



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:31 AM UTC

PDB ID : 3AZ9 / pdb_00003az9
Title : Beta-Hydroxyacyl-Acyl Carrier Protein Dehydratase (FabZ) from Plasmodium falciparum in complex with NAS91
Authors : Maity, K.; Venkata, B.S.; Kapoor, N.; Surolia, N.; Surolia, A.; Suguna, K.
Deposited on : 2011-05-21
Resolution : 2.75 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

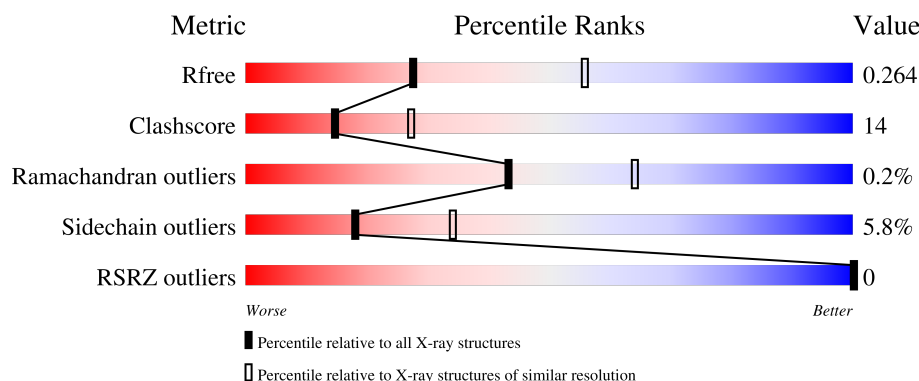
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

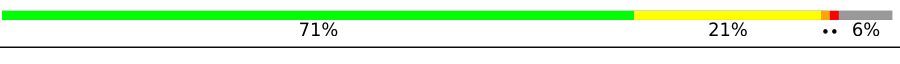
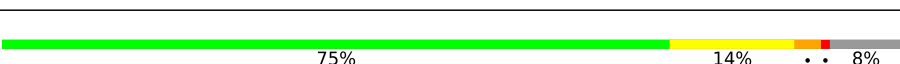
The reported resolution of this entry is 2.75 Å.

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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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 $\leq 5\%$. 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	
1	B	154	
1	C	154	
1	D	154	
1	E	154	

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Mol	Chain	Length	Quality of chain
1	F	154	
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
2	GOL	H	4	-	-	X	-
4	K91	C	2	-	-	X	-
4	K91	D	1	-	-	X	-
4	K91	E	3	-	-	X	-
4	K91	M	4	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	K91	N	5	-	-	X	-
4	K91	O	6	-	-	X	-
4	K91	P	7	-	-	X	-
4	K91	Q	8	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27414 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	146	Total	C	N	O	S	0	0	0
			1125	732	184	204	5			
1	B	145	Total	C	N	O	S	0	0	0
			1114	724	184	201	5			
1	C	144	Total	C	N	O	S	0	0	0
			1116	727	184	200	5			
1	D	144	Total	C	N	O	S	0	0	0
			1104	716	181	202	5			
1	E	142	Total	C	N	O	S	0	0	0
			1103	719	181	198	5			
1	F	146	Total	C	N	O	S	0	0	0
			1127	731	186	205	5			
1	G	147	Total	C	N	O	S	0	0	0
			1130	735	185	205	5			
1	H	145	Total	C	N	O	S	0	0	0
			1115	724	184	202	5			
1	I	144	Total	C	N	O	S	0	0	0
			1116	727	184	200	5			
1	J	144	Total	C	N	O	S	0	0	0
			1099	713	180	201	5			
1	K	142	Total	C	N	O	S	0	0	0
			1100	716	181	198	5			
1	L	146	Total	C	N	O	S	0	0	0
			1123	728	185	205	5			
1	M	146	Total	C	N	O	S	0	0	0
			1125	732	184	204	5			
1	N	145	Total	C	N	O	S	0	0	0
			1115	724	184	202	5			
1	O	144	Total	C	N	O	S	0	0	0
			1116	727	184	200	5			
1	P	144	Total	C	N	O	S	0	0	0
			1103	717	180	201	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	142	Total	C	N	O	S	0	0	0
			1097	713	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	0	0
			1125	732	184	204	5			
1	T	145	Total	C	N	O	S	0	0	0
			1118	727	184	202	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
			1103	717	180	201	5			
1	W	145	Total	C	N	O	S	0	0	0
			1120	728	184	203	5			
1	X	142	Total	C	N	O	S	0	0	0
			1098	714	182	197	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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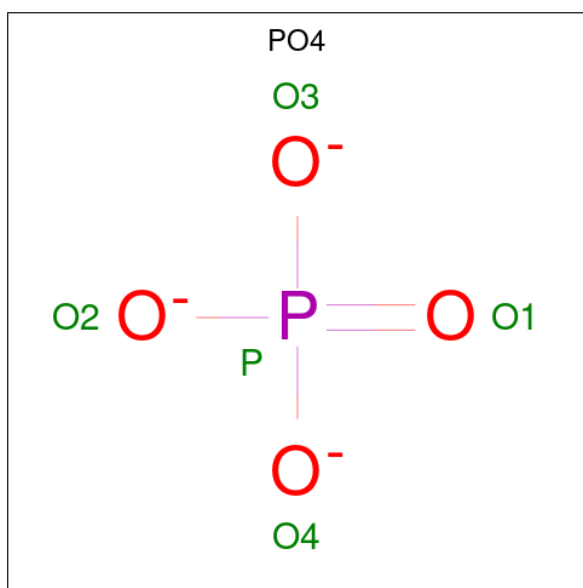
Chain	Residue	Modelled	Actual	Comment	Reference
Q	78	SER	-	expression tag	UNP Q965D7
Q	79	HIS	-	expression tag	UNP Q965D7
Q	80	MET	-	expression tag	UNP Q965D7
R	77	GLY	-	expression tag	UNP Q965D7
R	78	SER	-	expression tag	UNP Q965D7
R	79	HIS	-	expression tag	UNP Q965D7
R	80	MET	-	expression tag	UNP Q965D7
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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



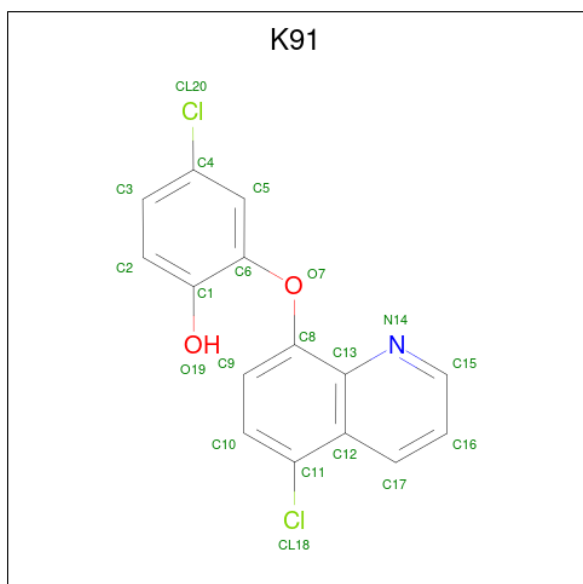
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		
2	L	1	Total	C	O	0	0
			6	3	3		
2	N	1	Total	C	O	0	0
			6	3	3		
2	P	1	Total	C	O	0	0
			6	3	3		
2	P	1	Total	C	O	0	0
			6	3	3		
2	Q	1	Total	C	O	0	0
			6	3	3		
2	S	1	Total	C	O	0	0
			6	3	3		
2	V	1	Total	C	O	0	0
			6	3	3		
2	W	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 4 is 4-chloro-2-[(5-chloroquinolin-8-yl)oxy]phenol (CCD ID: K91) (formula: C₁₅H₉Cl₂NO₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	Cl	N	O	0	0
			20	15	2	1	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total 20	C 15	Cl 2	N 1	O 2	0	0
4	E	1	Total 20	C 15	Cl 2	N 1	O 2	0	0
4	M	1	Total 20	C 15	Cl 2	N 1	O 2	0	0
4	N	1	Total 20	C 15	Cl 2	N 1	O 2	0	0
4	O	1	Total 20	C 15	Cl 2	N 1	O 2	0	0
4	P	1	Total 20	C 15	Cl 2	N 1	O 2	0	0
4	Q	1	Total 20	C 15	Cl 2	N 1	O 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	13	Total 13	O 13	0	0
5	B	17	Total 17	O 17	0	0
5	C	13	Total 13	O 13	0	0
5	D	15	Total 15	O 15	0	0
5	E	27	Total 27	O 27	0	0
5	F	29	Total 29	O 29	0	0
5	G	17	Total 17	O 17	0	0
5	H	18	Total 18	O 18	0	0
5	I	17	Total 17	O 17	0	0
5	J	15	Total 15	O 15	0	0
5	K	17	Total 17	O 17	0	0
5	L	23	Total 23	O 23	0	0

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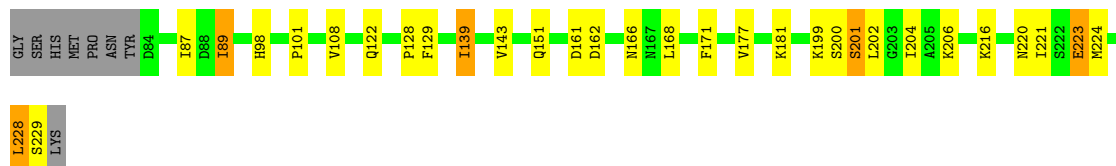
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	10	Total 10	O 10	0	0
5	N	23	Total 23	O 23	0	0
5	O	31	Total 31	O 31	0	0
5	P	9	Total 9	O 9	0	0
5	Q	15	Total 15	O 15	0	0
5	R	15	Total 15	O 15	0	0
5	S	13	Total 13	O 13	0	0
5	T	20	Total 20	O 20	0	0
5	U	14	Total 14	O 14	0	0
5	V	17	Total 17	O 17	0	0
5	W	20	Total 20	O 20	0	0
5	X	22	Total 22	O 22	0	0

3 Residue-property plots

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.

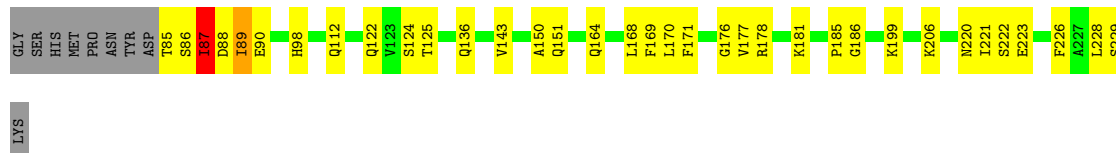
• Molecule 1: Beta-hydroxyacyl-ACP dehydratase

Chain A: 



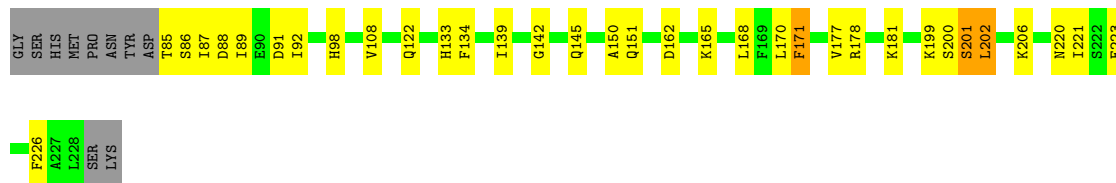
• Molecule 1: Beta-hydroxyacyl-ACP dehydratase

Chain B: 



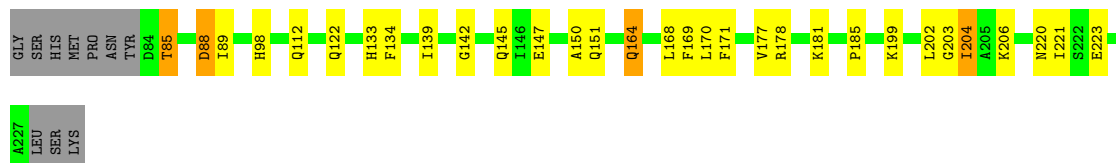
• Molecule 1: Beta-hydroxyacyl-ACP dehydratase

Chain C: 



• Molecule 1: Beta-hydroxyacyl-ACP dehydratase

Chain D: 



- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

Chain E:  75% 14% 8%



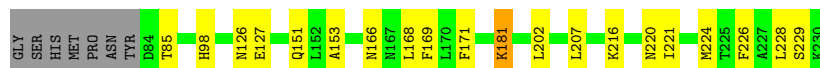
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

Chain F:  75% 18% 5%



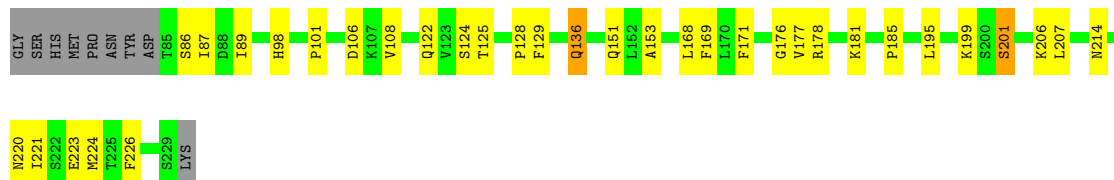
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

Chain G:  82% 12% 5%



- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

Chain H:  72% 21% 6%



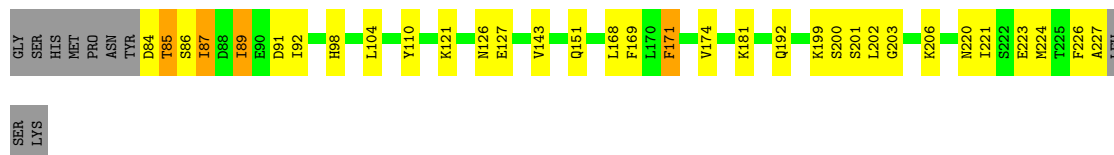
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

Chain I:  78% 15% 6%



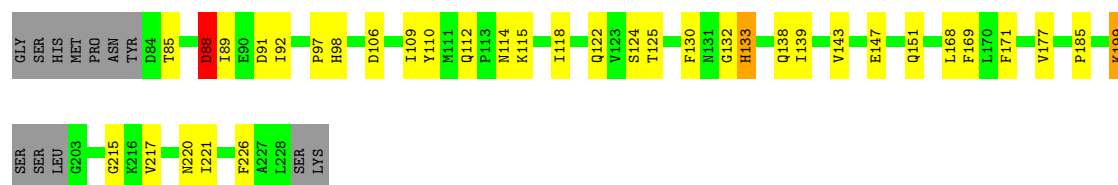
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

Chain J:  72% 19% 6%



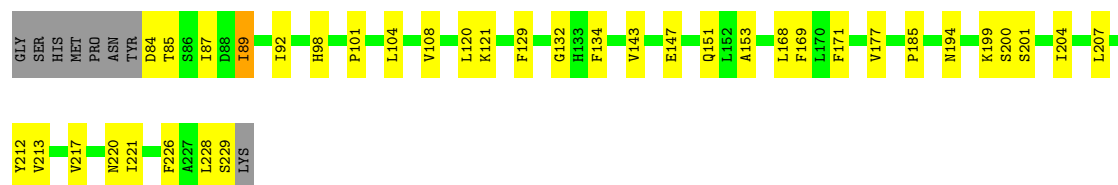
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

Chain K: 



• Molecule 1: Beta-hydroxyacyl-ACP dehydratase

Chain L: 



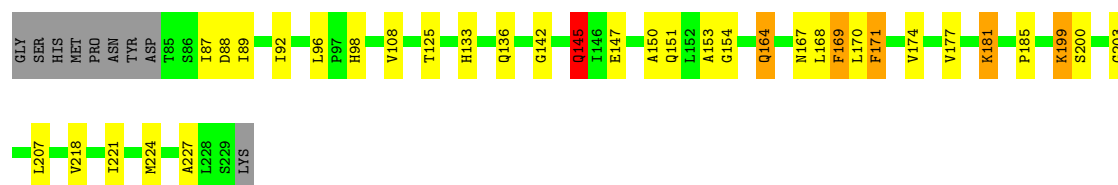
• Molecule 1: Beta-hydroxyacyl-ACP dehydratase

Chain M: 



• Molecule 1: Beta-hydroxyacyl-ACP dehydratase

Chain N: 



• Molecule 1: Beta-hydroxyacyl-ACP dehydratase

Chain O: 



• Molecule 1: Beta-hydroxyacyl-ACP dehydratase

Chain P: 



- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

Chain Q:  76% 14% 8%



- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

Chain R:  80% 14% 5%



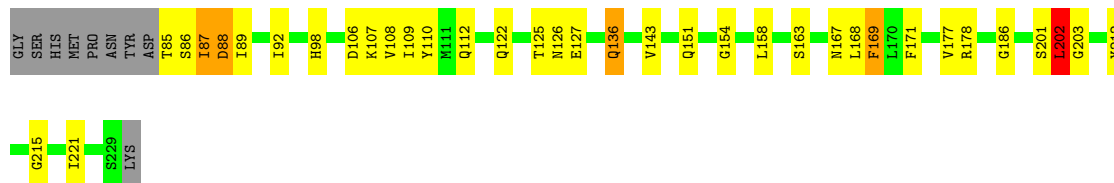
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

Chain S:  79% 13% 5%



- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

Chain T:  71% 20% 6%



- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

Chain U:  79% 12% 6%



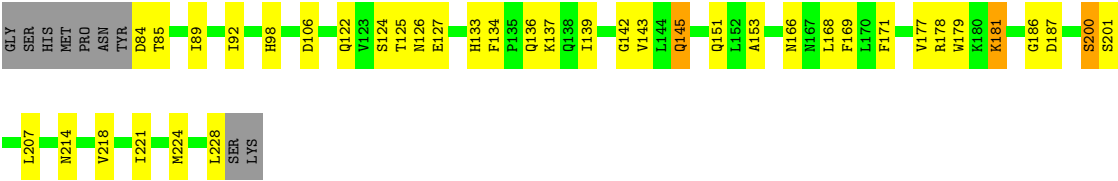
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

Chain V:  79% 13% 6%

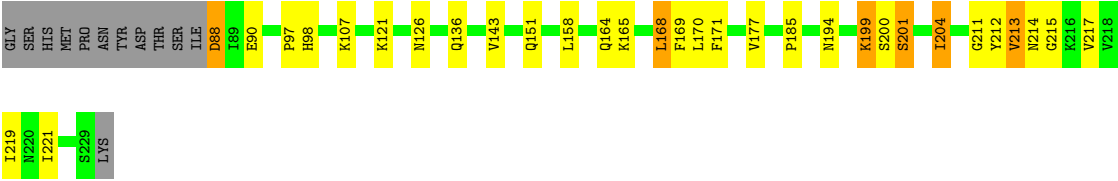


- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

Chain W:  69% 23% 6%



● Molecule 1: Beta-hydroxyacyl-ACP dehydratase



4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	216.68Å 216.68Å 156.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.58 – 2.75 51.58 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (51.58-2.75) 99.9 (51.58-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.234 , 0.282 0.232 , 0.264	Depositor DCC
R_{free} test set	4705 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 25.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.438 for -k,-h,-l	Xtriage
Reported twinning fraction	0.512 for H, K, L 0.488 for -H, K, -L	Depositor
Outliers	0 of 93851 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	27414	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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 29.71 % 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 1.4788e-03.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, GOL, K91

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	0.81	0/1147	0.89	2/1553 (0.1%)
1	B	0.90	1/1136 (0.1%)	0.97	4/1538 (0.3%)
1	C	0.85	0/1138	0.95	1/1539 (0.1%)
1	D	0.82	1/1126 (0.1%)	0.98	3/1527 (0.2%)
1	E	0.81	0/1124	0.97	3/1520 (0.2%)
1	F	0.77	0/1149	0.96	2/1554 (0.1%)
1	G	0.83	0/1152	0.90	0/1560
1	H	0.85	0/1137	0.92	1/1539 (0.1%)
1	I	0.84	0/1138	0.95	1/1539 (0.1%)
1	J	0.78	0/1121	0.95	2/1520 (0.1%)
1	K	0.86	1/1121 (0.1%)	0.95	1/1516 (0.1%)
1	L	0.92	1/1145 (0.1%)	0.96	2/1550 (0.1%)
1	M	0.83	2/1147 (0.2%)	0.88	0/1553
1	N	0.78	0/1137	0.90	3/1539 (0.2%)
1	O	0.79	0/1138	0.92	1/1539 (0.1%)
1	P	0.80	0/1125	0.95	1/1526 (0.1%)
1	Q	0.77	0/1117	0.93	1/1511 (0.1%)
1	R	0.80	0/1149	0.91	0/1554
1	S	0.78	0/1147	0.94	3/1553 (0.2%)
1	T	0.84	0/1140	0.98	2/1543 (0.1%)
1	U	0.77	0/1138	0.95	3/1539 (0.2%)
1	V	0.78	0/1125	0.86	1/1526 (0.1%)
1	W	0.85	0/1142	0.94	0/1546
1	X	0.83	0/1120	0.92	0/1514
All	All	0.82	6/27259 (0.0%)	0.93	37/36898 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	85	THR	CA-CB	8.37	1.62	1.53
1	L	204	ILE	CA-CB	8.33	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	145	GLN	CD-NE2	-6.73	1.19	1.33
1	M	85	THR	CA-CB	5.78	1.63	1.53
1	K	133	HIS	CA-CB	5.43	1.57	1.53
1	B	89	ILE	N-CA	5.36	1.52	1.46

