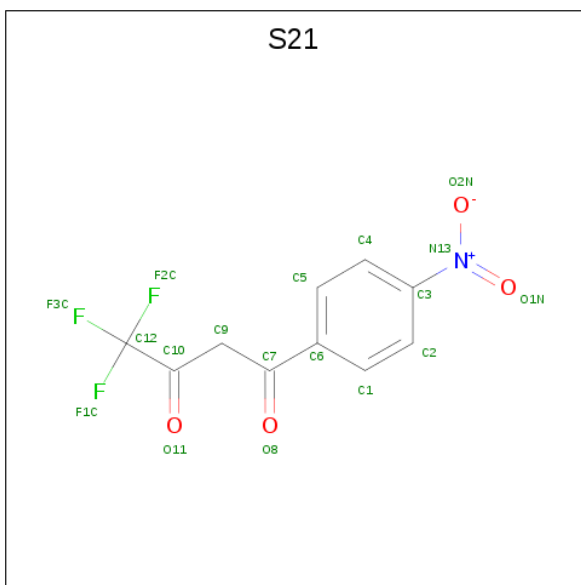
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Cl 1 1	0	0
4	J	1	Total Cl 1 1	0	0
4	K	1	Total Cl 1 1	0	0
4	H	1	Total Cl 1 1	0	0

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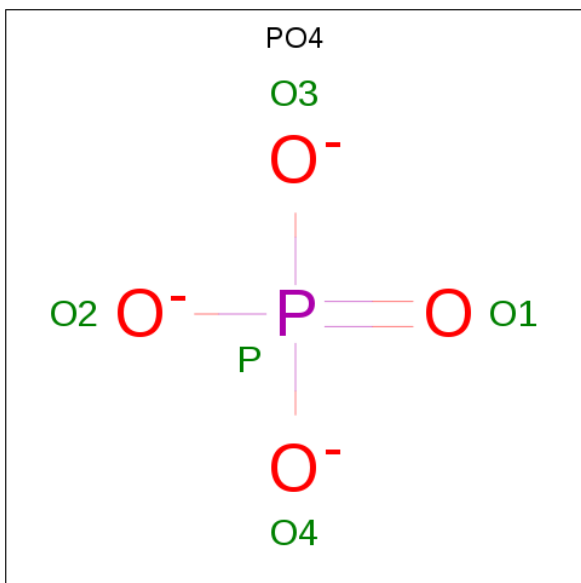
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	I	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		
4	V	1	Total	Cl	0	0
			1	1		
4	A	1	Total	Cl	0	0
			1	1		
4	T	1	Total	Cl	0	0
			1	1		
4	N	1	Total	Cl	0	0
			1	1		
4	U	1	Total	Cl	0	0
			1	1		
4	O	1	Total	Cl	0	0
			1	1		
4	R	1	Total	Cl	0	0
			1	1		
4	L	1	Total	Cl	0	0
			1	1		
4	S	1	Total	Cl	0	0
			1	1		
4	M	1	Total	Cl	0	0
			1	1		

- Molecule 5 is 4,4,4-trifluoro-1-(4-nitrophenyl)butane-1,3-dione (three-letter code: S21) (formula: C<sub>10</sub>H<sub>6</sub>F<sub>3</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	F	N	O	0	0
			18	10	3	1	4		
5	F	1	Total	C	F	N	O	0	0
			18	10	3	1	4		
5	P	1	Total	C	F	N	O	0	0
			18	10	3	1	4		
5	R	1	Total	C	F	N	O	0	0
			18	10	3	1	4		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	10	Total	O		0	0
			10	10			
7	B	21	Total	O		0	0
			21	21			
7	C	27	Total	O		0	0
			27	27			
7	D	19	Total	O		0	0
			19	19			
7	E	21	Total	O		0	0
			21	21			
7	F	25	Total	O		0	0
			25	25			
7	G	18	Total	O		0	0
			18	18			
7	H	16	Total	O		0	0
			16	16			
7	I	10	Total	O		0	0
			10	10			
7	J	23	Total	O		0	0
			23	23			
7	K	12	Total	O		0	0
			12	12			
7	L	15	Total	O		0	0
			15	15			
7	M	9	Total	O		0	0
			9	9			
7	N	18	Total	O		0	0
			18	18			
7	O	19	Total	O		0	0
			19	19			
7	P	22	Total	O		0	0
			22	22			
7	Q	16	Total	O		0	0
			16	16			
7	R	26	Total	O		0	0
			26	26			
7	S	9	Total	O		0	0
			9	9			

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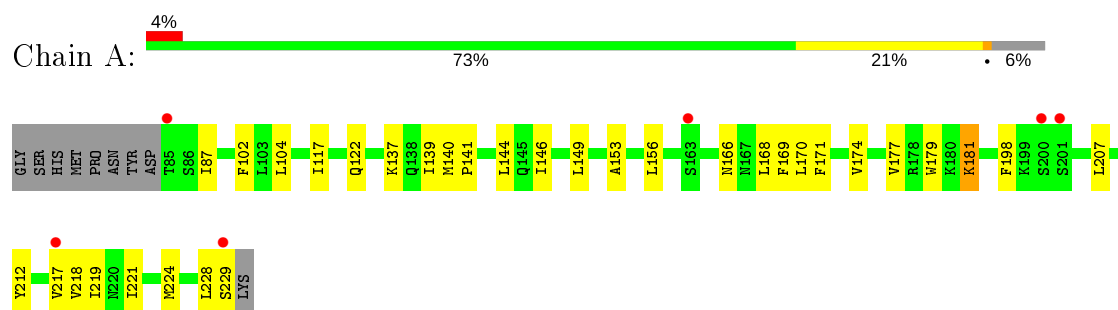
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	T	19	Total 19	O 19	0	0
7	U	18	Total 18	O 18	0	0
7	V	13	Total 13	O 13	0	0
7	W	12	Total 12	O 12	0	0
7	X	17	Total 17	O 17	0	0

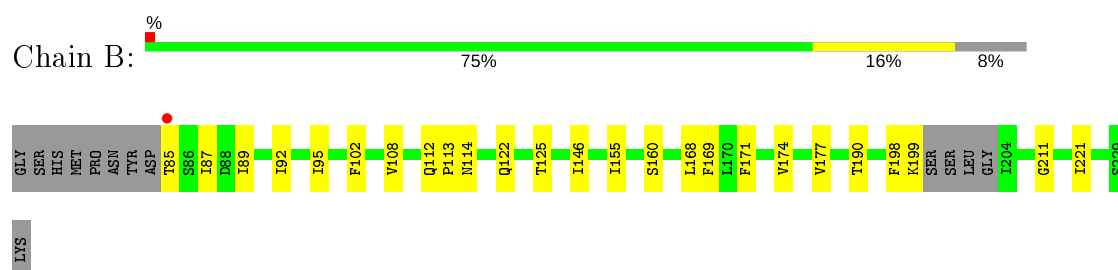
### 3 Residue-property plots [i](#)

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.

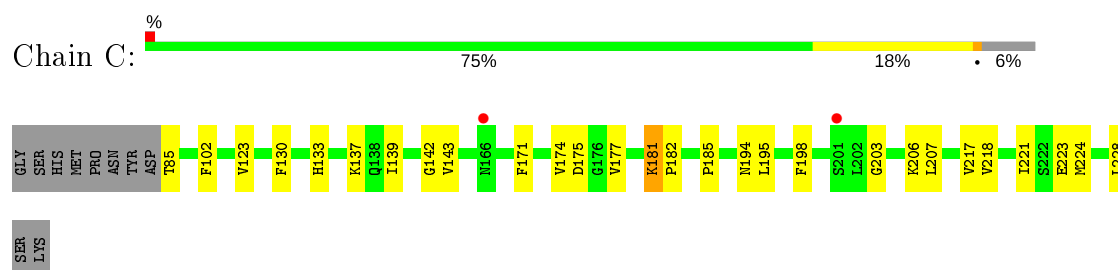
#### • Molecule 1: Beta-hydroxyacyl-ACP dehydratase



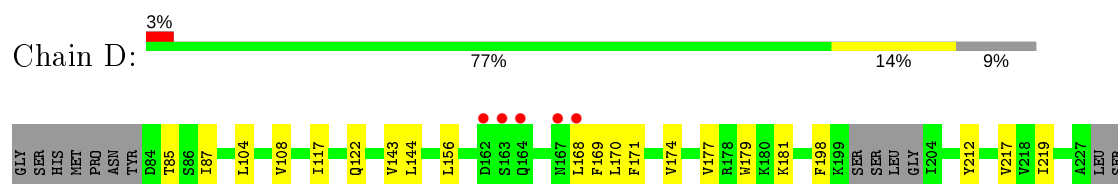
#### • Molecule 1: Beta-hydroxyacyl-ACP dehydratase



#### • Molecule 1: Beta-hydroxyacyl-ACP dehydratase

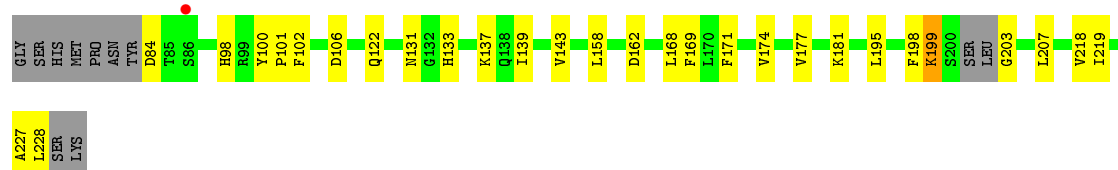
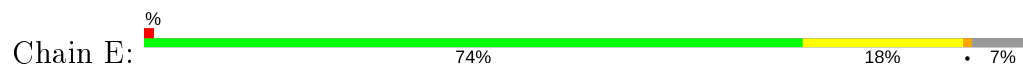


#### • Molecule 1: Beta-hydroxyacyl-ACP dehydratase

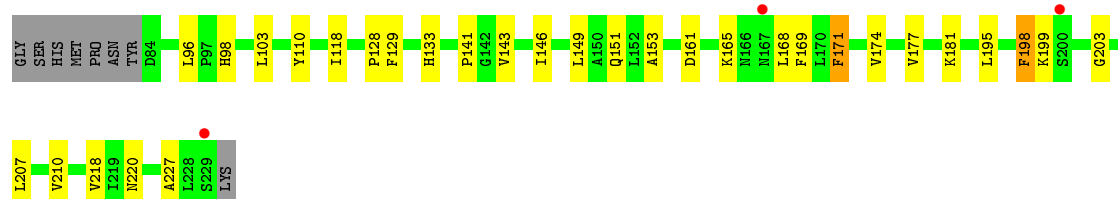
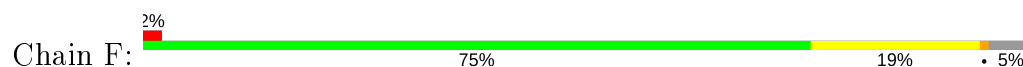


LYS

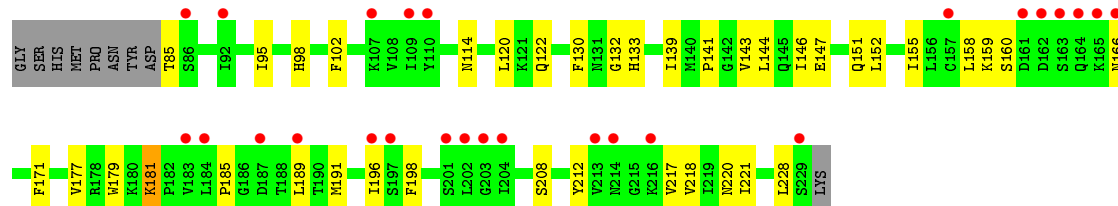
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



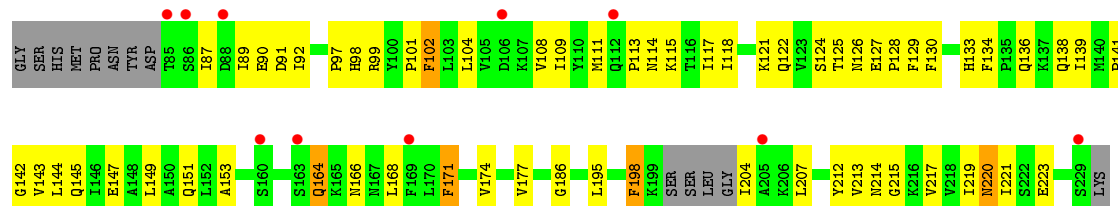
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



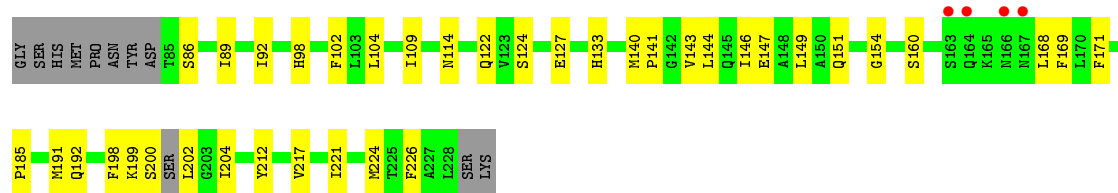
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



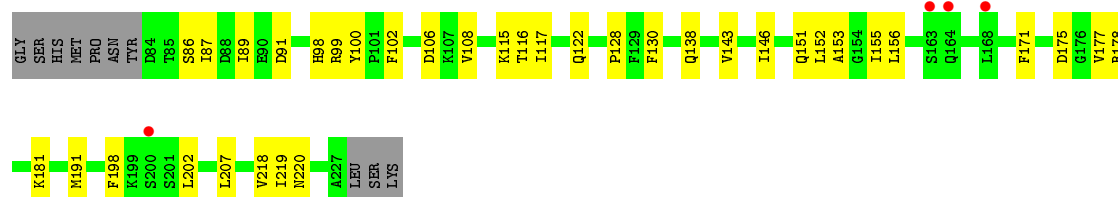
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



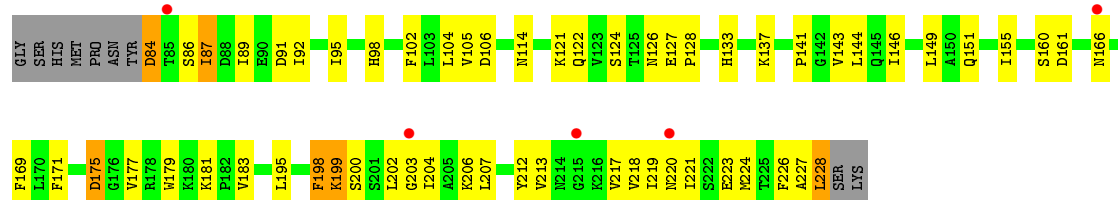




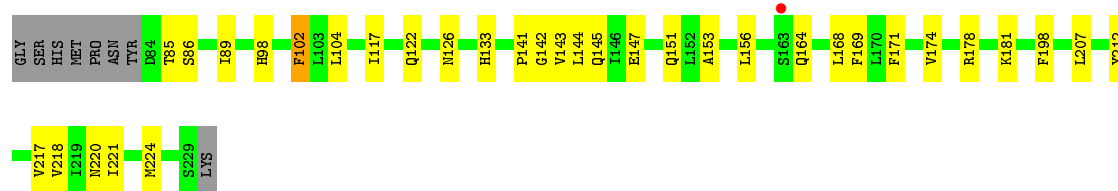
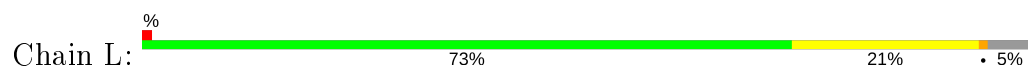
• Molecule 1: Beta-hydroxyacyl-ACP dehydratase



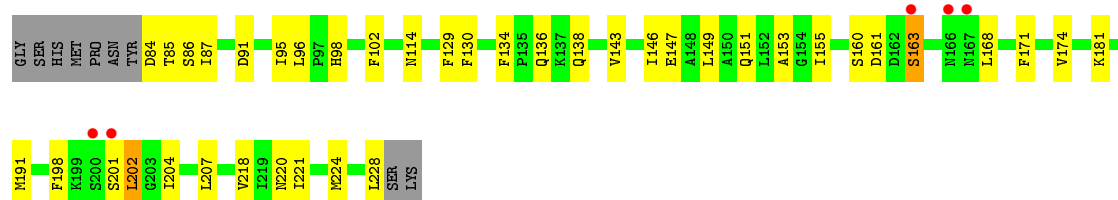
• Molecule 1: Beta-hydroxyacyl-ACP dehydratase



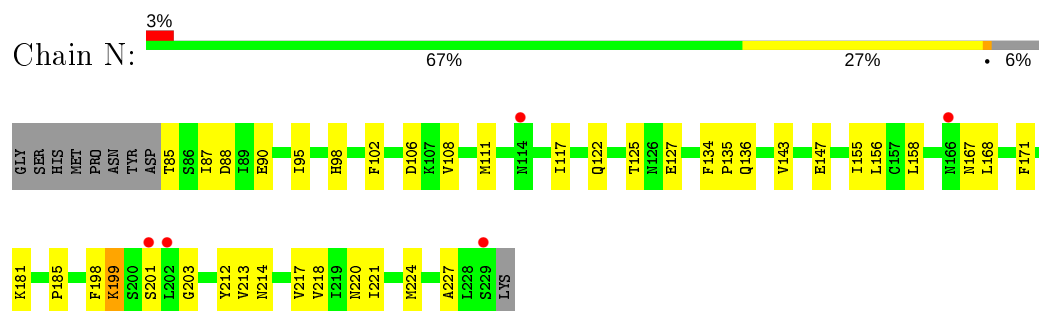
• Molecule 1: Beta-hydroxyacyl-ACP dehydratase



