



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 11:44 am BST

PDB ID : 3AZ9
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 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

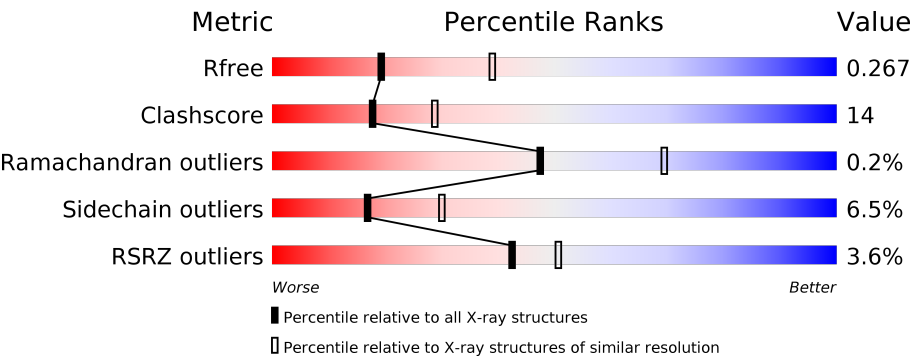
1 Overall quality at a glance i

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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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>5%</div><div><div></div><div>77%</div><div>17%</div><div>•• 5%</div></div></div>
1	B	154	<div><div>%</div><div><div></div><div>73%</div><div>21%</div><div>6%</div></div></div>
1	C	154	<div><div>3%</div><div><div></div><div>72%</div><div>20%</div><div>• 6%</div></div></div>
1	D	154	<div><div>3%</div><div><div></div><div>75%</div><div>16%</div><div>• 6%</div></div></div>
1	E	154	<div><div>%</div><div><div></div><div>75%</div><div>12%</div><div>5%</div><div>8%</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
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	-
4	K91	N	5	-	-	X	-
4	K91	O	6	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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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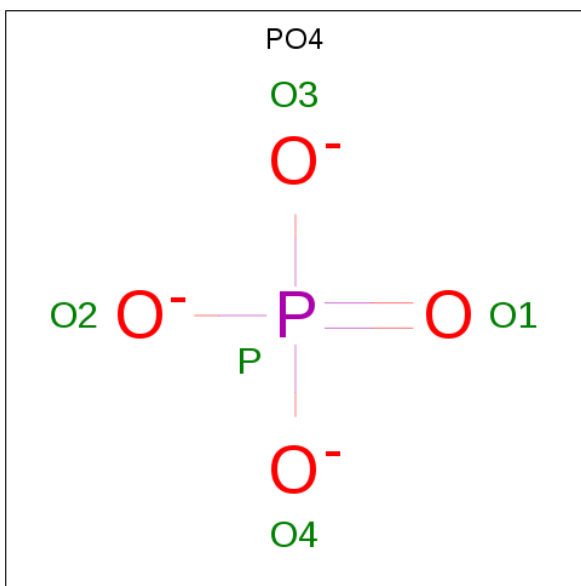
Chain	Residue	Modelled	Actual	Comment	Reference
Q	78	SER	-	EXPRESSION TAG	UNP Q965D7
Q	79	HIS	-	EXPRESSION TAG	UNP Q965D7
Q	80	MET	-	EXPRESSION TAG	UNP Q965D7
R	77	GLY	-	EXPRESSION TAG	UNP Q965D7
R	78	SER	-	EXPRESSION TAG	UNP Q965D7
R	79	HIS	-	EXPRESSION TAG	UNP Q965D7
R	80	MET	-	EXPRESSION TAG	UNP Q965D7
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 (three-letter code: GOL) (formula: $C_3H_8O_3$).



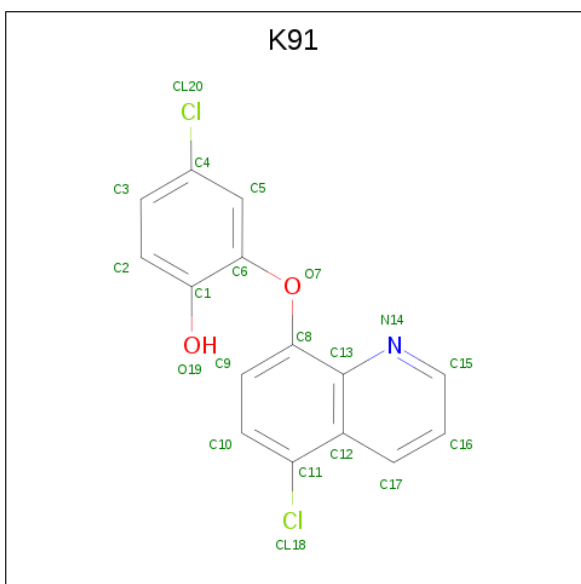
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		
2	L	1	Total	C	O	0	0
			6	3	3		
2	N	1	Total	C	O	0	0
			6	3	3		
2	P	1	Total	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 (three-letter code: 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 (three-letter code: 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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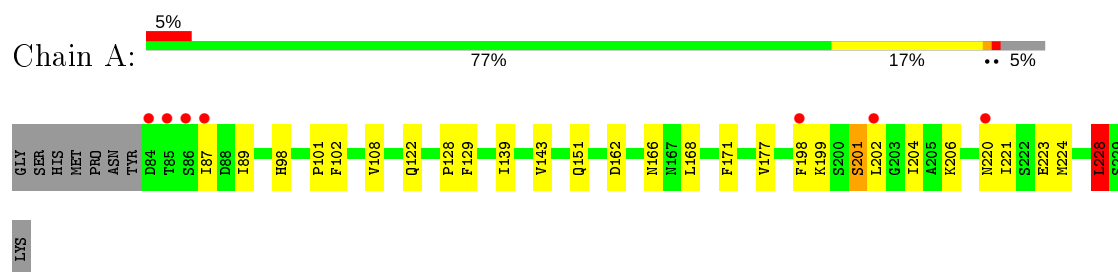
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	10	Total	O	0	0
			10	10		
5	N	23	Total	O	0	0
			23	23		
5	O	31	Total	O	0	0
			31	31		
5	P	9	Total	O	0	0
			9	9		
5	Q	15	Total	O	0	0
			15	15		
5	R	15	Total	O	0	0
			15	15		
5	S	13	Total	O	0	0
			13	13		
5	T	20	Total	O	0	0
			20	20		
5	U	14	Total	O	0	0
			14	14		
5	V	17	Total	O	0	0
			17	17		
5	W	20	Total	O	0	0
			20	20		
5	X	22	Total	O	0	0
			22	22		

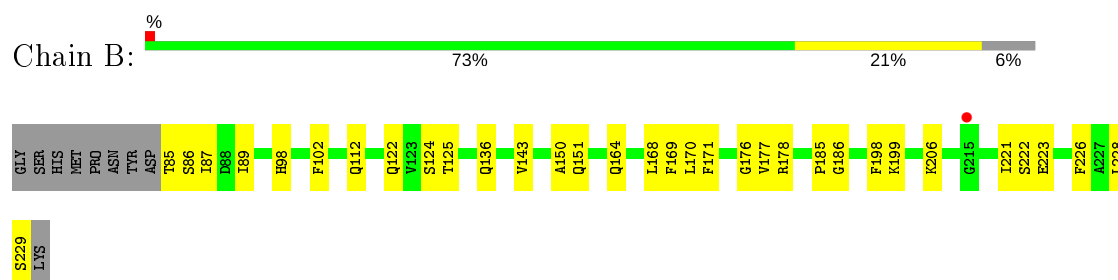
3 Residue-property plots [i](#)

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.

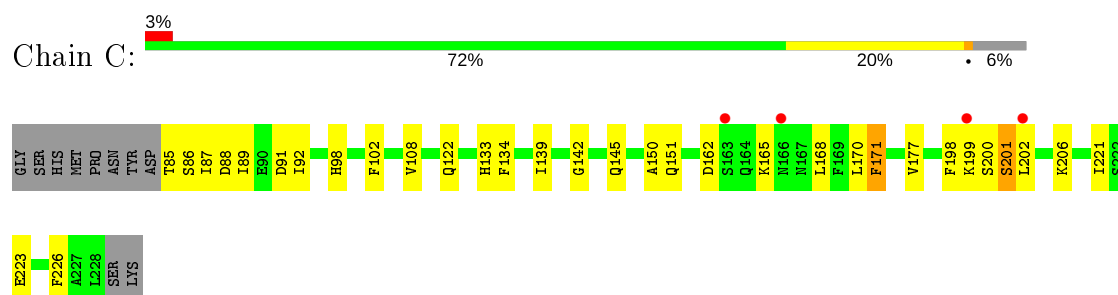
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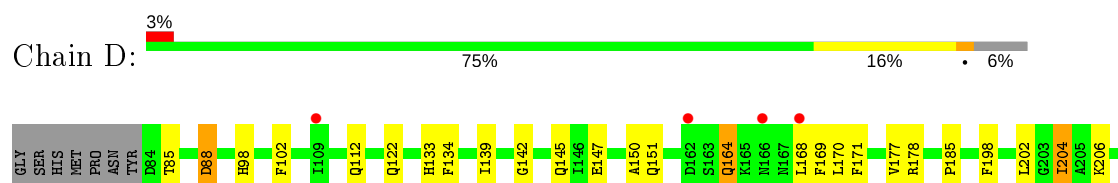
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

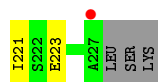


- Molecule 1: Beta-hydroxyacyl-ACP dehydratase

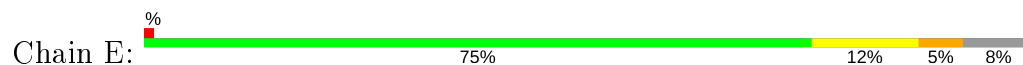


- Molecule 1: Beta-hydroxyacyl-ACP dehydratase





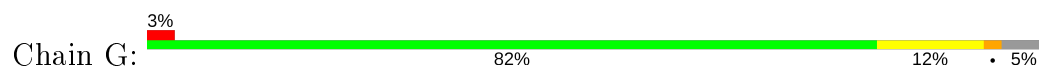
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



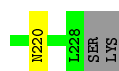
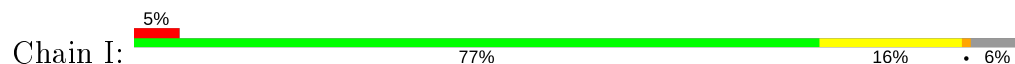
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



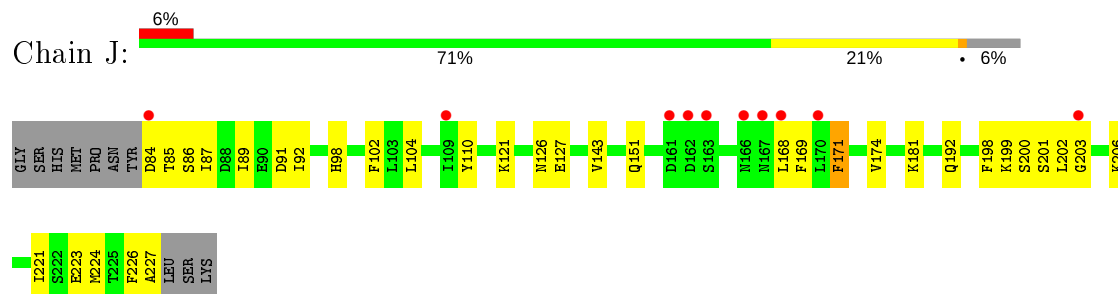
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



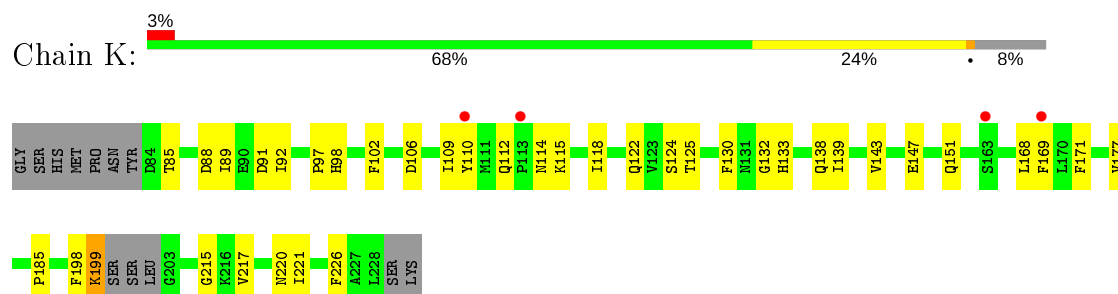
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



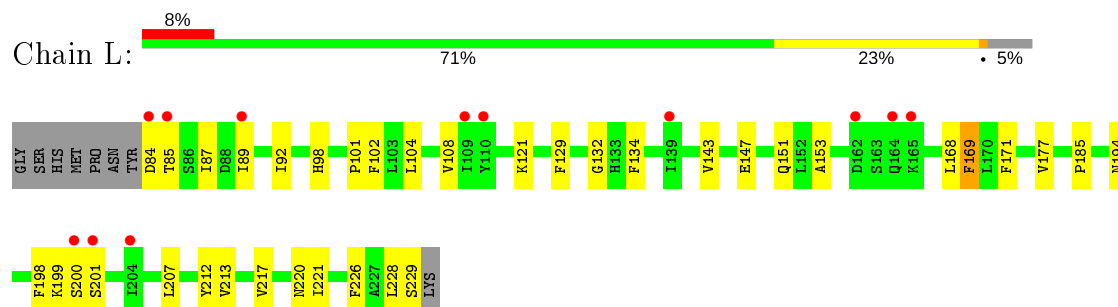
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