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	85	THR	N-CA-C	-10.64	96.19	110.55
1	J	85	THR	N-CA-C	-9.70	102.06	113.21
1	C	202	LEU	N-CA-C	-9.65	101.06	113.12
1	O	202	LEU	N-CA-C	-8.91	102.42	113.38
1	I	89	ILE	N-CA-C	8.81	119.61	110.72
1	U	202	LEU	N-CA-C	-8.22	102.14	114.64
1	P	86	SER	N-CA-C	8.18	120.47	110.41
1	B	87	ILE	N-CA-C	7.91	118.19	108.06
1	E	170	LEU	N-CA-C	7.81	121.83	110.28
1	S	89	ILE	N-CA-C	7.54	118.31	110.62
1	F	202	LEU	N-CA-C	-6.79	103.70	113.21
1	U	201	SER	N-CA-C	6.69	118.30	110.41
1	B	89	ILE	N-CA-C	6.46	117.99	110.62
1	D	203	GLY	N-CA-C	-6.12	106.51	115.63
1	N	200	SER	N-CA-C	6.11	123.80	110.80
1	D	199	LYS	N-CA-C	6.10	118.63	108.20
1	T	202	LEU	N-CA-C	-6.02	103.18	110.88
1	J	89	ILE	N-CA-C	5.90	116.64	110.62
1	F	86	SER	N-CA-C	-5.88	103.18	110.41
1	N	89	ILE	N-CA-C	5.76	117.28	111.00
1	U	200	SER	N-CA-C	5.68	122.91	110.80
1	A	89	ILE	N-CA-C	5.64	118.10	111.05
1	K	88	ASP	N-CA-C	5.56	117.09	110.19
1	B	88	ASP	CA-C-N	5.54	128.34	120.53
1	B	88	ASP	C-N-CA	5.54	128.34	120.53
1	S	203	GLY	N-CA-C	-5.53	107.37	115.72
1	S	204	ILE	N-CA-C	5.51	115.25	106.88
1	L	120	LEU	N-CA-C	5.50	117.76	109.23
1	E	169	PHE	CB-CA-C	-5.48	101.86	110.79
1	D	89	ILE	N-CA-C	5.40	116.03	110.36
1	T	136	GLN	CB-CG-CD	5.37	121.72	112.60
1	H	136	GLN	CB-CG-CD	5.32	121.64	112.60
1	V	204	ILE	N-CA-C	5.24	114.29	106.85
1	N	145	GLN	N-CA-C	-5.24	105.49	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	89	ILE	N-CA-C	5.21	119.39	111.89
1	A	223	GLU	N-CA-C	5.15	116.98	108.13
1	E	169	PHE	N-CA-C	5.01	116.85	107.99

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	1125	0	1165	28	0
1	B	1114	0	1146	35	0
1	C	1116	0	1164	46	0
1	D	1104	0	1124	46	0
1	E	1103	0	1144	37	0
1	F	1127	0	1164	28	0
1	G	1130	0	1167	15	0
1	H	1115	0	1149	35	0
1	I	1116	0	1164	16	0
1	J	1099	0	1117	24	0
1	K	1100	0	1135	93	0
1	L	1123	0	1153	21	0
1	M	1125	0	1165	44	0
1	N	1115	0	1149	66	0
1	O	1116	0	1164	33	0
1	P	1103	0	1127	43	0
1	Q	1097	0	1137	36	0
1	R	1127	0	1164	22	0
1	S	1125	0	1165	28	0
1	T	1118	0	1158	91	0
1	U	1116	0	1164	15	0
1	V	1103	0	1127	20	0
1	W	1120	0	1157	55	0
1	X	1098	0	1137	30	0
2	B	6	0	8	3	0
2	D	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	6	0	8	1	0
2	H	6	0	8	4	0
2	J	12	0	16	2	0
2	L	6	0	8	2	0
2	N	6	0	8	0	0
2	P	12	0	16	4	0
2	Q	6	0	8	3	0
2	S	6	0	8	1	0
2	V	6	0	8	1	0
2	W	6	0	8	0	0
3	B	5	0	0	0	0
4	C	20	0	9	30	0
4	D	20	0	8	33	0
4	E	20	0	8	32	0
4	M	20	0	9	26	0
4	N	20	0	9	37	0
4	O	20	0	8	31	0
4	P	20	0	8	25	0
4	Q	20	0	8	29	0
5	A	13	0	0	1	0
5	B	17	0	0	3	0
5	C	13	0	0	2	0
5	D	15	0	0	2	0
5	E	27	0	0	0	0
5	F	29	0	0	1	0
5	G	17	0	0	0	0
5	H	18	0	0	1	0
5	I	17	0	0	0	0
5	J	15	0	0	0	0
5	K	17	0	0	0	0
5	L	23	0	0	2	0
5	M	10	0	0	0	0
5	N	23	0	0	1	0
5	O	31	0	0	0	0
5	P	9	0	0	0	0
5	Q	15	0	0	0	0
5	R	15	0	0	0	0
5	S	13	0	0	2	0
5	T	20	0	0	0	0
5	U	14	0	0	1	0
5	V	17	0	0	2	0
5	W	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	X	22	0	0	4	0
All	All	27414	0	27785	760	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 14.

