Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2024 – 03:46 pm GMT

PDB ID	:	9FVE
Title	:	Crystal structure of VcSiaP W73A mutant in complex with sialic acid and a VHH antibody (VHH_VcP#2)
Authors	:	Schneberger, N.; Hagelueken, G.
Deposited on	:	2024-06-26
Resolution	:	2.81 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:

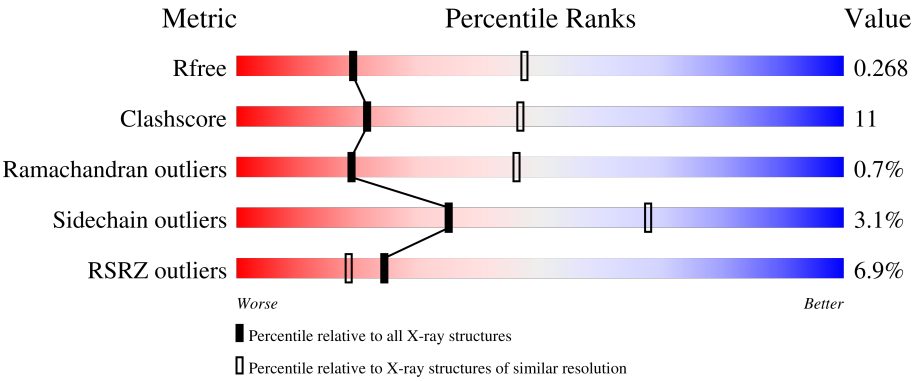
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.81 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}	164625	4293 (2.84-2.80)
Clashscore	180529	4801 (2.84-2.80)
Ramachandran outliers	177936	4739 (2.84-2.80)
Sidechain outliers	177891	4741 (2.84-2.80)
RSRZ outliers	164620	4295 (2.84-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	303	44% 51% 38% 8%
1	C	303	6% 76% 19%
1	E	303	2% 83% 14%
1	G	303	4% 77% 17%
1	I	303	4% 78% 17%

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Mol	Chain	Length	Quality of chain
1	K	303	9% 69% 24%
1	M	303	2% 82% 14%
1	O	303	5% 74% 21%
1	Q	303	% 86% 11%
1	U	303	2% 83% 12%
1	W	303	10% 77% 19%
1	Y	303	3% 82% 15%
2	B	123	6% 85% 10% 5%
2	D	123	6% 80% 13%
2	F	123	6% 89% 10%
2	H	123	6% 86% 10%
2	J	123	7% 83% 13%
2	L	123	4% 86% 9%
2	N	123	10% 82% 13%
2	P	123	2% 82% 15%
2	R	123	2% 88% 9%
2	T	123	5% 89% 8%
2	V	123	5% 89% 9%
2	X	123	2% 91% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 79063 atoms, of which 39084 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 Sialic acid-binding periplasmic protein SiaP.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	299	Total	C	H	N	O	S	0	0	0
			4701	1489	2341	396	460	15			
1	C	299	Total	C	H	N	O	S	0	0	0
			4696	1489	2336	396	460	15			
1	E	301	Total	C	H	N	O	S	0	0	0
			4717	1494	2348	398	462	15			
1	G	299	Total	C	H	N	O	S	0	0	0
			4700	1489	2340	396	460	15			
1	I	299	Total	C	H	N	O	S	0	0	0
			4702	1489	2342	396	460	15			
1	K	299	Total	C	H	N	O	S	0	0	0
			4701	1489	2341	396	460	15			
1	M	299	Total	C	H	N	O	S	0	0	0
			4701	1489	2341	396	460	15			
1	O	299	Total	C	H	N	O	S	0	0	0
			4700	1489	2340	396	460	15			
1	Q	299	Total	C	H	N	O	S	0	0	0
			4701	1489	2341	396	460	15			
1	U	299	Total	C	H	N	O	S	0	0	0
			4701	1489	2341	396	460	15			
1	W	299	Total	C	H	N	O	S	0	0	0
			4700	1489	2340	396	460	15			
1	Y	299	Total	C	H	N	O	S	0	0	0
			4700	1489	2340	396	460	15			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q9KR64
A	-2	ALA	-	expression tag	UNP Q9KR64
A	-1	MET	-	expression tag	UNP Q9KR64
A	0	GLY	ALA	conflict	UNP Q9KR64
A	73	ALA	TRP	engineered mutation	UNP Q9KR64

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP Q9KR64
C	-2	ALA	-	expression tag	UNP Q9KR64
C	-1	MET	-	expression tag	UNP Q9KR64
C	0	GLY	ALA	conflict	UNP Q9KR64
C	73	ALA	TRP	engineered mutation	UNP Q9KR64
E	-3	GLY	-	expression tag	UNP Q9KR64
E	-2	ALA	-	expression tag	UNP Q9KR64
E	-1	MET	-	expression tag	UNP Q9KR64
E	0	GLY	ALA	conflict	UNP Q9KR64
E	73	ALA	TRP	engineered mutation	UNP Q9KR64
G	-3	GLY	-	expression tag	UNP Q9KR64
G	-2	ALA	-	expression tag	UNP Q9KR64
G	-1	MET	-	expression tag	UNP Q9KR64
G	0	GLY	ALA	conflict	UNP Q9KR64
G	73	ALA	TRP	engineered mutation	UNP Q9KR64
I	-3	GLY	-	expression tag	UNP Q9KR64
I	-2	ALA	-	expression tag	UNP Q9KR64
I	-1	MET	-	expression tag	UNP Q9KR64
I	0	GLY	ALA	conflict	UNP Q9KR64
I	73	ALA	TRP	engineered mutation	UNP Q9KR64
K	-3	GLY	-	expression tag	UNP Q9KR64
K	-2	ALA	-	expression tag	UNP Q9KR64
K	-1	MET	-	expression tag	UNP Q9KR64
K	0	GLY	ALA	conflict	UNP Q9KR64
K	73	ALA	TRP	engineered mutation	UNP Q9KR64
M	-3	GLY	-	expression tag	UNP Q9KR64
M	-2	ALA	-	expression tag	UNP Q9KR64
M	-1	MET	-	expression tag	UNP Q9KR64
M	0	GLY	ALA	conflict	UNP Q9KR64
M	73	ALA	TRP	engineered mutation	UNP Q9KR64
O	-3	GLY	-	expression tag	UNP Q9KR64
O	-2	ALA	-	expression tag	UNP Q9KR64
O	-1	MET	-	expression tag	UNP Q9KR64
O	0	GLY	ALA	conflict	UNP Q9KR64
O	73	ALA	TRP	engineered mutation	UNP Q9KR64
Q	-3	GLY	-	expression tag	UNP Q9KR64
Q	-2	ALA	-	expression tag	UNP Q9KR64
Q	-1	MET	-	expression tag	UNP Q9KR64
Q	0	GLY	ALA	conflict	UNP Q9KR64
Q	73	ALA	TRP	engineered mutation	UNP Q9KR64
U	-3	GLY	-	expression tag	UNP Q9KR64
U	-2	ALA	-	expression tag	UNP Q9KR64