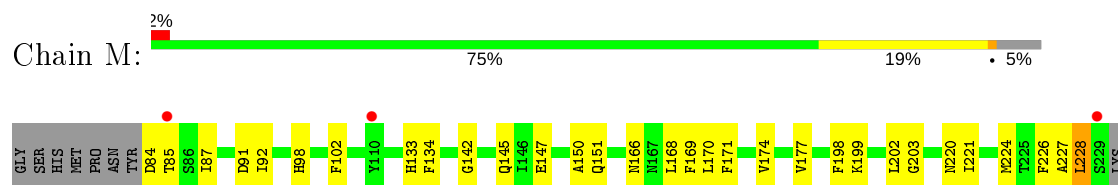
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



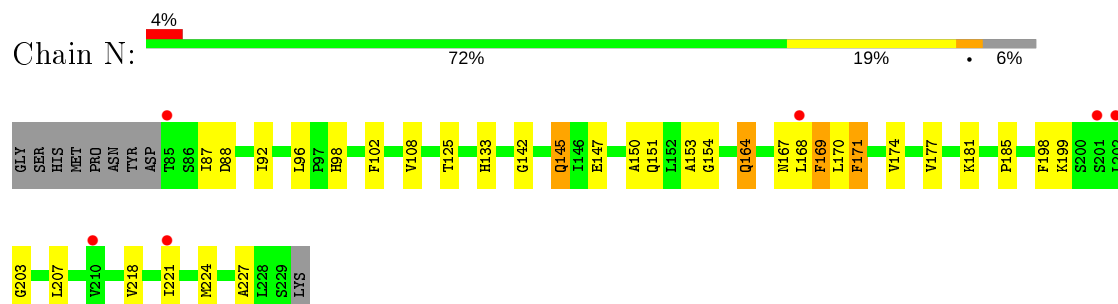
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



GLY	SER	HIS	MET	PRO	ASN	TYR	ASP
T95	S86	I87	D91	H98	F102	D106	Q122
H133	F134	G142	A150	Q151	K165	L168	F169
L170	F171	V177	K181	F198	K199	G203	I204
I221	N224	A227	L228	SER	LVS		

[illegible]

GLY	SER	HIS	NET	PRO	ASN	TYR	D84	S86	I87	D88	I89	I92	H98	P101	F102	D106	K107	V108	F129	E147	A150	Q151	Q164	F168	K199	SER	SER	SER	LEU	G203	I204	L228	SER	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	------	------	------	-----	-----

GLY	SER	HIS	MET	PRO	ASN	THR	D94	S86	I87	D91	H98	F102	V108	Q122	T125	H133	G142	V143	Q151	Q164	K165	L168	F171	K181	F198	S201	L202	G203	L204	V218	I221	M224	S229	L235
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

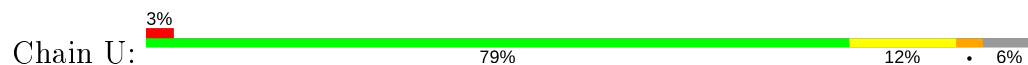
Gly	Ser	His	Met	Pro	Asn	Tyr
D84						
T85						
I89						
I92						
K93						
K94						
H98						
F102						
D106						
I109						
V110						
Q122						
N126						
E127						
P128						
F129						
E147						
Q151						
G154						
D162						
S163						
K164						
K165						
M166						
L167						
L168						
F169						
L170						
F171						
V177						
F198						
K199						
S200						
S201						
L202						
G203						
L204						
L221						



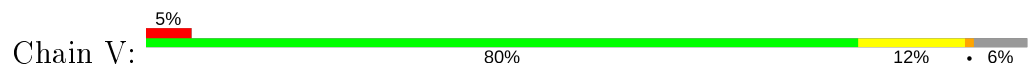
GLY	SER	HIS	MET	PRO	ASN	THR	ASP	S86	S85	T92	H98	F102	D106	K107	I108	Y110	F111	K112	Q122	T125	N126	E127	Q136	V143	Q151	G154	L158	S163	N167	L168	F169	L170	F171	V177	R178	G186	F198	K199	S200
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------



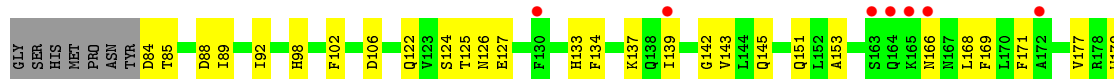
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



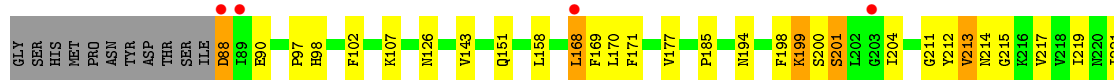
- Molecule 1: Beta-hydroxyacyl-ACP dehydratase



- 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, 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 0.233 , 0.267	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 , 14.7	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	0.89	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4, 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	0.63	0/1147	0.67	1/1553 (0.1%)
1	B	0.69	0/1136	0.67	0/1538
1	C	0.68	0/1138	0.71	0/1539
1	D	0.63	0/1126	0.69	0/1527
1	E	0.61	0/1124	0.71	1/1520 (0.1%)
1	F	0.61	0/1149	0.69	0/1554
1	G	0.67	0/1152	0.69	0/1560
1	H	0.66	0/1137	0.66	0/1539
1	I	0.67	0/1138	0.70	0/1539
1	J	0.61	0/1121	0.68	0/1520
1	K	0.68	0/1121	0.67	0/1516
1	L	0.71	0/1145	0.68	0/1550
1	M	0.68	1/1147 (0.1%)	0.66	1/1553 (0.1%)
1	N	0.61	0/1137	0.66	0/1539
1	O	0.65	0/1138	0.67	0/1539
1	P	0.60	0/1125	0.66	0/1526
1	Q	0.61	0/1117	0.68	1/1511 (0.1%)
1	R	0.62	0/1149	0.69	0/1554
1	S	0.62	0/1147	0.69	0/1553
1	T	0.68	0/1140	0.71	0/1543
1	U	0.63	0/1138	0.68	0/1539
1	V	0.62	0/1125	0.65	0/1526
1	W	0.69	0/1142	0.66	0/1546
1	X	0.66	0/1120	0.66	0/1514
All	All	0.65	1/27259 (0.0%)	0.68	4/36898 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	145	GLN	CD-NE2	-5.49	1.19	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	228	LEU	CA-CB-CG	5.86	128.78	115.30
1	Q	85	THR	N-CA-C	-5.49	96.19	111.00
1	A	228	LEU	CA-CB-CG	5.41	127.75	115.30
1	E	228	LEU	CA-CB-CG	5.21	127.29	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1125	0	1165	25	0
1	B	1114	0	1146	34	0
1	C	1116	0	1164	45	0
1	D	1104	0	1124	46	0
1	E	1103	0	1144	36	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	90	0
1	L	1123	0	1153	21	0
1	M	1125	0	1165	43	0
1	N	1115	0	1149	66	0
1	O	1116	0	1164	33	0
1	P	1103	0	1127	42	0
1	Q	1097	0	1137	35	0
1	R	1127	0	1164	23	0
1	S	1125	0	1165	28	0
1	T	1118	0	1158	88	0
1	U	1116	0	1164	15	0
1	V	1103	0	1127	19	0
1	W	1120	0	1157	54	0
1	X	1098	0	1137	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	6	0	8	3	0
2	D	6	0	8	0	0
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	36	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	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	V	17	0	0	2	0
5	W	20	0	0	0	0
5	X	22	0	0	4	0
All	All	27414	0	27785	745	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 (745) 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:N:169:PHE:CE1	4:N:5:K91:CL18	2.37	1.15
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:E:170:LEU:HD22	4:E:3:K91:H5	1.21	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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
1:O:150:ALA:HB3	4:O:6:K91:H16	1.32	1.03
4:E:3:K91:H9	1:F:134:PHE:HZ	1.18	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:T:158:LEU:HD11	1:T:169:PHE:CZ	1.94	1.01
1:Q:170:LEU:HD22	4:Q:8:K91:H5	1.37	1.01
4:C:2:K91:C2	1:D:142:GLY:N	2.23	1.01
1:M:150:ALA:CB	4:M:4:K91:C16	2.39	1.01
1:K:115:LYS:NZ	1:W:187:ASP:HA	1.75	1.01
1:K:115:LYS:CB	1:W:214:ASN:ND2	2.23	1.00
1:K:115:LYS:HZ3	1:W:187:ASP:HA	1.25	1.00
4:E:3:K91:C2	1:F:142:GLY:H	1.75	1.00
1:K:217:VAL:HG21	1:T:215:GLY:O	1.59	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:H:214:ASN:HD21	1:T:112:GLN:NE2	1.62	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:N:169:PHE:CD1	4:N:5:K91:CL18	2.56	0.95
1:K:110:TYR:CD2	1:T:109:ILE:HB	2.02	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:N	1:N:169:PHE:HD2	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:N	1:S:202:LEU:HD23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:214:ASN:HD21	1:T:112:GLN:HE21	1.15	0.90
1:S:202:LEU:H	1:S:202:LEU:HD23	1.35	0.90
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
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:M:134:PHE:HZ	4:N:5:K91:H9	1.38	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: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