All (760) 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:K:109:ILE:HB	1:T:110:TYR:CD1	1.38	1.57
1:C:150:ALA:CB	4:C:2:K91:H16	1.32	1.55
1:O:150:ALA:CB	4:O:6:K91:H16	1.40	1.50
1:N:150:ALA:CB	4:N:5:K91:H16	1.46	1.40
1:M:150:ALA:CB	4:M:4:K91:H16	1.51	1.39
1:B:112:GLN:NE2	1:T:163:SER:HB3	1.39	1.34
1:Q:150:ALA:CB	4:Q:8:K91:H16	1.57	1.33
1:K:115:LYS:CD	1:W:214:ASN:HD21	1.43	1.32
1:K:109:ILE:HD12	1:T:110:TYR:CG	1.65	1.30
1:K:118:ILE:HD11	1:T:109:ILE:CD1	1.62	1.29
1:C:150:ALA:HB1	4:C:2:K91:C16	1.61	1.29
1:K:109:ILE:HD12	1:T:110:TYR:CD2	1.67	1.29
1:K:118:ILE:CD1	1:T:109:ILE:HD12	1.63	1.27
1:K:115:LYS:HB2	1:W:214:ASN:ND2	1.50	1.26
1:K:115:LYS:HD2	1:W:214:ASN:ND2	1.52	1.24
1:T:158:LEU:HD11	1:T:169:PHE:CE2	1.72	1.23
1:K:114:ASN:O	1:W:214:ASN:HB3	1.32	1.22
4:C:2:K91:C2	1:D:142:GLY:H	1.54	1.21
1:E:150:ALA:CB	4:E:3:K91:H16	1.70	1.21
1:D:150:ALA:CB	4:D:1:K91:H16	1.70	1.20
4:Q:8:K91:H2	1:R:142:GLY:HA3	1.21	1.20
1:C:170:LEU:HD22	4:C:2:K91:CL20	1.79	1.19
4:O:6:K91:C2	1:P:142:GLY:H	1.56	1.18
1:O:142:GLY:HA3	4:P:7:K91:C2	1.75	1.16
1:P:150:ALA:CB	4:P:7:K91:H16	1.73	1.16
1:K:109:ILE:CB	1:T:110:TYR:CD1	2.29	1.16
1:C:150:ALA:CB	4:C:2:K91:C16	2.21	1.15
1:M:142:GLY:HA3	4:N:5:K91:H2	1.19	1.15
1:N:169:PHE:CE1	4:N:5:K91:CL18	2.37	1.15
1:E:170:LEU:HD22	4:E:3:K91:H5	1.21	1.14
1:K:110:TYR:CD1	1:T:86:SER:HB2	1.83	1.13
1:C:142:GLY:H	4:D:1:K91:C2	1.62	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:150:ALA:HB1	4:N:5:K91:H16	1.28	1.11
1:E:171:PHE:CD2	4:E:3:K91:H15	1.83	1.11
1:M:142:GLY:H	4:N:5:K91:C2	1.64	1.11
1:O:142:GLY:CA	4:P:7:K91:H2	1.79	1.10
4:Q:8:K91:C2	1:R:142:GLY:H	1.63	1.09
1:C:142:GLY:HA3	4:D:1:K91:H2	1.27	1.09
1:O:150:ALA:HB1	4:O:6:K91:C16	1.81	1.09
1:Q:150:ALA:HB3	4:Q:8:K91:C16	1.83	1.08
1:K:109:ILE:HB	1:T:110:TYR:CE1	1.89	1.07
1:N:150:ALA:HB3	4:N:5:K91:H16	1.15	1.07
4:Q:8:K91:H2	1:R:142:GLY:CA	1.84	1.07
1:O:142:GLY:H	4:P:7:K91:C2	1.68	1.06
1:M:142:GLY:CA	4:N:5:K91:H2	1.86	1.06
1:D:170:LEU:HD22	4:D:1:K91:H5	1.35	1.06
1:K:110:TYR:HB2	1:T:109:ILE:O	1.55	1.06
1:E:150:ALA:HB1	4:E:3:K91:C16	1.86	1.05
4:E:3:K91:H2	1:F:142:GLY:HA3	1.31	1.05
1:N:154:GLY:HA3	1:N:169:PHE:HE1	1.10	1.05
1:P:150:ALA:HB3	4:P:7:K91:H16	1.32	1.05
1:E:171:PHE:CD2	4:E:3:K91:C15	2.40	1.05
1:M:150:ALA:HB3	4:M:4:K91:H16	1.07	1.05
1:K:115:LYS:HG3	1:W:214:ASN:OD1	1.57	1.04
1:O:142:GLY:HA3	4:P:7:K91:H2	1.05	1.04
1:N:96:LEU:CD2	1:N:169:PHE:HZ	1.70	1.04
4:E:3:K91:H9	1:F:134:PHE:HZ	1.18	1.03
1:O:150:ALA:HB3	4:O:6:K91:H16	1.32	1.03
1:K:109:ILE:CG2	1:T:110:TYR:CE1	2.41	1.02
1:M:150:ALA:HB1	4:M:4:K91:H16	1.41	1.02
1:Q:150:ALA:CB	4:Q:8:K91:C16	2.38	1.02
4:O:6:K91:C2	1:P:142:GLY:N	2.22	1.01
1:Q:170:LEU:HD22	4:Q:8:K91:H5	1.37	1.01
1:T:158:LEU:HD11	1:T:169:PHE:CZ	1.94	1.01
4:C:2:K91:C2	1:D:142:GLY:N	2.23	1.01
1:K:115:LYS:NZ	1:W:187:ASP:HA	1.75	1.01
1:M:150:ALA:CB	4:M:4:K91:C16	2.39	1.01
1:K:115:LYS:CB	1:W:214:ASN:ND2	2.23	1.00
4:E:3:K91:C2	1:F:142:GLY:H	1.75	1.00
1:K:115:LYS:HZ3	1:W:187:ASP:HA	1.25	1.00
1:K:217:VAL:HG21	1:T:215:GLY:O	1.59	0.99
1:O:142:GLY:N	4:P:7:K91:C2	2.24	0.99
1:N:150:ALA:CB	4:N:5:K91:C16	2.41	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:142:GLY:CA	4:P:7:K91:C2	2.36	0.99
1:D:150:ALA:HB3	4:D:1:K91:H16	1.01	0.99
1:O:150:ALA:HB1	4:O:6:K91:H16	1.00	0.98
1:T:158:LEU:HD11	1:T:169:PHE:HE2	1.26	0.98
1:C:142:GLY:CA	4:D:1:K91:H2	1.92	0.98
1:H:214:ASN:HD21	1:T:112:GLN:NE2	1.62	0.97
4:M:4:K91:C2	1:N:142:GLY:H	1.77	0.97
1:P:170:LEU:HD22	4:P:7:K91:H5	1.45	0.97
1:C:142:GLY:N	4:D:1:K91:C2	2.25	0.97
1:O:150:ALA:CB	4:O:6:K91:C16	2.36	0.97
1:B:112:GLN:NE2	1:T:163:SER:CB	2.26	0.97
1:N:154:GLY:HA3	1:N:169:PHE:CE1	1.99	0.96
1:A:202:LEU:HD13	1:A:204:ILE:HD12	1.45	0.96
1:K:110:TYR:CD1	1:T:86:SER:CB	2.47	0.96
1:C:142:GLY:HA3	4:D:1:K91:C2	1.95	0.96
4:C:2:K91:H2	1:D:142:GLY:HA3	1.47	0.96
1:K:110:TYR:HD1	1:T:86:SER:CB	1.78	0.96
1:E:150:ALA:HB1	4:E:3:K91:H16	0.96	0.95
1:K:110:TYR:CD2	1:T:109:ILE:HB	2.02	0.95
1:N:169:PHE:CD1	4:N:5:K91:CL18	2.56	0.95
1:E:170:LEU:CD2	4:E:3:K91:H5	1.96	0.94
1:N:170:LEU:HD13	4:N:5:K91:CL20	2.05	0.94
1:N:170:LEU:HD22	4:N:5:K91:H5	1.48	0.94
1:M:150:ALA:HB1	4:M:4:K91:C16	1.96	0.93
4:E:3:K91:H9	1:F:134:PHE:CZ	2.03	0.93
1:Q:170:LEU:CD2	4:Q:8:K91:H5	1.98	0.93
1:C:150:ALA:HB3	4:C:2:K91:H16	1.49	0.93
1:N:169:PHE:HD2	1:N:169:PHE:N	1.66	0.93
1:E:170:LEU:HD13	4:E:3:K91:CL20	2.06	0.93
1:M:142:GLY:N	4:N:5:K91:C2	2.32	0.92
4:Q:8:K91:C2	1:R:142:GLY:N	2.31	0.92
1:T:98:HIS:CD2	1:T:151:GLN:HE21	1.87	0.92
4:E:3:K91:H2	1:F:142:GLY:CA	2.00	0.92
4:M:4:K91:C2	1:N:142:GLY:N	2.33	0.92
1:K:109:ILE:CB	1:T:110:TYR:CE1	2.51	0.91
1:S:202:LEU:HD23	1:S:202:LEU:N	1.86	0.91
4:C:2:K91:H2	1:D:142:GLY:CA	2.00	0.91
1:P:150:ALA:HB1	4:P:7:K91:H16	1.53	0.90
1:N:169:PHE:HD2	1:N:169:PHE:H	0.92	0.90
1:H:214:ASN:HD21	1:T:112:GLN:HE21	1.15	0.90
1:S:202:LEU:HD23	1:S:202:LEU:H	1.35	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:115:LYS:HD2	1:W:214:ASN:HD21	0.73	0.90
1:C:142:GLY:CA	4:D:1:K91:C2	2.50	0.90
1:B:112:GLN:HE21	1:T:163:SER:HB3	1.34	0.89
1:X:98:HIS:CD2	1:X:151:GLN:HE21	1.90	0.89
1:K:109:ILE:CD1	1:T:110:TYR:CG	2.56	0.89
1:E:169:PHE:O	4:E:3:K91:C10	2.20	0.89
1:K:109:ILE:HB	1:T:110:TYR:HD1	1.26	0.89
4:M:4:K91:H2	1:N:142:GLY:HA3	1.52	0.89
1:M:134:PHE:HZ	4:N:5:K91:H9	1.38	0.89
4:M:4:K91:C2	1:N:142:GLY:HA3	2.03	0.89
1:N:150:ALA:HB3	4:N:5:K91:C16	2.01	0.89
1:J:84:ASP:HB3	1:P:84:ASP:O	1.72	0.89
4:Q:8:K91:C2	1:R:142:GLY:HA3	2.01	0.89
1:K:109:ILE:HG21	1:T:110:TYR:CE1	2.09	0.88
1:K:118:ILE:CD1	1:T:109:ILE:CD1	2.36	0.88
1:O:142:GLY:H	4:P:7:K91:C1	1.86	0.88
4:M:4:K91:H2	1:N:142:GLY:CA	2.04	0.87
1:D:170:LEU:CD2	4:D:1:K91:H5	2.05	0.87
1:Q:150:ALA:HB3	4:Q:8:K91:H16	0.87	0.87
1:D:150:ALA:HB3	4:D:1:K91:C16	1.98	0.86
1:K:109:ILE:CD1	1:T:110:TYR:CD2	2.56	0.86
1:N:150:ALA:HB1	4:N:5:K91:C16	2.01	0.86
1:K:115:LYS:CB	1:W:214:ASN:CG	2.49	0.86
1:X:98:HIS:CD2	1:X:151:GLN:NE2	2.44	0.86
4:E:3:K91:C9	1:F:134:PHE:HZ	1.89	0.85
4:O:6:K91:H2	1:P:142:GLY:CA	2.06	0.85
1:T:158:LEU:CD1	1:T:169:PHE:CZ	2.58	0.85
1:M:150:ALA:HB3	4:M:4:K91:C16	2.02	0.85
1:H:214:ASN:ND2	1:T:112:GLN:HE21	1.75	0.85
1:B:176:GLY:HA3	1:H:178:ARG:HH12	1.41	0.84
4:Q:8:K91:C2	1:R:142:GLY:CA	2.55	0.84
1:Q:169:PHE:O	4:Q:8:K91:C10	2.26	0.83
1:X:211:GLY:O	1:X:212:TYR:CG	2.30	0.83
1:M:142:GLY:H	4:N:5:K91:C1	1.91	0.83
1:D:169:PHE:O	4:D:1:K91:C10	2.27	0.83
1:B:98:HIS:CD2	1:B:151:GLN:HE21	1.96	0.83
1:N:154:GLY:CA	1:N:169:PHE:HE1	1.91	0.83
1:M:98:HIS:CD2	1:M:151:GLN:HE21	1.97	0.82
1:E:170:LEU:HD22	4:E:3:K91:C5	2.06	0.82
4:M:4:K91:C2	1:N:142:GLY:CA	2.57	0.82
1:H:214:ASN:ND2	1:T:112:GLN:NE2	2.26	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:170:LEU:CD2	4:N:5:K91:H5	2.08	0.82
1:D:147:GLU:OE1	4:D:1:K91:C15	2.28	0.81
1:D:150:ALA:CB	4:D:1:K91:C16	2.55	0.81
1:T:158:LEU:CD1	1:T:169:PHE:CE2	2.60	0.80
4:E:3:K91:C2	1:F:142:GLY:N	2.44	0.80
4:O:6:K91:H2	1:P:142:GLY:HA3	1.62	0.80
1:K:110:TYR:CB	1:T:109:ILE:O	2.30	0.80
1:O:170:LEU:HD22	4:O:6:K91:H5	1.62	0.80
1:M:147:GLU:OE1	4:M:4:K91:C15	2.30	0.80
4:C:2:K91:H9	1:D:134:PHE:HZ	1.46	0.80
1:Q:170:LEU:HB3	4:Q:8:K91:CL20	2.19	0.80
1:K:115:LYS:CG	1:W:214:ASN:HD21	1.94	0.80
1:P:169:PHE:O	4:P:7:K91:H10	1.80	0.80
1:T:98:HIS:CD2	1:T:151:GLN:NE2	2.49	0.80
1:N:96:LEU:HD23	1:N:169:PHE:HZ	1.47	0.80
4:O:6:K91:C2	1:P:142:GLY:CA	2.59	0.80
1:K:115:LYS:CG	1:W:214:ASN:ND2	2.45	0.79
1:K:115:LYS:CG	1:W:214:ASN:OD1	2.29	0.79
1:D:204:ILE:HD11	1:D:206:LYS:HE3	1.64	0.79
1:K:115:LYS:HB2	1:W:214:ASN:CG	2.07	0.79
1:C:150:ALA:HB3	4:C:2:K91:C16	2.06	0.79
1:N:96:LEU:CD2	1:N:169:PHE:CZ	2.62	0.79
1:X:212:TYR:CE2	1:X:217:VAL:HG22	2.17	0.79
1:M:142:GLY:CA	4:N:5:K91:C2	2.61	0.78
1:Q:170:LEU:HD22	4:Q:8:K91:C5	2.13	0.78
1:Q:169:PHE:O	4:Q:8:K91:H10	1.83	0.78
1:J:84:ASP:C	1:J:86:SER:H	1.91	0.78
4:O:6:K91:C2	1:P:142:GLY:HA3	2.13	0.78
1:M:166:ASN:O	1:M:228:LEU:HD21	1.83	0.77
1:T:127:GLU:HG2	1:W:126:ASN:O	1.84	0.77
1:E:170:LEU:HB3	4:E:3:K91:CL20	2.20	0.77
1:D:170:LEU:HD22	4:D:1:K91:C5	2.12	0.77
1:D:170:LEU:HD13	4:D:1:K91:CL20	2.21	0.77
1:Q:147:GLU:OE1	4:Q:8:K91:H15	1.84	0.77
4:Q:8:K91:C1	1:R:142:GLY:H	1.97	0.77
1:K:110:TYR:CE2	1:T:109:ILE:HG22	2.18	0.77
1:Q:147:GLU:OE1	4:Q:8:K91:C15	2.33	0.77
1:Q:150:ALA:HB1	4:Q:8:K91:C16	2.14	0.77
1:E:150:ALA:CB	4:E:3:K91:C16	2.56	0.77
1:E:171:PHE:HD2	4:E:3:K91:H15	1.45	0.76
1:B:112:GLN:HE22	1:T:163:SER:HB3	1.45	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:GLU:OE1	4:D:1:K91:H15	1.85	0.76
1:M:147:GLU:OE1	4:M:4:K91:H15	1.85	0.76
1:B:98:HIS:CD2	1:B:151:GLN:NE2	2.54	0.76
1:M:169:PHE:CE2	1:M:228:LEU:HD23	2.20	0.75
4:E:3:K91:C2	1:F:142:GLY:HA3	2.15	0.75
1:V:201:SER:O	1:V:202:LEU:HB2	1.86	0.75
1:E:171:PHE:CE2	4:E:3:K91:H15	2.20	0.75
1:E:199:LYS:HG3	1:E:199:LYS:O	1.86	0.75
1:Q:87:ILE:HB	1:Q:108:VAL:HB	1.67	0.75
1:C:171:PHE:CD2	4:C:2:K91:C15	2.70	0.74
1:W:166:ASN:HB3	1:W:228:LEU:HD22	1.69	0.74
1:K:114:ASN:C	1:W:214:ASN:HB3	2.11	0.74
1:K:118:ILE:HD11	1:T:109:ILE:HD12	0.81	0.74
1:R:98:HIS:CD2	1:R:151:GLN:HE21	2.06	0.74
1:Q:169:PHE:O	4:Q:8:K91:C9	2.35	0.74
1:N:170:LEU:HD22	4:N:5:K91:C5	2.17	0.74
1:X:204:ILE:O	1:X:204:ILE:HG22	1.88	0.74
1:J:84:ASP:C	1:P:84:ASP:HB3	2.13	0.74
1:S:199:LYS:HB3	1:S:202:LEU:HG	1.69	0.74
1:S:202:LEU:HB2	1:S:204:ILE:HG13	1.70	0.74
4:C:2:K91:C3	1:D:142:GLY:H	2.01	0.74
1:U:98:HIS:CD2	1:U:151:GLN:NE2	2.56	0.74
1:O:169:PHE:O	4:O:6:K91:C10	2.36	0.73
1:B:176:GLY:HA3	1:H:178:ARG:NH1	2.02	0.73
1:I:98:HIS:CD2	1:I:151:GLN:HE21	2.06	0.73
1:C:142:GLY:H	4:D:1:K91:C1	2.00	0.73
1:S:166:ASN:HB3	1:S:228:LEU:HD11	1.70	0.73
1:P:169:PHE:O	4:P:7:K91:C10	2.36	0.73
1:C:170:LEU:CD2	4:C:2:K91:CL20	2.67	0.73
1:K:115:LYS:CG	1:W:214:ASN:CG	2.62	0.73
1:M:170:LEU:HD22	4:M:4:K91:H5	1.70	0.73
4:D:1:K91:O19	4:D:1:K91:N14	2.21	0.73
1:J:199:LYS:C	1:J:201:SER:H	1.97	0.72
1:M:166:ASN:HB3	1:M:228:LEU:HD21	1.70	0.72
1:L:98:HIS:CD2	1:L:151:GLN:HE21	2.06	0.72
1:R:165:LYS:HB2	1:R:165:LYS:NZ	2.03	0.72
1:O:150:ALA:HB3	4:O:6:K91:C16	2.14	0.72
1:Q:98:HIS:CD2	1:Q:151:GLN:HE21	2.07	0.72
1:O:169:PHE:O	4:O:6:K91:H10	1.90	0.72
1:N:169:PHE:CZ	4:N:5:K91:CL18	2.80	0.71
1:K:110:TYR:HD1	1:T:86:SER:HB3	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:98:HIS:CD2	1:W:151:GLN:HE21	2.08	0.71
1:D:145:GLN:NE2	5:D:278:HOH:O	2.20	0.71
1:M:133:HIS:NE2	4:N:5:K91:O7	2.24	0.71
1:Q:203:GLY:O	1:Q:228:LEU:HD12	1.91	0.71
1:S:201:SER:HB2	1:S:202:LEU:HD23	1.71	0.71
1:B:169:PHE:CE2	1:B:228:LEU:CB	2.74	0.71
4:C:2:K91:C2	1:D:142:GLY:CA	2.65	0.71
1:N:98:HIS:CD2	1:N:151:GLN:HE21	2.09	0.71
1:A:122:GLN:HB3	1:D:122:GLN:HB3	1.71	0.71
1:F:98:HIS:CD2	1:F:151:GLN:HE21	2.09	0.71
1:B:178:ARG:HH12	1:H:176:GLY:HA2	1.56	0.71
1:C:150:ALA:HB1	4:C:2:K91:H16	0.71	0.70
1:T:87:ILE:HD12	1:T:108:VAL:HG21	1.72	0.70
1:P:147:GLU:OE1	4:P:7:K91:C15	2.39	0.70
1:W:98:HIS:CD2	1:W:151:GLN:NE2	2.60	0.70
4:M:4:K91:C3	1:N:142:GLY:HA3	2.22	0.70
1:N:170:LEU:HB3	4:N:5:K91:CL20	2.28	0.70
1:K:112:GLN:OE1	1:T:107:LYS:NZ	2.24	0.69
1:N:169:PHE:O	4:N:5:K91:C10	2.40	0.69
1:L:87:ILE:HB	1:L:108:VAL:HB	1.73	0.69
1:F:87:ILE:HB	1:F:108:VAL:HB	1.74	0.69
1:S:98:HIS:CD2	1:S:151:GLN:HE21	2.10	0.69
4:E:3:K91:C1	1:F:142:GLY:H	2.05	0.69
4:O:6:K91:H2	1:P:142:GLY:N	2.08	0.69
1:K:114:ASN:O	1:W:214:ASN:CB	2.27	0.69
1:L:98:HIS:CD2	1:L:151:GLN:NE2	2.61	0.69
1:W:139:ILE:HD13	1:X:170:LEU:HD21	1.75	0.69
1:X:107:LYS:CG	5:X:410:HOH:O	2.40	0.69
1:A:139:ILE:HD13	1:B:170:LEU:HD21	1.73	0.69
1:V:206:LYS:NZ	5:V:293:HOH:O	2.26	0.69
1:X:211:GLY:O	1:X:212:TYR:CD1	2.46	0.69
1:S:202:LEU:CB	1:S:204:ILE:HG13	2.24	0.68
4:C:2:K91:C2	1:D:142:GLY:HA3	2.21	0.68
1:K:109:ILE:HG21	1:T:110:TYR:CZ	2.28	0.68
1:R:165:LYS:HB2	1:R:165:LYS:HZ3	1.58	0.68
1:I:98:HIS:CD2	1:I:151:GLN:NE2	2.62	0.68
1:K:199:LYS:C	1:K:199:LYS:HE3	2.18	0.68
1:S:202:LEU:N	1:S:202:LEU:CD2	2.57	0.68
1:B:178:ARG:HH12	1:H:176:GLY:CA	2.06	0.68
1:C:133:HIS:NE2	4:D:1:K91:O7	2.27	0.68
1:T:167:ASN:O	1:T:169:PHE:CE2	2.47	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:170:LEU:HD22	4:N:5:K91:CL20	2.31	0.67
1:N:171:PHE:CD2	4:N:5:K91:C15	2.77	0.67
1:M:166:ASN:HB3	1:M:228:LEU:HD11	1.76	0.67
4:O:6:K91:C3	1:P:142:GLY:HA3	2.24	0.67
1:N:167:ASN:O	1:N:169:PHE:CD2	2.48	0.67
1:C:170:LEU:HD13	4:C:2:K91:CL20	2.31	0.67
4:E:3:K91:O7	1:F:133:HIS:NE2	2.27	0.67
1:N:125:THR:HG22	1:Q:106:ASP:OD1	1.94	0.67
1:X:194:ASN:ND2	5:X:237:HOH:O	2.27	0.67
1:L:169:PHE:HD1	1:L:226:PHE:HB3	1.58	0.67
1:P:150:ALA:HB1	4:P:7:K91:C16	2.24	0.67
1:S:98:HIS:CD2	1:S:151:GLN:NE2	2.64	0.66
1:S:166:ASN:HB3	1:S:228:LEU:HD21	1.76	0.66
1:M:142:GLY:HA3	4:N:5:K91:C2	2.11	0.66
4:O:6:K91:O7	1:P:133:HIS:NE2	2.27	0.66
1:B:176:GLY:CA	1:H:178:ARG:HH12	2.08	0.66
1:M:134:PHE:CZ	4:N:5:K91:H9	2.27	0.66
1:U:98:HIS:CD2	1:U:151:GLN:HE21	2.13	0.65
1:A:202:LEU:CD1	1:A:204:ILE:HD12	2.26	0.65
1:C:98:HIS:CD2	1:C:151:GLN:HE21	2.13	0.65
1:B:86:SER:O	1:B:87:ILE:HG13	1.96	0.65
4:O:6:K91:H9	1:P:134:PHE:HZ	1.62	0.65
1:U:129:PHE:HB3	2:V:11:GOL:H11	1.78	0.65
1:E:169:PHE:O	4:E:3:K91:C11	2.45	0.65
4:O:6:K91:C3	1:P:142:GLY:H	2.08	0.65
1:V:87:ILE:HB	1:V:108:VAL:HB	1.79	0.64
1:K:147:GLU:HB2	1:L:143:VAL:HG21	1.78	0.64
1:P:192:GLN:NE2	2:P:14:GOL:H31	2.13	0.64
1:D:150:ALA:HB1	4:D:1:K91:H16	1.78	0.64
4:E:3:K91:C2	1:F:142:GLY:CA	2.71	0.64
4:Q:8:K91:N14	4:Q:8:K91:O19	2.30	0.64
1:F:98:HIS:CD2	1:F:151:GLN:NE2	2.66	0.64
1:Q:170:LEU:HD13	4:Q:8:K91:CL20	2.35	0.64
1:F:129:PHE:HB3	2:F:3:GOL:H31	1.80	0.64
1:P:192:GLN:HE22	2:P:14:GOL:H31	1.63	0.63
1:G:166:ASN:HB3	1:G:228:LEU:HD21	1.79	0.63
1:N:169:PHE:N	1:N:169:PHE:CD2	2.42	0.63
1:M:98:HIS:CD2	1:M:151:GLN:NE2	2.67	0.63
1:P:203:GLY:O	1:P:227:ALA:HA	1.99	0.63
4:P:7:K91:N14	4:P:7:K91:O19	2.31	0.63
1:D:202:LEU:CB	1:D:204:ILE:CG2	2.76	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:84:ASP:O	1:P:84:ASP:HB3	1.98	0.63
1:W:181:LYS:HG2	1:W:218:VAL:HG12	1.80	0.63
1:N:96:LEU:HD23	1:N:169:PHE:CZ	2.30	0.62
1:M:134:PHE:HZ	4:N:5:K91:C9	2.09	0.62
1:P:147:GLU:OE1	4:P:7:K91:H15	1.98	0.62
1:C:98:HIS:CD2	1:C:151:GLN:NE2	2.68	0.62
1:T:122:GLN:NE2	1:W:186:GLY:O	2.31	0.62
1:X:107:LYS:HG2	5:X:410:HOH:O	1.97	0.62
1:S:199:LYS:CB	1:S:202:LEU:HG	2.29	0.62
1:F:199:LYS:C	1:F:201:SER:H	2.08	0.62
1:O:98:HIS:CD2	1:O:151:GLN:HE21	2.18	0.62
1:G:98:HIS:CD2	1:G:151:GLN:HE21	2.18	0.62
1:K:110:TYR:CG	1:T:109:ILE:O	2.53	0.62
1:Q:98:HIS:CD2	1:Q:151:GLN:NE2	2.67	0.62
1:T:158:LEU:CD1	1:T:169:PHE:HZ	2.11	0.62
4:Q:8:K91:H2	1:R:142:GLY:N	2.03	0.61
1:C:171:PHE:CD2	4:C:2:K91:H15	2.36	0.61
2:P:14:GOL:O3	2:P:14:GOL:O1	2.17	0.61
1:E:171:PHE:HD2	4:E:3:K91:C15	2.07	0.61
1:N:88:ASP:O	1:N:92:ILE:HG13	2.01	0.61
1:O:142:GLY:N	4:P:7:K91:C1	2.58	0.61
1:N:203:GLY:O	1:N:227:ALA:HA	2.00	0.61
1:R:98:HIS:CD2	1:R:151:GLN:NE2	2.69	0.61
1:C:226:PHE:HE1	4:C:2:K91:C17	2.14	0.61
1:A:139:ILE:HD13	1:B:170:LEU:CD2	2.31	0.60
1:J:203:GLY:O	1:J:227:ALA:HA	2.00	0.60
1:Q:228:LEU:HD12	1:Q:228:LEU:N	2.15	0.60
1:Q:169:PHE:O	4:Q:8:K91:H9	2.01	0.60
4:Q:8:K91:O7	1:R:133:HIS:NE2	2.33	0.60
1:U:88:ASP:OD1	1:U:90:GLU:N	2.33	0.60
1:K:109:ILE:HD12	1:T:110:TYR:CD1	2.32	0.60
1:K:110:TYR:CE1	1:T:86:SER:HB2	2.35	0.60
1:M:84:ASP:O	1:M:85:THR:HG22	2.01	0.60
1:M:166:ASN:O	1:M:228:LEU:CD2	2.48	0.60
1:V:201:SER:O	1:V:202:LEU:HD22	2.01	0.60
1:X:212:TYR:HE2	1:X:217:VAL:HG22	1.66	0.60
1:B:222:SER:OG	1:H:178:ARG:NH1	2.35	0.60
1:D:170:LEU:HB3	4:D:1:K91:CL20	2.38	0.60
1:P:98:HIS:CD2	1:P:151:GLN:HE21	2.20	0.60
1:H:199:LYS:C	1:H:201:SER:H	2.09	0.60
1:T:98:HIS:HD2	1:T:151:GLN:HE21	1.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:107:LYS:NZ	5:V:238:HOH:O	2.31	0.60
1:W:169:PHE:CE2	1:W:228:LEU:CD2	2.85	0.59
1:A:98:HIS:CD2	1:A:151:GLN:HE21	2.20	0.59
1:C:145:GLN:NE2	5:C:259:HOH:O	2.35	0.59
1:V:201:SER:O	1:V:202:LEU:CB	2.50	0.59
1:S:106:ASP:OD1	1:V:125:THR:HG22	2.02	0.59
1:B:136:GLN:HG2	5:B:240:HOH:O	2.02	0.59
1:H:98:HIS:CD2	1:H:151:GLN:NE2	2.71	0.59
1:K:110:TYR:CE2	1:T:109:ILE:CG2	2.85	0.59
1:A:228:LEU:CD1	1:A:228:LEU:C	2.75	0.59
1:C:88:ASP:OD1	1:C:91:ASP:N	2.22	0.59
1:H:89:ILE:HG21	1:K:185:PRO:HG2	1.84	0.59
1:J:199:LYS:C	1:J:201:SER:N	2.60	0.59
1:C:134:PHE:HZ	4:D:1:K91:H9	1.67	0.58
1:N:87:ILE:HB	1:N:108:VAL:HB	1.85	0.58
1:Q:129:PHE:HB3	2:Q:9:GOL:H11	1.85	0.58
1:C:87:ILE:HD12	1:C:108:VAL:HG11	1.85	0.58
4:O:6:K91:C9	1:P:134:PHE:HZ	2.15	0.58
1:B:169:PHE:CD2	1:B:228:LEU:CB	2.86	0.58
1:C:165:LYS:C	5:C:329:HOH:O	2.47	0.58
1:N:154:GLY:CA	1:N:169:PHE:CE1	2.77	0.58
1:C:171:PHE:CE2	4:C:2:K91:H15	2.39	0.58
1:J:87:ILE:HG23	1:J:91:ASP:HB2	1.84	0.58
1:M:142:GLY:N	4:N:5:K91:H2	2.05	0.57
1:K:98:HIS:CD2	1:K:151:GLN:NE2	2.72	0.57
1:X:212:TYR:O	1:X:213:VAL:HG23	2.05	0.57
1:D:150:ALA:HB1	4:D:1:K91:C16	2.31	0.57
1:K:215:GLY:O	1:T:212:TYR:OH	2.21	0.57
1:B:178:ARG:NH1	1:H:176:GLY:CA	2.67	0.57
1:R:87:ILE:HB	1:R:108:VAL:HB	1.86	0.57
1:B:186:GLY:O	1:E:122:GLN:NE2	2.27	0.57
1:T:88:ASP:OD1	1:T:88:ASP:N	2.37	0.57
1:A:202:LEU:HD13	1:A:204:ILE:CD1	2.29	0.57
1:M:170:LEU:CD2	4:M:4:K91:H5	2.33	0.57
1:O:133:HIS:NE2	4:P:7:K91:O7	2.38	0.57
1:H:185:PRO:HG2	1:K:89:ILE:HG21	1.86	0.57
1:I:89:ILE:HG21	1:L:185:PRO:HG2	1.86	0.57