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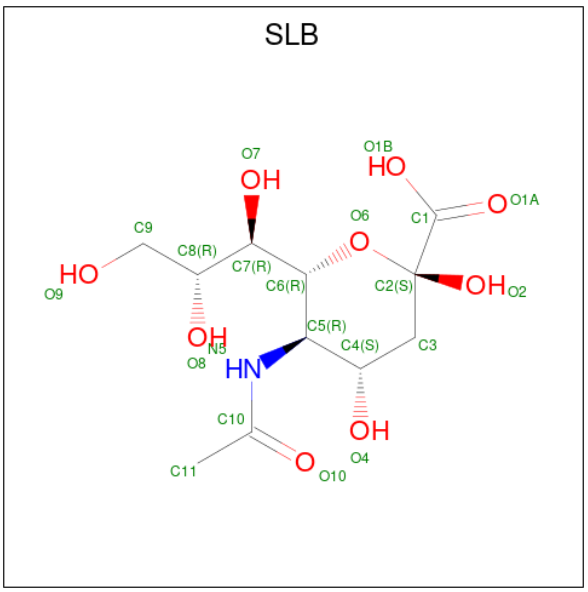
Chain	Residue	Modelled	Actual	Comment	Reference
U	-1	MET	-	expression tag	UNP Q9KR64
U	0	GLY	ALA	conflict	UNP Q9KR64
U	73	ALA	TRP	engineered mutation	UNP Q9KR64
W	-3	GLY	-	expression tag	UNP Q9KR64
W	-2	ALA	-	expression tag	UNP Q9KR64
W	-1	MET	-	expression tag	UNP Q9KR64
W	0	GLY	ALA	conflict	UNP Q9KR64
W	73	ALA	TRP	engineered mutation	UNP Q9KR64
Y	-3	GLY	-	expression tag	UNP Q9KR64
Y	-2	ALA	-	expression tag	UNP Q9KR64
Y	-1	MET	-	expression tag	UNP Q9KR64
Y	0	GLY	ALA	conflict	UNP Q9KR64
Y	73	ALA	TRP	engineered mutation	UNP Q9KR64

- Molecule 2 is a protein called VHH_VcP#2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	122	Total	C	H	N	O	S	0	0	0
			1836	590	891	168	183	4			
2	D	121	Total	C	H	N	O	S	0	0	0
			1826	587	887	167	181	4			
2	F	123	Total	C	H	N	O	S	0	0	0
			1845	592	896	169	184	4			
2	H	123	Total	C	H	N	O	S	0	0	0
			1845	592	896	169	184	4			
2	J	123	Total	C	H	N	O	S	0	0	0
			1845	592	896	169	184	4			
2	L	123	Total	C	H	N	O	S	0	0	0
			1847	592	898	169	184	4			
2	N	123	Total	C	H	N	O	S	0	0	0
			1845	592	896	169	184	4			
2	P	123	Total	C	H	N	O	S	0	0	0
			1846	592	897	169	184	4			
2	R	123	Total	C	H	N	O	S	0	0	0
			1845	592	896	169	184	4			
2	T	123	Total	C	H	N	O	S	0	0	0
			1845	592	896	169	184	4			
2	V	123	Total	C	H	N	O	S	0	0	0
			1845	592	896	169	184	4			
2	X	123	Total	C	H	N	O	S	0	0	0
			1845	592	896	169	184	4			

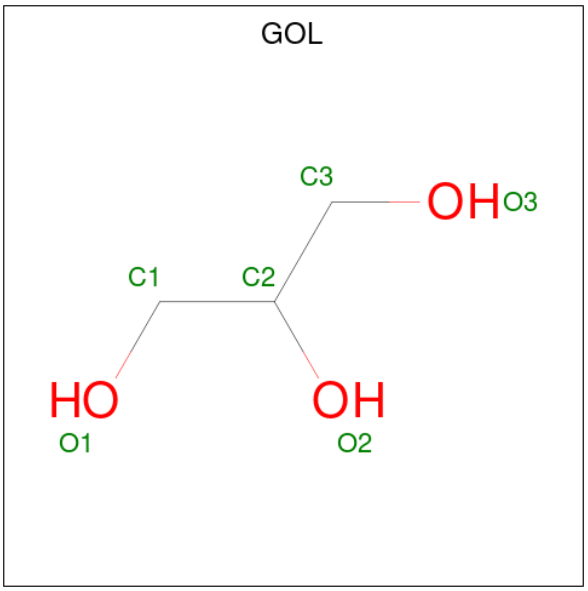
- Molecule 3 is N-acetyl-beta-neuraminic acid (three-letter code: SLB) (formula: $C_{11}H_{19}NO_9$)

(labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			37	11	17	1	8		
3	C	1	Total	C	H	N	O	0	0
			37	11	17	1	8		
3	E	1	Total	C	H	N	O	0	0
			37	11	17	1	8		
3	G	1	Total	C	H	N	O	0	0
			37	11	17	1	8		
3	I	1	Total	C	H	N	O	0	0
			37	11	17	1	8		
3	K	1	Total	C	H	N	O	0	0
			37	11	17	1	8		
3	M	1	Total	C	H	N	O	0	0
			37	11	17	1	8		
3	O	1	Total	C	H	N	O	0	0
			37	11	17	1	8		
3	Q	1	Total	C	H	N	O	0	0
			37	11	17	1	8		
3	U	1	Total	C	H	N	O	0	0
			37	11	17	1	8		
3	W	1	Total	C	H	N	O	0	0
			37	11	17	1	8		
3	Y	1	Total	C	H	N	O	0	0
			37	11	17	1	8		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