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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:H:214:ASN:ND2	1:T:112:GLN:NE2	2.26	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:K:115:LYS:CB	1:W:214:ASN:CG	2.49	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:P:169:PHE:O	4:P:7:K91:H10	1.80	0.80
1:K:115:LYS:CG	1:W:214:ASN:HD21	1.94	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: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
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:HD13	4:D:1:K91:CL20	2.21	0.77
1:D:170:LEU:HD22	4:D:1:K91:C5	2.12	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:O	1:E:199:LYS:HG3	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:K:115:LYS:HB2	1:W:214:ASN:CG	2.07	0.74
1:W:166:ASN:HB3	1:W:228:LEU:HD22	1.69	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: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:J:84:ASP:C	1:J:86:SER:H	1.91	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: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: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:NZ	1:R:165:LYS:HB2	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:114:ASN:C	1:W:214:ASN:HB3	2.11	0.70
1:N:169:PHE:O	4:N:5:K91:C10	2.40	0.69
1:K:112:GLN:OE1	1:T:107:LYS:NZ	2.24	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:J:84:ASP:C	1:P:84:ASP:HB3	2.13	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:X:107:LYS:CG	5:X:410:HOH:O	2.40	0.69
1:W:139:ILE:HD13	1:X:170:LEU:HD21	1.75	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:K:115:LYS:CG	1:W:214:ASN:CG	2.62	0.68
1:I:98:HIS:CD2	1:I:151:GLN:NE2	2.62	0.68
1:J:199:LYS:C	1:J:201:SER:H	1.97	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:O19	4:Q:8:K91:N14	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:K:199:LYS:HE3	1:K:199:LYS:C	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:LEU:CB	1:D:204:ILE:CG2	2.76	0.63
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: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:166:ASN:O	1:M:228:LEU:CD2	2.48	0.60
1:M:84:ASP:O	1:M:85:THR:HG22	2.01	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:D:170:LEU:HB3	4:D:1:K91:CL20	2.38	0.60
1:B:222:SER:OG	1:H:178:ARG:NH1	2.35	0.60
1:P:98:HIS:CD2	1:P:151:GLN:HE21	2.20	0.60
1:T:98:HIS:HD2	1:T:151:GLN:HE21	1.48	0.60
1:V:107:LYS:NZ	5:V:238:HOH:O	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:R:165:LYS:HZ3	1:R:165:LYS:HB2	1.68	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
1:A:128:PRO:HG2	2:B:1:GOL:H32	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:89:ILE:HG21	1:D:185:PRO:HG2	1.87	0.56
1:D:98:HIS:CD2	1:D:151:GLN:NE2	2.73	0.56
1:B:185:PRO:HG2	1:E:89:ILE:HG21	1.87	0.56
1:F:199:LYS:C	1:F:201:SER:H	2.08	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:169:PHE:HD1	1:K:226:PHE:HB3	1.72	0.55
1:K:110:TYR:OH	1:T:107:LYS:HD3	2.05	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:H:199:LYS:C	1:H:201:SER:H	2.09	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: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:K:110:TYR:CD2	1:T:109:ILE:CB	2.83	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:A:228:LEU:CD1	1:A:228:LEU:C	2.75	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: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:J:199:LYS:C	1:J:201:SER:N	2.60	0.54
1:G:181:LYS:HE2	1:G:216:LYS:HD2	1.89	0.54
1:K:88:ASP:N	1:K:88:ASP:OD2	2.33	0.54
1:S:94:LYS:NZ	5:S:40:HOH:O	2.30	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:U:147:GLU:O	1:U:151:GLN:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:169:PHE:CE2	1:W:228:LEU:HD23	2.42	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
1:C:165:LYS:C	5:C:329:HOH:O	2.47	0.52
4:O:6:K91:C3	1:P:142:GLY:CA	2.85	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:J:84:ASP:C	1:J:86:SER:N	2.62	0.52
1:M:87:ILE:HG23	1:M:91:ASP:HB2	1.90	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:V:201:SER:C	1:V:202:LEU:HD22	2.30	0.52
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:214:ASN:CG	1:T:112:GLN:NE2	2.65	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:D:147:GLU:CD	4:D:1:K91:C15	2.79	0.49
1:K:109:ILE:CD1	1:T:110:TYR:CE2	2.96	0.49
1:K:115:LYS:HA	1:W:214:ASN:CG	2.33	0.49
1:O:106:ASP:OD1	1:R:125:THR:HG22	2.12	0.49
1:T:154:GLY:HA3	1:T:169:PHE:HE1	1.76	0.49
1:U:164:GLN:OE1	1:U:164:GLN:HA	2.12	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
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:I:153:ALA:HB1	1:I:207:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:115:LYS:CA	1:W:214:ASN:CG	2.81	0.49
1:G:166:ASN:CG	1:G:228:LEU:HD21	2.34	0.49
1:Q:150:ALA:HB1	4:Q:8:K91:C17	2.43	0.49
1:R:165:LYS:HZ2	1:R:165:LYS:HB2	1.78	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:P:88:ASP:CG	1:P:89:ILE:N	2.66	0.48
1:M:147:GLU:CD	4:M:4:K91:C15	2.81	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: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: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:D:88:ASP:OD1	1:D:88:ASP:C	2.52	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: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:U:199:LYS:HB2	1:U:202:LEU:CD1	2.44	0.47
1:S:89:ILE:HG21	1:V:185:PRO:HG2	1.97	0.47
1:V:201:SER:O	1:V:202:LEU:CD2	2.62	0.47
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
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:W:177:VAL:HG22	1:W:221:ILE:HG12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:199:LYS:C	1:X:201:SER:H	2.17	0.47
1:F:199:LYS:C	1:F:201:SER:N	2.68	0.47
1:M:177:VAL:HB	1:N:174:VAL:HG12	1.97	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:206:LYS:HD3	1:B:223:GLU:OE2	2.15	0.47
1:B:124:SER:HB2	1:E:122:GLN:O	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: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: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: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
1:N:199:LYS:HE3	1:N:199:LYS:HB2	1.71	0.46
1:R:202:LEU:CB	1:R:204:ILE:HG13	2.46	0.46
1:K:115:LYS:HZ1	1:W:187:ASP:HA	1.72	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
4:O:6:K91:C3	1:P:142:GLY:N	2.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:133:HIS:CE1	4:P:7:K91:O7	2.69	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:O:221:ILE:HG21	1:O:224:MET:HG3	1.99	0.45
1:N:185:PRO:HG2	1:Q:89:ILE:HG21	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:W:200:SER:O	1:W:201:SER:C	2.55	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:A:199:LYS:C	1:A:201:SER:N	2.71	0.44
1:K:118:ILE:HD12	1:T:109:ILE:HG13	1.99	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:K:98:HIS:HA	1:L:132:GLY:O	2.18	0.44
1:X:211:GLY:HA3	1:X:219:ILE:HG22	2.00	0.44
1:X:177:VAL:HG22	1:X:221:ILE:HG12	2.00	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:199:LYS:C	1:H:201:SER:N	2.72	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:I:177:VAL:C	1:I:178:ARG:HG2	2.39	0.43
1:A:228:LEU:HD12	1:A:228:LEU:C	2.39	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:A:199:LYS:O	1:A:201:SER:N	2.52	0.43
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
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: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:Q:147:GLU:CD	4:Q:8:K91:C15	2.88	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: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
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:N	1:V:202:LEU:HD13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:P:221:ILE:HG21	1:P:224:MET:HG3	2.02	0.41
1:Q:84:ASP:OD2	1:Q:84:ASP:N	2.53	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:HG21	1:D:139:ILE:HD13	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:T:177:VAL:C	1:T:178:ARG:HG2	2.40	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:CA	1:U:164:GLN:OE1	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:K:215:GLY:C	1:T:212:TYR:HH	2.20	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:U:88:ASP:OD1	1:U:88:ASP:C	2.58	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
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: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:M:142:GLY:N	4:N:5:K91:C1	2.73	0.41
1:Q:228:LEU:CD1	1:Q:228:LEU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:226:PHE:CE1	4:E:3:K91:C17	3.04	0.40
1:C:206:LYS:HD3	1:C:223:GLU:OE2	2.21	0.40
1:C:89:ILE:HA	1:C:92:ILE:HD12	2.04	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
4:M:4:K91:C1	1:N:142:GLY:H	2.28	0.40
1:X:212:TYR:C	1:X:213:VAL:HG23	2.41	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%)	11	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	22	39
1	K	138/154 (90%)	130 (94%)	8 (6%)	0	100	100
1	L	144/154 (94%)	136 (94%)	7 (5%)	1 (1%)	22	39
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%)	22	39
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%)	11	19
All	All	3414/3696 (92%)	3160 (93%)	247 (7%)	7 (0%)	47	69

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	89	ILE
1	X	213	VAL
1	F	200	SER
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%)	119 (94%)	7 (6%)	21	36
1	B	123/135 (91%)	116 (94%)	7 (6%)	20	36
1	C	125/135 (93%)	118 (94%)	7 (6%)	21	36
1	D	122/135 (90%)	113 (93%)	9 (7%)	13	24
1	E	123/135 (91%)	115 (94%)	8 (6%)	17	30
1	F	126/135 (93%)	117 (93%)	9 (7%)	14	26
1	G	126/135 (93%)	117 (93%)	9 (7%)	14	26
1	H	124/135 (92%)	116 (94%)	8 (6%)	17	30
1	I	125/135 (93%)	118 (94%)	7 (6%)	21	36
1	J	121/135 (90%)	115 (95%)	6 (5%)	24	42
1	K	122/135 (90%)	115 (94%)	7 (6%)	20	36
1	L	125/135 (93%)	113 (90%)	12 (10%)	8	14
1	M	126/135 (93%)	119 (94%)	7 (6%)	21	36
1	N	124/135 (92%)	117 (94%)	7 (6%)	21	36
1	O	125/135 (93%)	118 (94%)	7 (6%)	21	36
1	P	122/135 (90%)	115 (94%)	7 (6%)	20	36
1	Q	122/135 (90%)	114 (93%)	8 (7%)	16	29
1	R	126/135 (93%)	117 (93%)	9 (7%)	14	26
1	S	126/135 (93%)	119 (94%)	7 (6%)	21	36
1	T	125/135 (93%)	113 (90%)	12 (10%)	8	14
1	U	125/135 (93%)	115 (92%)	10 (8%)	12	21
1	V	122/135 (90%)	116 (95%)	6 (5%)	25	43
1	W	125/135 (93%)	116 (93%)	9 (7%)	14	25
1	X	122/135 (90%)	114 (93%)	8 (7%)	16	29
All	All	2978/3240 (92%)	2785 (94%)	193 (6%)	17	30

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	PHE

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Mol	Chain	Res	Type
1	A	168	LEU
1	A	171	PHE
1	A	198	PHE
1	A	201	SER
1	A	220	ASN
1	A	228	LEU
1	B	102	PHE
1	B	164	GLN
1	B	168	LEU
1	B	171	PHE
1	B	198	PHE
1	B	199	LYS
1	B	229	SER
1	C	85	THR
1	C	86	SER
1	C	102	PHE
1	C	168	LEU
1	C	171	PHE
1	C	198	PHE
1	C	201	SER
1	D	85	THR
1	D	88	ASP
1	D	102	PHE
1	D	164	GLN
1	D	168	LEU
1	D	171	PHE
1	D	178	ARG
1	D	198	PHE
1	D	204	ILE
1	E	84	ASP
1	E	85	THR
1	E	102	PHE
1	E	168	LEU
1	E	169	PHE
1	E	171	PHE
1	E	198	PHE
1	E	199	LYS
1	F	85	THR
1	F	102	PHE
1	F	165	LYS
1	F	168	LEU
1	F	171	PHE

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Mol	Chain	Res	Type
1	F	198	PHE
1	F	201	SER
1	F	216	LYS
1	F	229	SER
1	G	102	PHE
1	G	168	LEU
1	G	169	PHE
1	G	171	PHE
1	G	181	LYS
1	G	198	PHE
1	G	202	LEU
1	G	220	ASN
1	G	229	SER
1	H	86	SER
1	H	102	PHE
1	H	136	GLN
1	H	168	LEU
1	H	171	PHE
1	H	198	PHE
1	H	201	SER
1	H	220	ASN
1	I	102	PHE
1	I	168	LEU
1	I	171	PHE
1	I	181	LYS
1	I	198	PHE
1	I	200	SER
1	I	220	ASN
1	J	102	PHE
1	J	168	LEU
1	J	171	PHE
1	J	181	LYS
1	J	198	PHE
1	J	202	LEU
1	K	85	THR
1	K	102	PHE
1	K	168	LEU
1	K	171	PHE
1	K	198	PHE
1	K	199	LYS
1	K	220	ASN
1	L	84	ASP

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Mol	Chain	Res	Type
1	L	85	THR
1	L	102	PHE
1	L	168	LEU
1	L	169	PHE
1	L	171	PHE
1	L	198	PHE
1	L	199	LYS
1	L	200	SER
1	L	201	SER
1	L	220	ASN
1	L	229	SER
1	M	102	PHE
1	M	168	LEU
1	M	171	PHE
1	M	198	PHE
1	M	199	LYS
1	M	202	LEU
1	M	220	ASN
1	N	102	PHE
1	N	145	GLN
1	N	164	GLN
1	N	168	LEU
1	N	169	PHE
1	N	171	PHE
1	N	198	PHE
1	O	85	THR
1	O	102	PHE
1	O	165	LYS
1	O	168	LEU
1	O	171	PHE
1	O	181	LYS
1	O	198	PHE
1	P	88	ASP
1	P	102	PHE
1	P	168	LEU
1	P	171	PHE
1	P	181	LYS
1	P	198	PHE
1	P	202	LEU
1	Q	84	ASP
1	Q	88	ASP
1	Q	102	PHE

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Mol	Chain	Res	Type
1	Q	168	LEU
1	Q	171	PHE
1	Q	198	PHE
1	Q	199	LYS
1	Q	228	LEU
1	R	84	ASP
1	R	85	THR
1	R	102	PHE
1	R	164	GLN
1	R	165	LYS
1	R	168	LEU
1	R	171	PHE
1	R	198	PHE
1	R	201	SER
1	S	85	THR
1	S	102	PHE
1	S	168	LEU
1	S	171	PHE
1	S	198	PHE
1	S	202	LEU
1	S	228	LEU
1	T	85	THR
1	T	86	SER
1	T	87	ILE
1	T	88	ASP
1	T	102	PHE
1	T	136	GLN
1	T	168	LEU
1	T	169	PHE
1	T	171	PHE
1	T	198	PHE
1	T	201	SER
1	T	202	LEU
1	U	85	THR
1	U	86	SER
1	U	89	ILE
1	U	102	PHE
1	U	164	GLN
1	U	168	LEU
1	U	171	PHE
1	U	198	PHE
1	U	200	SER

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Mol	Chain	Res	Type
1	U	202	LEU
1	V	102	PHE
1	V	168	LEU
1	V	171	PHE
1	V	198	PHE
1	V	201	SER
1	V	202	LEU
1	W	84	ASP
1	W	85	THR
1	W	88	ASP
1	W	102	PHE
1	W	168	LEU
1	W	171	PHE
1	W	181	LYS
1	W	198	PHE
1	W	200	SER
1	X	88	ASP
1	X	102	PHE
1	X	168	LEU
1	X	171	PHE
1	X	198	PHE
1	X	199	LYS
1	X	200	SER
1	X	201	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