1:N:98:HIS:CD2	1:N:151:GLN:NE2	2.73	0.56
1:D:170:LEU:HD22	4:D:1:K91:CL20	2.41	0.56
1:K:109:ILE:HG22	1:T:110:TYR:CE1	2.40	0.56
1:T:87:ILE:HG13	1:T:108:VAL:HB	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:201:SER:C	1:V:202:LEU:HD22	2.30	0.56
1:A:89:ILE:HG21	1:D:185:PRO:HG2	1.87	0.56
1:A:128:PRO:HG2	2:B:1:GOL:H32	1.86	0.56
1:B:185:PRO:HG2	1:E:89:ILE:HG21	1.87	0.56
1:D:98:HIS:CD2	1:D:151:GLN:NE2	2.73	0.56
1:G:166:ASN:CB	1:G:228:LEU:HD21	2.34	0.56
1:H:87:ILE:HB	1:H:108:VAL:HB	1.87	0.56
1:N:170:LEU:CD1	4:N:5:K91:CL20	2.86	0.56
4:O:6:K91:H3	1:P:142:GLY:HA3	1.87	0.56
1:P:169:PHE:HD1	1:P:226:PHE:HB3	1.70	0.56
1:H:122:GLN:O	1:K:124:SER:HB2	2.06	0.56
1:G:98:HIS:CD2	1:G:151:GLN:NE2	2.74	0.56
1:I:87:ILE:HG23	1:I:91:ASP:HB2	1.85	0.56
1:T:106:ASP:OD1	1:W:125:THR:HG22	2.06	0.56
1:K:98:HIS:CD2	1:K:151:GLN:HE21	2.23	0.55
1:D:169:PHE:O	4:D:1:K91:H10	2.05	0.55
1:H:124:SER:HB2	1:K:122:GLN:O	2.06	0.55
1:K:110:TYR:OH	1:T:107:LYS:HD3	2.05	0.55
1:K:169:PHE:HD1	1:K:226:PHE:HB3	1.72	0.55
1:K:115:LYS:CD	1:W:214:ASN:ND2	2.26	0.55
4:C:2:K91:O7	1:D:133:HIS:NE2	2.29	0.55
1:D:98:HIS:CD2	1:D:151:GLN:HE21	2.24	0.55
1:J:84:ASP:C	1:J:86:SER:N	2.62	0.55
1:Q:203:GLY:O	1:Q:228:LEU:CD1	2.54	0.55
1:D:169:PHE:O	4:D:1:K91:C9	2.55	0.55
1:H:214:ASN:CG	1:T:112:GLN:NE2	2.65	0.55
1:N:147:GLU:OE1	4:N:5:K91:C15	2.55	0.55
1:V:98:HIS:CD2	1:V:151:GLN:NE2	2.75	0.55
1:G:169:PHE:HD1	1:G:226:PHE:HB3	1.71	0.54
1:D:147:GLU:CD	4:D:1:K91:C15	2.79	0.54
1:K:110:TYR:CD2	1:T:109:ILE:CB	2.83	0.54
1:K:115:LYS:HA	1:W:214:ASN:CG	2.33	0.54
1:S:129:PHE:HB3	2:S:10:GOL:H31	1.89	0.54
1:W:169:PHE:HE2	1:W:228:LEU:CD2	2.20	0.54
1:J:98:HIS:CD2	1:J:151:GLN:HE21	2.25	0.54
1:K:109:ILE:CG1	1:T:110:TYR:CD1	2.89	0.54
1:K:115:LYS:CA	1:W:214:ASN:CG	2.81	0.54
1:T:169:PHE:N	1:T:169:PHE:CD2	2.76	0.54
1:U:89:ILE:HG21	1:X:185:PRO:HG2	1.90	0.54
1:J:98:HIS:CD2	1:J:151:GLN:NE2	2.76	0.54
1:G:181:LYS:HE2	1:G:216:LYS:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:88:ASP:OD2	1:K:88:ASP:N	2.33	0.54
1:S:94:LYS:NZ	5:S:40:HOH:O	2.30	0.53
1:G:166:ASN:CG	1:G:228:LEU:HD21	2.34	0.53
4:O:6:K91:N14	4:O:6:K91:O19	2.41	0.53
1:K:143:VAL:HG21	1:L:147:GLU:HB2	1.89	0.53
1:P:88:ASP:CG	1:P:89:ILE:N	2.66	0.53
1:U:147:GLU:O	1:U:151:GLN:HG3	2.08	0.53
1:W:169:PHE:CE2	1:W:228:LEU:HD23	2.42	0.53
1:M:147:GLU:CD	4:M:4:K91:C15	2.81	0.53
4:O:6:K91:C1	1:P:142:GLY:H	2.18	0.53
1:H:98:HIS:CD2	1:H:151:GLN:HE21	2.27	0.53
1:N:171:PHE:CD2	4:N:5:K91:H15	2.42	0.53
1:L:169:PHE:CD1	1:L:226:PHE:HB3	2.40	0.53
1:U:143:VAL:HB	1:V:143:VAL:HB	1.91	0.53
1:U:87:ILE:HB	1:U:108:VAL:HB	1.91	0.53
4:C:2:K91:H2	1:D:142:GLY:N	2.05	0.53
1:O:134:PHE:HZ	4:P:7:K91:C9	2.21	0.53
1:O:170:LEU:CD2	4:O:6:K91:H5	2.36	0.53
4:O:6:K91:C3	1:P:142:GLY:CA	2.85	0.52
1:D:88:ASP:C	1:D:88:ASP:OD1	2.52	0.52
1:E:98:HIS:CD2	1:E:151:GLN:HE21	2.27	0.52
1:I:87:ILE:HG22	1:I:88:ASP:O	2.08	0.52
1:G:166:ASN:HB3	1:G:228:LEU:HD11	1.89	0.52
1:N:167:ASN:O	1:N:169:PHE:CE2	2.62	0.52
1:X:204:ILE:O	1:X:204:ILE:CG2	2.57	0.52
1:O:98:HIS:CD2	1:O:151:GLN:NE2	2.77	0.52
1:F:178:ARG:NH1	5:F:231:HOH:O	2.43	0.52
1:I:143:VAL:HB	1:J:143:VAL:HB	1.92	0.52
1:U:199:LYS:HB2	1:U:202:LEU:HD12	1.91	0.52
1:B:178:ARG:NH1	1:H:176:GLY:HA3	2.24	0.52
1:M:87:ILE:HG23	1:M:91:ASP:HB2	1.90	0.52
4:N:5:K91:N14	4:N:5:K91:O19	2.39	0.52
1:B:122:GLN:HB3	1:E:122:GLN:HB3	1.92	0.52
1:V:177:VAL:HG22	1:V:221:ILE:HG12	1.92	0.52
1:F:169:PHE:CE2	1:F:228:LEU:CB	2.93	0.52
1:L:194:ASN:ND2	5:L:290:HOH:O	2.42	0.52
1:P:128:PRO:HG2	2:P:8:GOL:H12	1.91	0.52
1:X:199:LYS:C	1:X:201:SER:H	2.17	0.51
1:B:150:ALA:HB1	1:B:226:PHE:HZ	1.74	0.51
1:K:132:GLY:O	1:L:98:HIS:HA	2.11	0.51
1:H:106:ASP:OD1	1:K:125:THR:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:134:PHE:CD1	1:X:97:PRO:HG2	2.45	0.51
1:E:98:HIS:CD2	1:E:151:GLN:NE2	2.79	0.51
1:H:128:PRO:HG2	2:H:4:GOL:H32	1.92	0.51
1:K:109:ILE:CD1	1:T:110:TYR:CD1	2.92	0.51
1:C:122:GLN:HB3	1:F:122:GLN:HB3	1.93	0.51
1:K:177:VAL:HG22	1:K:221:ILE:HG12	1.91	0.51
1:J:89:ILE:HA	1:J:92:ILE:HD12	1.93	0.51
1:S:201:SER:CB	1:S:202:LEU:HD23	2.39	0.51
1:V:98:HIS:CD2	1:V:151:GLN:HE21	2.28	0.51
1:H:214:ASN:OD1	1:T:112:GLN:NE2	2.43	0.51
1:T:186:GLY:O	1:W:122:GLN:NE2	2.37	0.51
4:E:3:K91:O19	4:E:3:K91:N14	2.44	0.50
1:G:166:ASN:ND2	1:G:229:SER:O	2.44	0.50
4:M:4:K91:H3	1:N:142:GLY:HA3	1.93	0.50
1:O:87:ILE:HG23	1:O:91:ASP:HB2	1.94	0.50
1:F:87:ILE:HD12	1:F:108:VAL:HG11	1.93	0.50
1:K:109:ILE:HD12	1:T:110:TYR:CE2	2.37	0.50
4:M:4:K91:H2	1:N:142:GLY:N	2.17	0.50
1:G:166:ASN:OD1	1:G:228:LEU:HD21	2.11	0.50
1:I:87:ILE:CG2	1:I:91:ASP:HB2	2.42	0.50
1:S:122:GLN:O	1:V:124:SER:HB2	2.11	0.50
1:A:129:PHE:HB3	2:B:1:GOL:H31	1.94	0.50
1:L:177:VAL:HG22	1:L:221:ILE:HG12	1.93	0.50
1:R:221:ILE:HG21	1:R:224:MET:HG3	1.94	0.50
1:C:134:PHE:HZ	4:D:1:K91:C9	2.23	0.50
4:E:3:K91:H2	1:F:142:GLY:N	2.16	0.50
1:K:109:ILE:HD11	1:K:118:ILE:HG22	1.93	0.50
1:U:177:VAL:HG22	1:U:221:ILE:HG12	1.93	0.50
1:O:177:VAL:HG22	1:O:221:ILE:HG12	1.94	0.50
1:T:126:ASN:HB3	1:W:127:GLU:OE1	2.11	0.50
1:X:88:ASP:OD2	1:X:90:GLU:HG2	2.12	0.50
1:K:109:ILE:CD1	1:T:110:TYR:CE2	2.96	0.49
1:O:106:ASP:OD1	1:R:125:THR:HG22	2.12	0.49
1:W:200:SER:O	1:W:201:SER:C	2.55	0.49
1:T:154:GLY:HA3	1:T:169:PHE:HE1	1.76	0.49
1:U:127:GLU:HG2	1:X:126:ASN:O	2.11	0.49
1:K:88:ASP:OD2	1:K:91:ASP:OD2	2.31	0.49
1:W:145:GLN:NE2	1:W:179:TRP:HD1	2.09	0.49
1:A:87:ILE:HB	1:A:108:VAL:HB	1.94	0.49
1:I:177:VAL:HB	1:J:174:VAL:HG12	1.94	0.49
1:P:98:HIS:CD2	1:P:151:GLN:NE2	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:221:ILE:HG21	1:H:224:MET:HG3	1.94	0.49
1:J:192:GLN:NE2	2:J:13:GOL:H2	2.27	0.49
1:W:153:ALA:HB1	1:W:207:LEU:HD22	1.94	0.49
1:G:127:GLU:OE1	1:J:126:ASN:HB3	2.13	0.49
1:A:199:LYS:C	1:A:201:SER:N	2.71	0.49
1:I:153:ALA:HB1	1:I:207:LEU:HD22	1.94	0.49
1:J:192:GLN:HE22	2:J:13:GOL:H2	1.77	0.49
1:A:228:LEU:HD12	1:A:228:LEU:O	2.12	0.49
1:F:199:LYS:C	1:F:201:SER:N	2.68	0.49
1:Q:150:ALA:HB1	4:Q:8:K91:C17	2.43	0.49
1:J:169:PHE:HD1	1:J:226:PHE:HB3	1.77	0.48
1:B:125:THR:HG22	1:E:106:ASP:OD1	2.13	0.48
1:K:118:ILE:HD12	1:T:109:ILE:CG1	2.44	0.48
1:T:154:GLY:HA3	1:T:169:PHE:CE1	2.48	0.48
1:W:143:VAL:HB	1:X:143:VAL:HB	1.95	0.48
1:H:199:LYS:C	1:H:201:SER:N	2.72	0.48
1:T:158:LEU:HD12	1:T:169:PHE:HZ	1.78	0.48
1:D:202:LEU:CB	1:D:204:ILE:HG23	2.43	0.48
1:T:87:ILE:CG1	1:T:108:VAL:HB	2.43	0.48
1:W:169:PHE:HE2	1:W:228:LEU:HD21	1.78	0.48
1:B:85:THR:HG23	1:B:85:THR:O	2.14	0.48
1:W:145:GLN:NE2	1:W:179:TRP:CD1	2.82	0.48
1:I:177:VAL:C	1:I:178:ARG:HG2	2.39	0.48
1:I:185:PRO:HG2	1:L:89:ILE:HG21	1.94	0.48
1:D:164:GLN:H	1:D:164:GLN:HG2	1.23	0.48
1:G:166:ASN:CB	1:G:228:LEU:HD11	2.44	0.48
1:K:118:ILE:CD1	1:T:109:ILE:CG1	2.92	0.48
1:I:130:PHE:CD1	1:I:138:GLN:HB3	2.49	0.47
1:B:177:VAL:HG22	1:B:221:ILE:HG12	1.96	0.47
4:M:4:K91:C3	1:N:142:GLY:CA	2.90	0.47
1:A:162:ASP:N	5:A:311:HOH:O	2.20	0.47
1:A:228:LEU:C	1:A:228:LEU:HD12	2.39	0.47
1:N:164:GLN:HG3	5:N:333:HOH:O	2.13	0.47
4:O:6:K91:H9	1:P:134:PHE:CZ	2.45	0.47
1:D:202:LEU:CB	1:D:204:ILE:HG22	2.43	0.47
1:O:122:GLN:OE1	1:R:122:GLN:OE1	2.32	0.47
1:P:170:LEU:CD2	4:P:7:K91:H5	2.31	0.47
1:S:89:ILE:HG21	1:V:185:PRO:HG2	1.97	0.47
1:U:199:LYS:HB2	1:U:202:LEU:CD1	2.44	0.47
1:V:201:SER:O	1:V:202:LEU:CD2	2.62	0.47
1:Q:147:GLU:CD	4:Q:8:K91:C15	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:170:LEU:HD23	4:Q:8:K91:H5	1.90	0.47
1:E:199:LYS:HG2	1:E:204:ILE:HD12	1.95	0.47
1:M:177:VAL:HB	1:N:174:VAL:HG12	1.97	0.47
4:M:4:K91:O7	1:N:133:HIS:NE2	2.43	0.47
1:T:177:VAL:HG22	1:T:221:ILE:HG12	1.97	0.47
1:U:164:GLN:OE1	1:U:164:GLN:HA	2.12	0.47
1:W:177:VAL:HG22	1:W:221:ILE:HG12	1.95	0.47
1:H:195:LEU:O	5:H:247:HOH:O	2.21	0.47
1:L:101:PRO:HG2	2:L:6:GOL:H32	1.96	0.47
1:B:124:SER:HB2	1:E:122:GLN:O	2.15	0.47
1:B:206:LYS:HD3	1:B:223:GLU:OE2	2.15	0.47
1:E:143:VAL:HB	1:F:143:VAL:HB	1.95	0.47
1:K:215:GLY:HA2	1:T:212:TYR:OH	2.14	0.47
1:A:98:HIS:CD2	1:A:151:GLN:NE2	2.83	0.47
1:C:142:GLY:HA3	4:D:1:K91:C3	2.44	0.47
1:O:142:GLY:HA3	4:P:7:K91:C3	2.38	0.47
1:S:154:GLY:HA3	5:S:425:HOH:O	2.13	0.47
1:B:136:GLN:CG	5:B:240:HOH:O	2.60	0.46
1:D:177:VAL:HG22	1:D:221:ILE:HG12	1.97	0.46
1:H:125:THR:HG22	1:K:106:ASP:OD1	2.15	0.46
1:T:186:GLY:HA2	1:W:122:GLN:HG2	1.97	0.46
1:F:177:VAL:HG22	1:F:221:ILE:HG12	1.96	0.46
1:X:212:TYR:O	1:X:213:VAL:CG2	2.63	0.46
1:T:98:HIS:HD2	1:T:151:GLN:NE2	2.09	0.46
1:J:221:ILE:HG21	1:J:224:MET:HG3	1.98	0.46
1:X:212:TYR:HE2	1:X:217:VAL:CG2	2.27	0.46
1:B:112:GLN:HE21	1:T:163:SER:CB	2.11	0.46
1:T:177:VAL:C	1:T:178:ARG:HG2	2.40	0.46
1:E:226:PHE:HE1	4:E:3:K91:C16	2.29	0.46
1:N:96:LEU:HD22	1:N:169:PHE:HZ	1.72	0.46
1:E:169:PHE:CE2	1:E:228:LEU:HA	2.51	0.46
1:K:89:ILE:HA	1:K:92:ILE:HD12	1.97	0.46
1:M:174:VAL:HG12	1:N:177:VAL:HB	1.97	0.46
1:N:171:PHE:HD2	4:N:5:K91:C15	2.26	0.46
1:U:88:ASP:OD1	1:U:88:ASP:C	2.58	0.46
1:P:150:ALA:CB	4:P:7:K91:C16	2.67	0.46
1:G:221:ILE:HG21	1:G:224:MET:HG3	1.98	0.46
1:H:129:PHE:HB3	2:H:4:GOL:H31	1.96	0.46
1:K:115:LYS:HZ1	1:W:187:ASP:HA	1.72	0.46
1:K:130:PHE:CD1	1:K:138:GLN:HB3	2.51	0.46
1:M:84:ASP:O	1:M:85:THR:CG2	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:199:LYS:HB2	1:N:199:LYS:HE3	1.71	0.46
1:R:202:LEU:CB	1:R:204:ILE:HG13	2.46	0.46
1:X:107:LYS:HG3	5:X:410:HOH:O	2.07	0.46
1:J:206:LYS:HD3	1:J:223:GLU:OE2	2.16	0.45
4:C:2:K91:C6	1:D:133:HIS:HE2	2.26	0.45
1:O:133:HIS:CE1	4:P:7:K91:O7	2.69	0.45
4:O:6:K91:C3	1:P:142:GLY:N	2.71	0.45
1:X:158:LEU:HD21	1:X:169:PHE:CE2	2.51	0.45
1:F:206:LYS:HD3	1:F:223:GLU:OE2	2.16	0.45
1:O:171:PHE:CD2	4:O:6:K91:C15	3.00	0.45
1:S:202:LEU:HB3	1:S:204:ILE:HG13	1.99	0.45
1:B:89:ILE:HG21	1:E:185:PRO:HG2	1.96	0.45
1:L:129:PHE:HB3	2:L:6:GOL:H12	1.98	0.45
1:M:166:ASN:HB3	1:M:228:LEU:CD1	2.46	0.45
1:W:137:LYS:HB3	1:X:168:LEU:HD21	1.99	0.45
1:C:226:PHE:CE1	4:C:2:K91:C17	2.98	0.45
1:N:185:PRO:HG2	1:Q:89:ILE:HG21	1.99	0.45
1:O:221:ILE:HG21	1:O:224:MET:HG3	1.99	0.45
1:A:166:ASN:HB3	1:A:228:LEU:HD21	1.98	0.45
1:C:171:PHE:CE2	4:C:2:K91:C15	2.97	0.45
1:C:170:LEU:HD22	4:C:2:K91:C4	2.46	0.45
1:H:177:VAL:HG22	1:H:221:ILE:HG12	1.99	0.45
1:X:212:TYR:C	1:X:213:VAL:HG23	2.41	0.45
1:M:166:ASN:HB3	1:M:228:LEU:CD2	2.43	0.45
1:S:147:GLU:HB2	1:T:143:VAL:HG21	1.99	0.45
1:N:96:LEU:HD22	1:N:169:PHE:CZ	2.51	0.45
1:P:171:PHE:CD2	4:P:7:K91:C15	3.00	0.45
1:G:153:ALA:HB1	1:G:207:LEU:HD22	1.99	0.44
1:M:87:ILE:HG22	1:M:92:ILE:HG13	1.99	0.44
1:K:118:ILE:HD12	1:T:109:ILE:HG13	1.99	0.44
1:Q:177:VAL:C	1:Q:178:ARG:HG2	2.42	0.44
1:V:199:LYS:O	1:V:200:SER:C	2.60	0.44
1:W:181:LYS:CG	1:W:218:VAL:HG12	2.44	0.44
1:D:112:GLN:HG3	5:D:231:HOH:O	2.16	0.44
1:L:212:TYR:CE2	1:L:217:VAL:HG22	2.53	0.44
1:K:110:TYR:CE1	1:T:86:SER:CB	3.00	0.44
1:M:200:SER:O	1:M:201:SER:C	2.60	0.44
1:K:98:HIS:HA	1:L:132:GLY:O	2.18	0.44
1:X:177:VAL:HG22	1:X:221:ILE:HG12	2.00	0.44
1:X:211:GLY:HA3	1:X:219:ILE:HG22	2.00	0.44
1:K:112:GLN:CD	1:T:107:LYS:NZ	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:170:LEU:HD22	4:N:5:K91:C4	2.48	0.44
1:W:166:ASN:HB3	1:W:228:LEU:CD2	2.44	0.44
1:L:89:ILE:HA	1:L:92:ILE:HD12	1.99	0.44
1:H:101:PRO:O	2:H:4:GOL:O3	2.35	0.43
1:H:169:PHE:HD1	1:H:226:PHE:HB3	1.82	0.43
1:N:153:ALA:HB1	1:N:207:LEU:HD22	2.00	0.43
1:O:203:GLY:O	1:O:227:ALA:HA	2.17	0.43
1:Q:101:PRO:HG2	2:Q:9:GOL:H32	1.99	0.43
1:M:221:ILE:HG21	1:M:224:MET:HG3	1.99	0.43
1:L:213:VAL:O	5:L:280:HOH:O	2.21	0.43
1:C:177:VAL:HG22	1:C:221:ILE:HG12	2.01	0.43
1:N:221:ILE:HG21	1:N:224:MET:HG3	2.01	0.43
1:W:89:ILE:HA	1:W:92:ILE:HD12	2.00	0.43
1:A:166:ASN:HD21	1:A:229:SER:C	2.27	0.43
1:C:162:ASP:OD2	1:C:165:LYS:HD3	2.19	0.43
1:E:84:ASP:HB2	1:E:85:THR:H	1.37	0.43
1:K:112:GLN:NE2	1:T:107:LYS:HZ3	2.16	0.43
1:B:112:GLN:NE2	5:B:332:HOH:O	2.49	0.43
1:C:170:LEU:CD1	4:C:2:K91:CL20	3.03	0.43
4:C:2:K91:C3	1:D:142:GLY:N	2.73	0.43
1:K:215:GLY:C	1:T:212:TYR:HH	2.23	0.43
1:A:199:LYS:O	1:A:201:SER:N	2.52	0.43
1:P:88:ASP:OD1	1:P:88:ASP:C	2.62	0.43
1:W:177:VAL:C	1:W:178:ARG:HG2	2.43	0.43
1:C:88:ASP:OD1	1:C:88:ASP:C	2.61	0.42
1:Q:199:LYS:HG3	1:Q:204:ILE:HB	2.00	0.42
1:T:122:GLN:O	1:W:124:SER:HB2	2.20	0.42
5:U:306:HOH:O	1:X:121:LYS:NZ	2.40	0.42
1:A:87:ILE:HD12	1:A:108:VAL:HG11	2.01	0.42
1:J:104:LEU:O	1:J:121:LYS:HG3	2.19	0.42
1:K:199:LYS:C	1:K:199:LYS:CE	2.88	0.42
1:N:142:GLY:O	1:N:145:GLN:HB2	2.18	0.42
1:S:122:GLN:HB3	1:V:122:GLN:HB3	2.01	0.42
1:E:206:LYS:HD3	1:E:223:GLU:OE2	2.18	0.42
1:R:165:LYS:NZ	1:R:165:LYS:CB	2.79	0.42
1:K:97:PRO:HG2	1:L:134:PHE:CD1	2.54	0.42
1:B:90:GLU:CD	1:E:137:LYS:HA	2.44	0.42
1:E:218:VAL:HG23	1:E:219:ILE:HG22	2.01	0.42
1:H:153:ALA:HB1	1:H:207:LEU:HD22	2.02	0.42
1:S:126:ASN:ND2	1:V:128:PRO:HD2	2.35	0.42
1:C:200:SER:HB3	1:C:201:SER:H	1.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:85:THR:O	1:S:85:THR:OG1	2.35	0.42
1:S:127:GLU:HG2	1:V:126:ASN:O	2.19	0.42
1:V:202:LEU:HD13	1:V:202:LEU:N	2.34	0.42
1:E:102:PHE:CE2	1:E:147:GLU:HG2	2.55	0.42
1:G:126:ASN:HB3	1:J:127:GLU:OE1	2.19	0.42
1:I:212:TYR:CE2	1:I:217:VAL:HG22	2.55	0.42
4:M:4:K91:C3	1:N:142:GLY:H	2.29	0.42
1:Q:89:ILE:HA	1:Q:92:ILE:HD12	2.01	0.42
1:C:142:GLY:N	4:D:1:K91:C1	2.74	0.42
1:I:88:ASP:OD1	1:I:91:ASP:OD2	2.38	0.42
1:O:169:PHE:O	4:O:6:K91:C9	2.68	0.42
1:R:181:LYS:HB3	1:R:218:VAL:HG12	2.02	0.42
1:H:101:PRO:HG2	2:H:4:GOL:H11	2.02	0.42
1:L:104:LEU:O	1:L:121:LYS:HG3	2.19	0.42
1:N:181:LYS:HB3	1:N:218:VAL:HG12	2.00	0.42
1:A:221:ILE:HG21	1:A:224:MET:HG3	2.01	0.42
4:M:4:K91:N14	4:M:4:K91:O19	2.37	0.42
1:Q:101:PRO:HB2	2:Q:9:GOL:H32	2.00	0.42
1:W:142:GLY:O	1:W:145:GLN:HB2	2.20	0.42
1:X:213:VAL:O	1:X:214:ASN:HB2	2.20	0.42
1:A:199:LYS:O	1:A:200:SER:C	2.63	0.41
1:P:221:ILE:HG21	1:P:224:MET:HG3	2.02	0.41
1:W:139:ILE:CD1	1:X:170:LEU:HD21	2.46	0.41
1:C:199:LYS:CB	1:C:202:LEU:HD12	2.50	0.41
1:D:139:ILE:HD13	1:D:139:ILE:HG21	1.88	0.41
1:E:139:ILE:HD13	1:F:170:LEU:HD11	2.02	0.41
1:F:177:VAL:HA	1:F:220:ASN:O	2.20	0.41
1:H:206:LYS:HD3	1:H:223:GLU:OE2	2.20	0.41
1:K:114:ASN:O	1:W:214:ASN:O	2.38	0.41
1:K:109:ILE:HG22	1:T:110:TYR:HE1	1.81	0.41
1:U:164:GLN:OE1	1:U:164:GLN:CA	2.68	0.41
1:A:101:PRO:O	2:B:1:GOL:O3	2.35	0.41
1:A:206:LYS:HD3	1:A:223:GLU:OE2	2.20	0.41
1:R:87:ILE:HG23	1:R:91:ASP:HB2	2.02	0.41
1:S:89:ILE:HA	1:S:92:ILE:HD12	2.02	0.41
1:T:89:ILE:HA	1:T:92:ILE:HD12	2.02	0.41
1:W:221:ILE:HG21	1:W:224:MET:HG3	2.03	0.41
1:Q:147:GLU:HB2	1:R:143:VAL:HG21	2.00	0.41
1:L:153:ALA:HB1	1:L:207:LEU:HD22	2.01	0.41
1:S:177:VAL:HG22	1:S:221:ILE:HG12	2.02	0.41
1:T:125:THR:HG22	1:W:106:ASP:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:HIS:CE1	4:D:1:K91:O7	2.73	0.41
1:M:203:GLY:O	1:M:227:ALA:HA	2.21	0.41
1:T:202:LEU:O	1:T:203:GLY:C	2.63	0.41
1:M:142:GLY:N	4:N:5:K91:C1	2.73	0.41
1:M:169:PHE:HD1	1:M:226:PHE:HB3	1.86	0.41
1:N:170:LEU:CG	4:N:5:K91:CL20	3.06	0.41
1:Q:84:ASP:OD2	1:Q:84:ASP:N	2.53	0.41
1:Q:228:LEU:N	1:Q:228:LEU:CD1	2.84	0.41
1:C:134:PHE:CZ	4:D:1:K91:H9	2.53	0.41
1:P:87:ILE:HG23	1:P:91:ASP:HB2	2.03	0.41
1:W:133:HIS:ND1	1:W:139:ILE:O	2.47	0.41
1:A:143:VAL:HB	1:B:143:VAL:HB	2.03	0.40
1:A:161:ASP:C	1:A:161:ASP:OD1	2.64	0.40
1:E:226:PHE:CE1	4:E:3:K91:C17	3.04	0.40
1:C:89:ILE:HA	1:C:92:ILE:HD12	2.04	0.40
1:C:206:LYS:HD3	1:C:223:GLU:OE2	2.21	0.40
1:M:170:LEU:HB3	4:M:4:K91:CL20	2.58	0.40
1:A:177:VAL:HG22	1:A:221:ILE:HG12	2.04	0.40
1:C:139:ILE:HD13	1:C:139:ILE:HG21	1.87	0.40
1:D:206:LYS:HD3	1:D:223:GLU:OE2	2.22	0.40
4:E:3:K91:O7	1:F:133:HIS:CE1	2.75	0.40
4:C:2:K91:H9	1:D:134:PHE:CZ	2.38	0.40
1:E:169:PHE:HE2	1:E:228:LEU:HD23	1.87	0.40
1:K:215:GLY:C	1:T:212:TYR:OH	2.64	0.40
4:M:4:K91:C1	1:N:142:GLY:H	2.28	0.40
1:I:102:PHE:CE2	1:I:147:GLU:HG2	2.57	0.40
1:I:179:TRP:CE3	1:J:171:PHE:HB3	2.57	0.40
1:J:85:THR:OG1	1:J:110:TYR:HA	2.21	0.40
1:K:133:HIS:ND1	1:K:139:ILE:O	2.51	0.40
1:O:169:PHE:HB2	4:O:6:K91:CL18	2.59	0.40
1:S:166:ASN:CB	1:S:228:LEU:HD21	2.47	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	144/154 (94%)	131 (91%)	13 (9%)	0	100	100
1	B	143/154 (93%)	132 (92%)	11 (8%)	0	100	100
1	C	142/154 (92%)	128 (90%)	14 (10%)	0	100	100
1	D	142/154 (92%)	134 (94%)	8 (6%)	0	100	100
1	E	138/154 (90%)	130 (94%)	8 (6%)	0	100	100
1	F	144/154 (94%)	132 (92%)	10 (7%)	2 (1%)	9	17
1	G	145/154 (94%)	138 (95%)	7 (5%)	0	100	100
1	H	143/154 (93%)	132 (92%)	11 (8%)	0	100	100
1	I	142/154 (92%)	133 (94%)	9 (6%)	0	100	100
1	J	142/154 (92%)	129 (91%)	12 (8%)	1 (1%)	18	34
1	K	138/154 (90%)	130 (94%)	8 (6%)	0	100	100
1	L	144/154 (94%)	136 (94%)	7 (5%)	1 (1%)	18	34
1	M	144/154 (94%)	130 (90%)	14 (10%)	0	100	100
1	N	143/154 (93%)	129 (90%)	14 (10%)	0	100	100
1	O	142/154 (92%)	130 (92%)	12 (8%)	0	100	100
1	P	142/154 (92%)	132 (93%)	10 (7%)	0	100	100
1	Q	138/154 (90%)	130 (94%)	8 (6%)	0	100	100
1	R	144/154 (94%)	134 (93%)	10 (7%)	0	100	100
1	S	144/154 (94%)	134 (93%)	10 (7%)	0	100	100
1	T	143/154 (93%)	134 (94%)	9 (6%)	0	100	100
1	U	142/154 (92%)	131 (92%)	10 (7%)	1 (1%)	18	34
1	V	142/154 (92%)	130 (92%)	12 (8%)	0	100	100
1	W	143/154 (93%)	133 (93%)	10 (7%)	0	100	100
1	X	140/154 (91%)	128 (91%)	10 (7%)	2 (1%)	9	17
All	All	3414/3696 (92%)	3160 (93%)	247 (7%)	7 (0%)	43	64