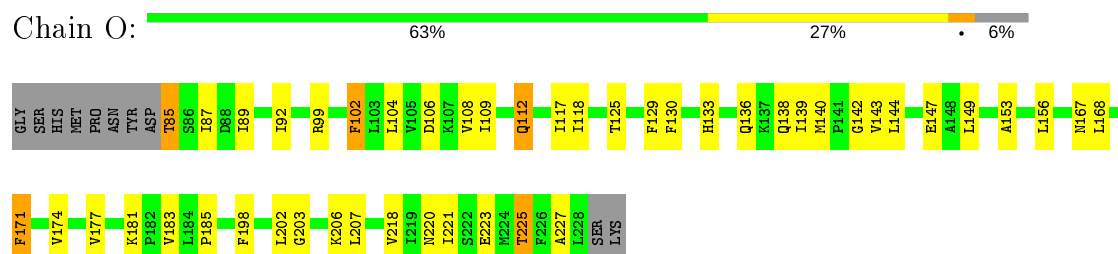
• Molecule 1: Beta-hydroxyacyl-ACP dehydratase



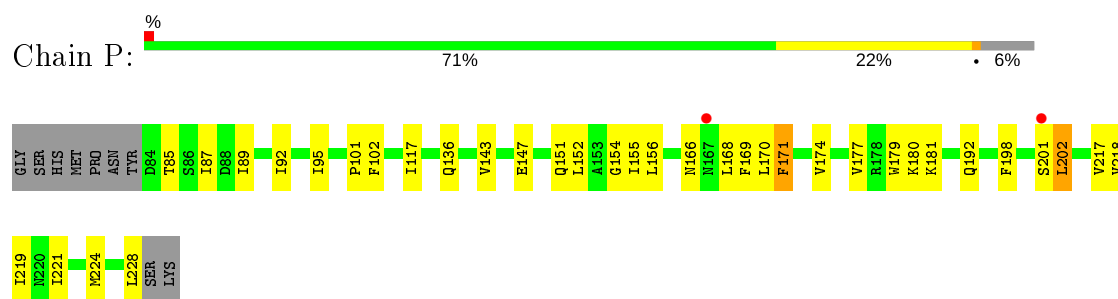
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



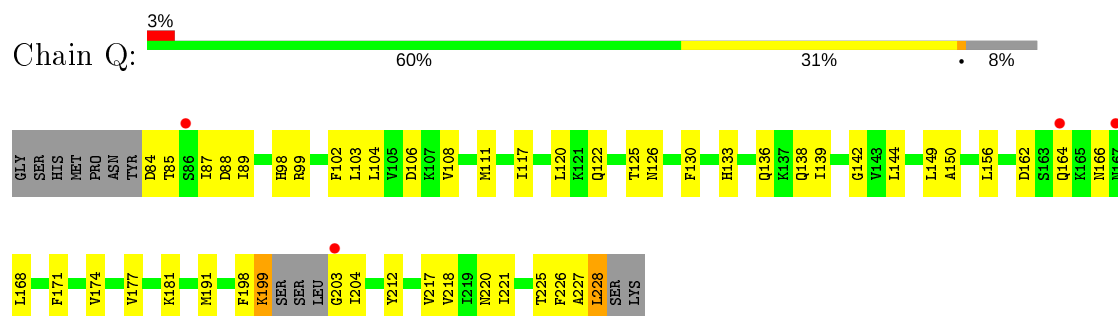
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



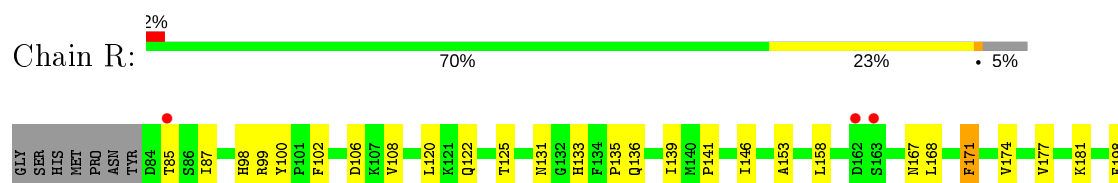
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

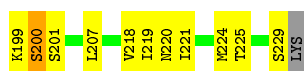


- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

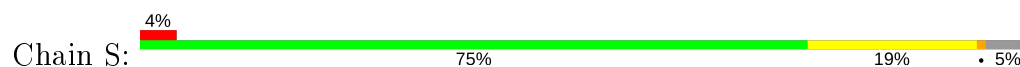


- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

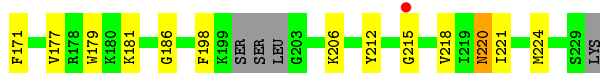




- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



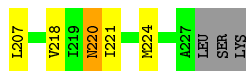
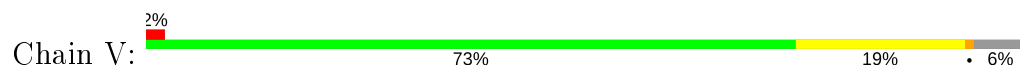
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

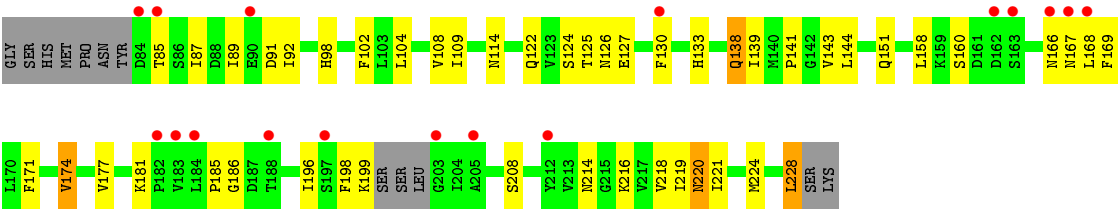


- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

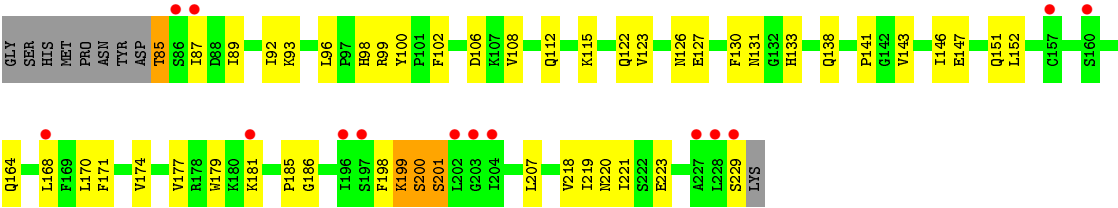


- Molecule 1: Beta-hydroxyacyl-ACP dehydratase





● Molecule 1: Beta-hydroxyacyl-ACP dehydratase



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	218.99Å 218.99Å 157.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.62 – 3.10 51.62 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (51.62-3.10) 99.6 (51.62-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.206 , 0.266 0.203 , 0.263	Depositor DCC
$R_{free}$ test set	3395 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.8	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 13.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.419 for -k,-h,-l	Xtriage
Reported twinning fraction	0.558 for H, K, L 0.442 for -H, K, -L	Depositor
Outliers	0 of 66978 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	27454	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6688e-04.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PEG, GOL, PO4, S21, CL

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	0.55	0/1143	0.57	0/1546
1	B	0.61	0/1115	0.58	0/1508
1	C	0.53	0/1138	0.60	0/1539
1	D	0.59	0/1096	0.60	0/1485
1	E	0.54	0/1130	0.61	0/1528
1	F	0.58	0/1158	0.60	0/1566
1	G	0.72	1/1132 (0.1%)	0.63	0/1533
1	H	0.65	0/1111	0.61	0/1504
1	I	0.57	0/1143	0.59	0/1544
1	J	0.67	0/1120	0.62	0/1520
1	K	0.63	0/1145	0.59	0/1550
1	L	0.57	0/1146	0.59	0/1550
1	M	0.62	0/1145	0.62	0/1550
1	N	0.57	0/1136	0.57	0/1538
1	O	0.54	0/1138	0.61	0/1539
1	P	0.60	0/1121	0.62	0/1520
1	Q	0.57	0/1124	0.62	0/1520
1	R	0.57	0/1149	0.63	0/1554
1	S	0.60	0/1159	0.61	0/1569
1	T	0.65	0/1119	0.60	0/1513
1	U	0.64	1/1138 (0.1%)	0.61	0/1539
1	V	0.61	0/1120	0.63	0/1519
1	W	0.73	0/1124	0.63	0/1520
1	X	0.67	1/1141 (0.1%)	0.59	0/1543
All	All	0.61	3/27191 (0.0%)	0.61	0/36797

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	U	166	ASN	CG-ND2	5.61	1.46	1.32
1	X	85	THR	N-CA	5.10	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	181	LYS	CE-NZ	5.08	1.61	1.49

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	1121	0	1172	18	0
1	B	1094	0	1133	13	0
1	C	1116	0	1164	22	0
1	D	1075	0	1092	14	0
1	E	1109	0	1149	23	0
1	F	1136	0	1171	24	0
1	G	1111	0	1154	33	0
1	H	1090	0	1122	59	0
1	I	1118	0	1167	26	0
1	J	1098	0	1112	20	0
1	K	1123	0	1166	45	0
1	L	1124	0	1155	19	0
1	M	1123	0	1166	26	0
1	N	1114	0	1146	24	0
1	O	1116	0	1164	37	0
1	P	1099	0	1113	33	0
1	Q	1103	0	1144	30	0
1	R	1127	0	1164	29	0
1	S	1133	0	1174	25	0
1	T	1098	0	1136	40	0
1	U	1116	0	1164	24	0
1	V	1098	0	1114	18	0
1	W	1103	0	1144	42	0
1	X	1119	0	1160	37	0
2	A	6	0	8	0	0
2	D	6	0	8	0	0
2	F	6	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	6	0	8	2	0
2	I	6	0	8	0	0
2	L	6	0	8	1	0
2	M	6	0	8	1	0
2	O	6	0	8	1	0
2	P	6	0	8	1	0
2	R	6	0	8	0	0
2	S	6	0	8	2	0
2	U	6	0	8	0	0
2	W	6	0	8	0	0
3	A	28	0	40	0	0
3	B	7	0	10	0	0
3	C	7	0	10	0	0
3	E	7	0	10	0	0
3	F	21	0	30	3	0
3	G	7	0	10	0	0
3	H	7	0	10	0	0
3	I	14	0	20	1	0
3	N	7	0	10	0	0
3	O	28	0	40	6	0
3	Q	21	0	30	1	0
3	R	14	0	20	0	0
3	S	28	0	40	8	0
3	U	7	0	10	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	G	1	0	0	1	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	R	1	0	0	0	0
4	S	1	0	0	1	0
4	T	1	0	0	0	0
4	U	1	0	0	0	0
4	V	1	0	0	0	0
5	D	18	0	6	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	18	0	6	10	0
5	P	18	0	6	11	0
5	R	18	0	6	12	0
6	E	5	0	0	1	0
7	A	10	0	0	0	0
7	B	21	0	0	2	0
7	C	27	0	0	2	0
7	D	19	0	0	0	0
7	E	21	0	0	1	0
7	F	25	0	0	0	0
7	G	18	0	0	0	0
7	H	16	0	0	1	0
7	I	10	0	0	0	0
7	J	23	0	0	0	0
7	K	12	0	0	1	0
7	L	15	0	0	0	0
7	M	9	0	0	0	0
7	N	18	0	0	0	0
7	O	19	0	0	1	0
7	P	22	0	0	1	0
7	Q	16	0	0	0	0
7	R	26	0	0	0	0
7	S	9	0	0	0	0
7	T	19	0	0	0	0
7	U	18	0	0	2	0
7	V	13	0	0	0	0
7	W	12	0	0	0	0
7	X	17	0	0	1	0
All	All	27454	0	27964	590	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 11.