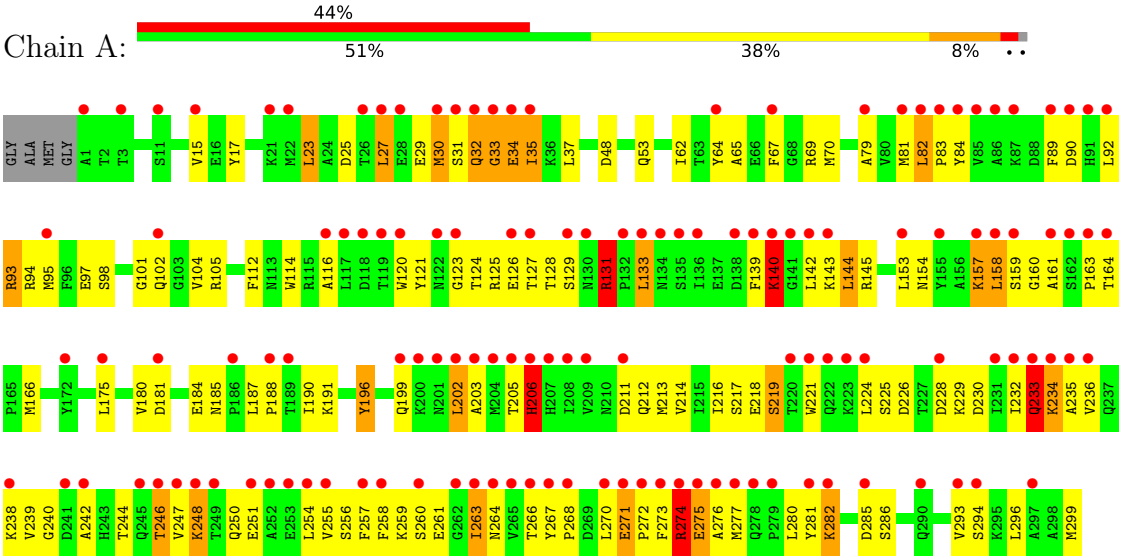
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	H	O	0	0
			14	3	8	3		
4	G	1	Total	C	H	O	0	0
			14	3	8	3		
4	Q	1	Total	C	H	O	0	0
			14	3	8	3		
4	U	1	Total	C	H	O	0	0
			14	3	8	3		
4	U	1	Total	C	H	O	0	0
			14	3	8	3		
4	U	1	Total	C	H	O	0	0
			14	3	8	3		

3 Residue-property plots (i)

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

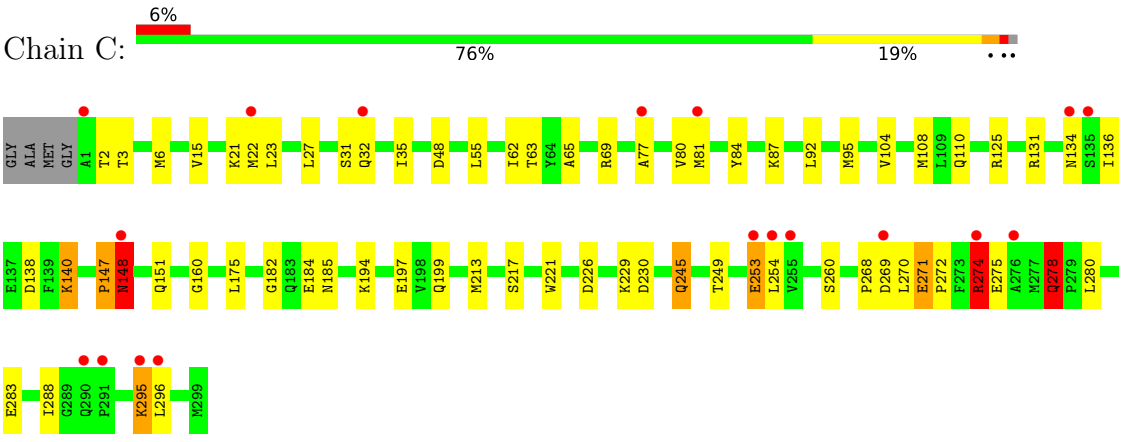
• Molecule 1: Sialic acid-binding periplasmic protein SiaP

Chain A:



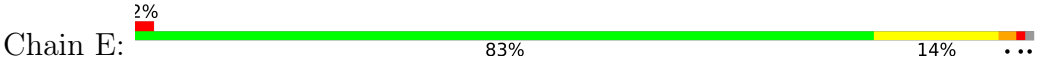
• Molecule 1: Sialic acid-binding periplasmic protein SiaP

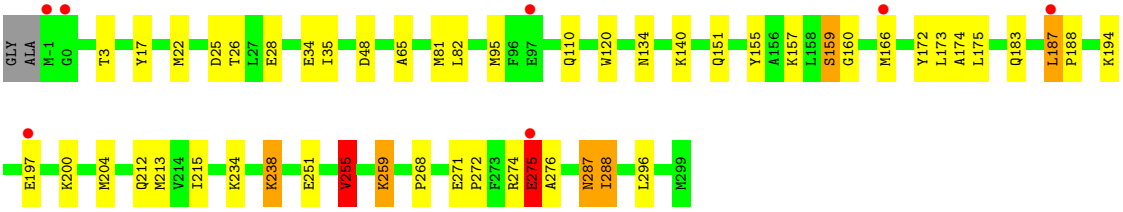
Chain C:



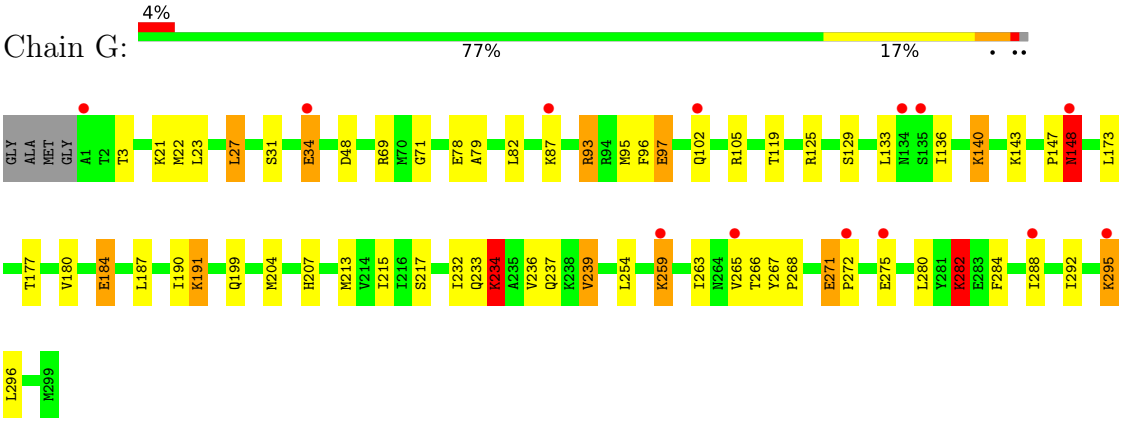
• Molecule 1: Sialic acid-binding periplasmic protein SiaP