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

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Mol	Chain	Res	Type
1	I	114	ASN
1	J	98	HIS
1	K	98	HIS
1	L	98	HIS
1	L	194	ASN
1	M	98	HIS
1	M	145	GLN
1	N	98	HIS
1	N	214	ASN
1	O	98	HIS
1	O	164	GLN
1	P	98	HIS
1	P	145	GLN
1	Q	98	HIS
1	Q	145	GLN
1	R	98	HIS
1	R	136	GLN
1	R	145	GLN
1	S	98	HIS
1	T	98	HIS
1	T	112	GLN
1	T	164	GLN
1	U	98	HIS
1	U	122	GLN
1	V	98	HIS
1	W	98	HIS
1	W	145	GLN
1	W	214	ASN
1	X	98	HIS
1	X	145	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	E	3	-	22,22,22	1.22	3 (13%)	29,31,31	1.27	5 (17%)
2	GOL	P	8	-	5,5,5	0.48	0	5,5,5	0.96	0
2	GOL	B	1	-	5,5,5	0.41	0	5,5,5	0.55	0
2	GOL	D	2	-	5,5,5	0.54	0	5,5,5	0.79	0
2	GOL	S	10	-	5,5,5	0.40	0	5,5,5	0.26	0
2	GOL	N	7	-	5,5,5	0.37	0	5,5,5	0.68	0
2	GOL	H	4	-	5,5,5	0.50	0	5,5,5	0.78	0
3	PO4	B	231	-	4,4,4	1.19	0	6,6,6	0.36	0
2	GOL	F	3	-	5,5,5	0.51	0	5,5,5	0.43	0
4	K91	O	6	-	22,22,22	1.22	3 (13%)	29,31,31	1.26	4 (13%)
2	GOL	Q	9	-	5,5,5	0.19	0	5,5,5	0.27	0
2	GOL	V	11	-	5,5,5	0.50	0	5,5,5	0.58	0
2	GOL	L	6	-	5,5,5	0.34	0	5,5,5	0.51	0
4	K91	Q	8	-	22,22,22	1.22	3 (13%)	29,31,31	1.26	5 (17%)
4	K91	P	7	-	22,22,22	1.22	3 (13%)	29,31,31	1.25	5 (17%)
2	GOL	P	14	-	5,5,5	0.41	0	5,5,5	1.00	0
2	GOL	J	5	-	5,5,5	0.40	0	5,5,5	0.51	0
4	K91	N	5	-	22,22,22	1.59	3 (13%)	29,31,31	1.58	6 (20%)
2	GOL	J	13	-	5,5,5	0.43	0	5,5,5	0.44	0
4	K91	C	2	-	22,22,22	1.71	4 (18%)	29,31,31	1.89	11 (37%)
4	K91	M	4	-	22,22,22	1.60	4 (18%)	29,31,31	1.77	9 (31%)
4	K91	D	1	-	22,22,22	1.22	3 (13%)	29,31,31	1.27	5 (17%)
2	GOL	W	12	-	5,5,5	0.47	0	5,5,5	0.62	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	E	3	-	-	2/4/4/4	0/3/3/3
2	GOL	P	8	-	-	1/4/4/4	-
2	GOL	B	1	-	-	2/4/4/4	-
2	GOL	D	2	-	-	2/4/4/4	-
2	GOL	S	10	-	-	1/4/4/4	-
2	GOL	N	7	-	-	4/4/4/4	-
2	GOL	H	4	-	-	2/4/4/4	-
2	GOL	F	3	-	-	4/4/4/4	-
4	K91	O	6	-	-	2/4/4/4	0/3/3/3
2	GOL	Q	9	-	-	4/4/4/4	-
2	GOL	V	11	-	-	0/4/4/4	-
2	GOL	L	6	-	-	4/4/4/4	-
4	K91	Q	8	-	-	0/4/4/4	0/3/3/3
4	K91	P	7	-	-	0/4/4/4	0/3/3/3
2	GOL	P	14	-	-	2/4/4/4	-
2	GOL	J	5	-	-	2/4/4/4	-
4	K91	N	5	-	-	0/4/4/4	0/3/3/3
2	GOL	J	13	-	-	4/4/4/4	-
4	K91	C	2	-	-	0/4/4/4	0/3/3/3
4	K91	M	4	-	-	0/4/4/4	0/3/3/3
4	K91	D	1	-	-	0/4/4/4	0/3/3/3
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	-5.05	1.36	1.42
4	M	4	K91	C8-C13	-4.38	1.36	1.42
4	N	5	K91	C4-CL20	3.88	1.82	1.74
4	N	5	K91	C8-C13	-3.54	1.38	1.42
4	C	2	K91	C4-CL20	2.88	1.80	1.74
4	C	2	K91	C11-CL18	2.75	1.81	1.74
4	D	1	K91	C8-C13	-2.52	1.39	1.42
4	P	7	K91	C4-CL20	2.52	1.80	1.74
4	E	3	K91	C8-C13	-2.52	1.39	1.42
4	O	6	K91	C4-CL20	2.51	1.80	1.74
4	E	3	K91	C4-CL20	2.51	1.80	1.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	7	K91	C8-C13	-2.51	1.39	1.42
4	O	6	K91	C8-C13	-2.50	1.39	1.42
4	Q	8	K91	C4-CL20	2.49	1.79	1.74
4	Q	8	K91	C8-C13	-2.49	1.39	1.42
4	D	1	K91	C4-CL20	2.48	1.79	1.74
4	C	2	K91	C17-C12	-2.32	1.37	1.42
4	M	4	K91	C17-C12	-2.27	1.37	1.42
4	N	5	K91	C11-CL18	2.18	1.80	1.74
4	M	4	K91	C11-CL18	2.15	1.80	1.74
4	Q	8	K91	C11-CL18	2.15	1.80	1.74
4	P	7	K91	C11-CL18	2.13	1.80	1.74
4	D	1	K91	C11-CL18	2.13	1.80	1.74
4	E	3	K91	C11-CL18	2.12	1.79	1.74
4	O	6	K91	C11-CL18	2.10	1.79	1.74
4	M	4	K91	C11-C12	-2.08	1.38	1.42

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2	K91	C11-C12-C13	4.45	121.98	117.39
4	M	4	K91	C11-C12-C13	3.67	121.18	117.39
4	M	4	K91	C16-C15-N14	-3.54	118.52	123.94
4	N	5	K91	C15-N14-C13	3.35	121.46	117.30
4	N	5	K91	C5-C4-CL20	3.30	123.28	119.15
4	C	2	K91	C5-C4-CL20	3.29	123.26	119.15
4	N	5	K91	C11-C12-C13	3.25	120.74	117.39
4	M	4	K91	C5-C4-CL20	3.18	123.13	119.15
4	C	2	K91	C16-C15-N14	-3.06	119.25	123.94
4	N	5	K91	C16-C15-N14	-3.06	119.26	123.94
4	M	4	K91	C15-N14-C13	3.05	121.10	117.30
4	C	2	K91	C17-C12-C11	-3.05	119.63	125.06
4	E	3	K91	C15-N14-C13	3.04	121.09	117.30
4	Q	8	K91	C15-N14-C13	3.03	121.08	117.30
4	D	1	K91	C15-N14-C13	3.03	121.07	117.30
4	P	7	K91	C15-N14-C13	3.02	121.05	117.30
4	O	6	K91	C15-N14-C13	3.01	121.05	117.30
4	M	4	K91	C17-C12-C11	-2.94	119.82	125.06
4	D	1	K91	C17-C12-C11	-2.73	120.19	125.06
4	E	3	K91	C17-C12-C11	-2.70	120.25	125.06
4	P	7	K91	C17-C12-C11	-2.70	120.26	125.06
4	E	3	K91	C11-C12-C13	2.69	120.17	117.39
4	O	6	K91	C11-C12-C13	2.69	120.17	117.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	6	K91	C17-C12-C11	-2.69	120.27	125.06
4	D	1	K91	C11-C12-C13	2.68	120.16	117.39
4	Q	8	K91	C17-C12-C11	-2.68	120.29	125.06
4	Q	8	K91	C11-C12-C13	2.66	120.13	117.39
4	P	7	K91	C11-C12-C13	2.62	120.10	117.39
4	C	2	K91	C8-C13-N14	-2.59	116.74	118.81
4	N	5	K91	C17-C12-C11	-2.59	120.45	125.06
4	M	4	K91	C3-C4-CL20	-2.46	115.50	119.35
4	N	5	K91	C3-C4-C5	-2.42	118.32	121.53
4	C	2	K91	C10-C11-C12	-2.41	117.83	121.66
4	M	4	K91	C12-C11-CL18	2.33	123.48	119.21
4	M	4	K91	C16-C17-C12	-2.31	117.69	120.89
4	C	2	K91	C3-C2-C1	2.24	122.81	120.50
4	C	2	K91	C8-C13-C12	2.19	120.47	118.74
4	C	2	K91	C16-C17-C12	-2.19	117.86	120.89
4	C	2	K91	C15-N14-C13	2.18	120.02	117.30
4	O	6	K91	C16-C15-N14	-2.15	120.64	123.94
4	E	3	K91	C16-C15-N14	-2.15	120.64	123.94
4	D	1	K91	C16-C15-N14	-2.15	120.65	123.94
4	C	2	K91	C17-C16-C15	2.14	121.69	118.93
4	Q	8	K91	C16-C15-N14	-2.14	120.67	123.94
4	P	7	K91	C16-C15-N14	-2.12	120.69	123.94
4	M	4	K91	C17-C16-C15	2.09	121.62	118.93
4	E	3	K91	O7-C6-C1	2.01	119.98	116.22
4	P	7	K91	O7-C6-C1	2.01	119.97	116.22
4	D	1	K91	O7-C6-C1	2.01	119.97	116.22
4	Q	8	K91	O7-C6-C1	2.00	119.96	116.22

There are no chirality outliers.

All (36) 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	N	7	GOL	O1-C1-C2-O2
2	N	7	GOL	O1-C1-C2-C3
2	N	7	GOL	C1-C2-C3-O3
2	F	3	GOL	C1-C2-C3-O3
2	Q	9	GOL	O1-C1-C2-C3
2	L	6	GOL	O1-C1-C2-O2
2	L	6	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	L	6	GOL	C1-C2-C3-O3
2	J	5	GOL	C1-C2-C3-O3
2	J	13	GOL	O1-C1-C2-C3
2	J	13	GOL	O1-C1-C2-O2
2	H	4	GOL	O1-C1-C2-C3
2	F	3	GOL	O1-C1-C2-C3
2	Q	9	GOL	C1-C2-C3-O3
2	P	14	GOL	O1-C1-C2-C3
2	J	13	GOL	C1-C2-C3-O3
2	B	1	GOL	O2-C2-C3-O3
2	F	3	GOL	O1-C1-C2-O2
2	F	3	GOL	O2-C2-C3-O3
2	Q	9	GOL	O1-C1-C2-O2
2	Q	9	GOL	O2-C2-C3-O3
2	L	6	GOL	O2-C2-C3-O3
2	P	14	GOL	O1-C1-C2-O2
2	J	5	GOL	O2-C2-C3-O3
2	P	8	GOL	O2-C2-C3-O3
2	N	7	GOL	O2-C2-C3-O3
4	E	3	K91	C13-C8-O7-C6
2	H	4	GOL	O1-C1-C2-O2
2	J	13	GOL	O2-C2-C3-O3
4	O	6	K91	C13-C8-O7-C6
2	S	10	GOL	O1-C1-C2-O2
4	E	3	K91	C9-C8-O7-C6
4	O	6	K91	C9-C8-O7-C6

There are no ring outliers.

18 monomers are involved in 263 short contacts:

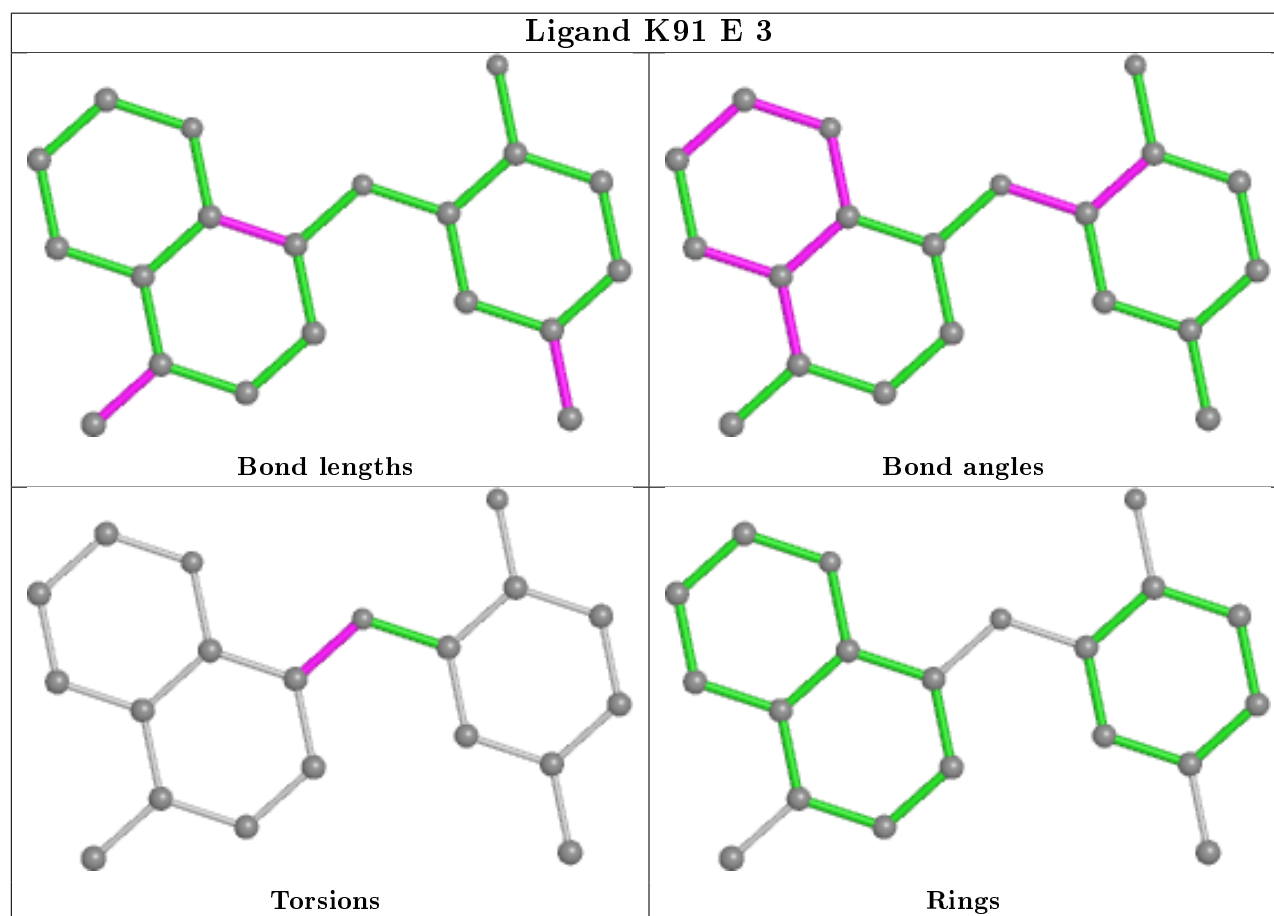
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	3	K91	32	0
2	P	8	GOL	1	0
2	B	1	GOL	3	0
2	S	10	GOL	1	0
2	H	4	GOL	4	0
2	F	3	GOL	1	0
4	O	6	K91	31	0
2	Q	9	GOL	3	0
2	V	11	GOL	1	0
2	L	6	GOL	2	0
4	Q	8	K91	29	0