All (590) 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:R:171:PHE:CB	5:R:1:S21:H5	1.61	1.31
1:R:171:PHE:HB2	5:R:1:S21:C5	1.69	1.21
1:F:171:PHE:HB2	5:F:231:S21:H5	1.13	1.08
1:J:87:ILE:HG23	1:J:91:ASP:HB2	1.42	1.02
1:M:84:ASP:O	1:M:85:THR:HG22	1.62	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:171:PHE:CB	5:F:231:S21:H5	1.93	0.98
1:Q:133:HIS:NE2	5:R:1:S21:H9A	1.84	0.92
1:H:166:ASN:HB2	7:H:241:HOH:O	1.67	0.92
1:P:169:PHE:HA	1:P:228:LEU:CA	2.00	0.91
1:P:169:PHE:CB	1:P:228:LEU:CA	2.48	0.91
1:J:87:ILE:CG2	1:J:91:ASP:HB2	2.01	0.90
1:X:181:LYS:HB3	1:X:218:VAL:HG12	1.53	0.90
1:S:192:GLN:HE22	3:S:8:PEG:H21	1.37	0.89
1:E:162:ASP:HB2	7:E:285:HOH:O	1.75	0.86
1:C:133:HIS:NE2	5:D:231:S21:H9A	1.90	0.85
1:J:98:HIS:CD2	1:J:151:GLN:HE21	1.94	0.84
1:F:171:PHE:HB2	5:F:231:S21:C5	2.06	0.84
1:W:166:ASN:HB3	1:W:228:LEU:HD21	1.60	0.83
1:R:181:LYS:HB3	1:R:218:VAL:HG12	1.62	0.81
1:V:153:ALA:HB1	1:V:207:LEU:HD13	1.62	0.81
1:W:181:LYS:HD2	1:W:216:LYS:HE2	1.63	0.80
1:L:122:GLN:HB3	1:L:122:GLN:HB3	1.62	0.80
1:X:146:ILE:HD11	1:X:177:VAL:HG11	1.64	0.79
1:Q:87:ILE:HB	1:Q:108:VAL:HB	1.66	0.78
1:M:84:ASP:O	1:M:85:THR:CG2	2.30	0.78
1:P:169:PHE:HB2	1:P:228:LEU:CA	2.14	0.78
1:U:143:VAL:HB	1:V:143:VAL:HB	1.66	0.77
1:X:96:LEU:HD22	1:X:98:HIS:CE1	2.20	0.77
1:L:117:ILE:HB	1:L:156:LEU:HD13	1.64	0.77
1:R:171:PHE:HB2	5:R:1:S21:H5	0.80	0.77
1:G:152:LEU:HA	1:G:155:ILE:HD12	1.67	0.76
1:E:133:HIS:NE2	5:F:231:S21:H9A	2.01	0.76
1:S:89:ILE:HG21	1:V:185:PRO:HG2	1.68	0.76
1:U:181:LYS:HB3	1:U:218:VAL:HG12	1.67	0.76
1:P:169:PHE:CA	1:P:228:LEU:CA	2.64	0.75
1:X:87:ILE:HB	1:X:108:VAL:HB	1.69	0.75
1:W:181:LYS:HB3	1:W:218:VAL:HG12	1.68	0.74
1:O:133:HIS:NE2	5:P:4:S21:C9	2.51	0.74
1:G:166:ASN:HB3	1:G:228:LEU:HD11	1.70	0.74
1:H:114:ASN:HB3	1:W:214:ASN:O	1.86	0.73
1:F:129:PHE:HB3	2:F:3:GOL:H31	1.68	0.73
1:M:143:VAL:HA	1:M:146:ILE:HD12	1.69	0.73
1:G:114:ASN:ND2	1:G:160:SER:HB3	2.04	0.73
1:N:199:LYS:HA	1:N:199:LYS:HE3	1.68	0.73
1:E:133:HIS:CE1	5:F:231:S21:H1	2.24	0.72
1:H:109:ILE:HD12	1:T:110:TYR:CD2	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:HIS:NE2	5:D:231:S21:C9	2.53	0.71
1:O:99:ARG:HE	3:O:10:PEG:H22	1.56	0.71
1:X:96:LEU:HD22	1:X:98:HIS:ND1	2.06	0.71
1:U:169:PHE:HB2	7:U:233:HOH:O	1.90	0.71
1:E:218:VAL:HG23	1:E:219:ILE:HG22	1.72	0.70
1:O:129:PHE:HB3	2:O:8:GOL:H31	1.72	0.70
1:U:87:ILE:HB	1:U:108:VAL:HB	1.72	0.70
1:J:117:ILE:HB	1:J:156:LEU:HD13	1.71	0.70
1:G:95:ILE:HD13	1:G:155:ILE:HG23	1.74	0.69
1:P:171:PHE:CB	5:P:4:S21:H5	2.22	0.69
1:J:98:HIS:CD2	1:J:151:GLN:NE2	2.61	0.69
1:R:120:LEU:HD13	1:R:122:GLN:HE21	1.57	0.69
1:E:139:ILE:HG22	5:F:231:S21:H2	1.73	0.68
1:H:130:PHE:CD1	1:H:138:GLN:HB3	2.28	0.68
1:W:177:VAL:HA	1:W:220:ASN:O	1.94	0.68
1:B:85:THR:HG21	7:B:235:HOH:O	1.93	0.68
3:O:28:PEG:H12	1:R:100:TYR:CE2	2.28	0.68
1:W:87:ILE:HB	1:W:108:VAL:HB	1.76	0.68
1:G:147:GLU:HB2	1:H:143:VAL:HG21	1.76	0.67
1:O:133:HIS:NE2	5:P:4:S21:H9	2.08	0.67
1:T:127:GLU:OE1	1:W:126:ASN:HB3	1.94	0.67
1:I:147:GLU:O	1:I:151:GLN:HG3	1.95	0.67
3:U:21:PEG:H12	3:U:21:PEG:H41	1.78	0.66
1:H:104:LEU:HD11	1:H:144:LEU:HD22	1.77	0.66
1:D:179:TRP:NE1	1:D:219:ILE:HD12	2.11	0.66
1:G:122:GLN:HB3	1:J:122:GLN:HB3	1.77	0.66
1:G:98:HIS:CD2	1:G:151:GLN:HE21	2.13	0.66
1:H:111:MET:HG3	1:H:117:ILE:HD12	1.78	0.66
1:U:127:GLU:HG2	1:X:126:ASN:O	1.95	0.66
1:Q:117:ILE:HB	1:Q:156:LEU:HD13	1.78	0.65
1:L:181:LYS:HB3	1:L:218:VAL:HG12	1.77	0.65
1:I:199:LYS:HB3	1:I:202:LEU:CD1	2.27	0.65
1:E:158:LEU:HD21	1:E:169:PHE:CE2	2.30	0.65
1:J:89:ILE:HD13	1:J:106:ASP:HA	1.77	0.65
1:P:95:ILE:HG21	1:P:155:ILE:HG23	1.77	0.65
1:G:146:ILE:HD11	1:G:179:TRP:CZ2	2.32	0.64
1:W:166:ASN:HB3	1:W:228:LEU:CD2	2.26	0.64
3:F:24:PEG:H31	3:F:25:PEG:H22	1.79	0.64
1:H:177:VAL:HG13	1:H:221:ILE:HG12	1.80	0.64
1:G:132:GLY:HA3	1:H:99:ARG:O	1.97	0.64
1:H:153:ALA:HB1	1:H:207:LEU:HD13	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:109:ILE:HB	1:T:110:TYR:CD1	2.33	0.63
1:R:120:LEU:HD13	1:R:122:GLN:NE2	2.13	0.63
1:W:133:HIS:ND1	1:W:139:ILE:O	2.24	0.63
1:K:95:ILE:HG21	1:K:155:ILE:HG23	1.81	0.63
1:S:129:PHE:HB3	2:S:10:GOL:H31	1.81	0.63
1:G:133:HIS:CG	1:G:141:PRO:HG3	2.33	0.62
1:S:147:GLU:OE2	4:S:15:CL:CL	2.54	0.62
1:X:102:PHE:CE2	1:X:147:GLU:HG2	2.34	0.62
1:R:171:PHE:CB	5:R:1:S21:C5	2.48	0.62
1:Q:203:GLY:O	1:Q:227:ALA:HA	2.00	0.62
1:A:166:ASN:HB3	1:A:228:LEU:HD21	1.80	0.62
1:O:133:HIS:NE2	5:P:4:S21:H9A	2.13	0.62
1:I:143:VAL:HB	1:J:143:VAL:HB	1.81	0.61
1:O:112:GLN:HG2	1:O:112:GLN:O	1.99	0.61
1:A:169:PHE:CE2	1:A:228:LEU:HD23	2.36	0.61
1:D:179:TRP:HE1	1:D:219:ILE:HD12	1.64	0.61
1:L:212:TYR:CE2	1:L:217:VAL:HG22	2.35	0.61
1:H:122:GLN:O	1:K:124:SER:HB2	2.01	0.61
1:P:171:PHE:HB2	5:P:4:S21:H5	1.82	0.61
1:B:87:ILE:HB	1:B:108:VAL:HB	1.83	0.60
1:C:177:VAL:HG22	1:C:221:ILE:HG12	1.84	0.60
1:B:177:VAL:HG22	1:B:221:ILE:HG12	1.84	0.60
1:E:98:HIS:NE2	6:E:1:PO4:O2	2.29	0.60
1:A:174:VAL:HG23	1:A:224:MET:HG2	1.84	0.60
1:S:100:TYR:HE2	3:S:13:PEG:H42	1.66	0.60
1:M:84:ASP:C	1:M:85:THR:HG22	2.22	0.60
1:O:203:GLY:O	1:O:227:ALA:HA	2.00	0.60
1:E:137:LYS:HE2	1:E:139:ILE:HD11	1.83	0.60
1:Q:111:MET:HG3	1:Q:117:ILE:HD12	1.83	0.60
1:T:87:ILE:CG2	1:T:91:ASP:HB2	2.31	0.60
1:X:123:VAL:HG12	1:X:185:PRO:HA	1.83	0.60
1:P:171:PHE:HB3	5:P:4:S21:H5	1.84	0.59
1:H:89:ILE:HA	1:H:92:ILE:HD12	1.83	0.59
1:R:133:HIS:CG	1:R:141:PRO:HG3	2.38	0.59
1:Q:120:LEU:HD13	1:Q:122:GLN:NE2	2.16	0.59
1:X:98:HIS:CD2	1:X:151:GLN:NE2	2.71	0.59
1:E:203:GLY:O	1:E:227:ALA:HA	2.03	0.59
1:F:153:ALA:HB1	1:F:207:LEU:HD22	1.85	0.59
1:F:210:VAL:HG22	1:F:220:ASN:ND2	2.16	0.59
1:W:139:ILE:HD13	1:X:170:LEU:HD11	1.84	0.59
1:H:87:ILE:HB	1:H:108:VAL:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:98:HIS:CD2	1:M:151:GLN:HE21	2.21	0.59
1:S:192:GLN:NE2	3:S:8:PEG:H21	2.16	0.59
1:Q:133:HIS:NE2	5:R:1:S21:C9	2.65	0.59
1:C:195:LEU:HA	1:C:207:LEU:HG	1.85	0.58
1:X:146:ILE:HG12	1:X:221:ILE:HD11	1.83	0.58
1:L:98:HIS:CD2	1:L:151:GLN:HE21	2.21	0.58
1:L:133:HIS:CG	1:L:141:PRO:HG3	2.39	0.58
1:M:202:LEU:HD12	1:M:204:ILE:HD13	1.83	0.58
1:N:181:LYS:HB3	1:N:218:VAL:HG12	1.85	0.58
3:O:28:PEG:H32	1:P:101:PRO:HG3	1.85	0.58
1:C:206:LYS:HD3	1:C:223:GLU:OE2	2.04	0.58
1:U:123:VAL:O	1:U:186:GLY:N	2.32	0.58
3:S:13:PEG:H11	1:X:131:ASN:HD22	1.69	0.58
1:A:177:VAL:HG22	1:A:221:ILE:HG12	1.85	0.57
1:G:212:TYR:CE2	1:G:217:VAL:HG22	2.39	0.57
1:I:199:LYS:HB3	1:I:202:LEU:HD13	1.87	0.57
1:T:149:LEU:HD13	1:T:221:ILE:HD12	1.87	0.57
1:V:130:PHE:CD1	1:V:138:GLN:HB3	2.40	0.57
1:A:146:ILE:HD11	1:A:179:TRP:CZ2	2.40	0.57
1:Q:142:GLY:H	5:R:1:S21:C1	2.18	0.57
1:P:181:LYS:HB3	1:P:218:VAL:HG12	1.86	0.56
1:N:185:PRO:HG2	1:Q:89:ILE:HG21	1.86	0.56
1:G:177:VAL:HG13	1:G:221:ILE:HG12	1.86	0.56
1:H:101:PRO:HG2	2:H:4:GOL:O3	2.05	0.56
1:K:181:LYS:HB3	1:K:218:VAL:HG12	1.87	0.56
1:O:153:ALA:HB1	1:O:207:LEU:HD22	1.88	0.56
1:O:143:VAL:HG11	1:P:147:GLU:HB2	1.87	0.56
1:S:87:ILE:CG2	1:S:91:ASP:HB2	2.36	0.56
1:K:133:HIS:CG	1:K:141:PRO:HG3	2.40	0.56
1:R:158:LEU:HD21	1:R:167:ASN:HA	1.86	0.56
1:T:126:ASN:HB3	1:W:127:GLU:OE1	2.06	0.55
1:U:112:GLN:OE1	1:U:115:LYS:HD3	2.05	0.55
1:K:199:LYS:HB3	1:K:204:ILE:HB	1.88	0.55
1:D:87:ILE:HB	1:D:108:VAL:HB	1.89	0.55
1:E:198:PHE:HD1	1:E:199:LYS:N	2.04	0.55
1:H:115:LYS:HB2	1:W:214:ASN:CG	2.27	0.55
1:G:143:VAL:HG21	1:H:147:GLU:HB2	1.88	0.55
1:M:87:ILE:HG23	1:M:91:ASP:HB2	1.87	0.55
1:X:133:HIS:CG	1:X:141:PRO:HG3	2.42	0.55
1:F:98:HIS:HB2	1:F:103:LEU:HD13	1.89	0.55
1:H:212:TYR:CE2	1:H:217:VAL:HG22	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:132:GLY:HA2	1:H:99:ARG:HB2	1.88	0.55
1:C:133:HIS:CE1	5:D:231:S21:H9A	2.41	0.55
1:C:221:ILE:HG21	1:C:224:MET:HG3	1.89	0.55
1:G:177:VAL:HG22	1:G:221:ILE:HG23	1.88	0.55
1:H:97:PRO:O	1:H:99:ARG:NH1	2.40	0.55
1:R:199:LYS:C	1:R:201:SER:H	2.09	0.55
1:I:169[B]:PHE:HD1	1:I:226:PHE:HB3	1.73	0.54
1:I:133:HIS:CG	1:I:141:PRO:HG3	2.42	0.54
1:H:127:GLU:OE1	1:K:126:ASN:HB3	2.06	0.54
1:R:87:ILE:HB	1:R:108:VAL:HB	1.89	0.54
1:I:89:ILE:HA	1:I:92:ILE:HD12	1.89	0.54
1:M:228:LEU:HD23	1:M:228:LEU:O	2.07	0.54
1:S:221:ILE:HG21	1:S:224:MET:HG3	1.90	0.54
1:S:147:GLU:HB2	1:T:143:VAL:HG21	1.90	0.54
1:E:139:ILE:CG2	5:F:231:S21:H2	2.38	0.54
1:W:143:VAL:HB	1:X:143:VAL:HB	1.88	0.54
1:K:98:HIS:CD2	1:K:151:GLN:HE21	2.26	0.54
1:P:169:PHE:HB3	1:P:228:LEU:CA	2.37	0.53
1:T:130:PHE:CD1	1:T:138:GLN:HB3	2.44	0.53
1:A:104:LEU:HD11	1:A:144:LEU:HD22	1.90	0.53
1:G:98:HIS:CD2	1:G:151:GLN:NE2	2.76	0.53
1:M:181:LYS:HB3	1:M:218:VAL:HG12	1.90	0.53
1:M:98:HIS:CD2	1:M:151:GLN:NE2	2.77	0.53
1:O:133:HIS:CE1	5:P:4:S21:H9A	2.43	0.53
1:O:177:VAL:HG22	1:O:221:ILE:HG12	1.90	0.53
1:O:130:PHE:CZ	1:O:185:PRO:HD3	2.43	0.53
1:U:174:VAL:HG12	1:V:177:VAL:HB	1.89	0.53
1:G:95:ILE:HD11	1:G:158:LEU:HB2	1.91	0.53
1:A:137:LYS:HE2	1:A:139:ILE:HD11	1.90	0.53
1:H:124:SER:HB2	1:K:122:GLN:O	2.09	0.53
1:B:95:ILE:HG21	1:B:155:ILE:HG23	1.89	0.53
1:K:92:ILE:HD13	1:K:105:VAL:HG12	1.91	0.53
1:A:177:VAL:HB	1:B:174:VAL:HG12	1.90	0.53
1:I:212:TYR:CE2	1:I:217:VAL:HG22	2.43	0.53
1:K:84:ASP:N	1:K:84:ASP:OD2	2.42	0.52
1:W:130:PHE:CD1	1:W:138:GLN:HB3	2.44	0.52
1:O:142:GLY:H	5:P:4:S21:C6	2.22	0.52
1:H:125:THR:HG22	1:K:106:ASP:OD1	2.10	0.52
1:K:221:ILE:HG21	1:K:224:MET:HG3	1.91	0.52
1:T:89:ILE:HG21	1:W:185:PRO:HG2	1.91	0.52
1:G:122:GLN:HA	1:G:122:GLN:OE1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:147:GLU:O	1:G:151:GLN:HG3	2.10	0.52
1:K:161:ASP:HB3	1:K:198:PHE:CZ	2.44	0.52
1:R:221:ILE:HG21	1:R:224:MET:HG3	1.92	0.52
1:W:221:ILE:HG21	1:W:224:MET:HG3	1.91	0.52
1:H:212:TYR:HE2	1:H:217:VAL:HG22	1.75	0.52
1:R:171:PHE:HB3	5:R:1:S21:H5	1.80	0.52
1:H:109:ILE:HD12	1:T:110:TYR:CE2	2.44	0.52
1:S:177:VAL:HG22	1:S:221:ILE:HG12	1.91	0.52
1:W:87:ILE:N	1:W:108:VAL:O	2.43	0.52
1:F:169:PHE:O	5:F:231:S21:O11	2.28	0.52
1:H:149:LEU:HD12	1:H:219:ILE:HD13	1.92	0.52
1:I:149:LEU:CD2	1:I:191:MET:HB3	2.39	0.52
1:J:87:ILE:HG21	1:J:91:ASP:HB2	1.90	0.52
1:M:174:VAL:HG12	1:N:177:VAL:HB	1.92	0.52
1:U:177:VAL:HA	1:U:220:ASN:O	2.09	0.52
1:W:214:ASN:C	1:W:216:LYS:H	2.13	0.52
1:T:177:VAL:HG22	1:T:221:ILE:HG12	1.92	0.52
1:T:181:LYS:HB3	1:T:218:VAL:HG12	1.91	0.52
1:I:199:LYS:HB2	1:I:202:LEU:HB2	1.91	0.51
1:G:144:LEU:HD11	1:H:102:PHE:CE1	2.45	0.51
1:C:194:ASN:ND2	7:C:239:HOH:O	2.31	0.51
1:S:122:GLN:HB2	1:V:124:SER:HB2	1.91	0.51
1:T:186:GLY:HA2	1:W:122:GLN:HG2	1.92	0.51
1:F:161:ASP:HB2	3:F:25:PEG:O4	2.10	0.51
1:K:177:VAL:HB	1:L:174:VAL:HG12	1.92	0.51
1:B:125:THR:HG22	1:E:106:ASP:OD1	2.11	0.51
1:J:181:LYS:HB3	1:J:218:VAL:HG12	1.93	0.51
1:K:87:ILE:HG23	1:K:91:ASP:HB2	1.92	0.51
1:H:121:LYS:NZ	1:H:122:GLN:O	2.35	0.51
1:R:133:HIS:ND1	1:R:139:ILE:O	2.42	0.51
1:X:98:HIS:O	1:X:99:ARG:NH1	2.41	0.51
1:N:199:LYS:HE3	1:N:199:LYS:CA	2.40	0.51
1:Q:177:VAL:HG22	1:Q:221:ILE:HG12	1.93	0.51
1:S:129:PHE:HB3	2:S:10:GOL:C3	2.41	0.51
1:W:158:LEU:HD21	1:W:167:ASN:HA	1.91	0.51
3:S:13:PEG:H11	1:X:131:ASN:ND2	2.26	0.51
1:H:207:LEU:O	1:H:223:GLU:HA	2.11	0.51
1:H:98:HIS:CD2	1:H:151:GLN:HE21	2.29	0.51
1:T:85:THR:N	1:T:111:MET:O	2.44	0.51
1:E:133:HIS:NE2	5:F:231:S21:C9	2.71	0.50
1:W:174:VAL:HG12	1:X:177:VAL:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:185:PRO:HG2	1:V:89:ILE:HG21	1.93	0.50
1:D:104:LEU:HD11	1:D:144:LEU:HD22	1.93	0.50
4:G:7:CL:CL	1:H:147:GLU:OE1	2.65	0.50
1:U:126:ASN:O	1:X:127:GLU:HG2	2.11	0.50
1:W:141:PRO:HG2	1:W:144:LEU:HD12	1.92	0.50
1:C:174:VAL:HG12	1:D:177:VAL:HB	1.93	0.50
1:F:203:GLY:O	1:F:227:ALA:HA	2.11	0.50
1:E:174:VAL:HG12	1:F:177:VAL:HB	1.94	0.50
1:G:146:ILE:HD11	1:G:179:TRP:HZ2	1.75	0.50
1:G:177:VAL:HB	1:H:174:VAL:HG12	1.93	0.50
1:O:181:LYS:HB3	1:O:218:VAL:HG12	1.94	0.50
1:P:117:ILE:HB	1:P:156:LEU:HD13	1.94	0.50
1:T:177:VAL:HA	1:T:220:ASN:O	2.11	0.50
1:N:158:LEU:HD21	1:N:167:ASN:HA	1.94	0.49
1:N:203:GLY:O	1:N:227:ALA:HA	2.11	0.49
1:P:174:VAL:HG23	1:P:224:MET:HG2	1.94	0.49
1:Q:142:GLY:H	5:R:1:S21:C6	2.25	0.49
1:G:212:TYR:HE2	1:G:217:VAL:HG22	1.76	0.49
1:Q:212:TYR:CE2	1:Q:217:VAL:HG22	2.47	0.49
1:I:154:GLY:HA3	1:I:169[A]:PHE:CZ	2.47	0.49
1:I:199:LYS:HB3	1:I:202:LEU:HD12	1.94	0.49
1:M:147:GLU:HB2	1:N:143:VAL:HG21	1.93	0.49
1:F:96:LEU:HB3	1:F:98:HIS:ND1	2.28	0.49
1:V:87:ILE:HG23	1:V:91:ASP:HB2	1.94	0.49
1:W:181:LYS:HD2	1:W:216:LYS:CE	2.39	0.49
1:D:169:PHE:O	5:D:231:S21:O11	2.30	0.49
1:C:177:VAL:HB	1:D:174:VAL:HG12	1.94	0.49
1:D:212:TYR:CE2	1:D:217:VAL:HG22	2.48	0.49
1:E:100:TYR:CD1	1:E:101:PRO:HA	2.47	0.49
1:N:125:THR:HG22	1:Q:106:ASP:OD1	2.11	0.49
1:Q:166:ASN:HB3	1:Q:228:LEU:HD21	1.94	0.49
1:E:177:VAL:HB	1:F:174:VAL:HG12	1.93	0.49
1:H:133:HIS:HA	1:H:134:PHE:CD1	2.48	0.49
1:I:98:HIS:CD2	1:I:151:GLN:NE2	2.80	0.49
1:K:169:PHE:HD1	1:K:226:PHE:HB3	1.76	0.49
1:X:179:TRP:HE1	1:X:219:ILE:HD12	1.77	0.49
1:H:118:ILE:HD11	1:T:109:ILE:HD12	1.93	0.49
1:A:181:LYS:HB2	1:A:218:VAL:HG12	1.95	0.49
1:N:127:GLU:HG2	1:Q:126:ASN:O	2.12	0.49
1:X:130:PHE:HB3	1:X:138:GLN:NE2	2.27	0.49
1:B:89:ILE:HA	1:B:92:ILE:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:158:LEU:HD21	1:E:169:PHE:CD2	2.48	0.49
1:G:130:PHE:CE1	1:G:185:PRO:HG3	2.48	0.49
1:H:122:GLN:HB3	1:K:122:GLN:HB3	1.95	0.49
1:X:93:LYS:HE3	1:X:99:ARG:CD	2.43	0.48
1:U:212:TYR:CE2	1:U:217:VAL:HG22	2.47	0.48
1:J:153:ALA:HB1	1:J:207:LEU:HD13	1.95	0.48
1:K:169:PHE:HA	1:K:228:LEU:C	2.33	0.48
1:O:89:ILE:HA	1:O:92:ILE:HD12	1.93	0.48
1:R:171:PHE:O	5:R:1:S21:H4	2.13	0.48
1:X:106:ASP:OD2	1:X:122:GLN:N	2.42	0.48
1:K:203:GLY:O	1:K:227:ALA:HA	2.12	0.48
1:M:95:ILE:HG21	1:M:155:ILE:HG23	1.96	0.48
1:O:117:ILE:HB	1:O:156:LEU:HD13	1.94	0.48
1:O:139:ILE:HG22	5:P:4:S21:H2	1.94	0.48
1:T:147:GLU:O	1:T:151:GLN:HG3	2.13	0.48
1:F:161:ASP:OD2	3:F:25:PEG:H32	2.13	0.48
1:I:149:LEU:HD23	1:I:191:MET:HB3	1.96	0.48
1:P:117:ILE:HG23	1:P:152:LEU:HG	1.95	0.48
1:V:89:ILE:HA	1:V:92:ILE:HD12	1.96	0.48
1:W:87:ILE:HG23	1:W:91:ASP:HB2	1.95	0.48
1:C:143:VAL:HB	1:D:143:VAL:HB	1.95	0.48
1:J:86:SER:HB2	1:J:108:VAL:O	2.14	0.48
1:H:126:ASN:HB3	1:K:127:GLU:OE1	2.14	0.48
1:P:147:GLU:O	1:P:151:GLN:HG3	2.14	0.48
1:O:139:ILE:CG2	5:P:4:S21:H2	2.43	0.48
1:T:124:SER:HB2	1:W:122:GLN:O	2.14	0.48
1:F:181:LYS:HB3	1:F:218:VAL:HG12	1.94	0.48
1:M:149:LEU:CD2	1:M:191:MET:HB3	2.43	0.48
1:U:177:VAL:HG22	1:U:221:ILE:HG12	1.96	0.48
1:X:123:VAL:O	1:X:186:GLY:N	2.37	0.48
1:H:133:HIS:ND1	1:H:139:ILE:O	2.42	0.48
1:D:170:LEU:HD22	5:D:231:S21:C1	2.44	0.47
1:P:221:ILE:HG21	1:P:224:MET:HG3	1.95	0.47
1:R:131:ASN:O	1:R:135:PRO:HG3	2.14	0.47
1:B:122:GLN:HB3	1:E:122:GLN:HB3	1.96	0.47
1:X:179:TRP:NE1	1:X:219:ILE:HD12	2.29	0.47
1:G:179:TRP:HB2	1:H:171:PHE:O	2.14	0.47
1:N:87:ILE:HB	1:N:108:VAL:HB	1.96	0.47
1:N:212:TYR:CE2	1:N:217:VAL:HG22	2.49	0.47
1:T:89:ILE:HA	1:T:92:ILE:HD12	1.97	0.47
1:F:110:TYR:HD2	1:F:118:ILE:HD12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:100:TYR:OH	1:J:128:PRO:HG3	2.14	0.47
1:N:88:ASP:OD1	1:N:90:GLU:N	2.47	0.47
1:O:167:ASN:HD21	3:O:23:PEG:H21	1.79	0.47
1:G:120:LEU:HA	1:G:189:LEU:O	2.15	0.47
1:H:129:PHE:HB3	2:H:4:GOL:O2	2.14	0.47
1:M:149:LEU:HD21	1:M:191:MET:HB3	1.96	0.47
1:S:110:TYR:HD2	1:S:118:ILE:HD12	1.78	0.47
1:F:98:HIS:CD2	1:F:151:GLN:NE2	2.82	0.47
1:G:95:ILE:HD12	1:G:159:LYS:HG2	1.95	0.47
1:W:141:PRO:CG	1:W:144:LEU:HD12	2.44	0.47
1:I:221:ILE:HG21	1:I:224:MET:HG3	1.96	0.47
1:X:200:SER:HB3	7:X:233:HOH:O	2.15	0.47
1:K:212:TYR:HE2	1:K:217:VAL:HG22	1.80	0.47
1:P:87:ILE:HG22	1:P:92:ILE:HG13	1.97	0.47
1:Q:150:ALA:HB1	1:Q:226:PHE:HZ	1.79	0.47
1:W:219:ILE:HG12	1:W:220:ASN:N	2.30	0.47
1:H:130:PHE:HD1	1:H:138:GLN:HB3	1.78	0.47
1:L:221:ILE:HG21	1:L:224:MET:HG3	1.96	0.47
1:N:122:GLN:HB3	1:Q:122:GLN:HB3	1.96	0.47
1:O:140:MET:HB3	1:O:183:VAL:HB	1.97	0.47
1:P:218:VAL:HG23	1:P:219:ILE:HG22	1.97	0.47
1:Q:130:PHE:CD1	1:Q:138:GLN:HB3	2.49	0.47
1:Q:174:VAL:HG12	1:R:177:VAL:HB	1.97	0.47
1:R:174:VAL:HG23	1:R:224:MET:HG2	1.96	0.47
1:S:212:TYR:CE1	3:S:19:PEG:H11	2.49	0.47
1:Q:133:HIS:ND1	1:Q:139:ILE:O	2.48	0.47
1:U:89:ILE:HG21	1:X:185:PRO:HG2	1.97	0.47
1:B:114:ASN:ND2	7:B:289:HOH:O	2.42	0.46
1:K:149:LEU:HD12	1:K:219:ILE:HD13	1.97	0.46
1:K:166:ASN:HB3	1:K:228:LEU:HD22	1.96	0.46
1:P:192:GLN:HE22	2:P:13:GOL:C1	2.28	0.46
1:T:87:ILE:HG22	1:T:91:ASP:HB2	1.96	0.46
1:N:117:ILE:HB	1:N:156:LEU:HD13	1.95	0.46
1:X:181:LYS:HD2	1:X:218:VAL:HG12	1.98	0.46
1:K:166:ASN:ND2	1:K:228:LEU:HD13	2.31	0.46
1:N:111:MET:HB2	1:N:117:ILE:HG13	1.96	0.46
1:H:177:VAL:HG13	1:H:221:ILE:CG1	2.44	0.46
1:H:217:VAL:HG21	1:T:215:GLY:O	2.14	0.46
1:J:152:LEU:HA	1:J:155:ILE:HD12	1.98	0.46
1:L:98:HIS:CD2	1:L:151:GLN:NE2	2.84	0.46
1:H:133:HIS:CG	1:H:141:PRO:HG3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:122:GLN:HA	1:K:122:GLN:OE1	2.16	0.46
1:T:146:ILE:HD11	1:T:179:TRP:CZ2	2.51	0.46
1:F:128:PRO:HG2	2:F:3:GOL:H32	1.98	0.46
1:Q:133:HIS:CE1	5:R:1:S21:H1	2.51	0.46
1:R:199:LYS:C	1:R:201:SER:N	2.68	0.46
1:T:85:THR:HG23	1:T:86:SER:N	2.29	0.46
1:U:186:GLY:O	1:X:122:GLN:NE2	2.48	0.46
1:H:87:ILE:HG23	1:H:91:ASP:HB2	1.97	0.46
1:I:199:LYS:CB	1:I:202:LEU:HB2	2.46	0.46
1:I:124:SER:HB2	1:L:122:GLN:O	2.16	0.46
1:R:98:HIS:O	1:R:99:ARG:NH1	2.40	0.46
1:U:127:GLU:OE1	1:X:126:ASN:HB3	2.16	0.46
1:G:181:LYS:HB3	1:G:218:VAL:HG12	1.98	0.46
1:M:143:VAL:HG21	1:N:147:GLU:HB2	1.98	0.46
1:Q:98:HIS:HB2	1:Q:103:LEU:HD13	1.97	0.46
1:T:122:GLN:HB2	1:W:124:SER:HB2	1.98	0.46
1:O:102:PHE:CE2	1:O:147:GLU:HG2	2.50	0.46
1:P:85:THR:HB	7:P:236:HOH:O	2.15	0.46
1:A:212:TYR:CE2	1:A:217:VAL:HG22	2.51	0.45
1:O:174:VAL:HG12	1:P:177:VAL:HB	1.97	0.45
1:T:127:GLU:HG2	1:W:126:ASN:O	2.16	0.45
1:U:121:LYS:NZ	1:U:122:GLN:O	2.48	0.45
1:W:89:ILE:HA	1:W:92:ILE:HD12	1.98	0.45
1:F:195:LEU:HA	1:F:207:LEU:HG	1.98	0.45
1:M:134:PHE:HE1	1:N:98:HIS:CE1	2.34	0.45
1:M:221:ILE:HG21	1:M:224:MET:HG3	1.98	0.45
1:S:143:VAL:HB	1:T:143:VAL:HB	1.98	0.45
1:X:207:LEU:O	1:X:223:GLU:HA	2.15	0.45
1:E:198:PHE:CD1	1:E:199:LYS:N	2.83	0.45
1:L:153:ALA:HB1	1:L:207:LEU:HD13	1.97	0.45
1:C:130:PHE:CE2	1:C:185:PRO:HG3	2.52	0.45
1:U:158:LEU:HD21	1:U:167:ASN:HA	1.98	0.45
1:G:146:ILE:HD11	1:G:177:VAL:HG11	1.99	0.45
1:K:143:VAL:HB	1:L:143:VAL:HB	1.99	0.45
1:O:167:ASN:ND2	3:O:23:PEG:C3	2.80	0.45
1:R:218:VAL:HG23	1:R:219:ILE:HG22	1.99	0.45
1:M:86:SER:O	1:M:87:ILE:HG13	2.16	0.45
1:J:89:ILE:HD13	1:J:106:ASP:O	2.17	0.45
1:R:146:ILE:HD11	1:R:177:VAL:HG11	1.99	0.45
1:H:177:VAL:HG22	1:H:221:ILE:HG12	1.99	0.45
1:N:221:ILE:HG21	1:N:224:MET:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:212:TYR:CE2	1:S:217:VAL:HG22	2.51	0.45
1:U:185:PRO:HG2	1:X:89:ILE:HG21	1.99	0.45
1:M:130:PHE:CD1	1:M:138:GLN:HB3	2.52	0.45
1:M:153:ALA:HB1	1:M:207:LEU:HD22	1.98	0.45
1:I:122:GLN:OE1	1:I:122:GLN:HA	2.16	0.44
1:L:104:LEU:HD11	1:L:144:LEU:HD22	1.99	0.44
1:N:95:ILE:HG21	1:N:155:ILE:HG23	1.98	0.44
1:Q:104:LEU:HD11	1:Q:144:LEU:HD22	1.98	0.44
1:C:133:HIS:NE2	5:D:231:S21:H9	2.31	0.44
1:K:104:LEU:HD11	1:K:144:LEU:HD22	1.99	0.44
1:M:161:ASP:OD1	1:M:163:SER:OG	2.35	0.44
1:O:87:ILE:HD12	1:O:108:VAL:HG11	1.97	0.44
1:W:196:ILE:HD11	1:W:208:SER:HB3	1.99	0.44
1:A:122:GLN:HB3	1:D:122:GLN:HB3	2.00	0.44
1:V:221:ILE:HG21	1:V:224:MET:HG3	1.98	0.44
1:C:142:GLY:HA3	5:D:231:S21:C5	2.47	0.44
1:C:142:GLY:H	5:D:231:S21:C6	2.30	0.44
1:I:127:GLU:OE1	1:L:126:ASN:HB3	2.17	0.44
1:O:206:LYS:HG2	1:O:225:THR:HG23	1.99	0.44
1:T:122:GLN:O	1:W:124:SER:HB2	2.17	0.44
1:W:177:VAL:HG22	1:W:221:ILE:HG12	1.99	0.44
1:K:114:ASN:ND2	1:K:160:SER:HB3	2.33	0.44
1:T:159:LYS:HD2	1:T:159:LYS:HA	1.84	0.44
1:I:104:LEU:HD11	1:I:144:LEU:HD22	1.99	0.44
1:I:185:PRO:HG2	1:L:89:ILE:HG21	2.00	0.44
1:Q:199:LYS:HA	1:Q:199:LYS:HD2	1.78	0.44
1:Q:181:LYS:HB3	1:Q:218:VAL:HG12	2.00	0.44
1:X:112:GLN:OE1	1:X:115:LYS:HD3	2.18	0.44
1:K:212:TYR:CE2	1:K:217:VAL:HG22	2.53	0.44
1:M:129:PHE:HB3	2:M:7:GOL:H11	1.99	0.44
1:W:104:LEU:HD11	1:W:144:LEU:HD22	1.99	0.44
1:E:198:PHE:HD1	1:E:199:LYS:H	1.65	0.44
1:U:221:ILE:HG21	1:U:224:MET:HG3	1.99	0.44
1:V:181:LYS:HB2	1:V:218:VAL:HG12	2.00	0.44
1:W:114:ASN:ND2	1:W:160:SER:HB3	2.33	0.44
1:M:174:VAL:HG23	1:M:224:MET:HG2	2.00	0.43
1:N:213:VAL:O	1:N:214:ASN:HB2	2.17	0.43
1:O:149:LEU:HD13	1:O:221:ILE:HD12	2.00	0.43
1:P:154:GLY:HA3	1:P:169:PHE:CZ	2.53	0.43
1:C:123:VAL:HG12	1:C:185:PRO:HA	2.00	0.43
1:S:99:ARG:HG3	3:S:12:PEG:H21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:196:ILE:HD11	1:G:208:SER:HB3	2.00	0.43
1:J:130:PHE:CD1	1:J:138:GLN:HB3	2.53	0.43
1:H:90:GLU:CD	1:K:137:LYS:HA	2.39	0.43
1:K:202:LEU:CD2	1:P:166:ASN:HB2	2.48	0.43
1:B:146:ILE:HD11	1:B:177:VAL:HG11	2.01	0.43
1:E:143:VAL:HB	1:F:143:VAL:HB	1.99	0.43
1:H:215:GLY:O	1:T:212:TYR:OH	2.28	0.43
1:J:152:LEU:HD22	1:J:191:MET:HB2	2.01	0.43
1:Q:99:ARG:HH21	3:Q:9:PEG:H41	1.84	0.43
1:H:124:SER:OG	1:K:121:LYS:NZ	2.52	0.43
1:N:135:PRO:HB2	1:N:136:GLN:OE1	2.18	0.43
1:X:108:VAL:HG22	1:X:152:LEU:HD11	2.01	0.43
1:A:146:ILE:HD11	1:A:179:TRP:HZ2	1.81	0.43
1:C:203:GLY:HA3	1:C:228:LEU:CB	2.49	0.43
1:I:143:VAL:O	1:I:146:ILE:HB	2.18	0.43
1:O:125:THR:HG22	1:R:106:ASP:OD1	2.18	0.43
7:U:13:HOH:O	1:X:100:TYR:HB2	2.18	0.43
1:C:181:LYS:HB3	1:C:218:VAL:HG12	2.01	0.43
1:K:183:VAL:HG22	1:K:213:VAL:HG21	2.00	0.43
1:L:102:PHE:HE1	2:L:6:GOL:HO3	1.65	0.43
1:G:146:ILE:CD1	1:G:179:TRP:HZ2	2.32	0.43
1:H:121:LYS:NZ	1:K:124:SER:OG	2.52	0.43
1:K:207:LEU:O	1:K:223:GLU:HA	2.19	0.43
1:L:102:PHE:CE2	1:L:147:GLU:HG2	2.54	0.43
1:H:115:LYS:HB2	1:W:214:ASN:ND2	2.33	0.43
1:H:128:PRO:HD3	1:K:128:PRO:HD3	2.00	0.43
1:W:138:GLN:HG2	1:W:138:GLN:H	1.59	0.43
1:A:149:LEU:HD13	1:A:221:ILE:HD12	2.01	0.43
1:Q:150:ALA:HB1	1:Q:226:PHE:CZ	2.54	0.43
1:T:186:GLY:HA2	1:W:122:GLN:CG	2.48	0.43
1:V:104:LEU:HD11	1:V:144:LEU:HD22	2.01	0.43
1:E:195:LEU:HA	1:E:207:LEU:HG	2.01	0.42
1:F:198:PHE:HD1	1:F:199:LYS:N	2.16	0.42
1:T:206:LYS:HA	1:T:224:MET:O	2.18	0.42
1:O:130:PHE:CD1	1:O:138:GLN:HB3	2.55	0.42
1:N:106:ASP:OD1	1:Q:125:THR:HG22	2.19	0.42
1:S:86:SER:HB2	1:S:109:ILE:HA	2.01	0.42
1:V:152:LEU:HA	1:V:155:ILE:HD12	2.01	0.42
1:A:140:MET:HA	1:A:141:PRO:HD3	1.91	0.42
1:A:219:ILE:HD11	1:A:221:ILE:HD11	2.00	0.42
1:H:142:GLY:HA2	1:H:145:GLN:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:142:GLY:HA2	1:L:145:GLN:NE2	2.35	0.42
1:F:98:HIS:CD2	1:F:151:GLN:HE21	2.38	0.42
1:H:186:GLY:O	1:K:122:GLN:NE2	2.53	0.42
1:K:166:ASN:HB3	1:K:228:LEU:CD2	2.49	0.42
1:P:180:LYS:HG3	1:P:217:VAL:HG12	2.01	0.42
1:T:186:GLY:O	1:W:122:GLN:NE2	2.51	0.42
1:P:169:PHE:HB3	1:P:228:LEU:O	2.20	0.42
1:T:104:LEU:HD11	1:T:144:LEU:HD22	2.02	0.42
1:X:170:LEU:HD12	1:X:229:SER:OG	2.19	0.42
1:A:170:LEU:HA	1:A:170:LEU:HD23	1.92	0.42
1:D:117:ILE:HB	1:D:156:LEU:HD13	2.02	0.42
1:H:213:VAL:O	1:H:214:ASN:HB2	2.19	0.42
1:M:96:LEU:HB3	1:M:98:HIS:ND1	2.34	0.42
1:O:112:GLN:CG	1:O:112:GLN:O	2.64	0.42
1:O:106:ASP:OD1	1:R:125:THR:HG22	2.19	0.42
1:B:112:GLN:HA	1:B:113:PRO:HD3	1.90	0.42
1:C:181:LYS:HG2	1:C:182:PRO:HD2	2.02	0.42
1:C:195:LEU:HD12	1:C:207:LEU:HG	2.01	0.42
1:D:170:LEU:HD22	5:D:231:S21:C2	2.50	0.42
1:O:109:ILE:HD11	1:O:118:ILE:HG22	2.01	0.42
1:P:177:VAL:HG22	1:P:221:ILE:HG12	2.01	0.42
1:B:190:THR:O	1:B:211:GLY:HA2	2.19	0.42
1:H:164:GLN:H	1:H:164:GLN:HG2	1.59	0.42
1:U:197:SER:HB2	1:U:199:LYS:NZ	2.35	0.42
1:C:137:LYS:HD3	1:C:139:ILE:HD11	2.01	0.41
1:D:117:ILE:HG22	1:D:156:LEU:HD22	2.00	0.41
1:O:85:THR:N	7:O:234:HOH:O	2.52	0.41
1:T:87:ILE:HD12	1:T:108:VAL:HG21	2.02	0.41
1:T:140:MET:HA	1:T:141:PRO:HD3	1.91	0.41
1:V:98:HIS:CD2	1:V:151:GLN:HE21	2.38	0.41
1:O:171:PHE:CD1	1:P:179:TRP:HZ3	2.38	0.41
1:R:153:ALA:HB1	1:R:207:LEU:HD22	2.02	0.41
1:S:192:GLN:HE22	3:S:8:PEG:C2	2.21	0.41
1:T:106:ASP:OD1	1:W:125:THR:HG22	2.20	0.41
1:F:133:HIS:CG	1:F:141:PRO:HG3	2.55	0.41
1:N:134:PHE:O	1:N:135:PRO:C	2.58	0.41
1:O:104:LEU:HD11	1:O:144:LEU:HD22	2.02	0.41
1:T:86:SER:HB2	1:T:109:ILE:O	2.20	0.41
1:G:152:LEU:HD22	1:G:191:MET:HB2	2.01	0.41
1:H:195:LEU:HD21	1:H:198:PHE:HD2	1.85	0.41
1:P:89:ILE:HA	1:P:92:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:149:LEU:CD2	1:Q:191:MET:HB3	2.50	0.41
1:X:199:LYS:C	1:X:201:SER:H	2.24	0.41
1:G:139:ILE:O	1:G:141:PRO:HD3	2.20	0.41
1:L:178:ARG:HD3	1:L:178:ARG:HA	1.89	0.41
1:O:206:LYS:HD3	1:O:223:GLU:OE2	2.20	0.41
1:P:170:LEU:HA	5:P:4:S21:O11	2.20	0.41
1:S:112:GLN:OE1	1:S:115:LYS:HD3	2.20	0.41
1:S:98:HIS:CD2	1:S:151:GLN:HE21	2.38	0.41
1:W:98:HIS:CD2	1:W:151:GLN:HE21	2.38	0.41
1:E:133:HIS:HE1	5:F:231:S21:H1	1.78	0.41
1:I:114:ASN:ND2	1:I:160:SER:HB3	2.36	0.41
1:I:140:MET:HA	1:I:141:PRO:HD3	1.94	0.41
1:J:178:ARG:O	1:J:219:ILE:HA	2.21	0.41
1:K:104:LEU:HD22	1:K:121:LYS:HE2	2.03	0.41
1:O:143:VAL:HB	1:P:143:VAL:HB	2.01	0.41
1:T:221:ILE:HG21	1:T:224:MET:HG3	2.03	0.41
1:U:184:LEU:HB3	1:U:185:PRO:HD2	2.02	0.41
1:V:102:PHE:CE2	1:V:147:GLU:HG2	2.56	0.41
1:T:122:GLN:NE2	1:W:186:GLY:O	2.46	0.41
1:J:115:LYS:HG2	1:J:116:THR:HG22	2.02	0.41
1:R:221:ILE:HG21	1:R:224:MET:CG	2.51	0.41
1:M:114:ASN:ND2	1:M:160:SER:HB3	2.35	0.41
1:P:202:LEU:HD23	1:P:202:LEU:H	1.86	0.41
1:V:177:VAL:HA	1:V:220:ASN:O	2.20	0.41
1:B:114:ASN:ND2	1:B:160:SER:HB3	2.36	0.41
1:H:128:PRO:HD2	1:K:126:ASN:O	2.21	0.41
1:P:117:ILE:O	1:P:117:ILE:HG23	2.21	0.41
1:S:181:LYS:HE2	1:S:216:LYS:HD3	2.03	0.41
1:T:85:THR:HG23	1:T:86:SER:H	1.86	0.41
1:H:177:VAL:HA	1:H:220:ASN:O	2.21	0.41
1:K:89:ILE:HA	1:K:92:ILE:HD12	2.03	0.41
1:U:87:ILE:HG22	1:U:92:ILE:HG13	2.03	0.41
1:X:89:ILE:HA	1:X:92:ILE:HD12	2.02	0.41
1:F:146:ILE:HD11	1:F:177:VAL:HG11	2.03	0.40
1:J:146:ILE:HD11	1:J:177:VAL:HG11	2.02	0.40
1:K:175:ASP:HB2	7:K:301:HOH:O	2.20	0.40
1:V:117:ILE:HG23	1:V:152:LEU:HG	2.03	0.40
1:A:117:ILE:HG22	1:A:156:LEU:HD22	2.03	0.40
1:H:113:PRO:O	1:H:114:ASN:HB2	2.20	0.40
1:I:192:GLN:HE22	3:I:11:PEG:H42	1.86	0.40
1:K:98:HIS:CD2	1:K:151:GLN:NE2	2.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:87:ILE:HG22	1:S:91:ASP:HB2	2.04	0.40
1:U:97:PRO:HG2	1:V:134:PHE:CE1	2.55	0.40
1:A:153:ALA:HB1	1:A:207:LEU:HD13	2.02	0.40
1:K:195:LEU:HD12	1:K:206:LYS:O	2.21	0.40
1:C:217:VAL:HB	7:C:47:HOH:O	2.21	0.40
1:K:146:ILE:HD11	1:K:179:TRP:CZ2	2.56	0.40
1:O:167:ASN:HD21	3:O:23:PEG:C2	2.34	0.40
1:Q:177:VAL:HB	1:R:174:VAL:HG12	2.03	0.40
1:R:98:HIS:NE2	5:R:1:S21:F3C	2.40	0.40
1:U:200:SER:HB3	1:U:201:SER:H	1.66	0.40
1:S:166:ASN:HB3	1:S:228:LEU:HD11	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	143/154 (93%)	134 (94%)	9 (6%)	0	100	100
1	B	137/154 (89%)	127 (93%)	10 (7%)	0	100	100
1	C	142/154 (92%)	132 (93%)	10 (7%)	0	100	100
1	D	136/154 (88%)	127 (93%)	9 (7%)	0	100	100
1	E	139/154 (90%)	130 (94%)	9 (6%)	0	100	100
1	F	145/154 (94%)	133 (92%)	11 (8%)	1 (1%)	22	57
1	G	143/154 (93%)	133 (93%)	10 (7%)	0	100	100
1	H	137/154 (89%)	122 (89%)	15 (11%)	0	100	100
1	I	140/154 (91%)	131 (94%)	9 (6%)	0	100	100
1	J	142/154 (92%)	130 (92%)	12 (8%)	0	100	100
1	K	143/154 (93%)	134 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	144/154 (94%)	134 (93%)	10 (7%)	0	100	100
1	M	143/154 (93%)	127 (89%)	15 (10%)	1 (1%)	22	57
1	N	143/154 (93%)	131 (92%)	12 (8%)	0	100	100
1	O	142/154 (92%)	128 (90%)	14 (10%)	0	100	100
1	P	143/154 (93%)	132 (92%)	11 (8%)	0	100	100
1	Q	138/154 (90%)	128 (93%)	10 (7%)	0	100	100
1	R	144/154 (94%)	134 (93%)	9 (6%)	1 (1%)	22	57
1	S	145/154 (94%)	132 (91%)	13 (9%)	0	100	100
1	T	138/154 (90%)	127 (92%)	11 (8%)	0	100	100
1	U	142/154 (92%)	125 (88%)	17 (12%)	0	100	100
1	V	142/154 (92%)	130 (92%)	12 (8%)	0	100	100
1	W	138/154 (90%)	128 (93%)	10 (7%)	0	100	100
1	X	143/154 (93%)	134 (94%)	9 (6%)	0	100	100
All	All	3392/3696 (92%)	3123 (92%)	266 (8%)	3 (0%)	51	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	201	SER
1	R	200	SER
1	F	168	LEU