Chain E:

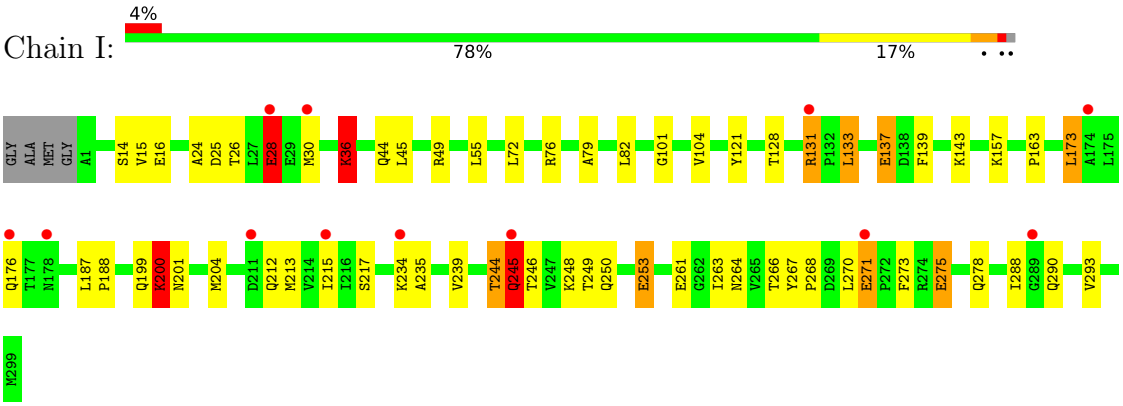




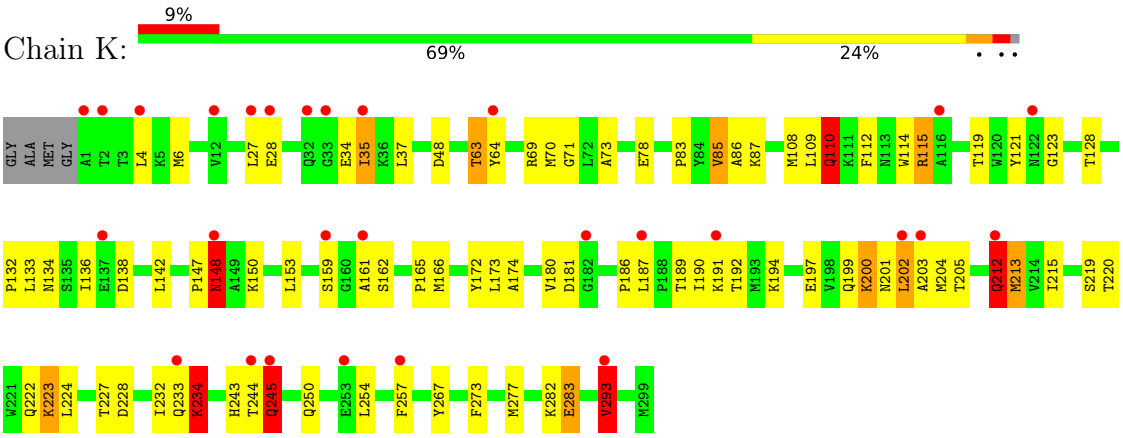
• Molecule 1: Sialic acid-binding periplasmic protein SiaP



• Molecule 1: Sialic acid-binding periplasmic protein SiaP

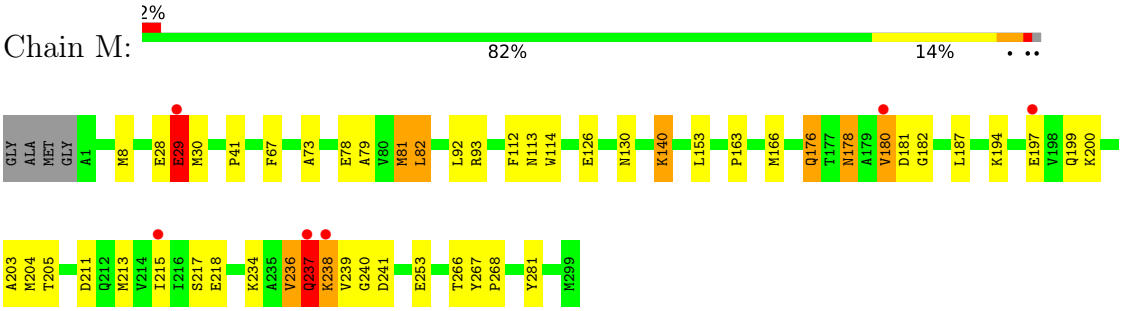


• Molecule 1: Sialic acid-binding periplasmic protein SiaP



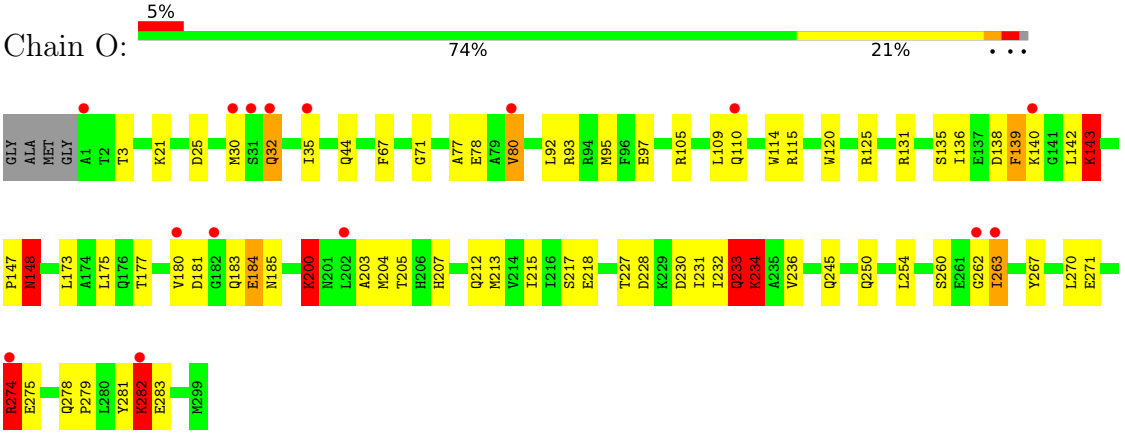
• Molecule 1: Sialic acid-binding periplasmic protein SiaP