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	89	ILE
1	X	213	VAL
1	F	200	SER

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Mol	Chain	Res	Type
1	J	200	SER
1	L	228	LEU
1	U	200	SER
1	X	215	GLY

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%)	118 (94%)	8 (6%)	16	30
1	B	123/135 (91%)	115 (94%)	8 (6%)	15	29
1	C	125/135 (93%)	117 (94%)	8 (6%)	16	29
1	D	122/135 (90%)	113 (93%)	9 (7%)	13	24
1	E	123/135 (91%)	116 (94%)	7 (6%)	18	35
1	F	126/135 (93%)	117 (93%)	9 (7%)	13	25
1	G	126/135 (93%)	120 (95%)	6 (5%)	23	44
1	H	124/135 (92%)	117 (94%)	7 (6%)	19	36
1	I	125/135 (93%)	120 (96%)	5 (4%)	28	50
1	J	121/135 (90%)	115 (95%)	6 (5%)	22	42
1	K	122/135 (90%)	116 (95%)	6 (5%)	22	43
1	L	125/135 (93%)	116 (93%)	9 (7%)	13	25
1	M	126/135 (93%)	120 (95%)	6 (5%)	23	44
1	N	124/135 (92%)	116 (94%)	8 (6%)	15	29
1	O	125/135 (93%)	118 (94%)	7 (6%)	19	36
1	P	122/135 (90%)	117 (96%)	5 (4%)	27	49
1	Q	122/135 (90%)	115 (94%)	7 (6%)	18	35
1	R	126/135 (93%)	119 (94%)	7 (6%)	19	36
1	S	126/135 (93%)	119 (94%)	7 (6%)	19	36
1	T	125/135 (93%)	116 (93%)	9 (7%)	13	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	125/135 (93%)	117 (94%)	8 (6%)	16	29
1	V	122/135 (90%)	118 (97%)	4 (3%)	33	57
1	W	125/135 (93%)	117 (94%)	8 (6%)	16	29
1	X	122/135 (90%)	112 (92%)	10 (8%)	10	20
All	All	2978/3240 (92%)	2804 (94%)	174 (6%)	18	34

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	ILE
1	A	168	LEU
1	A	171	PHE
1	A	181	LYS
1	A	201	SER
1	A	216	LYS
1	A	220	ASN
1	A	228	LEU
1	B	87	ILE
1	B	164	GLN
1	B	168	LEU
1	B	171	PHE
1	B	181	LYS
1	B	199	LYS
1	B	220	ASN
1	B	229	SER
1	C	85	THR
1	C	86	SER
1	C	168	LEU
1	C	171	PHE
1	C	178	ARG
1	C	181	LYS
1	C	201	SER
1	C	220	ASN
1	D	85	THR
1	D	88	ASP
1	D	164	GLN
1	D	168	LEU
1	D	171	PHE
1	D	178	ARG
1	D	181	LYS
1	D	204	ILE

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Mol	Chain	Res	Type
1	D	220	ASN
1	E	84	ASP
1	E	85	THR
1	E	168	LEU
1	E	169	PHE
1	E	171	PHE
1	E	199	LYS
1	E	220	ASN
1	F	85	THR
1	F	165	LYS
1	F	168	LEU
1	F	171	PHE
1	F	178	ARG
1	F	201	SER
1	F	216	LYS
1	F	220	ASN
1	F	229	SER
1	G	85	THR
1	G	168	LEU
1	G	171	PHE
1	G	181	LYS
1	G	202	LEU
1	G	220	ASN
1	H	86	SER
1	H	136	GLN
1	H	168	LEU
1	H	171	PHE
1	H	181	LYS
1	H	201	SER
1	H	220	ASN
1	I	168	LEU
1	I	171	PHE
1	I	181	LYS
1	I	200	SER
1	I	220	ASN
1	J	87	ILE
1	J	168	LEU
1	J	171	PHE
1	J	181	LYS
1	J	202	LEU
1	J	220	ASN
1	K	85	THR

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Mol	Chain	Res	Type
1	K	88	ASP
1	K	168	LEU
1	K	171	PHE
1	K	199	LYS
1	K	220	ASN
1	L	84	ASP
1	L	85	THR
1	L	168	LEU
1	L	171	PHE
1	L	199	LYS
1	L	200	SER
1	L	201	SER
1	L	220	ASN
1	L	229	SER
1	M	168	LEU
1	M	171	PHE
1	M	181	LYS
1	M	199	LYS
1	M	202	LEU
1	M	220	ASN
1	N	136	GLN
1	N	145	GLN
1	N	164	GLN
1	N	168	LEU
1	N	169	PHE
1	N	171	PHE
1	N	181	LYS
1	N	199	LYS
1	O	85	THR
1	O	112	GLN
1	O	165	LYS
1	O	168	LEU
1	O	171	PHE
1	O	181	LYS
1	O	202	LEU
1	P	88	ASP
1	P	168	LEU
1	P	171	PHE
1	P	181	LYS
1	P	202	LEU
1	Q	88	ASP
1	Q	168	LEU

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Mol	Chain	Res	Type
1	Q	171	PHE
1	Q	178	ARG
1	Q	199	LYS
1	Q	220	ASN
1	Q	228	LEU
1	R	84	ASP
1	R	85	THR
1	R	164	GLN
1	R	165	LYS
1	R	168	LEU
1	R	171	PHE
1	R	201	SER
1	S	85	THR
1	S	168	LEU
1	S	171	PHE
1	S	178	ARG
1	S	202	LEU
1	S	204	ILE
1	S	228	LEU
1	T	85	THR
1	T	87	ILE
1	T	88	ASP
1	T	136	GLN
1	T	168	LEU
1	T	169	PHE
1	T	171	PHE
1	T	201	SER
1	T	202	LEU
1	U	85	THR
1	U	86	SER
1	U	89	ILE
1	U	164	GLN
1	U	168	LEU
1	U	171	PHE
1	U	200	SER
1	U	202	LEU
1	V	168	LEU
1	V	171	PHE
1	V	201	SER
1	V	202	LEU
1	W	84	ASP
1	W	85	THR

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Mol	Chain	Res	Type
1	W	136	GLN
1	W	145	GLN
1	W	168	LEU
1	W	171	PHE
1	W	181	LYS
1	W	200	SER
1	X	88	ASP
1	X	136	GLN
1	X	164	GLN
1	X	165	LYS
1	X	168	LEU
1	X	171	PHE
1	X	199	LYS
1	X	200	SER
1	X	201	SER
1	X	204	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	HIS
1	A	112	GLN
1	A	136	GLN
1	B	112	GLN
1	B	126	ASN
1	B	145	GLN
1	B	164	GLN
1	C	98	HIS
1	C	114	ASN
1	C	138	GLN
1	D	98	HIS
1	D	114	ASN
1	D	136	GLN
1	E	98	HIS
1	E	114	ASN
1	E	136	GLN
1	E	145	GLN
1	F	98	HIS
1	F	114	ASN
1	F	194	ASN
1	G	98	HIS
1	G	126	ASN

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Mol	Chain	Res	Type
1	G	136	GLN
1	G	138	GLN
1	H	98	HIS
1	H	114	ASN
1	H	126	ASN
1	H	145	GLN
1	I	98	HIS
1	I	126	ASN
1	I	136	GLN
1	J	98	HIS
1	J	126	ASN
1	J	136	GLN
1	J	138	GLN
1	J	192	GLN
1	K	98	HIS
1	K	126	ASN
1	K	136	GLN
1	K	192	GLN
1	K	194	ASN
1	L	98	HIS
1	L	136	GLN
1	L	138	GLN
1	L	194	ASN
1	L	220	ASN
1	M	98	HIS
1	M	126	ASN
1	M	136	GLN
1	M	145	GLN
1	N	98	HIS
1	N	136	GLN
1	N	214	ASN
1	O	98	HIS
1	O	112	GLN
1	O	138	GLN
1	O	164	GLN
1	P	98	HIS
1	P	192	GLN
1	Q	98	HIS
1	Q	145	GLN
1	R	98	HIS
1	R	136	GLN
1	R	145	GLN

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Mol	Chain	Res	Type
1	S	98	HIS
1	S	220	ASN
1	T	98	HIS
1	T	112	GLN
1	T	126	ASN
1	T	164	GLN
1	U	98	HIS
1	U	122	GLN
1	U	126	ASN
1	U	145	GLN
1	V	98	HIS
1	V	138	GLN
1	V	194	ASN
1	W	98	HIS
1	W	138	GLN
1	W	145	GLN
1	W	214	ASN
1	X	98	HIS
1	X	126	ASN
1	X	138	GLN
1	X	145	GLN
1	X	220	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

23 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	K91	C	2	-	22,22,22	1.66	4 (18%)	31,31,31	1.75	9 (29%)
2	GOL	P	8	-	5,5,5	0.48	0	5,5,5	1.01	0
2	GOL	V	11	-	5,5,5	0.51	0	5,5,5	0.61	0
2	GOL	S	10	-	5,5,5	0.41	0	5,5,5	0.30	0
3	PO4	B	231	-	4,4,4	1.24	0	6,6,6	0.37	0
2	GOL	J	5	-	5,5,5	0.42	0	5,5,5	0.53	0
2	GOL	D	2	-	5,5,5	0.57	0	5,5,5	0.85	0
4	K91	O	6	-	22,22,22	1.19	3 (13%)	31,31,31	1.23	4 (12%)
2	GOL	B	1	-	5,5,5	0.42	0	5,5,5	0.58	0
4	K91	D	1	-	22,22,22	1.19	3 (13%)	31,31,31	1.24	5 (16%)
2	GOL	Q	9	-	5,5,5	0.18	0	5,5,5	0.27	0
4	K91	M	4	-	22,22,22	1.57	4 (18%)	31,31,31	1.73	9 (29%)
2	GOL	L	6	-	5,5,5	0.34	0	5,5,5	0.55	0
2	GOL	F	3	-	5,5,5	0.52	0	5,5,5	0.48	0
4	K91	Q	8	-	22,22,22	1.19	3 (13%)	31,31,31	1.23	4 (12%)
4	K91	P	7	-	22,22,22	1.19	3 (13%)	31,31,31	1.23	5 (16%)
2	GOL	N	7	-	5,5,5	0.38	0	5,5,5	0.72	0
4	K91	E	3	-	22,22,22	1.19	3 (13%)	31,31,31	1.24	5 (16%)
4	K91	N	5	-	22,22,22	1.55	3 (13%)	31,31,31	1.55	6 (19%)
2	GOL	P	14	-	5,5,5	0.43	0	5,5,5	1.07	0
2	GOL	H	4	-	5,5,5	0.52	0	5,5,5	0.82	0
2	GOL	J	13	-	5,5,5	0.44	0	5,5,5	0.48	0
2	GOL	W	12	-	5,5,5	0.48	0	5,5,5	0.66	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	K91	C	2	-	-	0/4/4/4	0/3/3/3
2	GOL	P	8	-	-	1/4/4/4	-
2	GOL	V	11	-	-	0/4/4/4	-
2	GOL	S	10	-	-	2/4/4/4	-
2	GOL	J	5	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	D	2	-	-	2/4/4/4	-
4	K91	O	6	-	-	2/4/4/4	0/3/3/3
2	GOL	B	1	-	-	2/4/4/4	-
4	K91	D	1	-	-	0/4/4/4	0/3/3/3
2	GOL	Q	9	-	-	4/4/4/4	-
4	K91	M	4	-	-	1/4/4/4	0/3/3/3
2	GOL	L	6	-	-	4/4/4/4	-
2	GOL	F	3	-	-	4/4/4/4	-
4	K91	Q	8	-	-	0/4/4/4	0/3/3/3
4	K91	P	7	-	-	1/4/4/4	0/3/3/3
2	GOL	N	7	-	-	4/4/4/4	-
4	K91	E	3	-	-	2/4/4/4	0/3/3/3
4	K91	N	5	-	-	0/4/4/4	0/3/3/3
2	GOL	P	14	-	-	2/4/4/4	-
2	GOL	H	4	-	-	2/4/4/4	-
2	GOL	J	13	-	-	4/4/4/4	-
2	GOL	W	12	-	-	0/4/4/4	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2	K91	C8-C13	-4.73	1.36	1.42
4	M	4	K91	C8-C13	-4.10	1.36	1.42
4	N	5	K91	C4-CL20	3.65	1.82	1.74
4	N	5	K91	C8-C13	-3.32	1.38	1.42
4	C	2	K91	C11-CL18	2.88	1.81	1.74
4	C	2	K91	C4-CL20	2.71	1.80	1.74
4	C	2	K91	C17-C12	-2.39	1.37	1.42
4	P	7	K91	C4-CL20	2.38	1.80	1.74
4	O	6	K91	C4-CL20	2.37	1.80	1.74
4	E	3	K91	C4-CL20	2.37	1.80	1.74
4	D	1	K91	C8-C13	-2.36	1.39	1.42
4	E	3	K91	C8-C13	-2.36	1.39	1.42
4	Q	8	K91	C4-CL20	2.36	1.79	1.74
4	P	7	K91	C8-C13	-2.35	1.39	1.42
4	O	6	K91	C8-C13	-2.35	1.39	1.42
4	M	4	K91	C17-C12	-2.34	1.37	1.42
4	D	1	K91	C4-CL20	2.34	1.79	1.74
4	Q	8	K91	C8-C13	-2.33	1.39	1.42
4	N	5	K91	C11-CL18	2.28	1.80	1.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	4	K91	C11-CL18	2.25	1.80	1.74
4	Q	8	K91	C11-CL18	2.25	1.80	1.74
4	P	7	K91	C11-CL18	2.23	1.80	1.74
4	D	1	K91	C11-CL18	2.23	1.80	1.74
4	E	3	K91	C11-CL18	2.22	1.79	1.74
4	O	6	K91	C11-CL18	2.20	1.79	1.74
4	M	4	K91	C11-C12	-2.02	1.38	1.41