### 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	126/135 (93%)	119 (94%)	7 (6%)	21	52
1	B	122/135 (90%)	116 (95%)	6 (5%)	25	57
1	C	125/135 (93%)	119 (95%)	6 (5%)	25	58
1	D	118/135 (87%)	113 (96%)	5 (4%)	30	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	124/135 (92%)	116 (94%)	8 (6%)	17	47
1	F	127/135 (94%)	123 (97%)	4 (3%)	40	70
1	G	124/135 (92%)	119 (96%)	5 (4%)	31	65
1	H	121/135 (90%)	113 (93%)	8 (7%)	16	47
1	I	125/135 (93%)	117 (94%)	8 (6%)	17	48
1	J	119/135 (88%)	112 (94%)	7 (6%)	19	50
1	K	126/135 (93%)	115 (91%)	11 (9%)	10	36
1	L	125/135 (93%)	116 (93%)	9 (7%)	14	44
1	M	126/135 (93%)	118 (94%)	8 (6%)	18	48
1	N	123/135 (91%)	114 (93%)	9 (7%)	14	43
1	O	125/135 (93%)	115 (92%)	10 (8%)	12	40
1	P	119/135 (88%)	112 (94%)	7 (6%)	19	50
1	Q	123/135 (91%)	108 (88%)	15 (12%)	5	19
1	R	126/135 (93%)	116 (92%)	10 (8%)	12	40
1	S	127/135 (94%)	123 (97%)	4 (3%)	40	70
1	T	122/135 (90%)	114 (93%)	8 (7%)	16	47
1	U	125/135 (93%)	118 (94%)	7 (6%)	21	52
1	V	120/135 (89%)	113 (94%)	7 (6%)	20	51
1	W	123/135 (91%)	111 (90%)	12 (10%)	8	29
1	X	125/135 (93%)	115 (92%)	10 (8%)	12	40
All	All	2966/3240 (92%)	2775 (94%)	191 (6%)	17	48