Chain M:



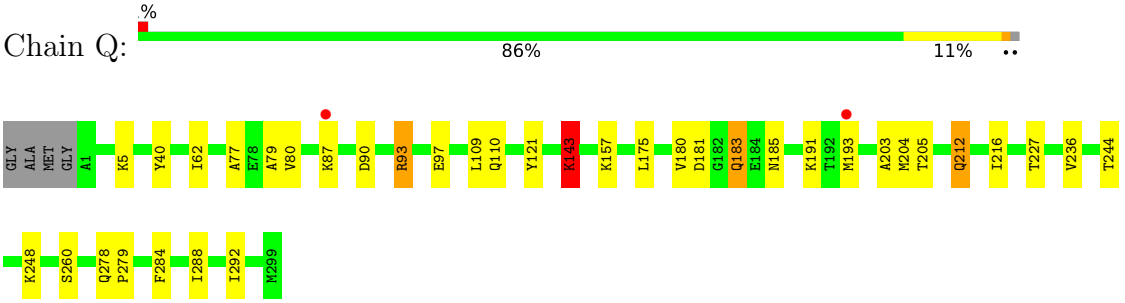
• Molecule 1: Sialic acid-binding periplasmic protein SiaP

Chain O:



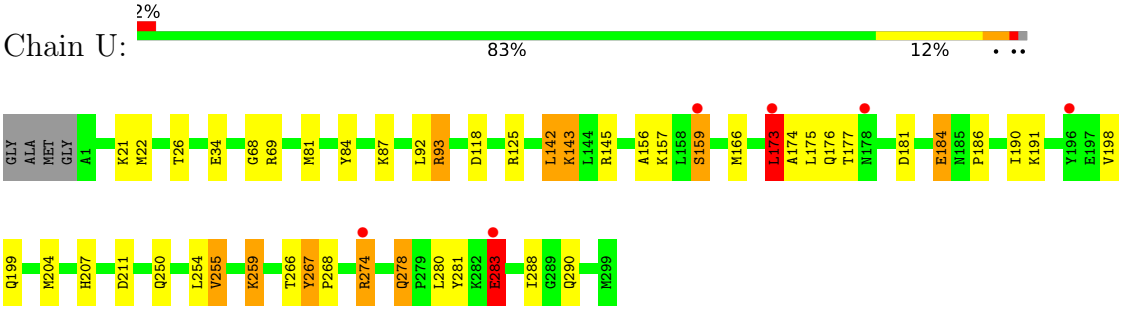
• Molecule 1: Sialic acid-binding periplasmic protein SiaP

Chain Q:



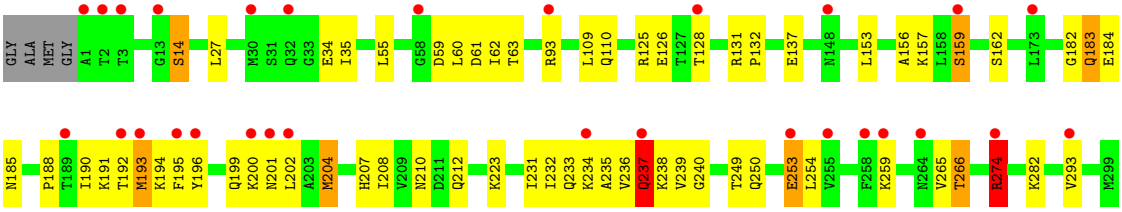
• Molecule 1: Sialic acid-binding periplasmic protein SiaP

Chain U:

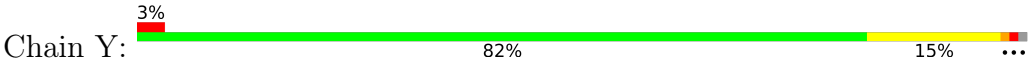


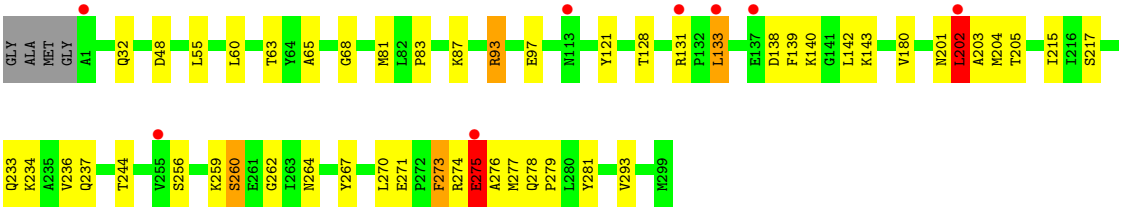
• Molecule 1: Sialic acid-binding periplasmic protein SiaP

Chain W:

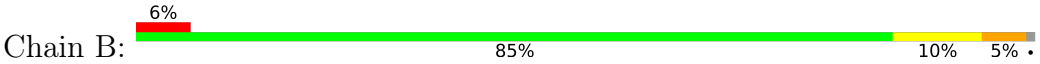


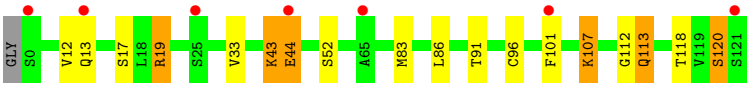
• Molecule 1: Sialic acid-binding periplasmic protein SiaP