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2	K91	C11-C12-C13	3.86	121.98	117.40
4	M	4	K91	C16-C15-N14	-3.71	118.52	123.97
4	N	5	K91	C15-N14-C13	3.52	121.46	117.31
4	N	5	K91	C5-C4-CL20	3.27	123.28	119.17
4	C	2	K91	C5-C4-CL20	3.26	123.26	119.17
4	M	4	K91	C15-N14-C13	3.22	121.10	117.31
4	C	2	K91	C16-C15-N14	-3.21	119.25	123.97
4	N	5	K91	C16-C15-N14	-3.21	119.26	123.97
4	E	3	K91	C15-N14-C13	3.21	121.09	117.31
4	Q	8	K91	C15-N14-C13	3.19	121.08	117.31
4	D	1	K91	C15-N14-C13	3.19	121.07	117.31
4	M	4	K91	C11-C12-C13	3.18	121.18	117.40
4	P	7	K91	C15-N14-C13	3.18	121.05	117.31
4	O	6	K91	C15-N14-C13	3.17	121.05	117.31
4	M	4	K91	C5-C4-CL20	3.16	123.13	119.17
4	C	2	K91	C17-C12-C11	-3.13	119.63	125.07
4	M	4	K91	C17-C12-C11	-3.02	119.82	125.07
4	N	5	K91	C11-C12-C13	2.81	120.74	117.40
4	D	1	K91	C17-C12-C11	-2.81	120.19	125.07
4	E	3	K91	C17-C12-C11	-2.78	120.25	125.07
4	P	7	K91	C17-C12-C11	-2.77	120.26	125.07
4	O	6	K91	C17-C12-C11	-2.76	120.27	125.07
4	Q	8	K91	C17-C12-C11	-2.75	120.29	125.07
4	N	5	K91	C17-C12-C11	-2.66	120.45	125.07
4	M	4	K91	C3-C4-CL20	-2.61	115.50	119.36
4	M	4	K91	C12-C11-CL18	2.49	123.48	119.25
4	N	5	K91	C3-C4-C5	-2.45	118.32	121.53
4	M	4	K91	C16-C17-C12	-2.39	117.69	120.91
4	E	3	K91	C11-C12-C13	2.33	120.17	117.40
4	O	6	K91	C11-C12-C13	2.33	120.17	117.40
4	D	1	K91	C11-C12-C13	2.32	120.16	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2	K91	C10-C11-C12	-2.32	117.83	121.61
4	C	2	K91	C3-C2-C1	2.31	122.81	120.50
4	Q	8	K91	C11-C12-C13	2.30	120.13	117.40
4	C	2	K91	C15-N14-C13	2.30	120.02	117.31
4	P	7	K91	C11-C12-C13	2.27	120.10	117.40
4	O	6	K91	C16-C15-N14	-2.27	120.64	123.97
4	E	3	K91	C16-C15-N14	-2.26	120.64	123.97
4	C	2	K91	C16-C17-C12	-2.26	117.86	120.91
4	D	1	K91	C16-C15-N14	-2.26	120.65	123.97
4	Q	8	K91	C16-C15-N14	-2.25	120.67	123.97
4	P	7	K91	C16-C15-N14	-2.24	120.69	123.97
4	C	2	K91	C17-C16-C15	2.22	121.69	118.92
4	M	4	K91	C17-C16-C15	2.17	121.62	118.92
4	E	3	K91	O7-C6-C1	2.01	119.98	116.59
4	D	1	K91	O7-C6-C1	2.00	119.97	116.59
4	P	7	K91	O7-C6-C1	2.00	119.97	116.59

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	GOL	C1-C2-C3-O3
2	D	2	GOL	C1-C2-C3-O3
2	D	2	GOL	O2-C2-C3-O3
2	F	3	GOL	C1-C2-C3-O3
2	J	5	GOL	C1-C2-C3-O3
2	J	13	GOL	O1-C1-C2-C3
2	L	6	GOL	O1-C1-C2-O2
2	L	6	GOL	O1-C1-C2-C3
2	L	6	GOL	C1-C2-C3-O3
2	N	7	GOL	O1-C1-C2-O2
2	N	7	GOL	O1-C1-C2-C3
2	N	7	GOL	C1-C2-C3-O3
2	Q	9	GOL	O1-C1-C2-C3
2	J	13	GOL	O1-C1-C2-O2
2	F	3	GOL	O1-C1-C2-C3
2	H	4	GOL	O1-C1-C2-C3
2	J	13	GOL	C1-C2-C3-O3
2	P	14	GOL	O1-C1-C2-C3
2	Q	9	GOL	C1-C2-C3-O3
2	B	1	GOL	O2-C2-C3-O3
2	F	3	GOL	O1-C1-C2-O2

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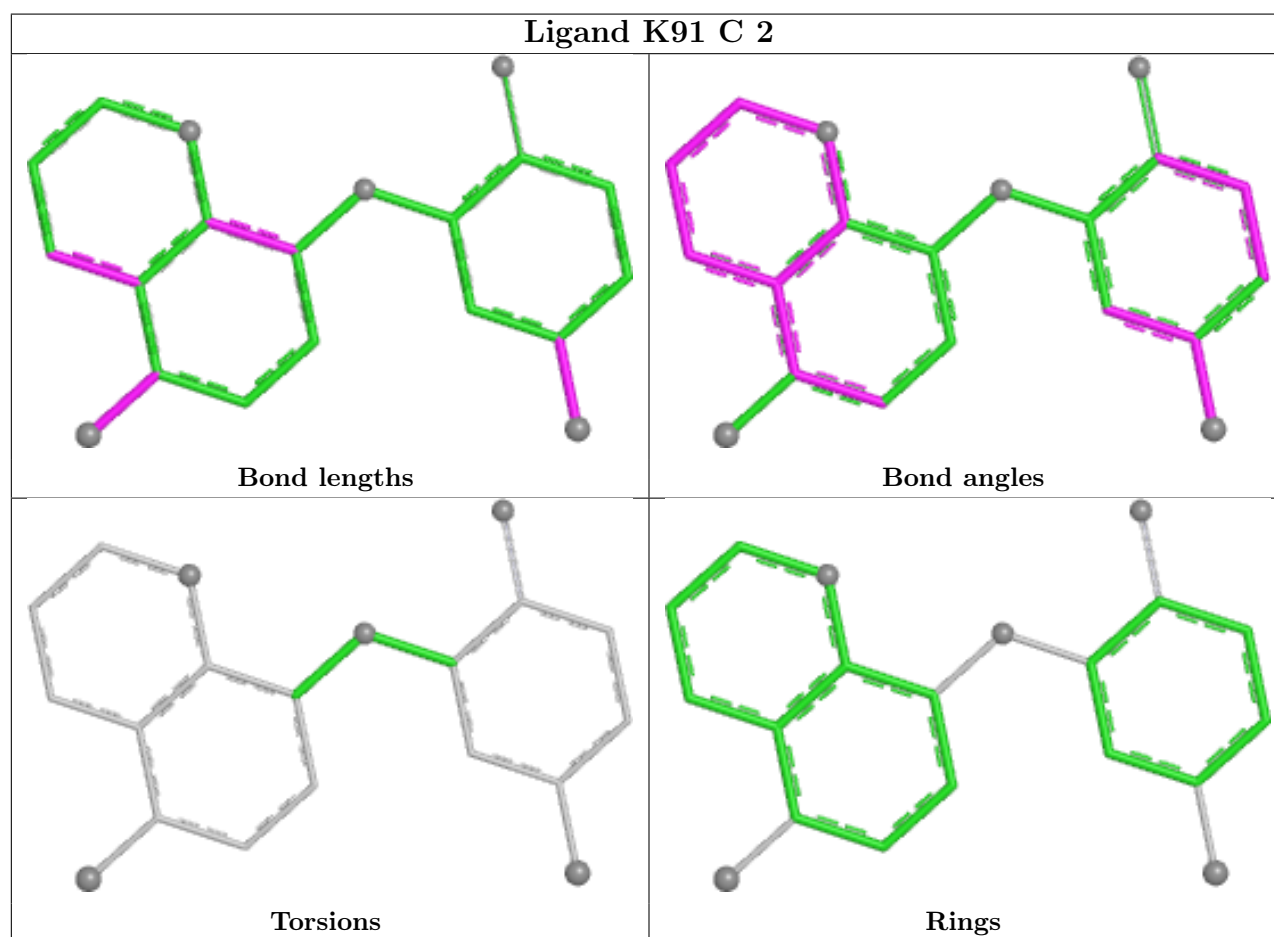
Mol	Chain	Res	Type	Atoms
2	F	3	GOL	O2-C2-C3-O3
2	J	5	GOL	O2-C2-C3-O3
2	L	6	GOL	O2-C2-C3-O3
2	P	14	GOL	O1-C1-C2-O2
2	Q	9	GOL	O1-C1-C2-O2
2	Q	9	GOL	O2-C2-C3-O3
2	N	7	GOL	O2-C2-C3-O3
2	P	8	GOL	O2-C2-C3-O3
4	E	3	K91	C13-C8-O7-C6
4	O	6	K91	C13-C8-O7-C6
2	H	4	GOL	O1-C1-C2-O2
2	J	13	GOL	O2-C2-C3-O3
4	E	3	K91	C9-C8-O7-C6
2	S	10	GOL	O1-C1-C2-O2
4	O	6	K91	C9-C8-O7-C6
4	M	4	K91	C13-C8-O7-C6
4	P	7	K91	C13-C8-O7-C6
2	S	10	GOL	O2-C2-C3-O3

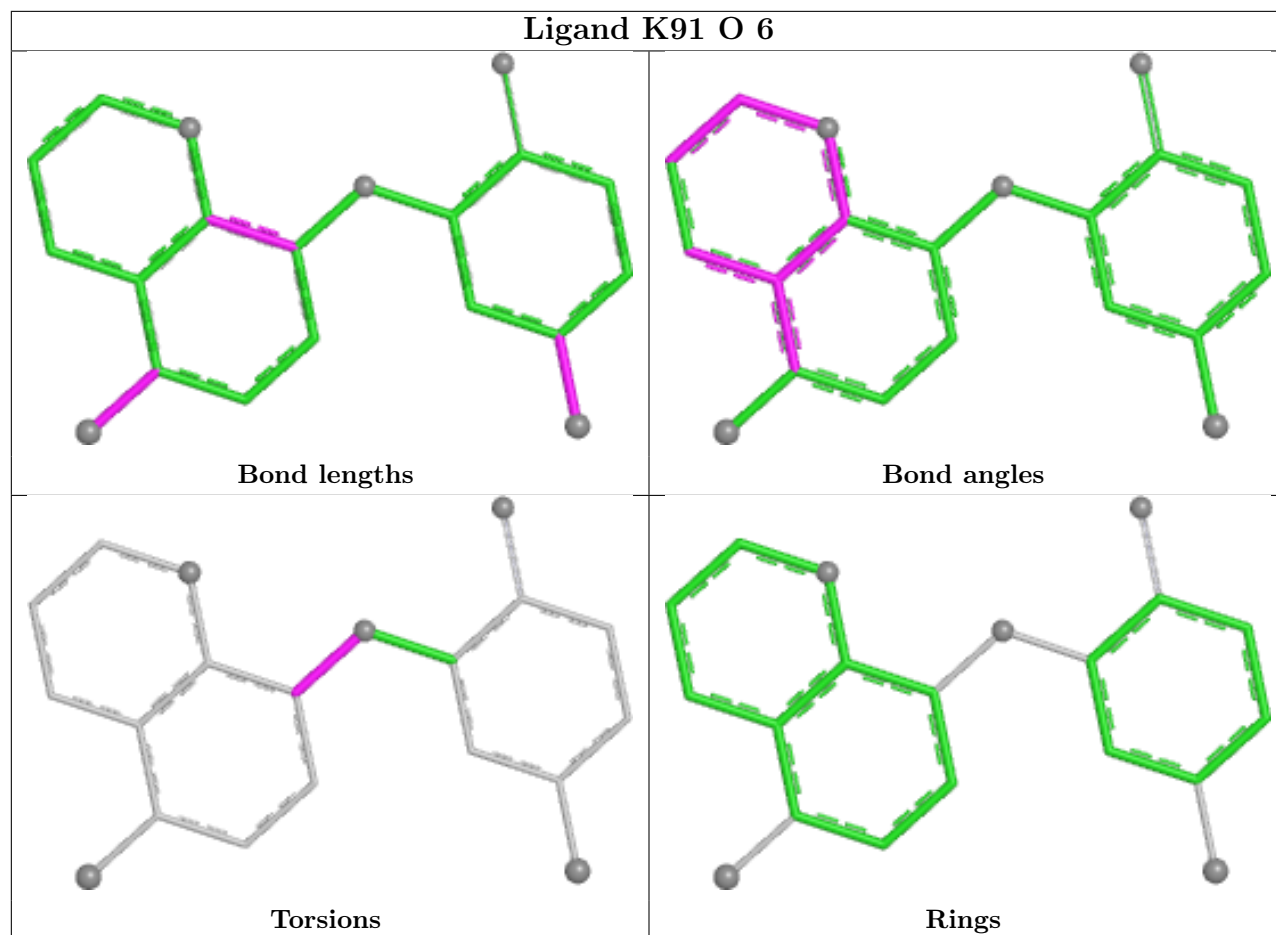
There are no ring outliers.

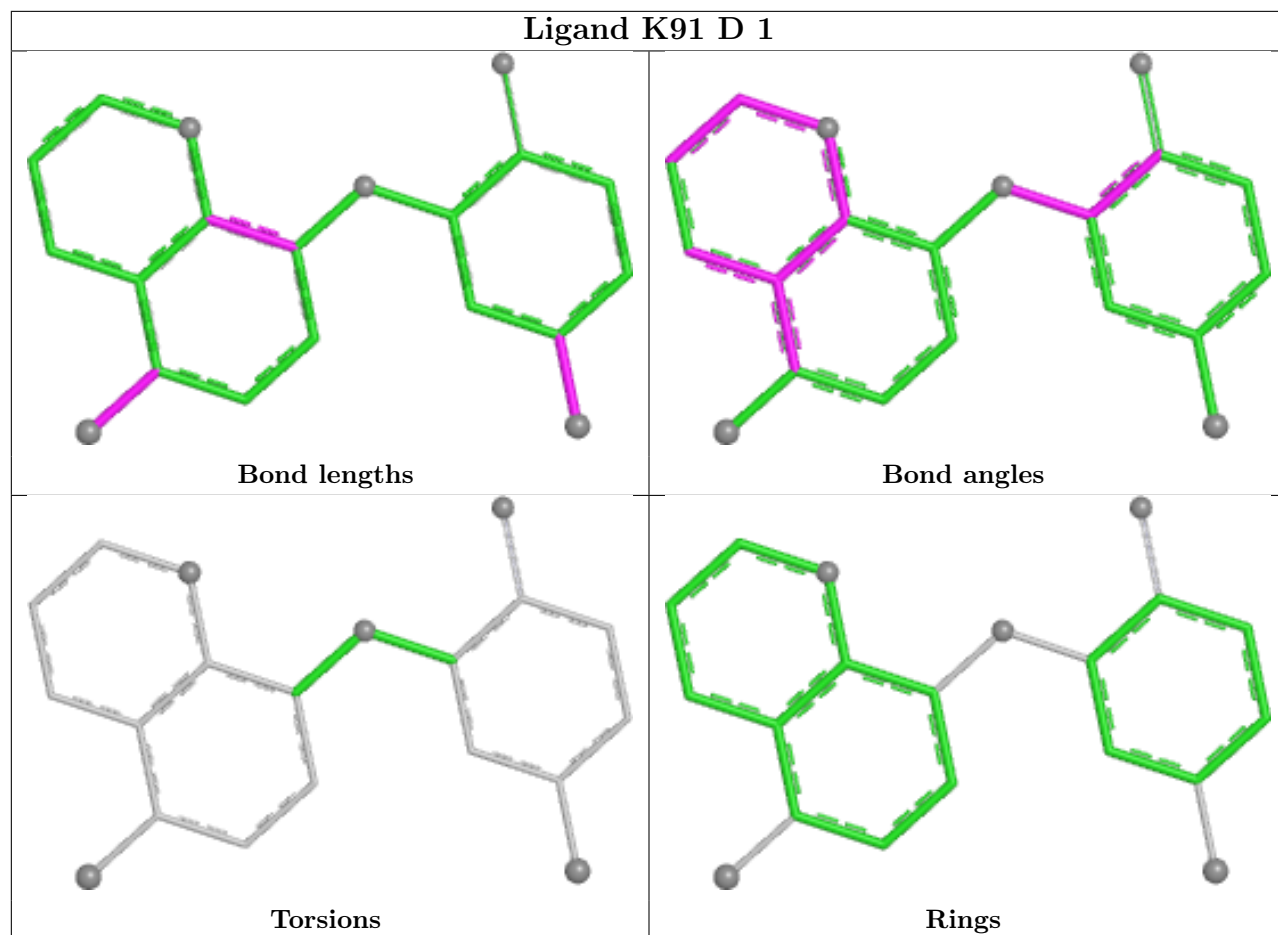
18 monomers are involved in 264 short contacts:

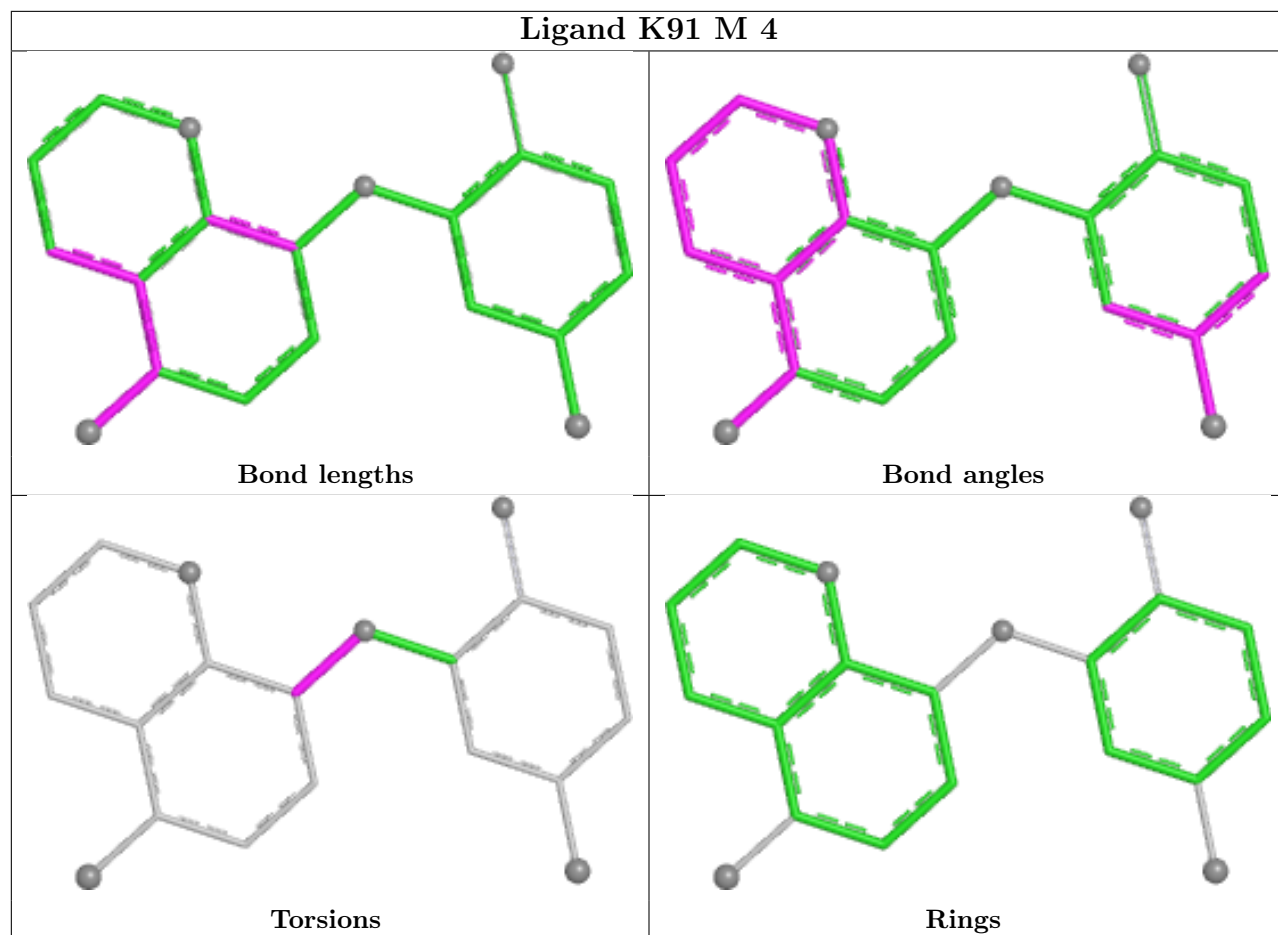
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2	K91	30	0
2	P	8	GOL	1	0
2	V	11	GOL	1	0
2	S	10	GOL	1	0
4	O	6	K91	31	0
2	B	1	GOL	3	0
4	D	1	K91	33	0
2	Q	9	GOL	3	0
4	M	4	K91	26	0
2	L	6	GOL	2	0
2	F	3	GOL	1	0
4	Q	8	K91	29	0
4	P	7	K91	25	0
4	E	3	K91	32	0
4	N	5	K91	37	0
2	P	14	GOL	3	0
2	H	4	GOL	4	0
2	J	13	GOL	2	0

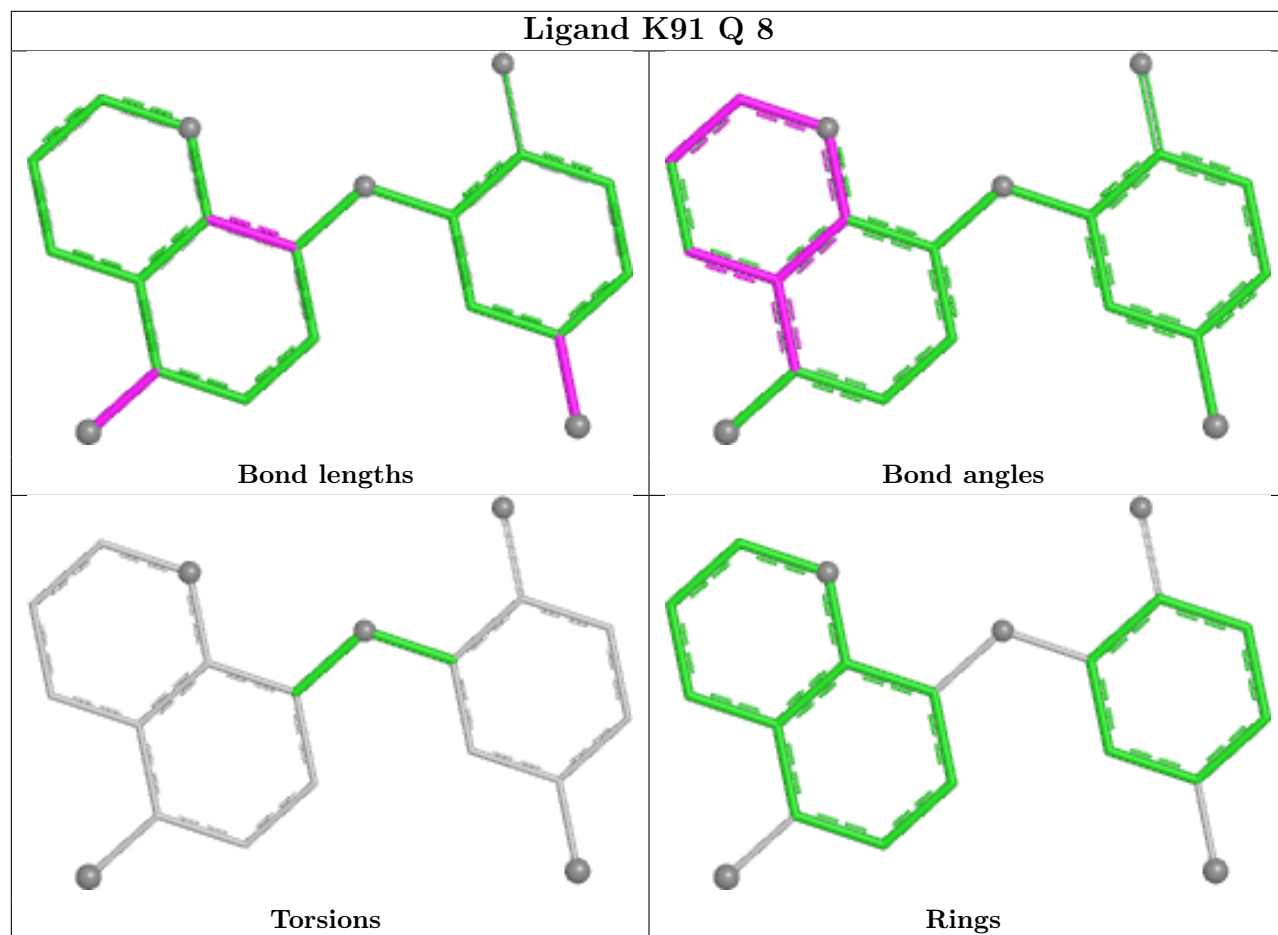
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

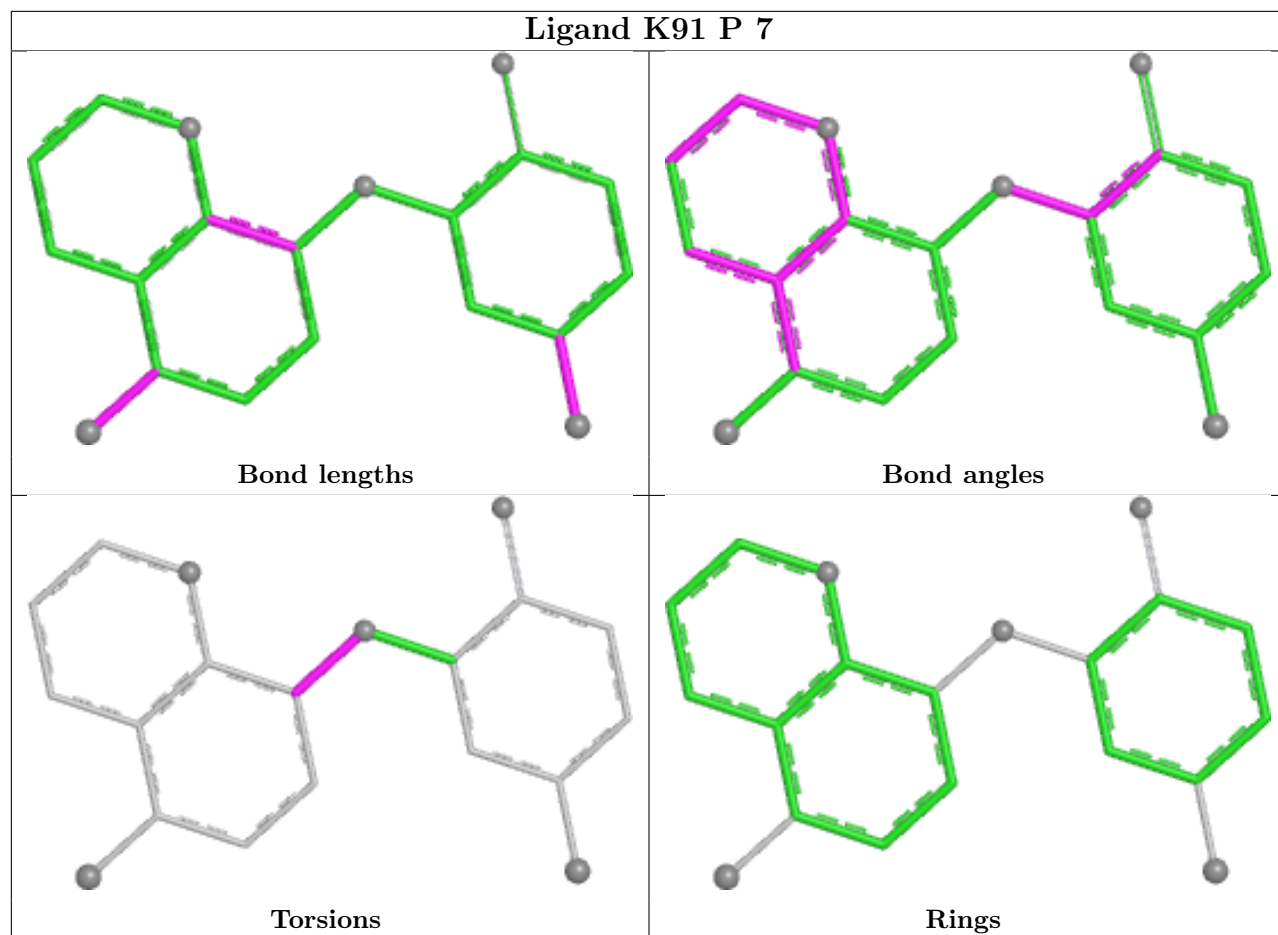


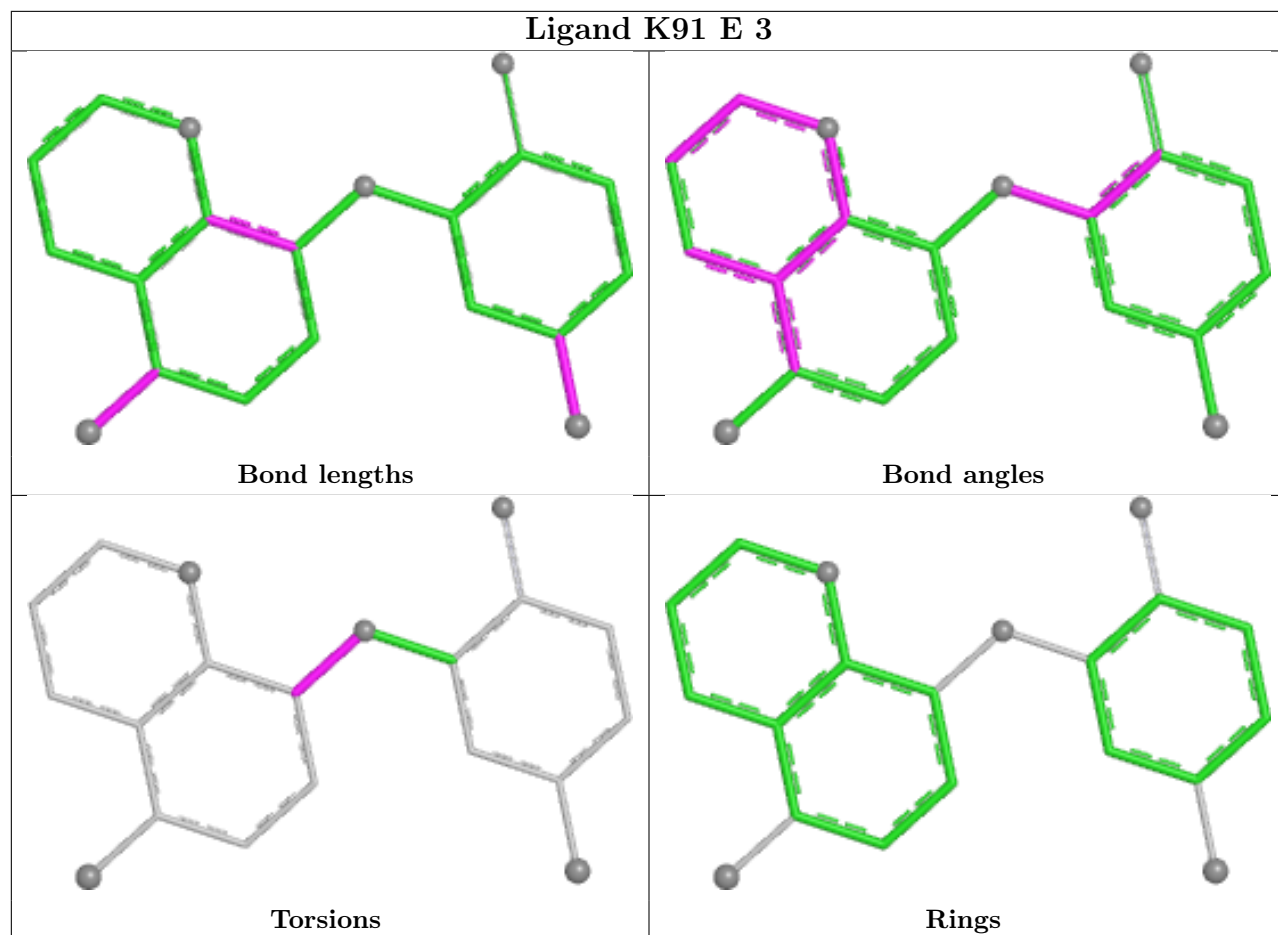


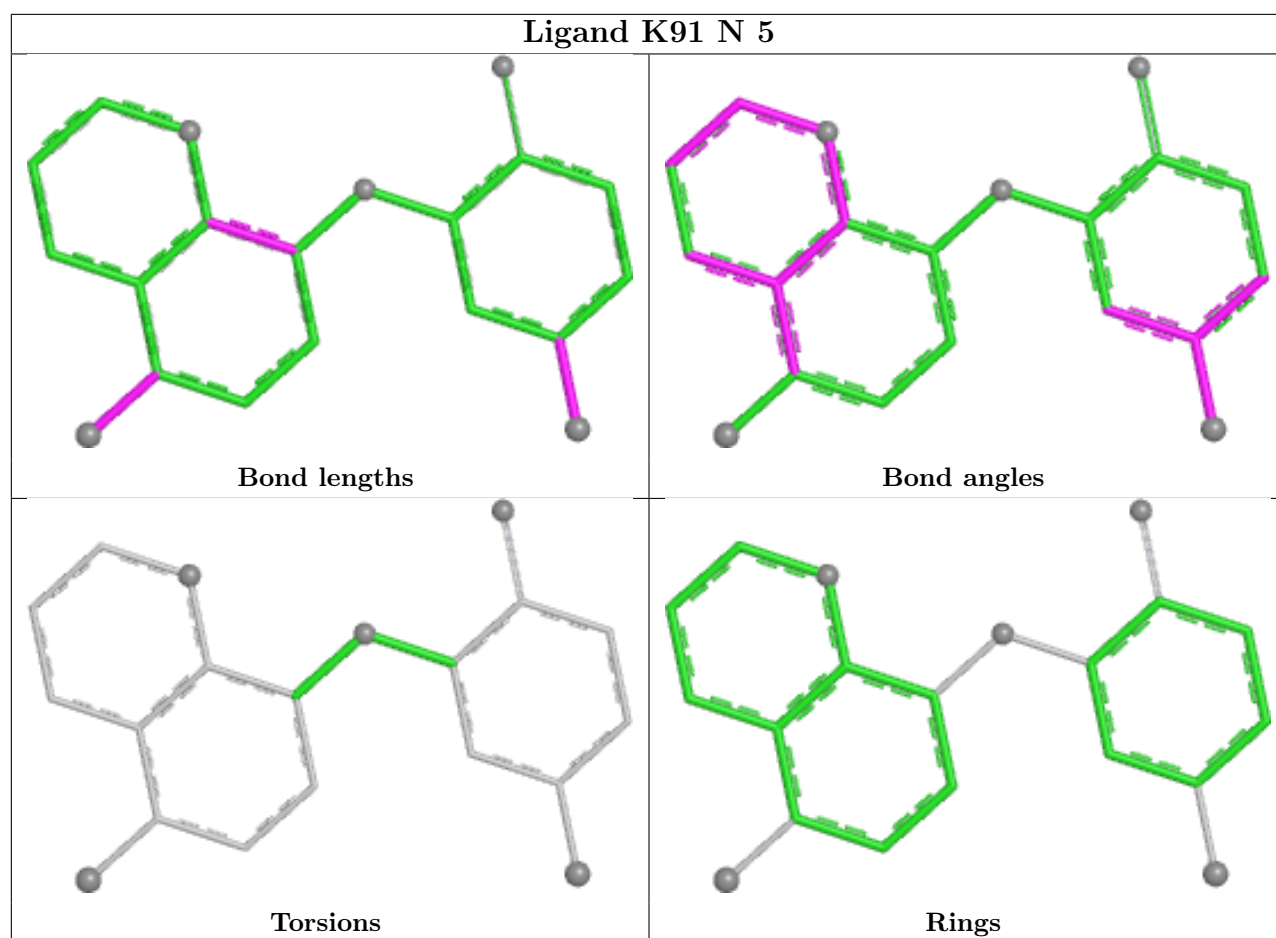












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	146/154 (94%)	-1.50	0 100 100	28, 41, 58, 68	0
1	B	145/154 (94%)	-1.50	0 100 100	28, 41, 57, 60	0
1	C	144/154 (93%)	-1.55	0 100 100	27, 40, 56, 60	0
1	D	144/154 (93%)	-1.50	0 100 100	28, 40, 56, 60	1 (0%)
1	E	142/154 (92%)	-1.52	0 100 100	28, 40, 57, 60	0
1	F	146/154 (94%)	-1.57	0 100 100	28, 41, 57, 60	0
1	G	147/154 (95%)	-1.49	0 100 100	28, 41, 57, 60	0
1	H	145/154 (94%)	-1.50	0 100 100	28, 41, 56, 61	0
1	I	144/154 (93%)	-1.44	0 100 100	28, 41, 57, 61	0
1	J	144/154 (93%)	-1.53	0 100 100	28, 41, 58, 62	1 (0%)
1	K	142/154 (92%)	-1.42	0 100 100	28, 41, 58, 61	0
1	L	146/154 (94%)	-1.37	0 100 100	28, 41, 57, 59	0
1	M	146/154 (94%)	-1.55	0 100 100	28, 41, 57, 60	0
1	N	145/154 (94%)	-1.50	0 100 100	28, 41, 57, 61	0
1	O	144/154 (93%)	-1.53	0 100 100	28, 41, 56, 61	0
1	P	144/154 (93%)	-1.52	0 100 100	28, 40, 56, 60	1 (0%)
1	Q	142/154 (92%)	-1.54	0 100 100	28, 40, 56, 62	0
1	R	146/154 (94%)	-1.55	0 100 100	28, 40, 57, 61	0
1	S	146/154 (94%)	-1.49	0 100 100	28, 41, 57, 60	0
1	T	145/154 (94%)	-1.44	0 100 100	28, 41, 56, 60	0
1	U	144/154 (93%)	-1.56	0 100 100	28, 41, 56, 60	0
1	V	144/154 (93%)	-1.48	0 100 100	28, 41, 58, 64	1 (0%)
1	W	145/154 (94%)	-1.44	0 100 100	28, 41, 56, 60	0
1	X	142/154 (92%)	-1.40	0 100 100	28, 41, 56, 60	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3468/3696 (93%)	-1.50	0 100 100	27, 41, 57, 68	4 (0%)

There are no RSRZ outliers to report.