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	ILE
1	A	102	PHE
1	A	168	LEU
1	A	171	PHE
1	A	181	LYS
1	A	198	PHE
1	A	229	SER
1	B	102	PHE
1	B	168	LEU
1	B	169	PHE

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Mol	Chain	Res	Type
1	B	171	PHE
1	B	198	PHE
1	B	199	LYS
1	C	85	THR
1	C	102	PHE
1	C	171	PHE
1	C	175	ASP
1	C	181	LYS
1	C	198	PHE
1	D	85	THR
1	D	168	LEU
1	D	171	PHE
1	D	181	LYS
1	D	198	PHE
1	E	84	ASP
1	E	102	PHE
1	E	131	ASN
1	E	168	LEU
1	E	171	PHE
1	E	181	LYS
1	E	199	LYS
1	E	228	LEU
1	F	149	LEU
1	F	165	LYS
1	F	171	PHE
1	F	198	PHE
1	G	85	THR
1	G	102	PHE
1	G	171	PHE
1	G	198	PHE
1	G	220	ASN
1	H	102	PHE
1	H	136	GLN
1	H	164	GLN
1	H	168	LEU
1	H	171	PHE
1	H	198	PHE
1	H	204	ILE
1	H	220	ASN
1	I	86	SER
1	I	102	PHE
1	I	109	ILE

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Mol	Chain	Res	Type
1	I	168	LEU
1	I	171	PHE
1	I	198	PHE
1	I	200	SER
1	I	204	ILE
1	J	99	ARG
1	J	102	PHE
1	J	171	PHE
1	J	175	ASP
1	J	198	PHE
1	J	202	LEU
1	J	220	ASN
1	K	84	ASP
1	K	86	SER
1	K	87	ILE
1	K	102	PHE
1	K	171	PHE
1	K	175	ASP
1	K	198	PHE
1	K	199	LYS
1	K	200	SER
1	K	220	ASN
1	K	228	LEU
1	L	85	THR
1	L	86	SER
1	L	102	PHE
1	L	164	GLN
1	L	168	LEU
1	L	169	PHE
1	L	171	PHE
1	L	198	PHE
1	L	220	ASN
1	M	102	PHE
1	M	136	GLN
1	M	163	SER
1	M	168	LEU
1	M	171	PHE
1	M	198	PHE
1	M	202	LEU
1	M	220	ASN
1	N	85	THR
1	N	102	PHE

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Mol	Chain	Res	Type
1	N	168	LEU
1	N	171	PHE
1	N	175	ASP
1	N	198	PHE
1	N	199	LYS
1	N	201	SER
1	N	220	ASN
1	O	85	THR
1	O	102	PHE
1	O	112	GLN
1	O	136	GLN
1	O	168	LEU
1	O	171	PHE
1	O	198	PHE
1	O	202	LEU
1	O	220	ASN
1	O	225	THR
1	P	102	PHE
1	P	136	GLN
1	P	168	LEU
1	P	171	PHE
1	P	198	PHE
1	P	201	SER
1	P	202	LEU
1	Q	84	ASP
1	Q	85	THR
1	Q	88	ASP
1	Q	102	PHE
1	Q	136	GLN
1	Q	162	ASP
1	Q	164	GLN
1	Q	168	LEU
1	Q	171	PHE
1	Q	198	PHE
1	Q	199	LYS
1	Q	204	ILE
1	Q	220	ASN
1	Q	225	THR
1	Q	228	LEU
1	R	85	THR
1	R	102	PHE
1	R	136	GLN

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Mol	Chain	Res	Type
1	R	168	LEU
1	R	171	PHE
1	R	198	PHE
1	R	200	SER
1	R	220	ASN
1	R	225	THR
1	R	229	SER
1	S	168	LEU
1	S	171	PHE
1	S	181	LYS
1	S	198	PHE
1	T	85	THR
1	T	86	SER
1	T	102	PHE
1	T	164	GLN
1	T	168	LEU
1	T	171	PHE
1	T	198	PHE
1	T	220	ASN
1	U	86	SER
1	U	168	LEU
1	U	171	PHE
1	U	181	LYS
1	U	198	PHE
1	U	202	LEU
1	U	220	ASN
1	V	102	PHE
1	V	168	LEU
1	V	169	PHE
1	V	171	PHE
1	V	198	PHE
1	V	200	SER
1	V	220	ASN
1	W	85	THR
1	W	102	PHE
1	W	109	ILE
1	W	138	GLN
1	W	168	LEU
1	W	169	PHE
1	W	171	PHE
1	W	174	VAL
1	W	198	PHE

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Mol	Chain	Res	Type
1	W	199	LYS
1	W	220	ASN
1	W	228	LEU
1	X	85	THR
1	X	164	GLN
1	X	168	LEU
1	X	171	PHE
1	X	174	VAL
1	X	198	PHE
1	X	199	LYS
1	X	200	SER
1	X	201	SER
1	X	220	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	B	112	GLN
1	B	114	ASN
1	B	220	ASN
1	C	114	ASN
1	D	192	GLN
1	E	114	ASN
1	F	214	ASN
1	F	220	ASN
1	G	98	HIS
1	G	114	ASN
1	G	133	HIS
1	H	98	HIS
1	H	112	GLN
1	H	114	ASN
1	H	145	GLN
1	H	164	GLN
1	H	220	ASN
1	I	114	ASN
1	I	138	GLN
1	I	192	GLN
1	J	98	HIS
1	J	114	ASN
1	J	214	ASN
1	K	98	HIS