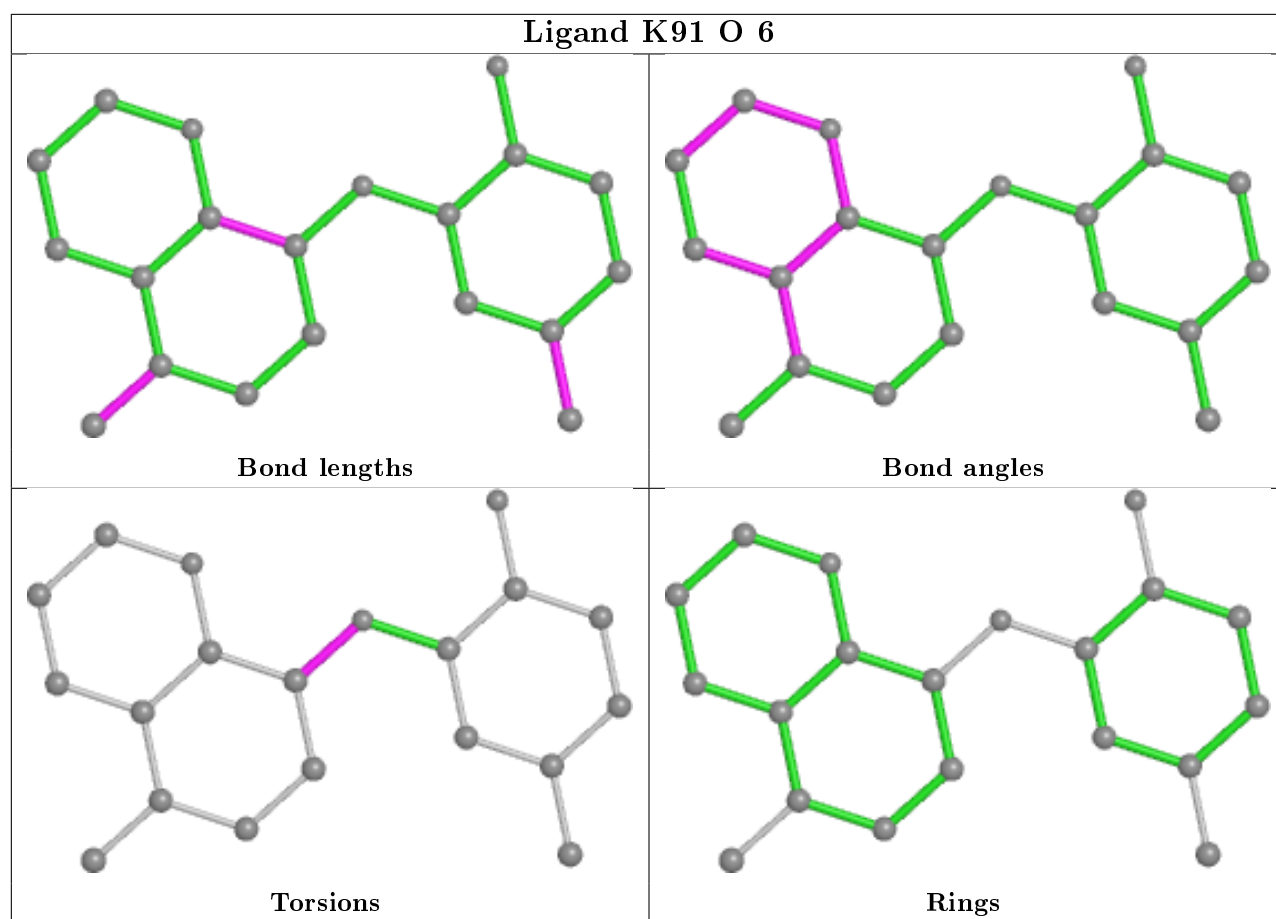
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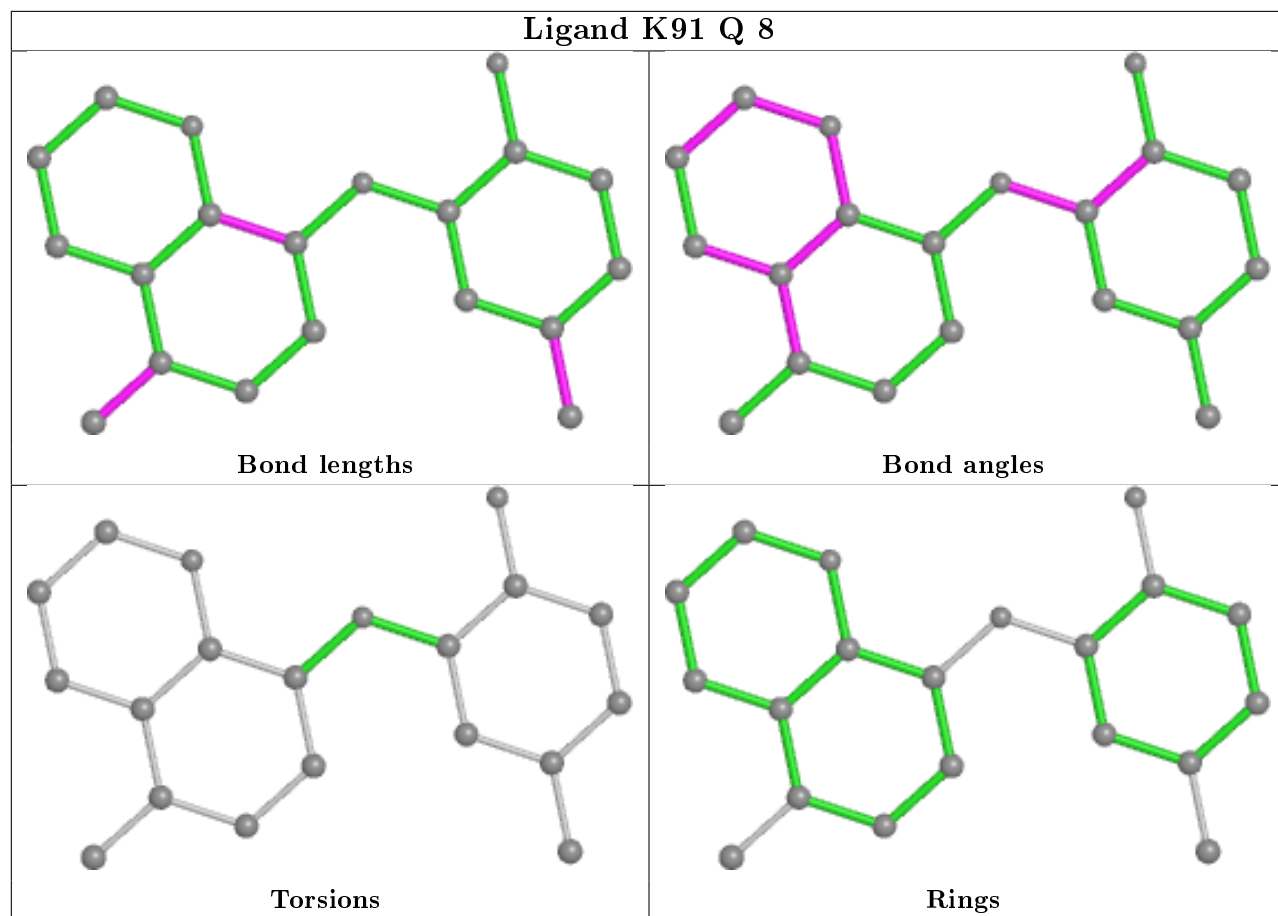
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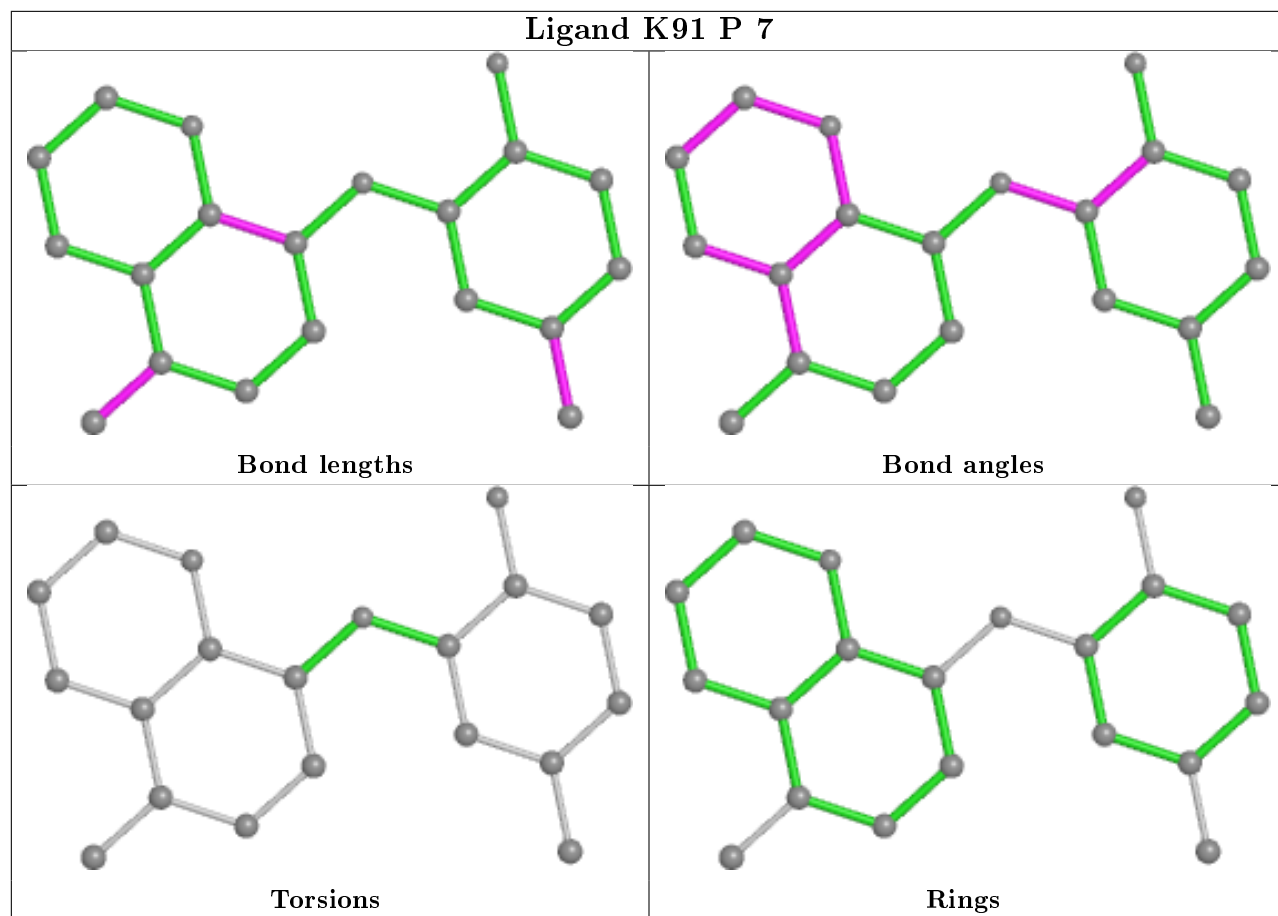
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	P	7	K91	25	0
2	P	14	GOL	3	0
4	N	5	K91	36	0
2	J	13	GOL	2	0
4	C	2	K91	30	0
4	M	4	K91	26	0
4	D	1	K91	33	0