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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

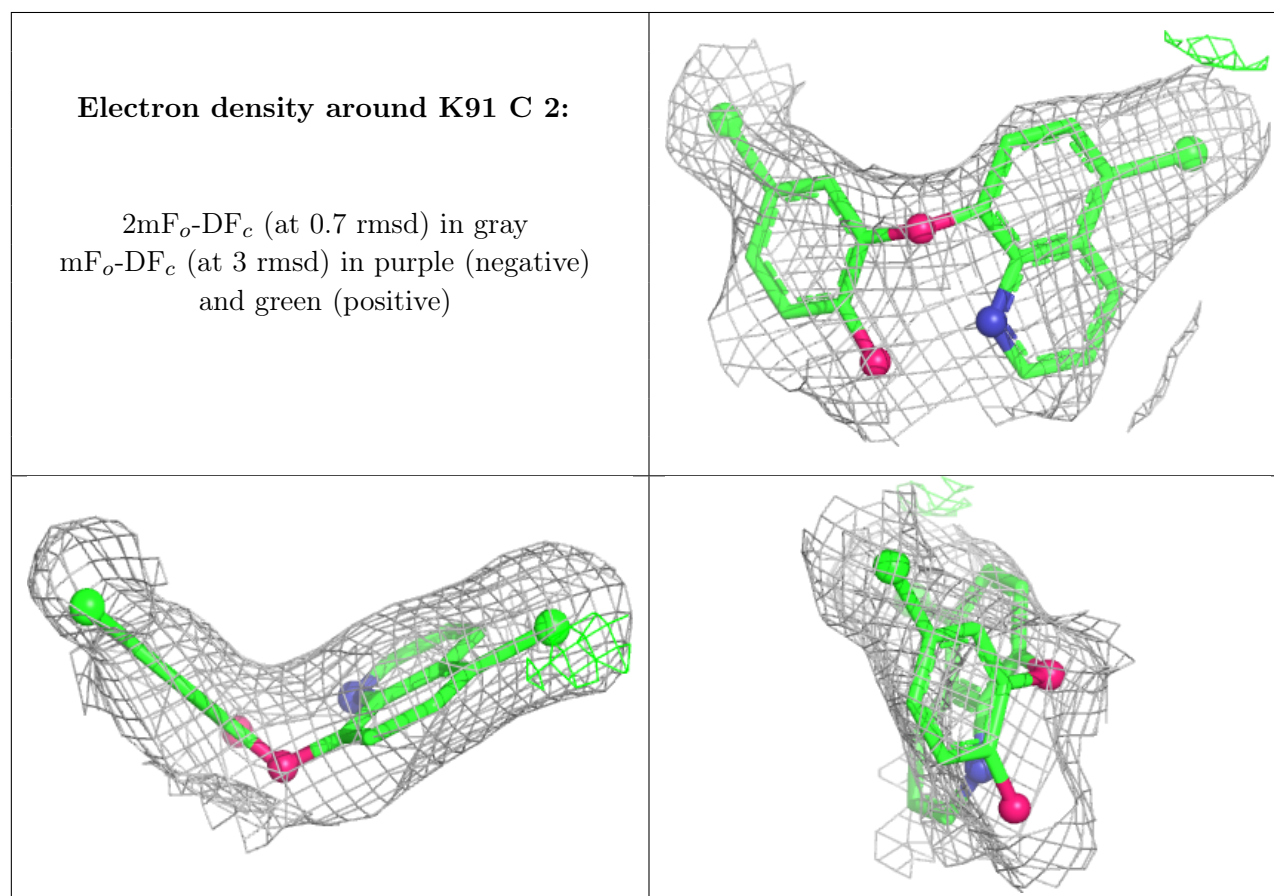
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	H	4	6/6	0.98	0.07	46,49,51,51	0
2	GOL	J	5	6/6	0.98	0.05	24,27,28,29	0
2	GOL	B	1	6/6	0.99	0.03	26,29,32,34	0
2	GOL	D	2	6/6	0.99	0.03	27,27,29,31	0
2	GOL	J	13	6/6	0.99	0.03	28,31,31,33	0
2	GOL	L	6	6/6	0.99	0.05	44,46,47,48	0
2	GOL	N	7	6/6	0.99	0.03	37,38,38,40	0
2	GOL	P	8	6/6	0.99	0.05	33,34,35,37	0
2	GOL	P	14	6/6	0.99	0.04	27,28,30,30	0
2	GOL	Q	9	6/6	0.99	0.04	35,38,41,42	0
2	GOL	S	10	6/6	0.99	0.04	36,37,39,40	0
2	GOL	W	12	6/6	0.99	0.04	43,45,48,48	0
3	PO4	B	231	5/5	0.99	0.04	41,42,44,44	0
4	K91	C	2	20/20	0.99	0.03	34,37,39,45	0
4	K91	D	1	20/20	0.99	0.03	29,35,38,41	0
4	K91	E	3	20/20	0.99	0.05	36,38,44,45	0
4	K91	M	4	20/20	0.99	0.03	34,37,39,39	0
4	K91	N	5	20/20	0.99	0.03	34,38,39,44	0
4	K91	O	6	20/20	0.99	0.03	34,38,41,41	0

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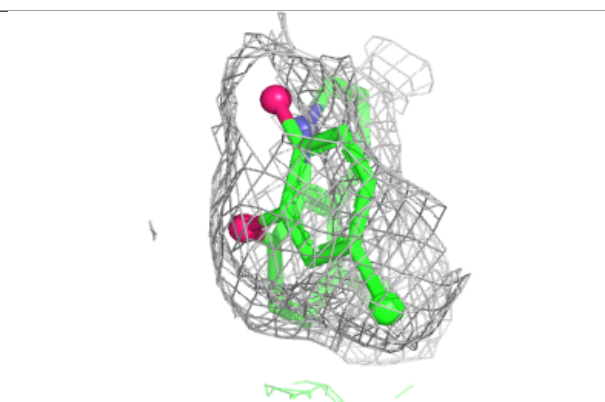
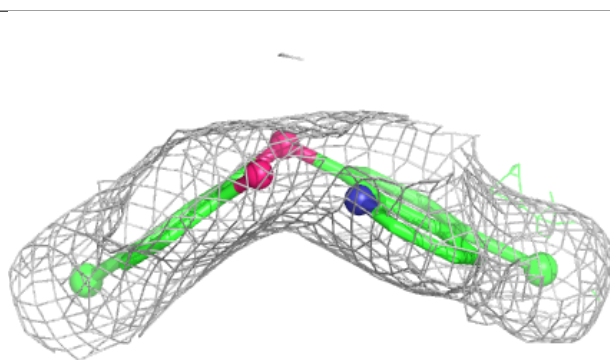
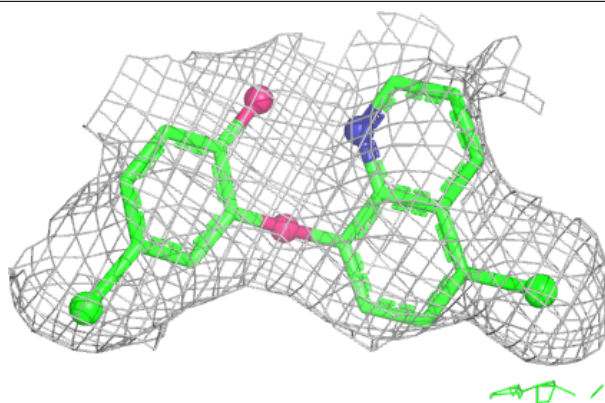
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	K91	P	7	20/20	0.99	0.03	34,38,40,43	0
2	GOL	V	11	6/6	1.00	0.03	13,21,24,26	0
2	GOL	F	3	6/6	1.00	0.03	29,34,35,36	0
4	K91	Q	8	20/20	1.00	0.03	35,39,44,45	0

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.

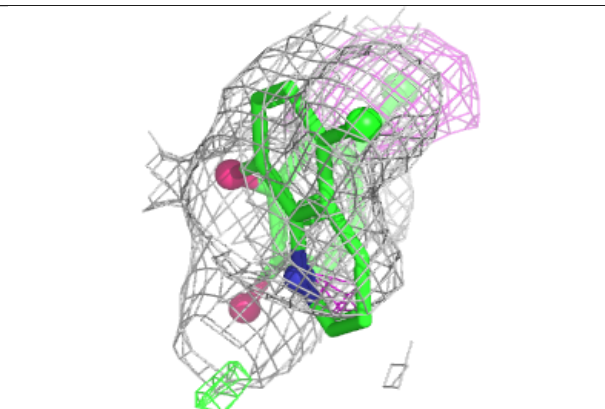
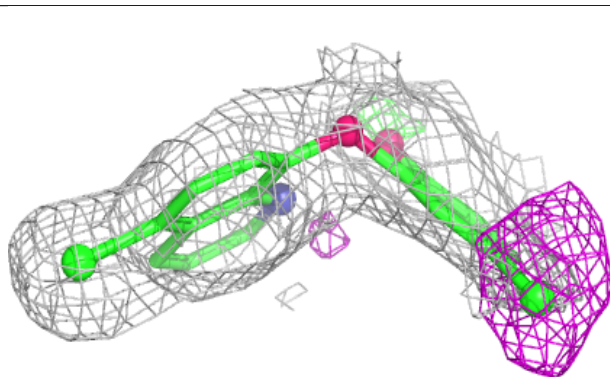
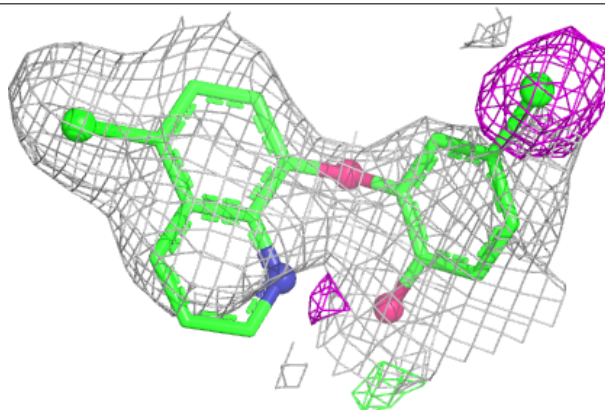


Electron density around K91 D 1:

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

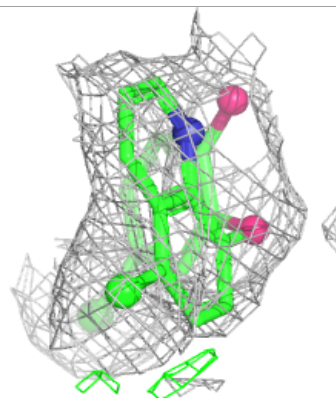
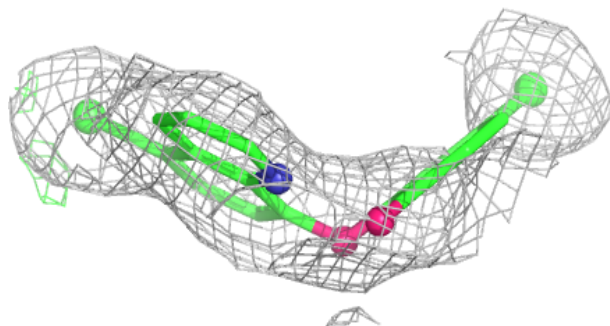
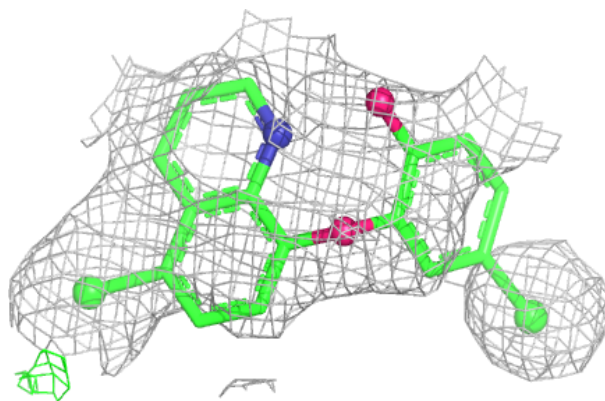
**Electron density around K91 E 3:**

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

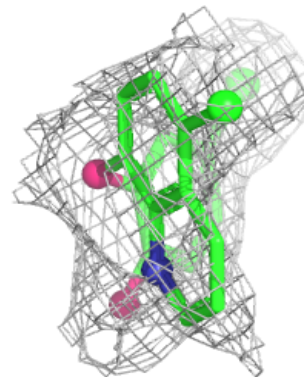
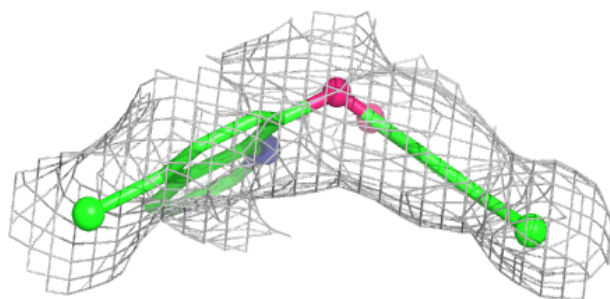
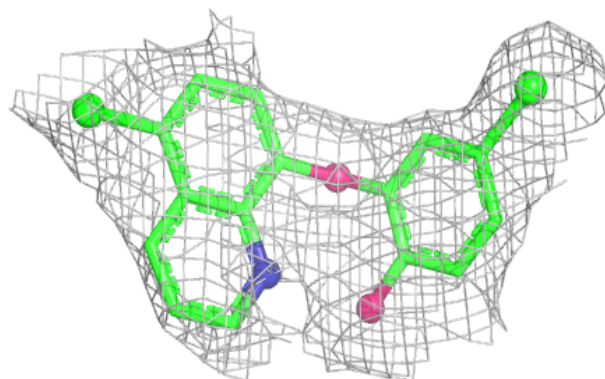


Electron density around K91 M 4:

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

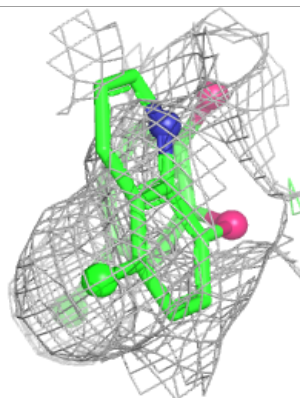
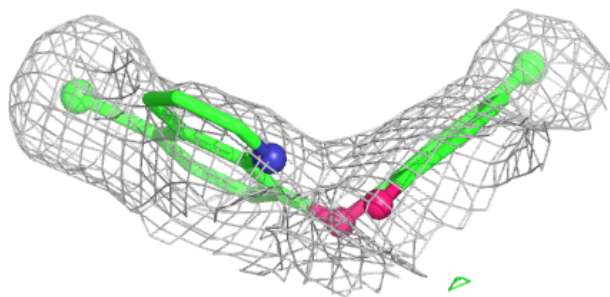
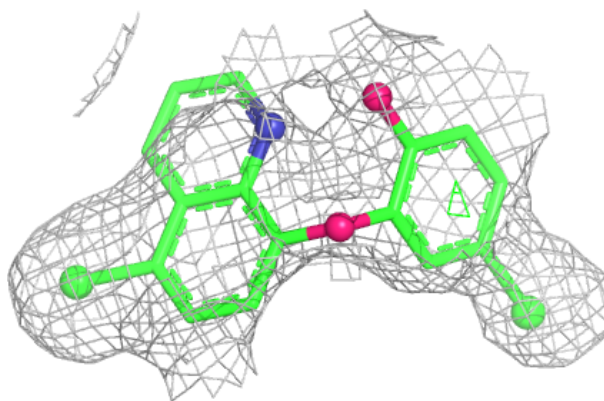
**Electron density around K91 N 5:**

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

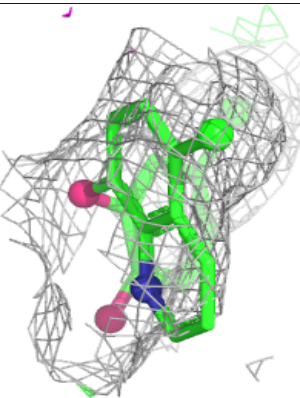
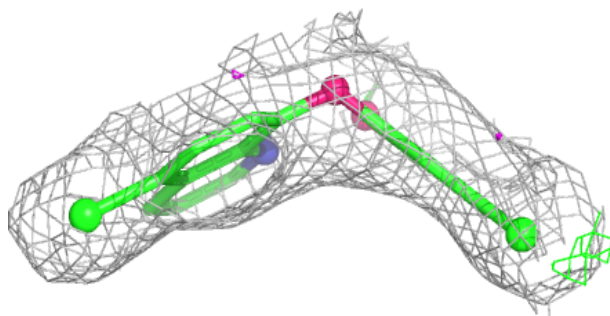
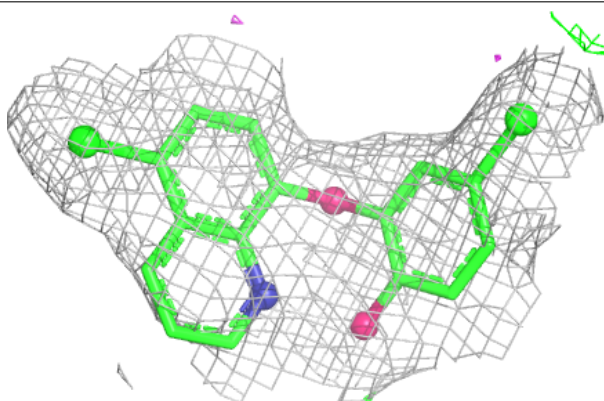


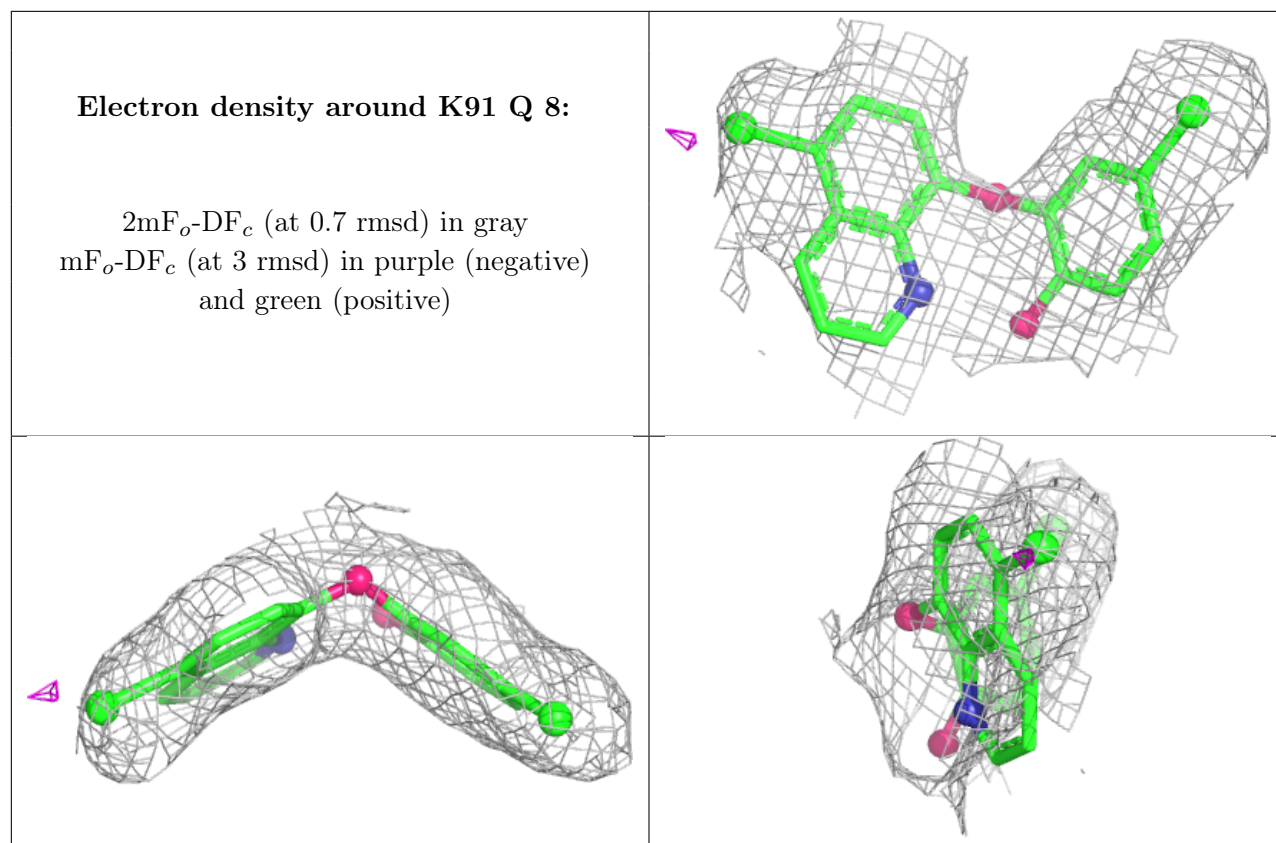
Electron density around K91 O 6:

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

**Electron density around K91 P 7:**

$2mF_o-DF_c$ (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.