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Mol	Chain	Res	Type
1	K	114	ASN
1	K	164	GLN
1	K	220	ASN
1	L	98	HIS
1	L	114	ASN
1	L	145	GLN
1	L	164	GLN
1	M	98	HIS
1	M	114	ASN
1	O	164	GLN
1	O	167	ASN
1	P	138	GLN
1	R	164	GLN
1	S	192	GLN
1	T	98	HIS
1	T	112	GLN
1	T	114	ASN
1	U	214	ASN
1	W	114	ASN
1	X	114	ASN
1	X	138	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 64 ligands modelled in this entry, 17 are monoatomic - leaving 47 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
3	PEG	A	27	-	6,6,6	0.64	0	5,5,5	0.33	0
2	GOL	S	10	-	5,5,5	0.45	0	5,5,5	0.99	0
3	PEG	E	17	-	6,6,6	0.66	0	5,5,5	0.23	0
3	PEG	F	2	-	6,6,6	0.64	0	5,5,5	0.22	0
5	S21	P	4	-	17,18,18	0.71	0	22,26,26	0.92	0
3	PEG	A	18	-	6,6,6	0.57	0	5,5,5	0.32	0
3	PEG	R	29	-	6,6,6	0.73	0	5,5,5	0.19	0
5	S21	D	231	-	17,18,18	0.85	0	22,26,26	1.05	1 (4%)
5	S21	R	1	-	17,18,18	0.62	0	22,26,26	1.16	2 (9%)
2	GOL	F	3	-	5,5,5	0.29	0	5,5,5	0.50	0
2	GOL	R	9	-	5,5,5	0.33	0	5,5,5	0.40	0
2	GOL	O	8	-	5,5,5	0.37	0	5,5,5	0.34	0
3	PEG	S	12	-	6,6,6	0.56	0	5,5,5	0.49	0
2	GOL	I	5	-	5,5,5	0.36	0	5,5,5	0.37	0
2	GOL	A	1	-	5,5,5	0.33	0	5,5,5	0.41	0
3	PEG	O	22	-	6,6,6	0.62	0	5,5,5	0.28	0
2	GOL	U	11	-	5,5,5	0.35	0	5,5,5	0.33	0
3	PEG	I	20	-	6,6,6	0.38	0	5,5,5	0.31	0
2	GOL	W	12	-	5,5,5	0.30	0	5,5,5	0.41	0
3	PEG	S	13	-	6,6,6	0.49	0	5,5,5	0.36	0
2	GOL	P	13	-	5,5,5	0.38	0	5,5,5	0.62	0
5	S21	F	231	-	17,18,18	0.76	0	22,26,26	1.25	3 (13%)
3	PEG	A	5	-	6,6,6	0.59	0	5,5,5	0.26	0
3	PEG	Q	9	-	6,6,6	0.59	0	5,5,5	0.21	0
3	PEG	B	3	-	6,6,6	0.56	0	5,5,5	0.27	0
3	PEG	H	231	-	6,6,6	0.51	0	5,5,5	0.39	0
3	PEG	N	14	-	6,6,6	0.73	0	5,5,5	0.40	0
3	PEG	F	24	-	6,6,6	0.59	0	5,5,5	0.30	0
2	GOL	D	2	-	5,5,5	0.27	0	5,5,5	0.53	0
3	PEG	G	6	-	6,6,6	0.58	0	5,5,5	0.41	0
3	PEG	S	19	-	6,6,6	0.69	0	5,5,5	0.22	0
3	PEG	Q	16	-	6,6,6	0.78	0	5,5,5	0.45	0
3	PEG	S	8	-	6,6,6	0.69	0	5,5,5	0.45	0
2	GOL	L	6	-	5,5,5	0.38	0	5,5,5	0.21	0
3	PEG	U	21	-	6,6,6	0.81	0	5,5,5	0.50	0
3	PEG	F	25	-	6,6,6	0.60	0	5,5,5	0.32	0
3	PEG	I	11	-	6,6,6	0.52	0	5,5,5	0.28	0
3	PEG	O	23	-	6,6,6	0.59	0	5,5,5	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PEG	A	26	-	6,6,6	0.64	0	5,5,5	0.30	0
6	PO4	E	1	-	4,4,4	0.61	0	6,6,6	0.59	0
3	PEG	R	15	-	6,6,6	0.53	0	5,5,5	0.49	0
3	PEG	Q	7	-	6,6,6	0.69	0	5,5,5	0.31	0
2	GOL	H	4	-	5,5,5	0.45	0	5,5,5	0.34	0
2	GOL	M	7	-	5,5,5	0.37	0	5,5,5	0.31	0
3	PEG	O	10	-	6,6,6	0.57	0	5,5,5	0.39	0
3	PEG	O	28	-	6,6,6	0.43	0	5,5,5	0.31	0
3	PEG	C	1	-	6,6,6	0.69	0	5,5,5	0.23	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	A	27	-	-	3/4/4/4	-
2	GOL	S	10	-	-	2/4/4/4	-
3	PEG	E	17	-	-	3/4/4/4	-
3	PEG	F	2	-	-	2/4/4/4	-
5	S21	P	4	-	-	8/16/18/18	0/1/1/1
3	PEG	A	18	-	-	4/4/4/4	-
3	PEG	R	29	-	-	3/4/4/4	-
5	S21	D	231	-	-	5/16/18/18	0/1/1/1
5	S21	R	1	-	-	11/16/18/18	0/1/1/1
2	GOL	F	3	-	-	0/4/4/4	-
2	GOL	R	9	-	-	4/4/4/4	-
2	GOL	O	8	-	-	0/4/4/4	-
3	PEG	S	12	-	-	2/4/4/4	-
2	GOL	I	5	-	-	2/4/4/4	-
2	GOL	A	1	-	-	2/4/4/4	-
3	PEG	O	22	-	-	2/4/4/4	-
2	GOL	U	11	-	-	2/4/4/4	-
3	PEG	I	20	-	-	3/4/4/4	-
2	GOL	W	12	-	-	4/4/4/4	-
3	PEG	S	13	-	-	3/4/4/4	-
2	GOL	P	13	-	-	2/4/4/4	-
5	S21	F	231	-	-	12/16/18/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	A	5	-	-	0/4/4/4	-
3	PEG	Q	9	-	-	3/4/4/4	-
3	PEG	B	3	-	-	4/4/4/4	-
3	PEG	H	231	-	-	2/4/4/4	-
3	PEG	N	14	-	-	2/4/4/4	-
3	PEG	F	24	-	-	4/4/4/4	-
2	GOL	D	2	-	-	2/4/4/4	-
3	PEG	G	6	-	-	3/4/4/4	-
3	PEG	S	19	-	-	3/4/4/4	-
3	PEG	Q	16	-	-	1/4/4/4	-
3	PEG	S	8	-	-	3/4/4/4	-
2	GOL	L	6	-	-	2/4/4/4	-
3	PEG	U	21	-	-	1/4/4/4	-
3	PEG	F	25	-	-	3/4/4/4	-
3	PEG	I	11	-	-	3/4/4/4	-
3	PEG	O	23	-	-	3/4/4/4	-
3	PEG	A	26	-	-	3/4/4/4	-
3	PEG	R	15	-	-	3/4/4/4	-
3	PEG	Q	7	-	-	2/4/4/4	-
2	GOL	H	4	-	-	0/4/4/4	-
2	GOL	M	7	-	-	0/4/4/4	-
3	PEG	O	10	-	-	3/4/4/4	-
3	PEG	O	28	-	-	2/4/4/4	-
3	PEG	C	1	-	-	1/4/4/4	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	231	S21	C2-C3-N13	2.95	121.60	119.38
5	R	1	S21	C2-C3-N13	2.71	121.42	119.38
5	F	231	S21	C4-C3-N13	2.60	121.33	119.38
5	F	231	S21	C2-C3-N13	2.34	121.14	119.38
5	R	1	S21	O8-C7-C9	-2.21	118.06	120.56
5	F	231	S21	O8-C7-C9	-2.05	118.25	120.56

There are no chirality outliers.

All (132) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	S	10	GOL	O1-C1-C2-C3
5	D	231	S21	C2-C3-N13-O1N
5	D	231	S21	C4-C3-N13-O1N
5	R	1	S21	C2-C3-N13-O1N
5	R	1	S21	C4-C3-N13-O1N
2	R	9	GOL	O1-C1-C2-C3
2	R	9	GOL	C1-C2-C3-O3
2	R	9	GOL	O2-C2-C3-O3
5	P	4	S21	C2-C3-N13-O1N
5	P	4	S21	C4-C3-N13-O1N
5	P	4	S21	C6-C7-C9-C10
2	U	11	GOL	O1-C1-C2-C3
2	W	12	GOL	O1-C1-C2-C3
2	W	12	GOL	C1-C2-C3-O3
5	F	231	S21	C2-C3-N13-O1N
5	F	231	S21	C4-C3-N13-O1N
5	F	231	S21	C6-C7-C9-C10
2	L	6	GOL	O1-C1-C2-O2
2	L	6	GOL	O1-C1-C2-C3
3	R	15	PEG	C1-C2-O2-C3
5	R	1	S21	C1-C6-C7-O8
5	R	1	S21	C5-C6-C7-O8
5	R	1	S21	C1-C6-C7-C9
5	R	1	S21	C5-C6-C7-C9
3	S	8	PEG	O2-C3-C4-O4
3	R	15	PEG	O1-C1-C2-O2
5	F	231	S21	C1-C6-C7-O8
2	R	9	GOL	O1-C1-C2-O2
2	A	1	GOL	O2-C2-C3-O3
2	U	11	GOL	O1-C1-C2-O2
3	O	22	PEG	O1-C1-C2-O2
3	H	231	PEG	O1-C1-C2-O2
3	G	6	PEG	O1-C1-C2-O2
3	F	25	PEG	O1-C1-C2-O2
3	O	10	PEG	O1-C1-C2-O2
5	F	231	S21	C5-C6-C7-O8
3	A	27	PEG	O1-C1-C2-O2
3	E	17	PEG	O1-C1-C2-O2
3	Q	9	PEG	O2-C3-C4-O4
3	I	11	PEG	O1-C1-C2-O2
3	I	11	PEG	O2-C3-C4-O4
3	O	23	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	26	PEG	O2-C3-C4-O4
3	O	28	PEG	O2-C3-C4-O4
2	I	5	GOL	O1-C1-C2-C3
2	A	1	GOL	C1-C2-C3-O3
2	P	13	GOL	O1-C1-C2-C3
3	I	20	PEG	O2-C3-C4-O4
3	G	6	PEG	O2-C3-C4-O4
3	U	21	PEG	O1-C1-C2-O2
5	F	231	S21	C1-C6-C7-C9
2	S	10	GOL	O1-C1-C2-O2
2	I	5	GOL	O1-C1-C2-O2
3	I	20	PEG	O1-C1-C2-O2
3	N	14	PEG	O1-C1-C2-O2
3	F	24	PEG	O1-C1-C2-O2
3	F	24	PEG	O2-C3-C4-O4
5	F	231	S21	C5-C6-C7-C9
3	E	17	PEG	O2-C3-C4-O4
3	S	13	PEG	O2-C3-C4-O4
3	B	3	PEG	O2-C3-C4-O4
3	R	29	PEG	O2-C3-C4-O4
3	S	12	PEG	O1-C1-C2-O2
3	S	12	PEG	O2-C3-C4-O4
3	O	22	PEG	O2-C3-C4-O4
3	Q	9	PEG	O1-C1-C2-O2
3	B	3	PEG	O1-C1-C2-O2
3	S	19	PEG	O1-C1-C2-O2
3	S	19	PEG	O2-C3-C4-O4
3	F	2	PEG	O2-C3-C4-O4
3	A	18	PEG	O2-C3-C4-O4
3	F	25	PEG	O2-C3-C4-O4
2	W	12	GOL	O1-C1-C2-O2
3	A	18	PEG	O1-C1-C2-O2
3	R	29	PEG	O1-C1-C2-O2
3	O	10	PEG	O2-C3-C4-O4
3	N	14	PEG	C1-C2-O2-C3
3	S	8	PEG	C4-C3-O2-C2
5	P	4	S21	O8-C7-C9-C10
5	F	231	S21	O8-C7-C9-C10
3	O	23	PEG	C1-C2-O2-C3
5	R	1	S21	O11-C10-C12-F1C
5	R	1	S21	O11-C10-C12-F3C
3	A	18	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
3	A	26	PEG	C1-C2-O2-C3
5	D	231	S21	O11-C10-C9-C7
5	R	1	S21	O11-C10-C9-C7
5	P	4	S21	O11-C10-C9-C7
2	P	13	GOL	O1-C1-C2-O2
5	F	231	S21	O11-C10-C9-C7
2	D	2	GOL	O2-C2-C3-O3
3	O	28	PEG	O1-C1-C2-O2
3	Q	16	PEG	C1-C2-O2-C3
3	Q	7	PEG	C4-C3-O2-C2
2	D	2	GOL	C1-C2-C3-O3
5	R	1	S21	C6-C7-C9-C10
3	G	6	PEG	C4-C3-O2-C2
3	O	23	PEG	C4-C3-O2-C2
3	R	15	PEG	O2-C3-C4-O4
3	A	27	PEG	C4-C3-O2-C2
3	B	3	PEG	C1-C2-O2-C3
3	R	29	PEG	C1-C2-O2-C3
2	W	12	GOL	O2-C2-C3-O3
3	C	1	PEG	C1-C2-O2-C3
3	S	13	PEG	C1-C2-O2-C3
3	F	24	PEG	C4-C3-O2-C2
3	I	11	PEG	C4-C3-O2-C2
3	S	13	PEG	C4-C3-O2-C2
3	O	10	PEG	C1-C2-O2-C3
3	F	2	PEG	C4-C3-O2-C2
3	F	24	PEG	C1-C2-O2-C3
3	S	8	PEG	C1-C2-O2-C3
3	Q	9	PEG	C1-C2-O2-C3
3	S	19	PEG	C1-C2-O2-C3
5	P	4	S21	C9-C10-C12-F1C
5	P	4	S21	C9-C10-C12-F2C
5	P	4	S21	C9-C10-C12-F3C
5	F	231	S21	C9-C10-C12-F1C
5	F	231	S21	C9-C10-C12-F2C
5	F	231	S21	C9-C10-C12-F3C
3	A	27	PEG	O2-C3-C4-O4
3	F	25	PEG	C4-C3-O2-C2
3	B	3	PEG	C4-C3-O2-C2
5	R	1	S21	O11-C10-C12-F2C
3	I	20	PEG	C1-C2-O2-C3
3	A	26	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
5	D	231	S21	C6-C7-C9-C10
3	Q	7	PEG	O1-C1-C2-O2
3	H	231	PEG	O2-C3-C4-O4
3	A	18	PEG	C1-C2-O2-C3
3	E	17	PEG	C4-C3-O2-C2
5	D	231	S21	C1-C6-C7-O8

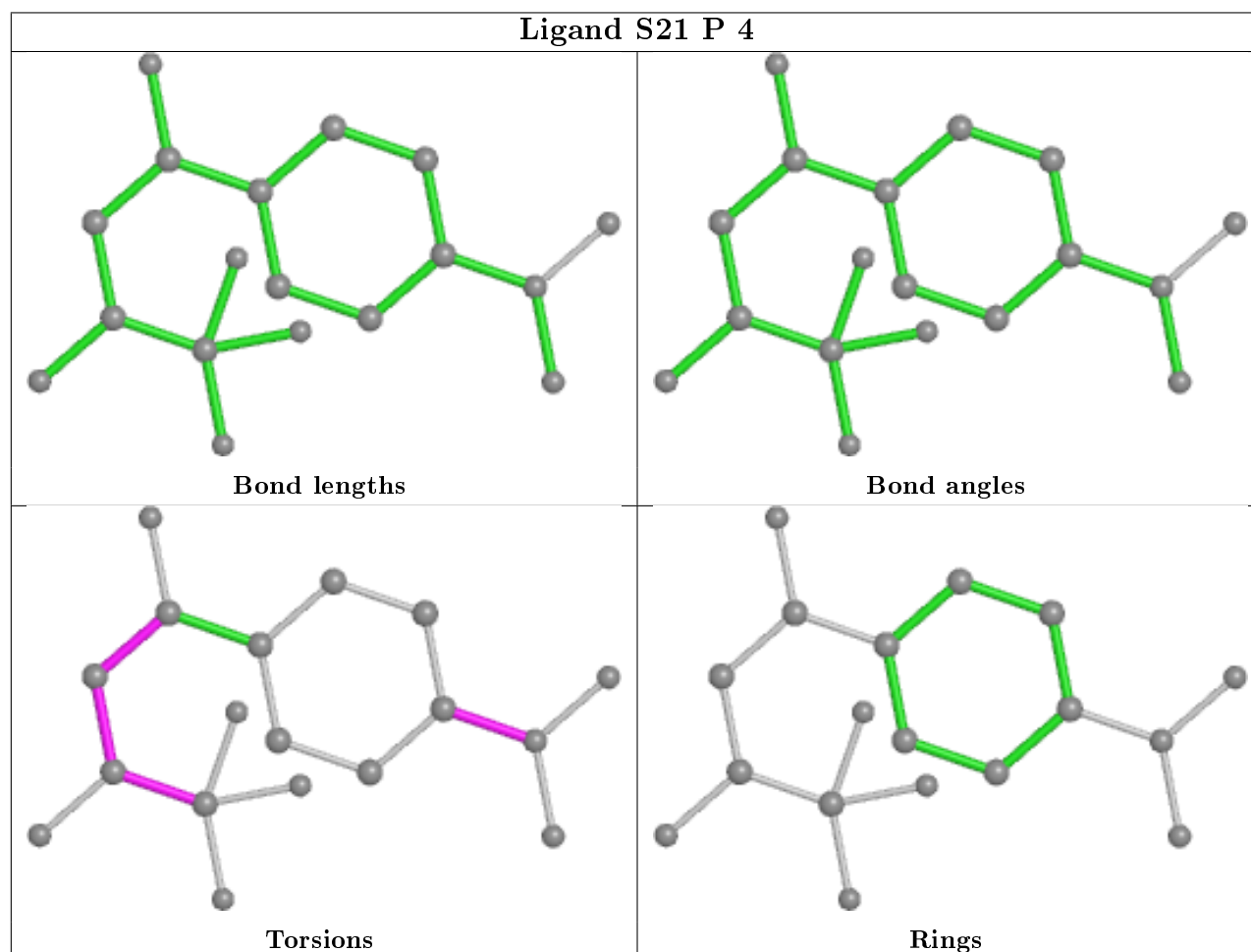
There are no ring outliers.