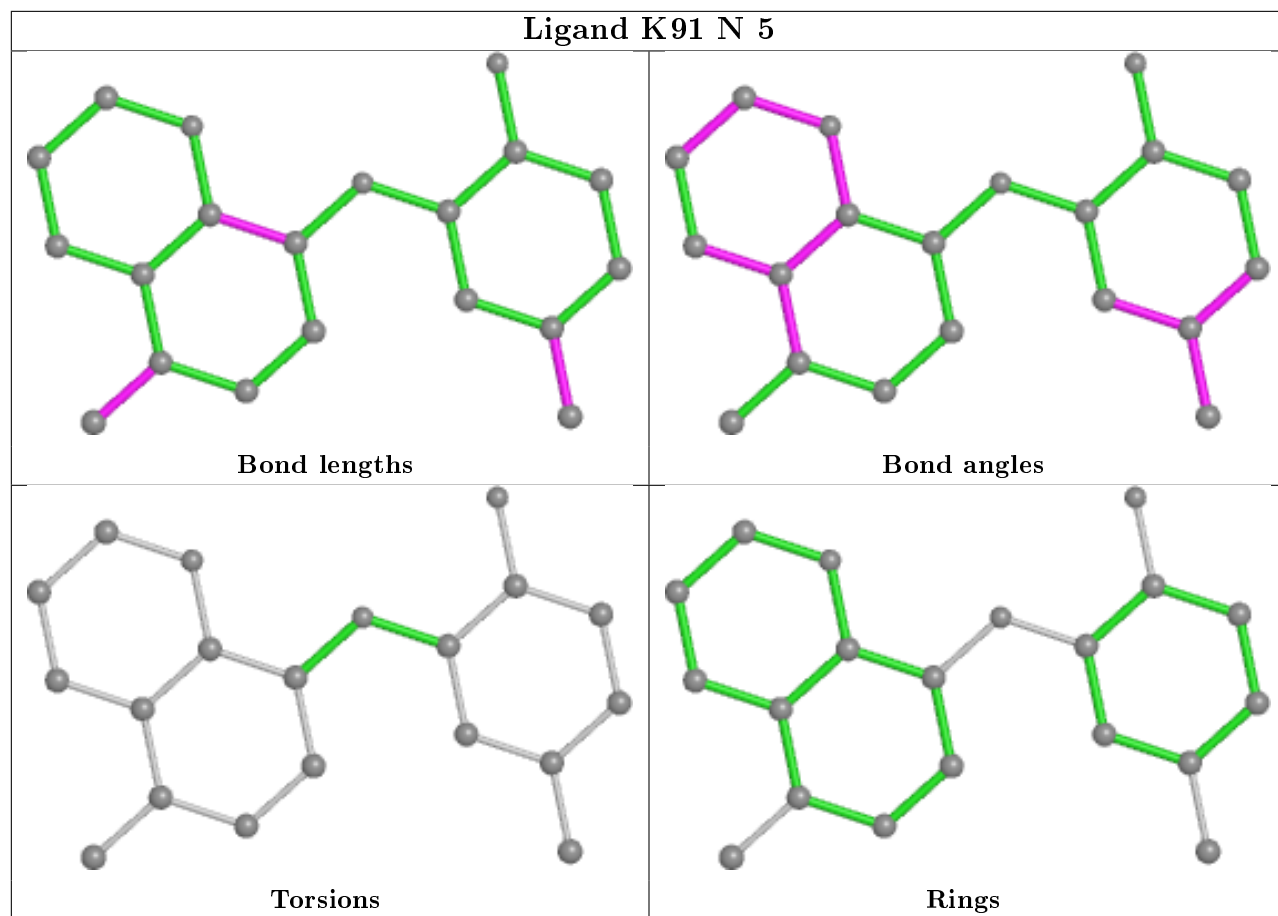
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