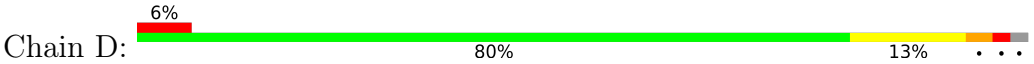


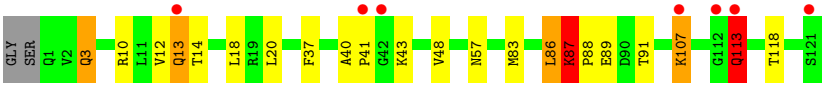
• Molecule 2: VHH_VcP#2



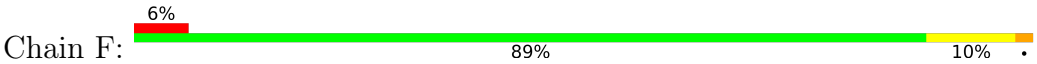


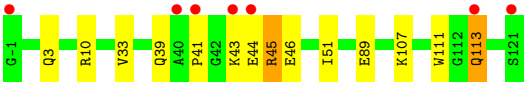
• Molecule 2: VHH_VcP#2



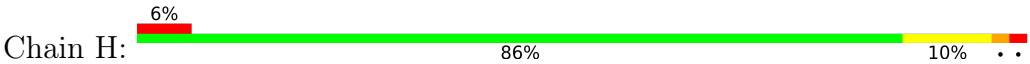


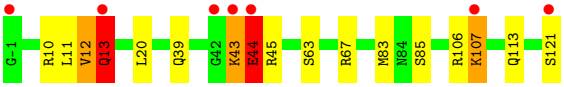
• Molecule 2: VHH_VcP#2





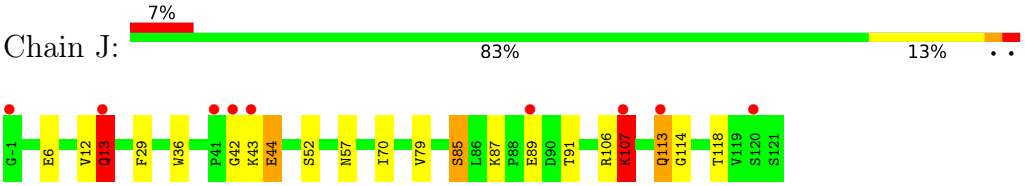
• Molecule 2: VHH_VcP#2





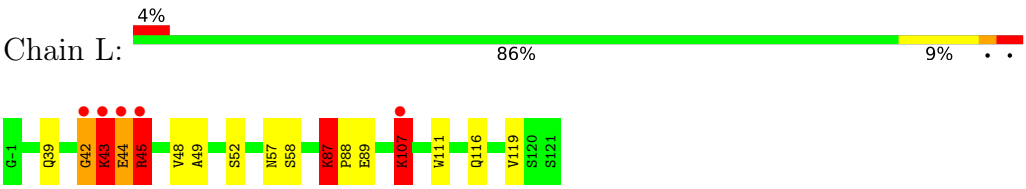
• Molecule 2: VHH_VcP#2

Chain J:



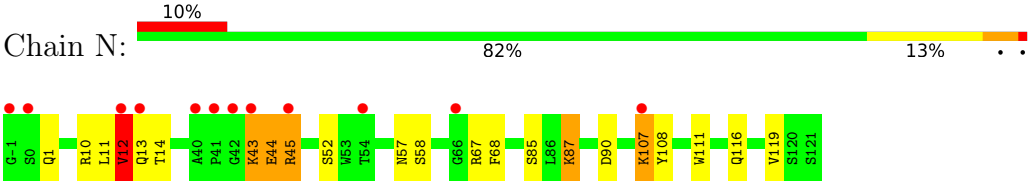
• Molecule 2: VHH_VcP#2

Chain L:



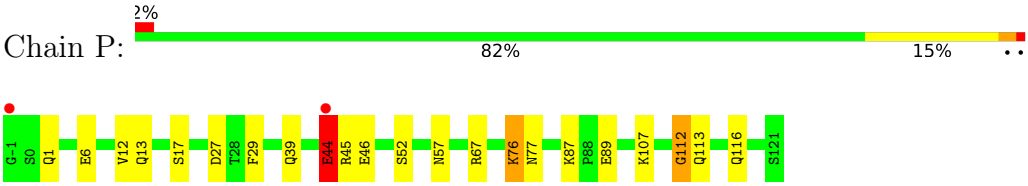
• Molecule 2: VHH_VcP#2

Chain N:



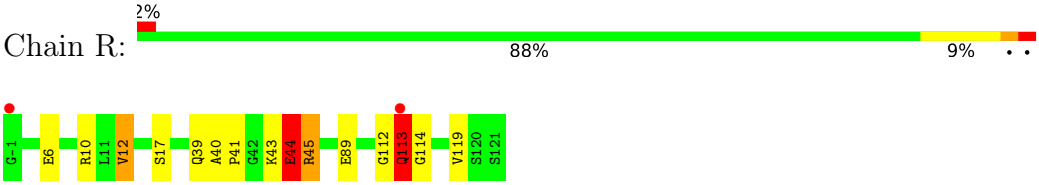
• Molecule 2: VHH_VcP#2

Chain P:



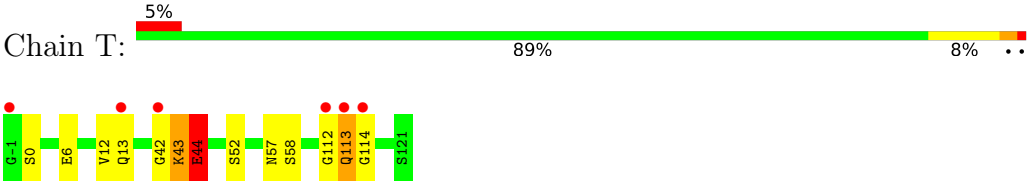
• Molecule 2: VHH_VcP#2

Chain R:



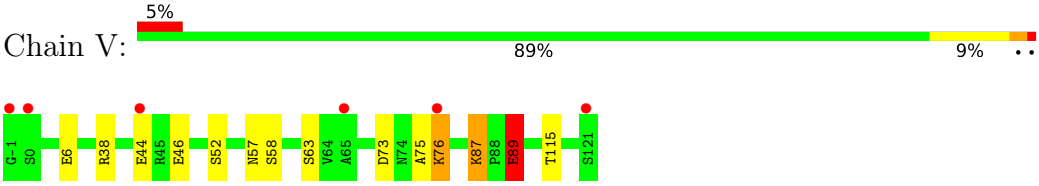
• Molecule 2: VHH_VcP#2

Chain T:



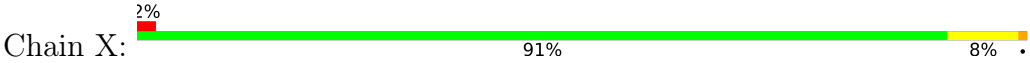
• Molecule 2: VHH_VcP#2

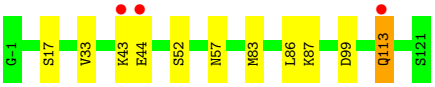
Chain V:



• Molecule 2: VHH_VcP#2

Chain X:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	223.57Å 153.11Å 210.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.24 – 2.81 34.24 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.1 (34.24-2.81) 99.0 (34.24-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.234 , 0.267 0.233 , 0.268	Depositor DCC
R_{free} test set	170340 reflections (1.17%)	wwPDB-VP
Wilson B-factor (Å^2)	44.9	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 38.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.008 for -h,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	79063	wwPDB-VP
Average B, all atoms (Å^2)	51.0	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 27.07 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3500e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.80	9/2404 (0.4%)	1.18	24/3248 (0.7%)
1	C	0.61	7/2404 (0.3%)	0.86	12/3248 (0.4%)
1	E	0.70	13/2413 (0.5%)	0.85	12/3260 (0.4%)
1	G	0.92	16/2404 (0.7%)	0.97	19/3248 (0.6%)
1	I	0.94	14/2404 (0.6%)	1.11	27/3248 (0.8%)
1	K	0.86	14/2404 (0.6%)	1.15	34/3248 (1.0%)
1	M	0.67	7/2404 (0.3%)	1.02	13/3248 (0.4%)
1	O	0.83	13/2404 (0.5%)	1.02	25/3248 (0.8%)
1	Q	0.38	1/2404 (0.0%)	0.70	8/3248 (0.2%)
1	U	0.66	7/2404 (0.3%)	0.83	11/3248 (0.3%)
1	W	0.58	6/2404 (0.2%)	0.92	17/3248 (0.5%)
1	Y	0.51	4/2404 (0.2%)	0.79	12/3248 (0.4%)
2	B	1.23	7/967 (0.7%)	1.03	5/1311 (0.4%)
2	D	0.65	4/961 (0.4%)	1.02	8/1303 (0.6%)
2	F	0.71	4/971 (0.4%)	1.09	14/1316 (1.1%)
2	H	0.85	4/971 (0.4%)	0.90	8/1316 (0.6%)
2	J	0.62	3/971 (0.3%)	0.85	4/1316 (0.3%)
2	L	0.70	4/971 (0.4%)	0.95	9/1316 (0.7%)
2	N	0.95	5/971 (0.5%)	1.00	8/1316 (0.6%)
2	P	0.74	5/971 (0.5%)	1.05	10/1316 (0.8%)
2	R	0.81	5/971 (0.5%)	0.91	7/1316 (0.5%)
2	T	0.38	0/971	0.74	2/1316 (0.2%)
2	V	0.68	5/971 (0.5%)	0.75	3/1316 (0.2%)
2	X	0.53	3/971 (0.3%)	0.68	2/1316 (0.2%)
All	All	0.74	160/40495 (0.4%)	0.95	294/54762 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	C	0	3
1	E	0	2
1	G	0	2
1	I	0	2
1	K	0	3
1	M	0	5
1	O	0	6
1	U	0	3
1	W	0	5
1	Y	0	3
2	B	0	1
2	D	0	3
2	H	0	1
2	J	0	2
2	L	0	3
2	N	0	1
2	P	0	3
2	R	0	3
2	T	0	1
All	All	0	57