24 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	S	10	GOL	2	0
5	P	4	S21	11	0
5	D	231	S21	9	0
5	R	1	S21	12	0
2	F	3	GOL	2	0
2	O	8	GOL	1	0
3	S	12	PEG	1	0
3	S	13	PEG	3	0
2	P	13	GOL	1	0
5	F	231	S21	10	0
3	Q	9	PEG	1	0
3	F	24	PEG	1	0
3	S	19	PEG	1	0
3	S	8	PEG	3	0
2	L	6	GOL	1	0
3	U	21	PEG	1	0
3	F	25	PEG	3	0
3	I	11	PEG	1	0
3	O	23	PEG	3	0
6	E	1	PO4	1	0
2	H	4	GOL	2	0
2	M	7	GOL	1	0
3	O	10	PEG	1	0
3	O	28	PEG	2	0

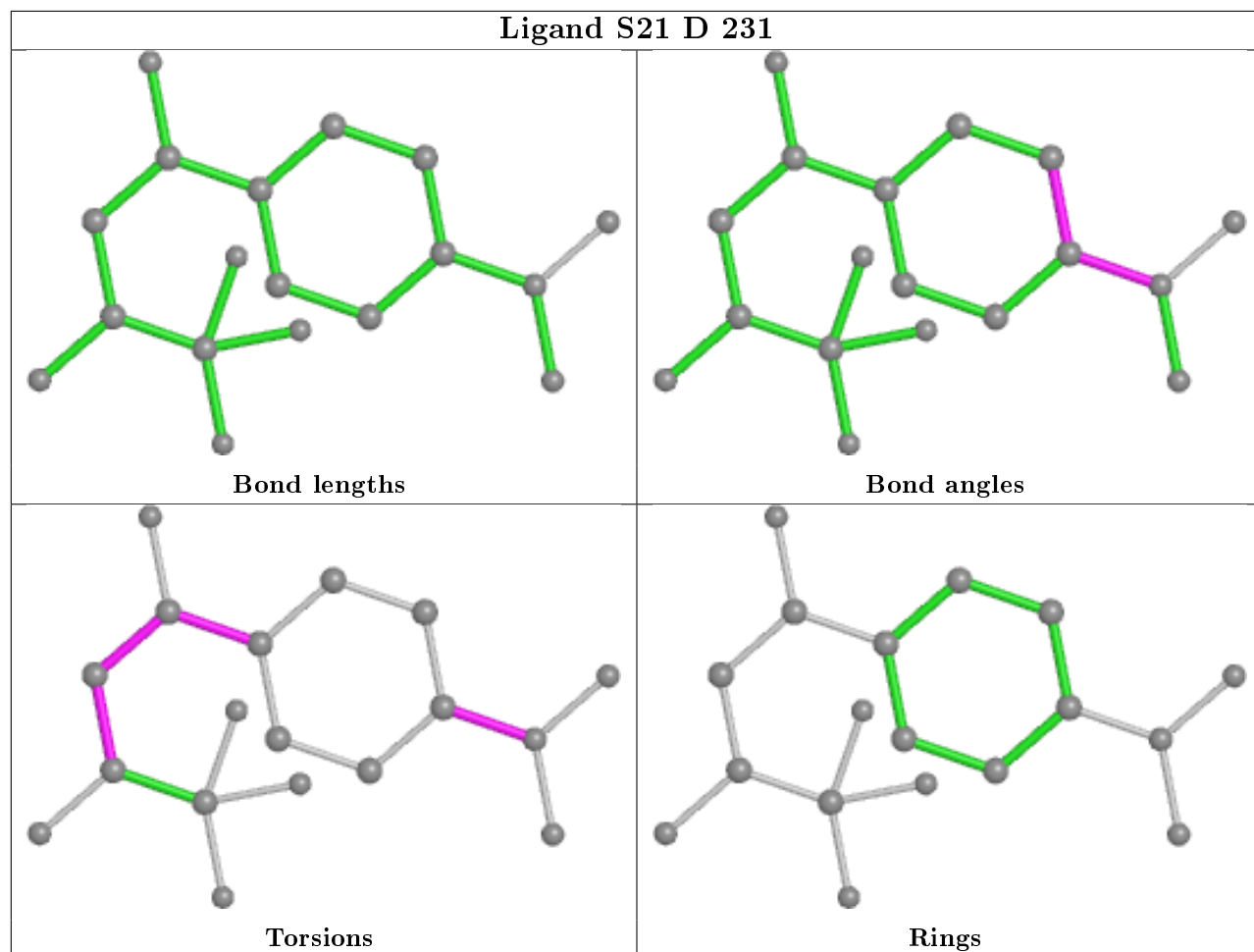
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

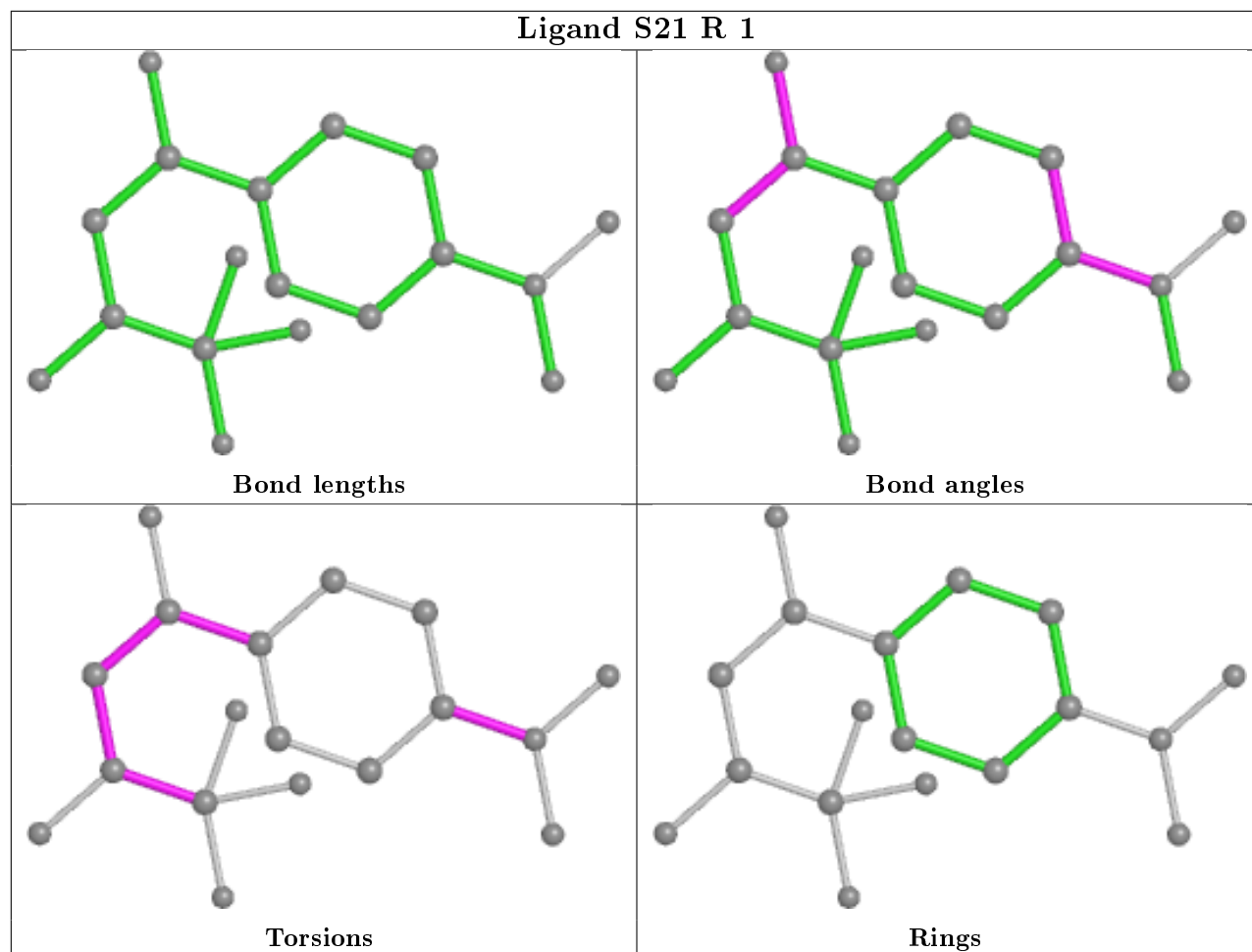
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

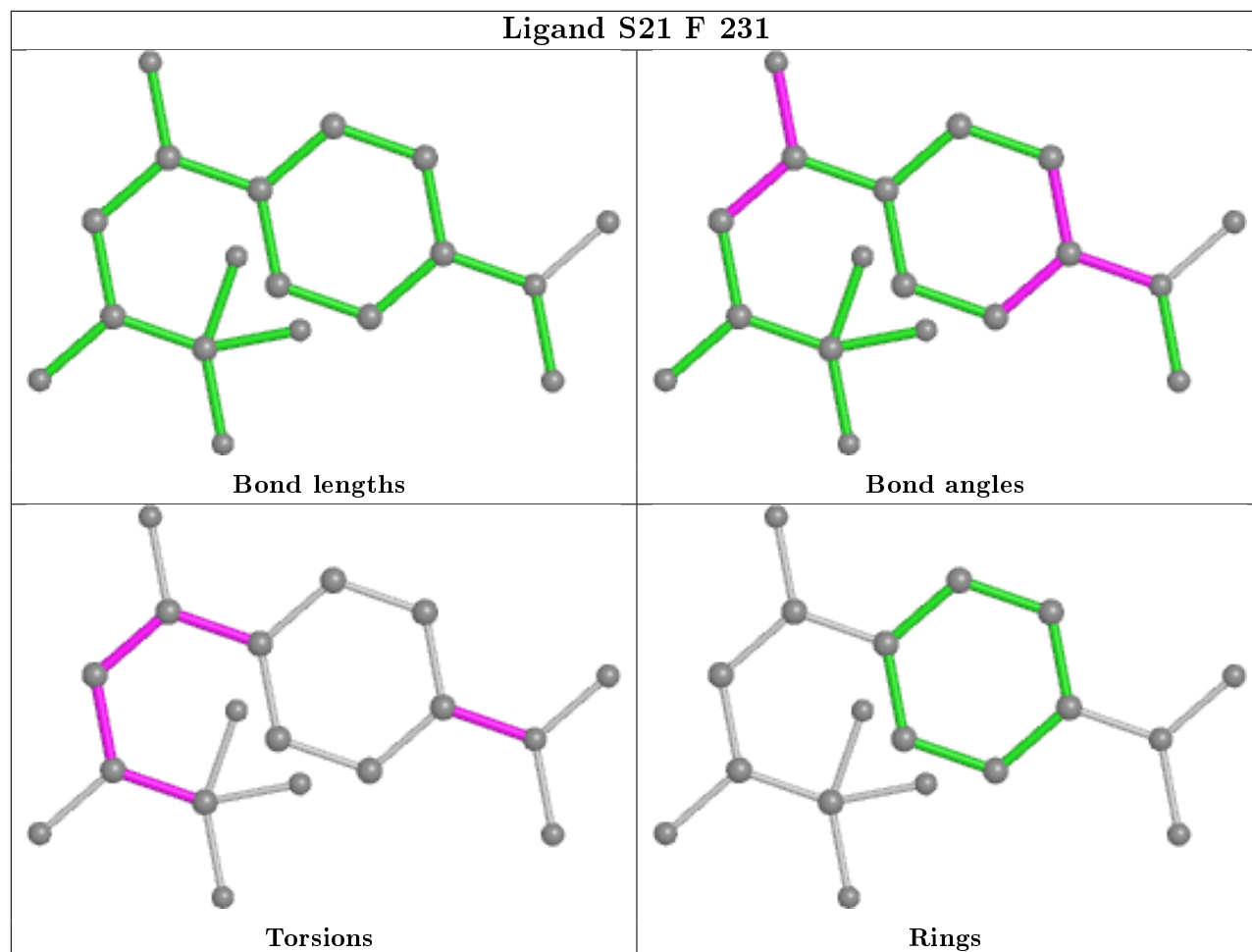




## Ligand S21 D 231







## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	145/154 (94%)	0.08	6 (4%) 37 18	32, 56, 71, 72	0
1	B	141/154 (91%)	-0.05	1 (0%) 87 75	33, 56, 72, 77	0
1	C	144/154 (93%)	-0.15	2 (1%) 75 56	28, 41, 65, 70	0
1	D	140/154 (90%)	-0.13	5 (3%) 42 22	32, 46, 67, 71	1 (0%)
1	E	143/154 (92%)	-0.16	1 (0%) 87 75	28, 42, 65, 71	0
1	F	146/154 (94%)	-0.09	3 (2%) 63 43	29, 44, 64, 73	0
1	G	145/154 (94%)	0.78	26 (17%) 1 0	49, 61, 73, 79	0
1	H	141/154 (91%)	0.31	10 (7%) 16 6	48, 61, 74, 77	0
1	I	143/154 (92%)	-0.08	4 (2%) 53 30	41, 53, 71, 77	0
1	J	144/154 (93%)	0.29	4 (2%) 53 30	45, 59, 73, 78	1 (0%)
1	K	145/154 (94%)	0.20	5 (3%) 45 24	46, 58, 73, 78	0
1	L	146/154 (94%)	0.15	1 (0%) 87 75	42, 61, 76, 80	0
1	M	145/154 (94%)	-0.01	5 (3%) 45 24	35, 55, 70, 73	0
1	N	145/154 (94%)	0.04	5 (3%) 45 24	31, 52, 71, 74	0
1	O	144/154 (93%)	-0.17	0 100 100	29, 44, 62, 68	0
1	P	145/154 (94%)	-0.11	2 (1%) 75 56	33, 50, 66, 73	1 (0%)
1	Q	142/154 (92%)	-0.06	4 (2%) 53 30	26, 44, 67, 73	0
1	R	146/154 (94%)	-0.09	3 (2%) 63 43	30, 47, 69, 76	0
1	S	146/154 (94%)	0.09	6 (4%) 37 18	39, 51, 73, 79	0
1	T	142/154 (92%)	0.09	3 (2%) 63 43	41, 59, 73, 79	0
1	U	144/154 (93%)	0.07	2 (1%) 75 56	41, 57, 72, 76	0
1	V	144/154 (93%)	0.03	3 (2%) 63 43	40, 55, 74, 79	1 (0%)
1	W	142/154 (92%)	0.68	17 (11%) 4 2	48, 63, 78, 85	0
1	X	145/154 (94%)	0.43	14 (9%) 7 2	46, 62, 77, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3453/3696 (93%)	0.09	132 (3%)	40	20	26, 54, 72, 85	4 (0%)