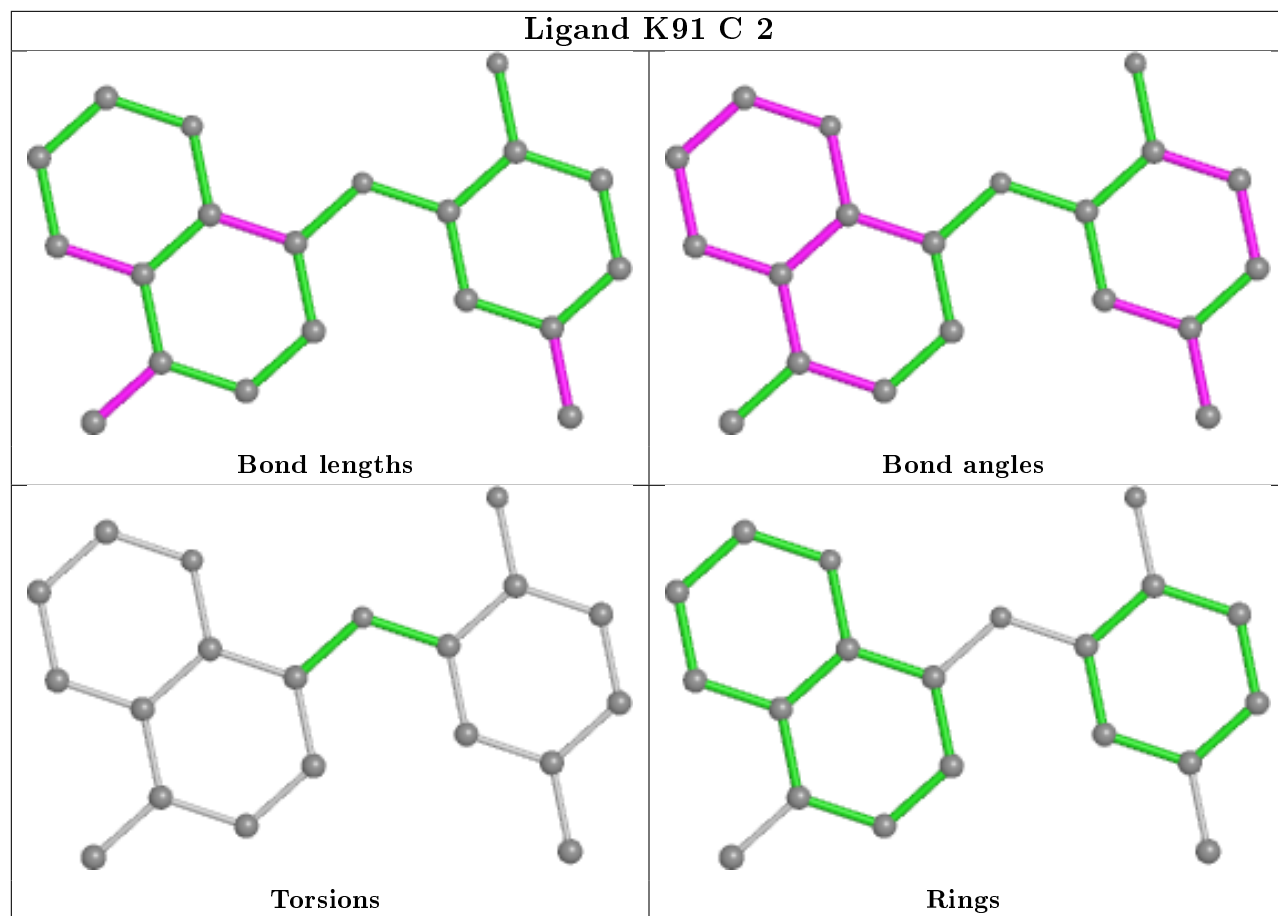


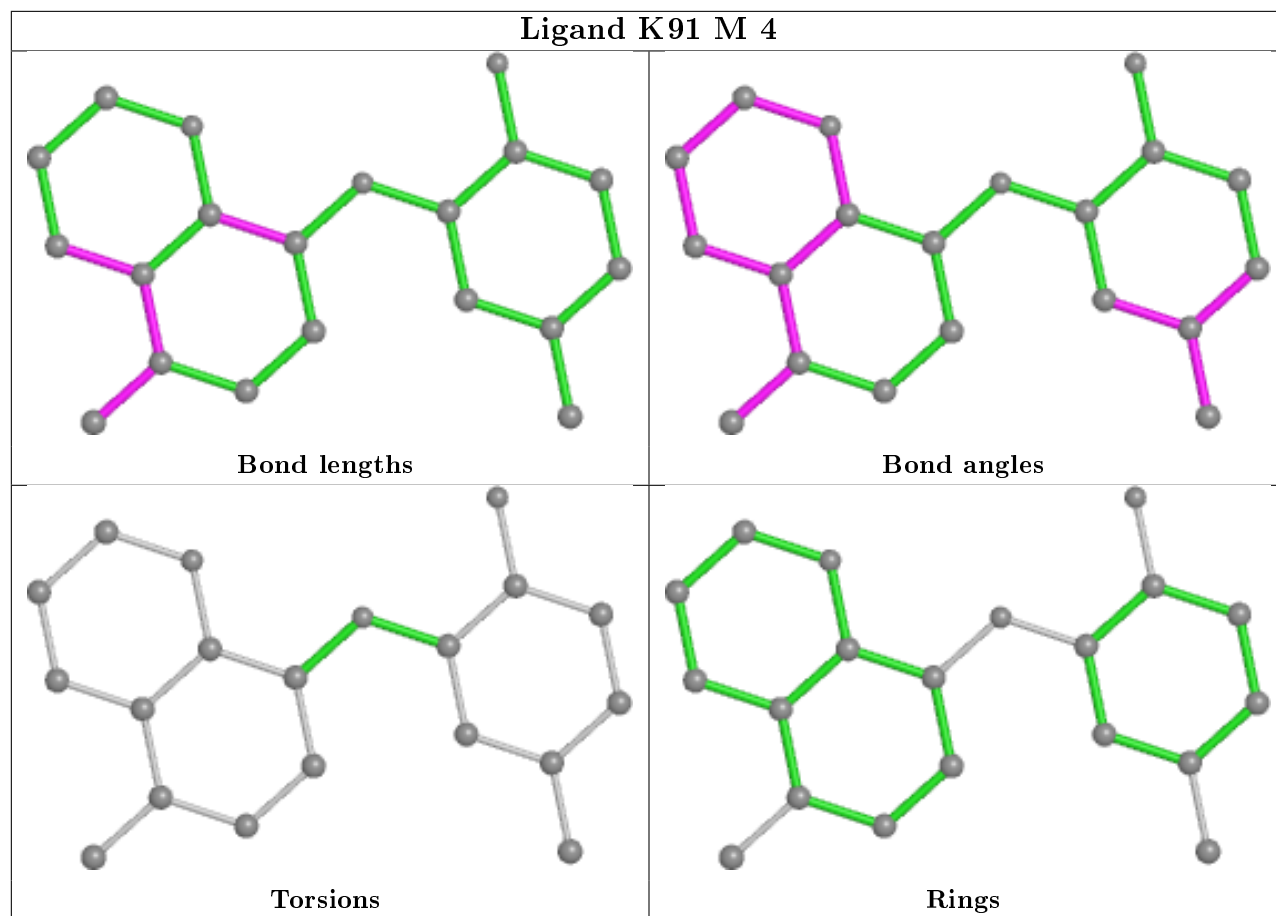


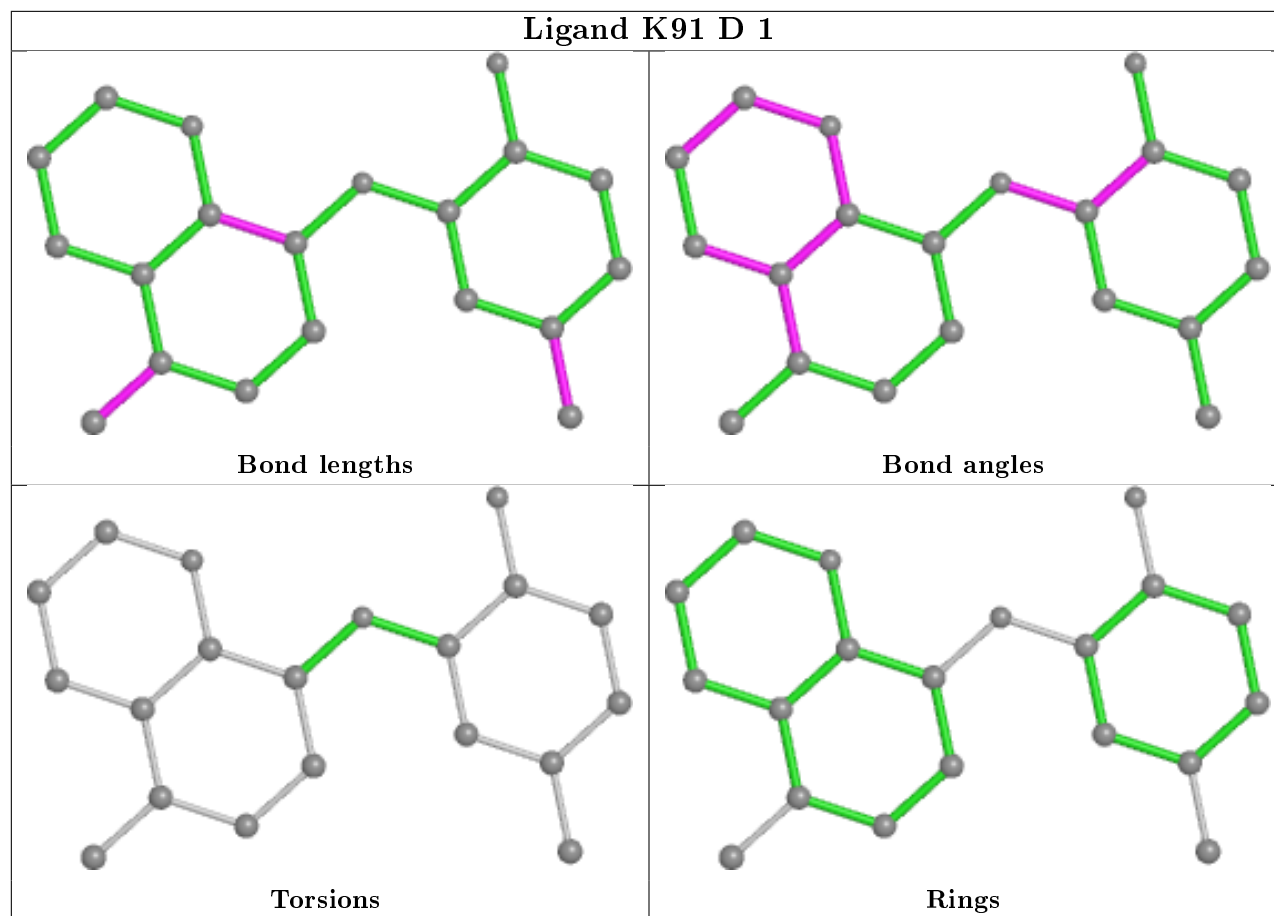












5.7 Other polymers [i](#)

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%)	0.29	7 (4%) 30 36	28, 41, 58, 68	0
1	B	145/154 (94%)	0.16	1 (0%) 87 91	28, 41, 57, 60	0
1	C	144/154 (93%)	0.19	4 (2%) 53 62	27, 40, 57, 60	0
1	D	144/154 (93%)	0.19	5 (3%) 44 52	28, 41, 56, 60	1 (0%)
1	E	142/154 (92%)	0.14	1 (0%) 87 91	28, 40, 57, 60	0
1	F	146/154 (94%)	0.18	3 (2%) 63 72	28, 41, 57, 60	0
1	G	147/154 (95%)	0.23	4 (2%) 54 63	28, 41, 57, 60	0
1	H	145/154 (94%)	0.19	6 (4%) 37 44	28, 41, 56, 61	0
1	I	144/154 (93%)	0.39	8 (5%) 24 29	28, 41, 57, 61	0
1	J	144/154 (93%)	0.16	10 (6%) 16 20	28, 41, 58, 62	1 (0%)
1	K	142/154 (92%)	0.33	4 (2%) 53 62	28, 41, 58, 61	0
1	L	146/154 (94%)	0.53	12 (8%) 11 14	28, 41, 57, 59	0
1	M	146/154 (94%)	0.17	3 (2%) 63 72	28, 41, 57, 60	0
1	N	145/154 (94%)	0.19	6 (4%) 37 44	28, 41, 57, 61	0
1	O	144/154 (93%)	0.20	2 (1%) 75 82	28, 41, 56, 61	0
1	P	144/154 (93%)	0.22	4 (2%) 53 62	28, 40, 56, 60	1 (0%)
1	Q	142/154 (92%)	0.15	3 (2%) 63 72	28, 40, 56, 62	0
1	R	146/154 (94%)	0.16	0 100 100	28, 40, 57, 61	0
1	S	146/154 (94%)	0.23	11 (7%) 14 17	28, 41, 57, 60	0
1	T	145/154 (94%)	0.34	4 (2%) 53 62	29, 41, 56, 60	0
1	U	144/154 (93%)	0.18	5 (3%) 44 52	28, 41, 56, 60	0
1	V	144/154 (93%)	0.31	8 (5%) 24 29	28, 41, 58, 64	1 (0%)
1	W	145/154 (94%)	0.42	8 (5%) 25 30	29, 41, 56, 60	0
1	X	142/154 (92%)	0.37	5 (3%) 44 52	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%)	0.25	124 (3%)	42	51	27, 41, 58, 68	4 (0%)

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	201	SER	6.2
1	N	168	LEU	4.5
1	V	200	SER	4.5
1	I	204	ILE	4.3
1	S	168	LEU	4.2
1	K	169	PHE	4.2
1	J	167	ASN	4.1
1	H	85	THR	4.1
1	J	168	LEU	3.9
1	J	162	ASP	3.9
1	K	110	TYR	3.7
1	W	183	VAL	3.7
1	L	201	SER	3.6
1	U	168	LEU	3.6
1	S	166	ASN	3.6
1	S	163	SER	3.6
1	Q	203	GLY	3.6
1	T	204	ILE	3.6
1	L	200	SER	3.5
1	W	165	LYS	3.5
1	G	204	ILE	3.4
1	T	200	SER	3.4
1	D	166	ASN	3.3
1	O	204	ILE	3.3
1	Q	164	GLN	3.3
1	D	168	LEU	3.3
1	J	109	ILE	3.3
1	S	170	LEU	3.2
1	X	89	ILE	3.2
1	A	85	THR	3.2
1	U	85	THR	3.1
1	M	229	SER	3.1
1	J	203	GLY	3.1
1	S	164	GLN	3.1
1	W	164	GLN	3.1
1	A	86	SER	3.0
1	V	199	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	I	198	PHE	3.0
1	L	164	GLN	3.0
1	O	199	LYS	3.0
1	H	169	PHE	2.9
1	N	221	ILE	2.9
1	T	109	ILE	2.9
1	M	110	TYR	2.9
1	J	170	LEU	2.8
1	A	198	PHE	2.8
1	D	162	ASP	2.8
1	F	166	ASN	2.8
1	N	202	LEU	2.7
1	L	165	LYS	2.7
1	V	198	PHE	2.7
1	S	167	ASN	2.7
1	G	200	SER	2.7
1	P	168	LEU	2.7
1	W	139	ILE	2.7
1	S	162	ASP	2.7
1	L	85	THR	2.6
1	V	222	SER	2.6
1	I	86	SER	2.6
1	P	110	TYR	2.6
1	K	113	PRO	2.6
1	L	110	TYR	2.6
1	X	228	LEU	2.6
1	J	163	SER	2.6
1	P	162	ASP	2.5
1	H	229	SER	2.5
1	I	164	GLN	2.5
1	A	84	ASP	2.4
1	A	87	ILE	2.4
1	V	168	LEU	2.4
1	U	226	PHE	2.4
1	I	170	LEU	2.4
1	M	85	THR	2.4
1	V	112	GLN	2.4
1	W	172	ALA	2.4
1	L	109	ILE	2.4
1	X	168	LEU	2.4
1	A	202	LEU	2.3
1	H	168	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	199	LYS	2.3
1	C	202	LEU	2.3
1	J	161	ASP	2.3
1	N	210	VAL	2.3
1	F	165	LYS	2.3
1	I	166	ASN	2.3
1	W	163	SER	2.3
1	S	203	GLY	2.3
1	V	159	LYS	2.3
1	H	202	LEU	2.3
1	H	166	ASN	2.3
1	L	89	ILE	2.3
1	S	109	ILE	2.2
1	V	111	MET	2.2
1	X	88	ASP	2.2
1	D	109	ILE	2.2
1	W	166	ASN	2.2
1	G	205	ALA	2.2
1	W	130	PHE	2.2
1	L	204	ILE	2.2
1	J	166	ASN	2.2
1	X	203	GLY	2.2
1	L	139	ILE	2.1
1	B	215	GLY	2.1
1	D	227	ALA	2.1
1	U	165	LYS	2.1
1	L	84	ASP	2.1
1	E	85	THR	2.1
1	C	166	ASN	2.1
1	P	167	ASN	2.1
1	G	163	SER	2.1
1	I	87	ILE	2.1
1	I	199	LYS	2.1
1	A	220	ASN	2.1
1	K	163	SER	2.1
1	Q	199	LYS	2.1
1	S	110	TYR	2.1
1	N	85	THR	2.1
1	J	84	ASP	2.1
1	U	170	LEU	2.1
1	L	162	ASP	2.1
1	C	163	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	110	TYR	2.0
1	S	229	SER	2.0
1	T	202	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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, 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.

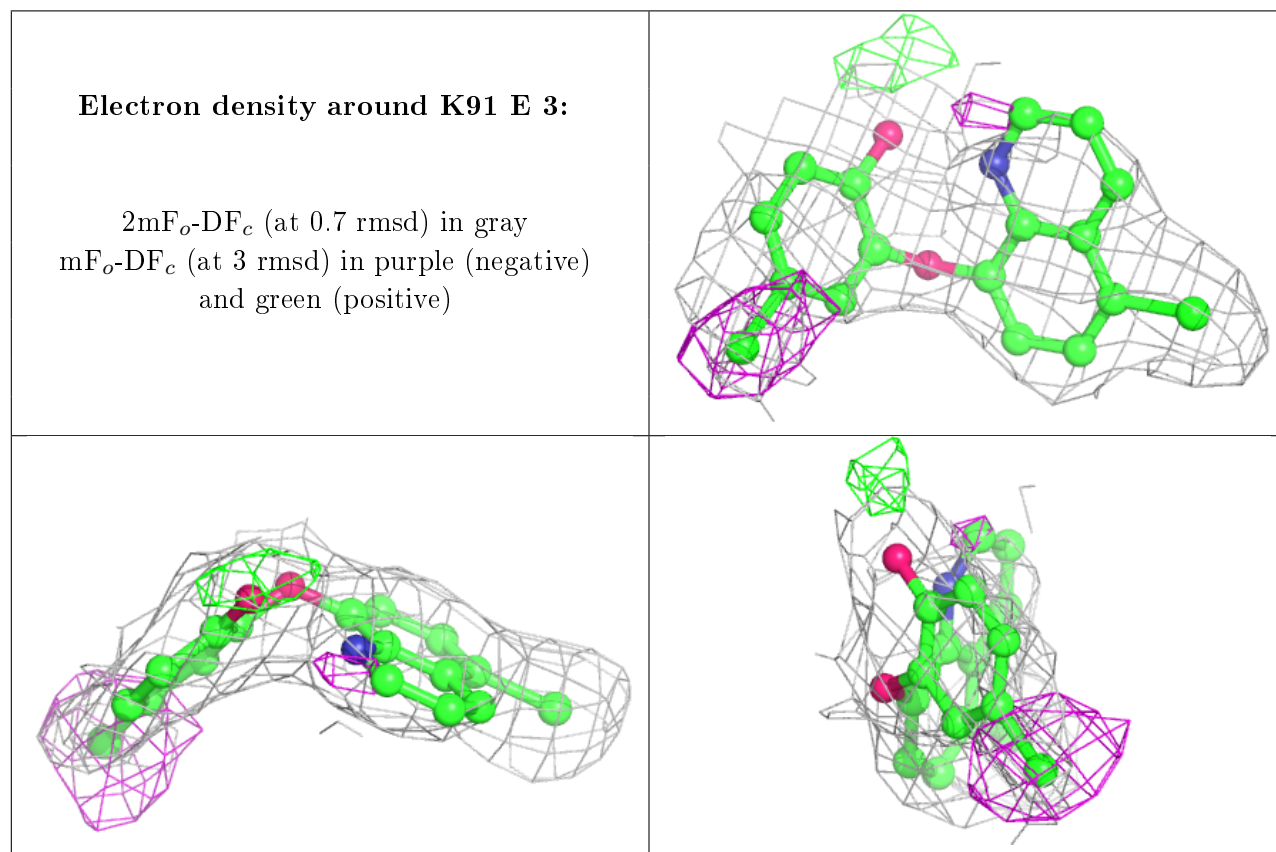
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	K91	E	3	20/20	0.83	0.28	36,38,44,45	0
2	GOL	H	4	6/6	0.83	0.18	46,49,51,51	0
4	K91	O	6	20/20	0.87	0.18	34,38,41,41	0
2	GOL	L	6	6/6	0.87	0.25	44,46,47,48	0
4	K91	Q	8	20/20	0.88	0.22	35,39,44,45	0
4	K91	C	2	20/20	0.88	0.19	34,37,39,45	0
4	K91	P	7	20/20	0.89	0.21	34,38,40,43	0
2	GOL	W	12	6/6	0.89	0.22	43,45,48,48	0
4	K91	M	4	20/20	0.90	0.17	34,37,39,39	0
2	GOL	P	8	6/6	0.90	0.17	33,34,35,37	0
4	K91	D	1	20/20	0.91	0.20	29,35,38,41	0
2	GOL	P	14	6/6	0.92	0.20	27,28,30,30	0
2	GOL	N	7	6/6	0.93	0.18	37,38,38,40	0
2	GOL	Q	9	6/6	0.93	0.19	35,38,41,42	0
2	GOL	D	2	6/6	0.93	0.16	27,27,29,31	0
2	GOL	J	13	6/6	0.93	0.17	28,31,31,33	0
4	K91	N	5	20/20	0.94	0.15	34,38,39,44	0
2	GOL	B	1	6/6	0.94	0.18	26,29,32,34	0
2	GOL	S	10	6/6	0.94	0.17	36,37,39,40	0
2	GOL	V	11	6/6	0.95	0.14	13,21,24,26	0

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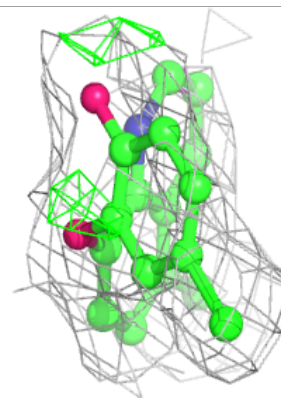
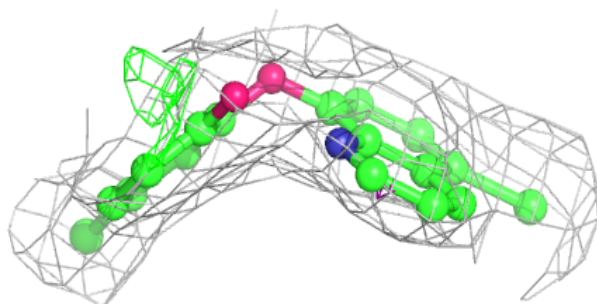
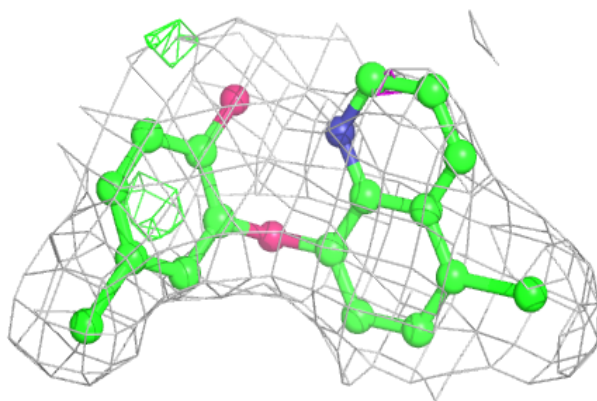
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GOL	F	3	6/6	0.96	0.21	29,34,35,36	0
3	PO4	B	231	5/5	0.96	0.15	41,42,44,44	0
2	GOL	J	5	6/6	0.96	0.15	24,27,28,29	0

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.