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	167	ASN	6.6
1	S	168	LEU	5.8
1	G	163	SER	5.4
1	A	201	SER	5.4
1	W	167	ASN	5.1
1	N	202	LEU	5.1
1	G	216	LYS	5.0
1	G	202	LEU	4.6
1	X	203	GLY	4.5
1	G	213	VAL	4.5
1	W	183	VAL	4.3
1	Q	86	SER	4.3
1	G	203	GLY	4.0
1	S	229	SER	4.0
1	U	201	SER	4.0
1	K	166	ASN	3.8
1	W	162	ASP	3.8
1	M	200	SER	3.8
1	X	196	ILE	3.7
1	W	163	SER	3.6
1	G	214	ASN	3.6
1	D	167	ASN	3.5
1	N	229	SER	3.5
1	X	227	ALA	3.5
1	K	203	GLY	3.4
1	A	163	SER	3.4
1	N	166	ASN	3.4
1	A	85	THR	3.4
1	I	166	ASN	3.4
1	G	166	ASN	3.3
1	G	162	ASP	3.3
1	W	166	ASN	3.2
1	U	200	SER	3.2
1	B	85	THR	3.2
1	G	110	TYR	3.2
1	X	197	SER	3.2
1	V	201	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	165	LYS	3.1
1	I	163	SER	3.1
1	D	168	LEU	3.1
1	H	86	SER	3.1
1	W	203	GLY	3.1
1	G	201	SER	3.1
1	X	229	SER	3.1
1	H	160	SER	3.0
1	T	88	ASP	3.0
1	E	86	SER	3.0
1	W	168	LEU	3.0
1	G	164	GLN	2.9
1	T	162	ASP	2.9
1	P	167	ASN	2.9
1	F	167	ASN	2.9
1	I	167	ASN	2.9
1	X	228	LEU	2.8
1	W	197	SER	2.8
1	S	162	ASP	2.8
1	W	184	LEU	2.7
1	X	168	LEU	2.7
1	G	161	ASP	2.7
1	H	229	SER	2.7
1	X	160	SER	2.7
1	W	84	ASP	2.7
1	C	166	ASN	2.6
1	F	229	SER	2.6
1	X	86	SER	2.6
1	W	188	THR	2.6
1	G	183	VAL	2.6
1	H	112	GLN	2.6
1	G	196	ILE	2.6
1	D	162	ASP	2.6
1	R	163	SER	2.6
1	K	85	THR	2.5
1	G	189	LEU	2.5
1	G	107	LYS	2.5
1	X	87	ILE	2.5
1	M	167	ASN	2.5
1	W	182	PRO	2.5
1	G	109	ILE	2.5
1	G	184	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	X	204	ILE	2.4
1	G	197	SER	2.4
1	H	163	SER	2.4
1	H	169	PHE	2.4
1	L	163	SER	2.4
1	Q	167	ASN	2.4
1	Q	203	GLY	2.4
1	H	106	ASP	2.4
1	H	88	ASP	2.3
1	K	215	GLY	2.3
1	I	164	GLN	2.3
1	N	114	ASN	2.3
1	V	167	ASN	2.3
1	R	162	ASP	2.3
1	G	157	CYS	2.3
1	Q	164	GLN	2.3
1	W	212	TYR	2.3
1	G	187	ASP	2.3
1	A	200	SER	2.3
1	N	201	SER	2.3
1	M	166	ASN	2.3
1	W	130	PHE	2.2
1	P	201	SER	2.2
1	W	205	ALA	2.2
1	W	90	GLU	2.2
1	A	217	VAL	2.2
1	K	220	ASN	2.2
1	J	163	SER	2.2
1	J	200	SER	2.2
1	X	202	LEU	2.2
1	D	163	SER	2.2
1	R	85	THR	2.2
1	S	86	SER	2.2
1	F	200	SER	2.2
1	D	164	GLN	2.2
1	J	168	LEU	2.1
1	V	200	SER	2.1
1	X	181	LYS	2.1
1	S	166	ASN	2.1
1	G	92	ILE	2.1
1	A	229	SER	2.1
1	C	201	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	T	215	GLY	2.1
1	G	86	SER	2.1
1	G	229	SER	2.1
1	G	204	ILE	2.1
1	J	164	GLN	2.0
1	X	157	CYS	2.0
1	H	205	ALA	2.0
1	W	85	THR	2.0
1	M	201	SER	2.0
1	H	85	THR	2.0
1	M	163	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	PEG	F	25	7/7	0.72	0.25	63,63,64,64	0
3	PEG	I	20	7/7	0.73	0.37	74,74,74,75	0
5	S21	F	231	18/18	0.74	0.30	66,70,73,73	6
4	CL	B	4	1/1	0.76	0.14	49,49,49,49	0
3	PEG	A	5	7/7	0.76	0.24	57,58,58,59	0
3	PEG	S	19	7/7	0.78	0.31	34,37,39,39	0
3	PEG	A	26	7/7	0.81	0.26	51,52,53,53	0
4	CL	G	7	1/1	0.82	0.12	57,57,57,57	0
3	PEG	A	18	7/7	0.85	0.20	53,56,58,58	0
3	PEG	S	8	7/7	0.85	0.23	55,56,56,56	0
3	PEG	B	3	7/7	0.86	0.17	40,41,41,41	0
3	PEG	R	29	7/7	0.86	0.23	40,43,43,43	0

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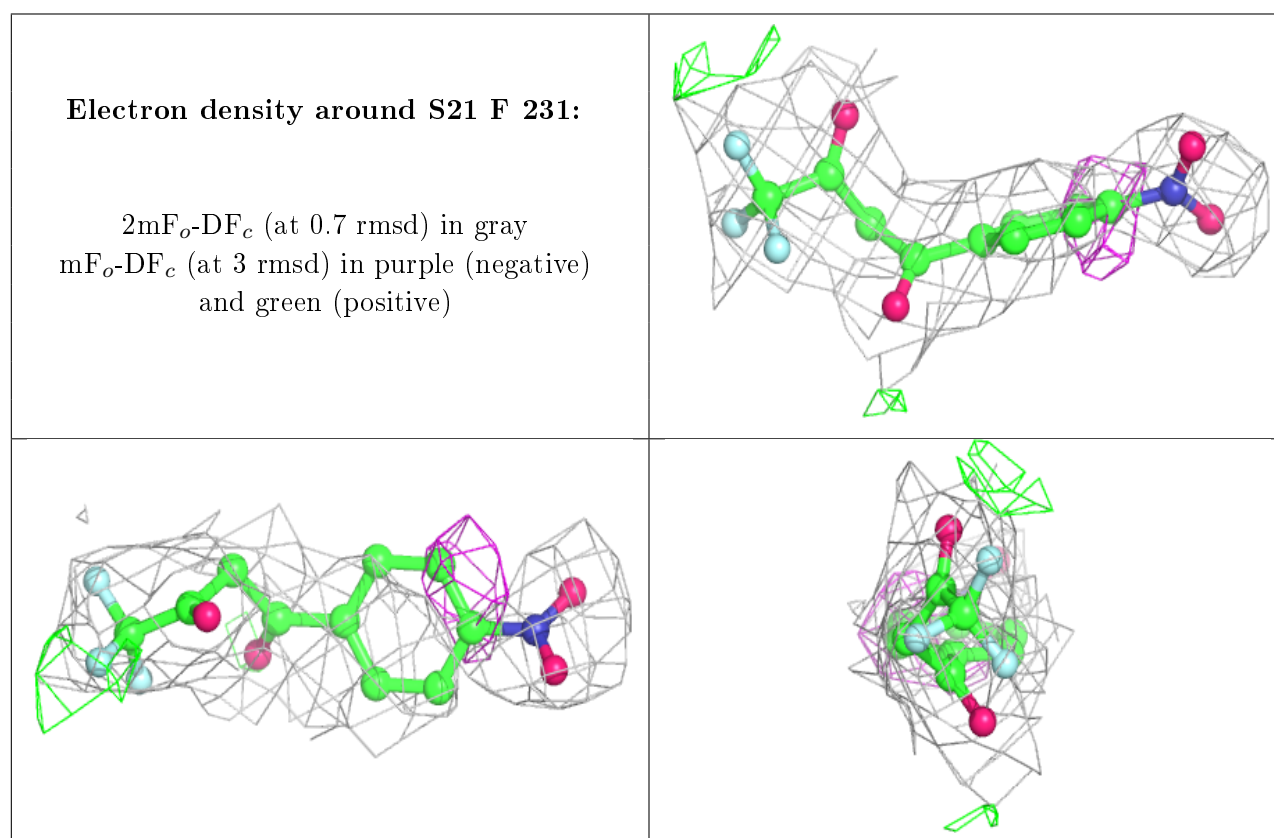
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PEG	Q	9	7/7	0.86	0.21	40,41,42,42	0
3	PEG	U	21	7/7	0.88	0.18	37,40,41,42	0
3	PEG	Q	16	7/7	0.88	0.20	48,49,50,50	0
5	S21	P	4	18/18	0.88	0.26	63,65,66,67	0
5	S21	D	231	18/18	0.89	0.25	50,55,57,57	0
3	PEG	E	17	7/7	0.89	0.19	59,60,60,60	0
3	PEG	A	27	7/7	0.89	0.19	52,54,55,55	0
3	PEG	F	2	7/7	0.89	0.18	42,42,43,43	0
2	GOL	W	12	6/6	0.89	0.28	54,55,55,56	0
3	PEG	O	22	7/7	0.90	0.21	52,53,54,55	0
3	PEG	Q	7	7/7	0.90	0.16	56,58,59,59	0
3	PEG	F	24	7/7	0.90	0.20	38,41,42,42	0
4	CL	K	10	1/1	0.90	0.17	53,53,53,53	0
2	GOL	A	1	6/6	0.90	0.24	45,46,46,46	0
3	PEG	O	28	7/7	0.90	0.23	29,30,32,33	0
3	PEG	H	231	7/7	0.91	0.14	52,52,55,55	0
4	CL	J	9	1/1	0.91	0.17	49,49,49,49	0
4	CL	L	11	1/1	0.91	0.21	50,50,50,50	0
3	PEG	I	11	7/7	0.91	0.22	51,51,53,53	0
2	GOL	U	11	6/6	0.91	0.25	40,41,42,43	0
3	PEG	R	15	7/7	0.91	0.18	36,40,43,44	0
3	PEG	C	1	7/7	0.91	0.17	36,37,39,39	0
3	PEG	O	10	7/7	0.91	0.22	46,47,48,48	0
5	S21	R	1	18/18	0.91	0.25	44,46,52,53	0
3	PEG	S	13	7/7	0.92	0.25	46,47,47,48	0
4	CL	S	15	1/1	0.93	0.15	43,43,43,43	0
4	CL	T	16	1/1	0.93	0.17	50,50,50,50	0
3	PEG	O	23	7/7	0.93	0.25	27,32,37,38	0
3	PEG	S	12	7/7	0.93	0.15	28,28,30,31	0
2	GOL	F	3	6/6	0.94	0.23	27,29,29,29	0
3	PEG	G	6	7/7	0.94	0.13	29,29,30,30	0
2	GOL	P	13	6/6	0.94	0.15	27,30,30,31	0
2	GOL	S	10	6/6	0.95	0.20	36,37,38,39	0
2	GOL	I	5	6/6	0.95	0.16	58,59,60,60	0
4	CL	V	17	1/1	0.95	0.19	39,39,39,39	0
6	PO4	E	1	5/5	0.95	0.18	42,43,44,44	0
2	GOL	O	8	6/6	0.95	0.18	23,24,25,26	0
4	CL	O	1	1/1	0.95	0.19	45,45,45,45	0
4	CL	A	3	1/1	0.95	0.19	55,55,55,55	0
2	GOL	H	4	6/6	0.95	0.27	25,28,29,29	0
2	GOL	D	2	6/6	0.95	0.19	29,30,30,30	0
2	GOL	L	6	6/6	0.95	0.17	35,38,38,39	0

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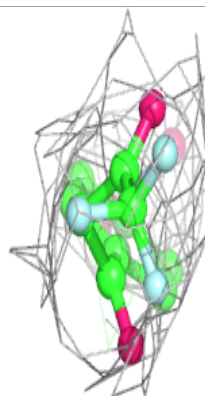
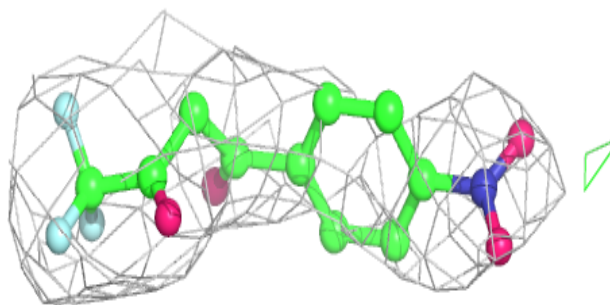
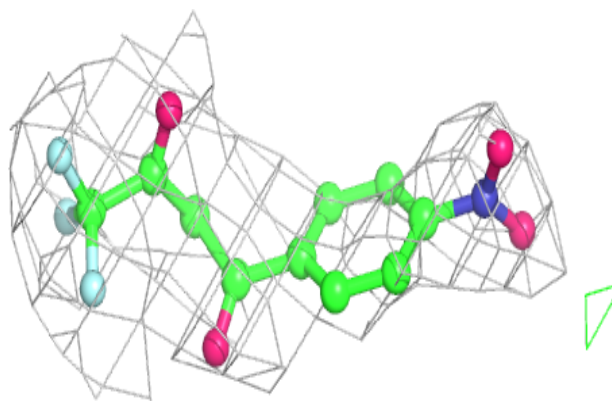
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	C	5	1/1	0.96	0.24	51,51,51,51	0
3	PEG	N	14	7/7	0.96	0.10	29,34,35,36	0
2	GOL	M	7	6/6	0.96	0.15	29,30,30,31	0
4	CL	I	8	1/1	0.96	0.15	46,46,46,46	0
4	CL	U	2	1/1	0.96	0.20	52,52,52,52	0
4	CL	M	12	1/1	0.97	0.16	39,39,39,39	0
4	CL	N	13	1/1	0.97	0.15	66,66,66,66	0
2	GOL	R	9	6/6	0.97	0.22	28,29,31,33	0
4	CL	R	14	1/1	0.98	0.11	54,54,54,54	0
4	CL	H	6	1/1	0.98	0.15	44,44,44,44	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

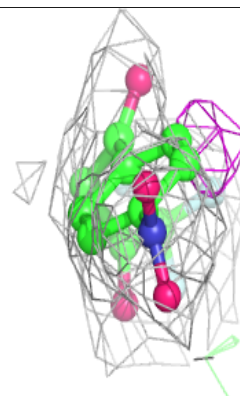
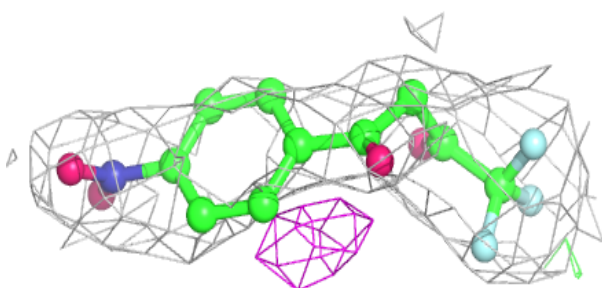
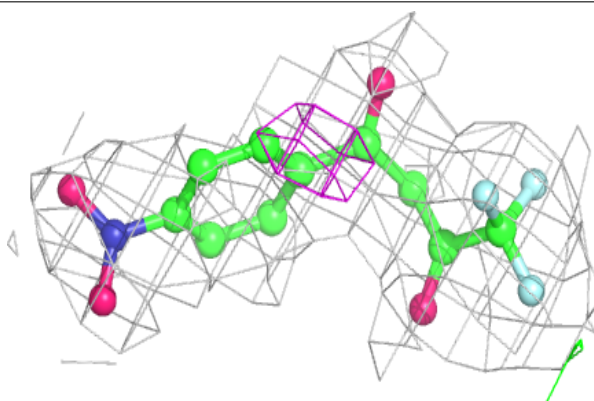


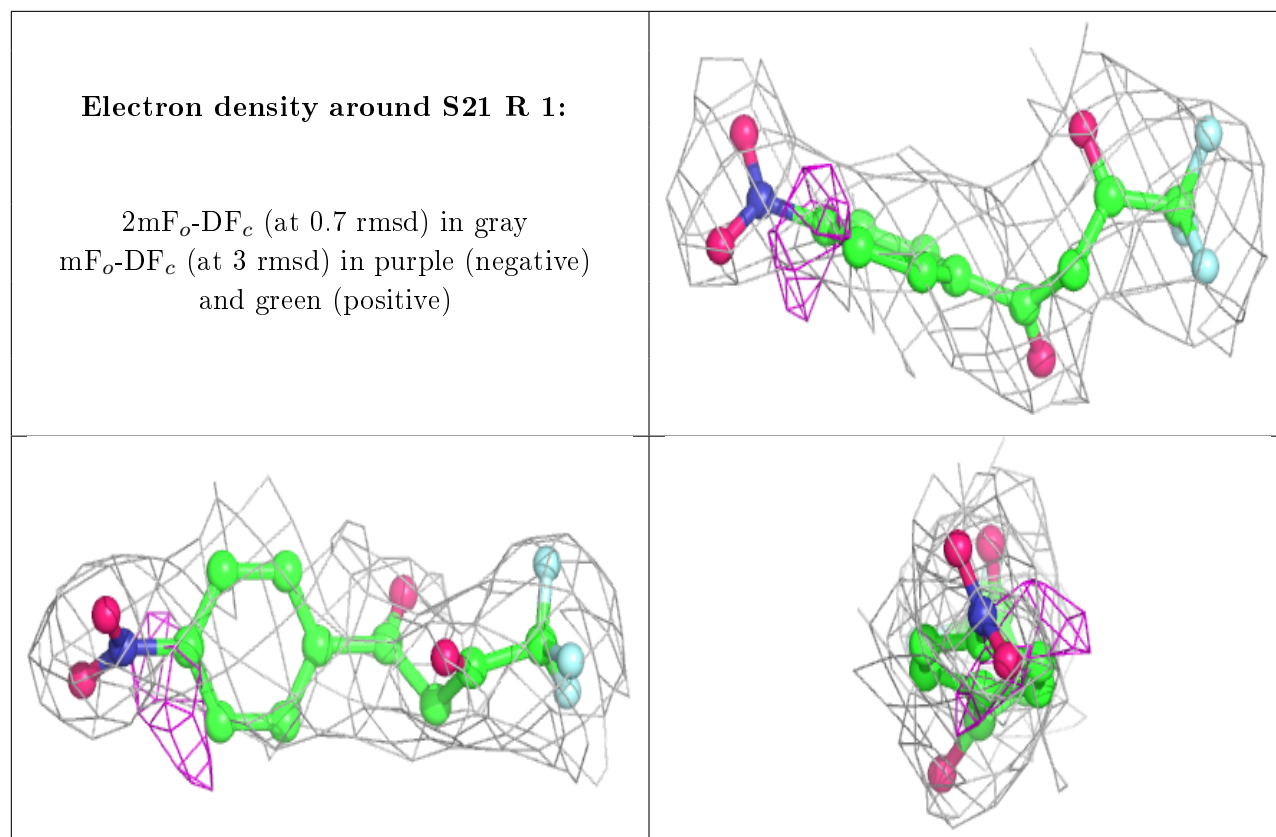
**Electron density around S21 P 4:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around S21 D 231:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.