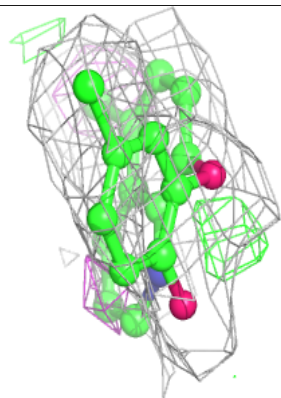
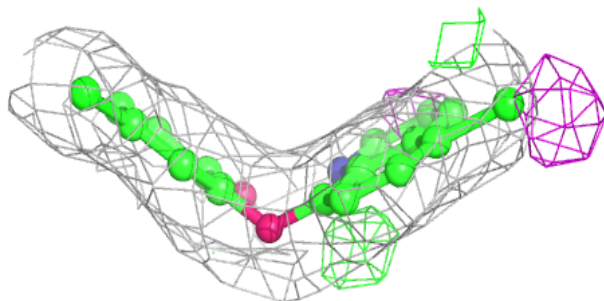
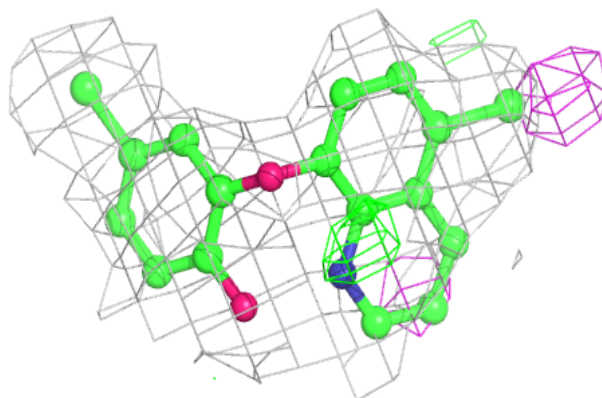


Electron density around K91 O 6:

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

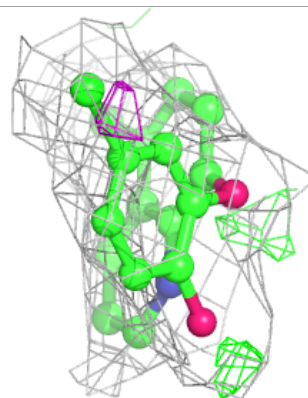
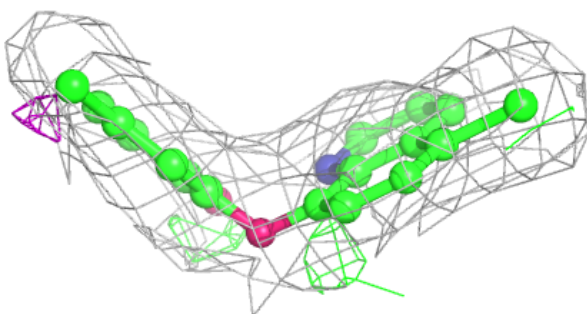
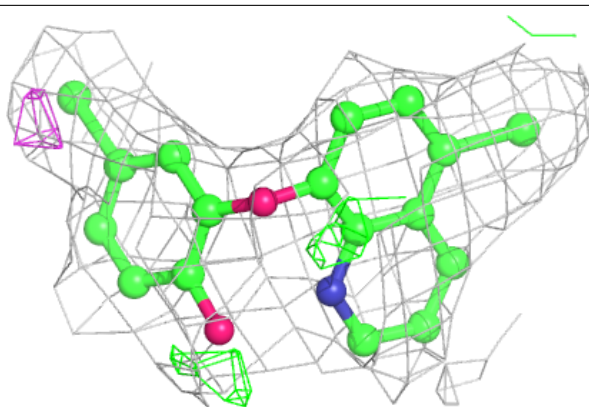
**Electron density around K91 Q 8:**

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

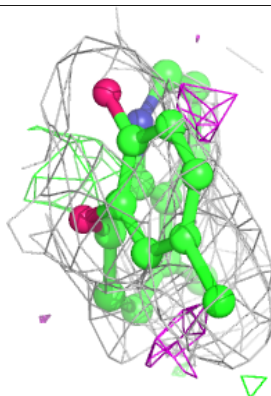
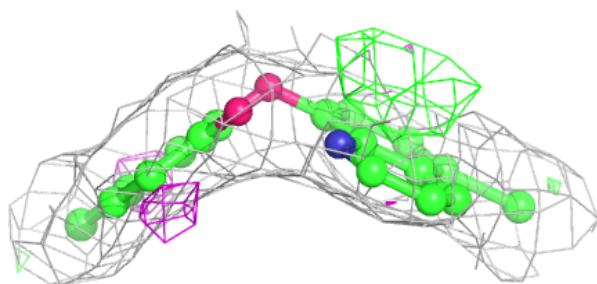
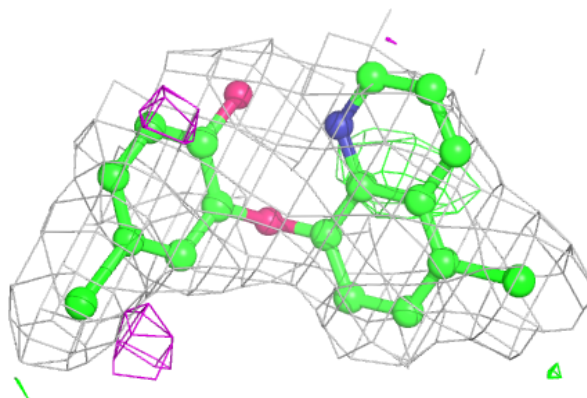


Electron density around K91 C 2:

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

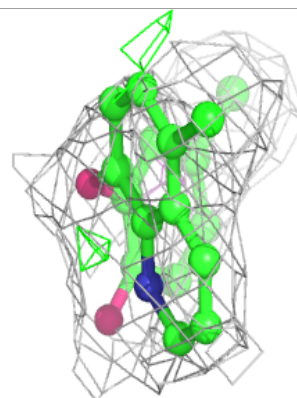
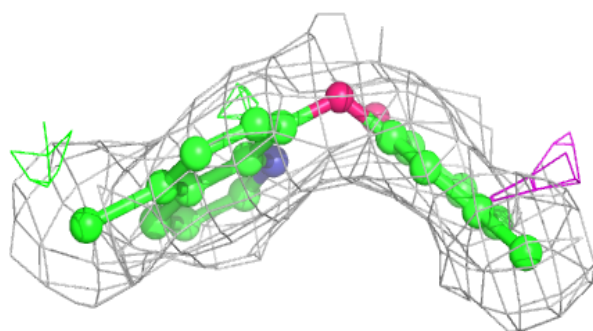
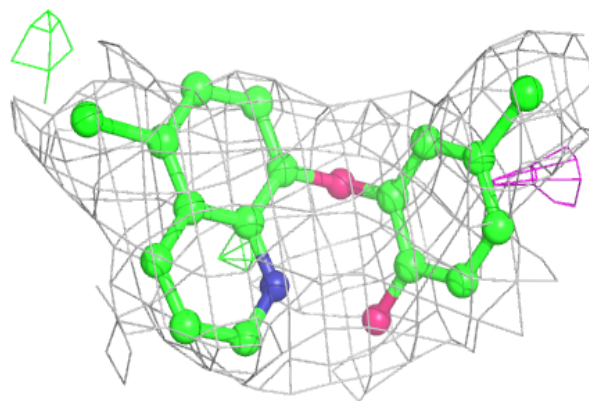
**Electron density around K91 P 7:**

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

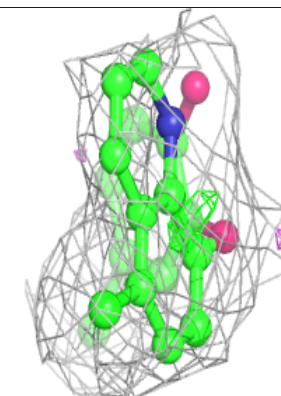
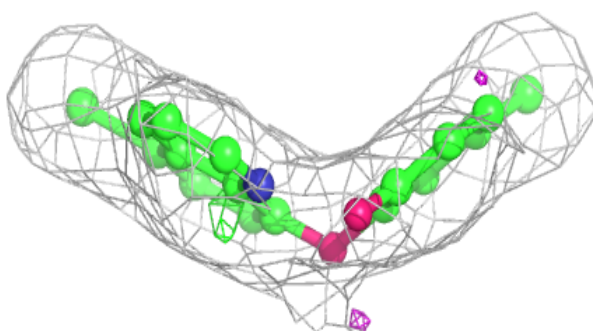
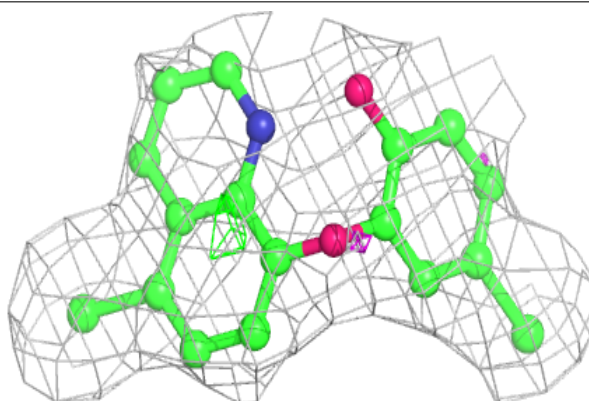


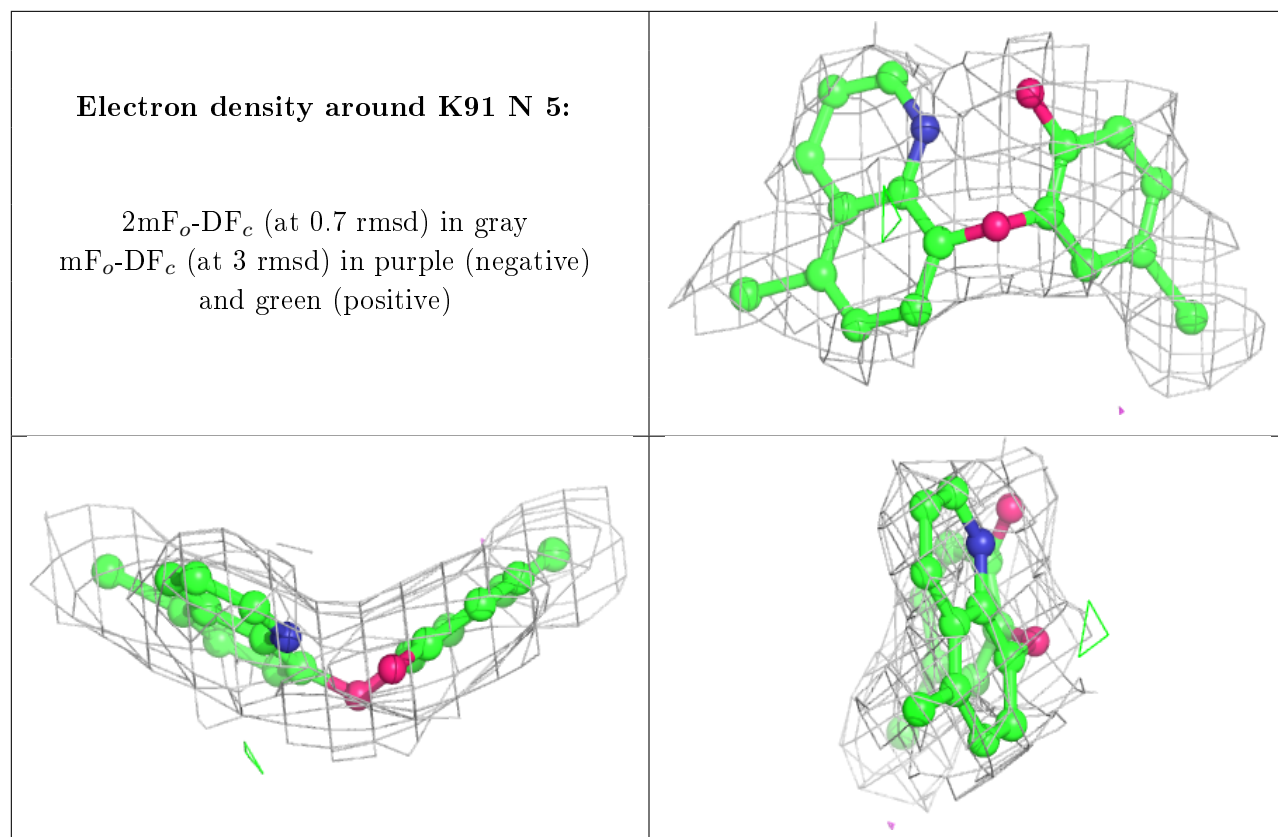
Electron density around K91 M 4:

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

**Electron density around K91 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.