All (160) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	107	LYS	CE-NZ	29.34	2.22	1.49
1	I	271	GLU	CD-OE2	22.21	1.50	1.25
1	I	271	GLU	CD-OE1	18.72	1.46	1.25
2	N	107	LYS	CD-CE	16.91	1.93	1.51
1	K	234	LYS	CD-CE	15.20	1.89	1.51
1	O	200	LYS	CE-NZ	14.80	1.86	1.49
2	H	44	GLU	CD-OE1	14.16	1.41	1.25
2	H	44	GLU	CD-OE2	13.99	1.41	1.25
2	R	44	GLU	CD-OE1	13.94	1.41	1.25
1	U	173	LEU	CG-CD1	13.65	2.02	1.51
1	G	191	LYS	CE-NZ	13.21	1.82	1.49
2	N	107	LYS	CB-CG	12.68	1.86	1.52
1	K	293	VAL	CB-CG2	12.42	1.78	1.52
1	E	187	LEU	CG-CD1	12.33	1.97	1.51
1	G	234	LYS	CE-NZ	12.20	1.79	1.49
1	M	180	VAL	CB-CG2	12.05	1.78	1.52
1	U	173	LEU	CG-CD2	11.88	1.95	1.51
2	F	44	GLU	CB-CG	11.73	1.74	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	140	LYS	CE-NZ	11.65	1.78	1.49
1	M	140	LYS	CD-CE	11.61	1.80	1.51
1	G	34	GLU	CD-OE1	-11.60	1.12	1.25
2	B	43	LYS	CD-CE	11.30	1.79	1.51
2	N	107	LYS	CG-CD	11.27	1.90	1.52
1	G	259	LYS	CE-NZ	11.14	1.76	1.49
2	L	87	LYS	CE-NZ	11.10	1.76	1.49
1	E	187	LEU	CG-CD2	10.71	1.91	1.51
1	M	29	GLU	CD-OE2	10.65	1.37	1.25
2	R	44	GLU	CD-OE2	10.41	1.37	1.25
1	G	239	VAL	CB-CG1	10.37	1.74	1.52
1	K	212	GLN	CB-CG	10.27	1.80	1.52
1	O	80	VAL	CB-CG2	-10.26	1.31	1.52
1	I	137	GLU	CB-CG	9.92	1.71	1.52
1	A	234	LYS	CD-CE	-9.90	1.26	1.51
1	G	34	GLU	CG-CD	-9.89	1.37	1.51
1	O	282	LYS	CE-NZ	9.86	1.73	1.49
1	W	293	VAL	CB-CG2	9.81	1.73	1.52
1	Y	202	LEU	CG-CD2	9.81	1.88	1.51
1	G	191	LYS	CD-CE	9.78	1.75	1.51
2	R	113	GLN	CG-CD	9.78	1.73	1.51
2	V	89	GLU	CD-OE1	9.72	1.36	1.25
1	G	140	LYS	CG-CD	9.43	1.84	1.52
1	W	293	VAL	CB-CG1	9.42	1.72	1.52
1	I	36	LYS	CE-NZ	9.37	1.72	1.49
2	B	12	VAL	CB-CG2	9.34	1.72	1.52
1	I	275	GLU	CD-OE2	9.26	1.35	1.25
1	K	283	GLU	CD-OE2	9.14	1.35	1.25
1	O	282	LYS	CG-CD	8.97	1.82	1.52
1	K	293	VAL	CB-CG1	8.90	1.71	1.52
1	G	234	LYS	CD-CE	8.84	1.73	1.51
1	O	80	VAL	CB-CG1	8.82	1.71	1.52
1	A	234	LYS	CB-CG	8.69	1.76	1.52
2	B	43	LYS	CG-CD	8.40	1.81	1.52
2	V	89	GLU	CG-CD	8.39	1.64	1.51
1	M	237	GLN	CG-CD	8.38	1.70	1.51
1	G	34	GLU	CD-OE2	-8.35	1.16	1.25
1	U	143	LYS	CD-CE	8.34	1.72	1.51
2	L	43	LYS	CB-CG	8.31	1.75	1.52
1	O	143	LYS	CE-NZ	8.29	1.69	1.49
2	J	107	LYS	CD-CE	8.27	1.72	1.51
1	O	110	GLN	CD-NE2	-8.24	1.12	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	29	GLU	CB-CG	8.22	1.67	1.52
1	I	131	ARG	CB-CG	8.21	1.74	1.52
1	G	140	LYS	CD-CE	8.16	1.71	1.51
2	D	12	VAL	CB-CG2	8.00	1.69	1.52
1	I	271	GLU	CG-CD	7.99	1.64	1.51
1	E	255	VAL	CB-CG2	7.96	1.69	1.52
2	P	76	LYS	CD-CE	7.91	1.71	1.51
1	O	32	GLN	CB-CG	7.88	1.73	1.52
2	B	12	VAL	CB-CG1	7.63	1.68	1.52
1	E	238	LYS	CE-NZ	7.61	1.68	1.49
2	P	44	GLU	CB-CG	7.61	1.66	1.52
1	A	248	LYS	CE-NZ	7.61	1.68	1.49
1	C	295	LYS	CE-NZ	7.60	1.68	1.49
1	K	223	LYS	CB-CG	7.52	1.72	1.52
1	K	162	SER	CB-OG	-7.50	1.32	1.42
2	H	12	VAL	CB-CG1	7.50	1.68	1.52
1	O	140	LYS	CB-CG	7.43	1.72	1.52
2	V	76	LYS	CB-CG	7.38	1.72	1.52
1	A	234	LYS	CE-NZ	-7.36	1.30	1.49
1	O	110	GLN	CB-CG	7.36	1.72	1.52
1	E	275	GLU	CB-CG	7.33	1.66	1.52
1	Y	275	GLU	CB-CG	7.29	1.66	1.52
1	I	253	GLU	CB-CG	7.27	1.66	1.52
1	E	157	LYS	CE-NZ	7.26	1.67	1.49
2	P	44	GLU	CD-OE2	7.22	1.33	1.25
1	K	234	LYS	CG-CD	7.16	1.76	1.52
1	O	200	LYS	CD-CE	7.13	1.69	1.51
1	E	259	LYS	CE-NZ	7.13	1.66	1.49
2	X	44	GLU	CB-CG	7.05	1.65	1.52
1	C	22	MET	CG-SD	7.02	1.99	1.81
1	E	255	VAL	CB-CG1	7.00	1.67	1.52
1	C	271	GLU	CB-CG	6.95	1.65	1.52
1	O	234	LYS	CD-CE	-6.86	1.34	1.51
1	K	115	ARG	CG-CD	6.82	1.69	1.51
2	N	12	VAL	CB-CG2	6.78	1.67	1.52
2	L	89	GLU	CG-CD	6.69	1.61	1.51
1	K	114	TRP	CB-CG	-6.62	1.38	1.50
1	U	278	GLN	CD-NE2	6.60	1.49	1.32
2	J	87	LYS	N-CA	-6.58	1.33	1.46
1	Q	87	LYS	CB-CG	6.57	1.70	1.52
1	K	283	GLU	CB-CG	6.56	1.64	1.52
1	A	34	GLU	CD-OE2	-6.51	1.18	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	89	GLU	CD-OE2	6.51	1.32	1.25
1	I	271	GLU	CB-CG	-6.48	1.39	1.52
1	A	263	ILE	CB-CG2	6.47	1.73	1.52
1	G	87	LYS	CB-CG	6.47	1.70	1.52
1	C	253	GLU	CD-OE1	6.43	1.32	1.25
1	U	259	LYS	CB-CG	6.43	1.70	1.52
1	C	22	MET	CB-CG	6.37	1.71	1.51
1	W	234	LYS	CD-CE	6.37	1.67	1.51
2	L	43	LYS	CE-NZ	6.34	1.64	1.49
2	P	113	GLN	CB-CG	6.33	1.69	1.52
1	K	223	LYS	CG-CD	6.28	1.73	1.52
2	N	44	GLU	CD-OE2	6.23	1.32	1.25
1	E	275	GLU	CG-CD	-6.22	1.42	1.51
2	R	12	VAL	CB-CG1	6.19	1.65	1.52
1	G	27	LEU	CG-CD2	6.10	1.74	1.51
1	C	254	LEU	CG-CD1	6.09	1.74	1.51
1	M	29	GLU	CD-OE1	6.08	1.32	1.25
2	R	12	VAL	CB-CG2	6.05	1.65	1.52
1	M	253	GLU	CD-OE2	-6.00	1.19	1.25
1	W	157	LYS	CD-CE	5.99	1.66	1.51
2	J	107	LYS	CE-NZ	5.98	1.64	1.49
1	G	140	LYS	CE-NZ	5.95	1.64	1.49
2	H	12	VAL	CB-CG2	5.93	1.65	1.52
1	U	283	GLU	CB-CG	5.93	1.63	1.52
1	K	234	LYS	CE-NZ	5.91	1.63	1.49
1	E	259	LYS	CD-CE	5.90	1.66	1.51
1	U	278	GLN	CB-CG	5.86	1.68	1.52
1	A	164	THR	CB-CG2	5.86	1.71	1.52
1	O	283	GLU	CG-CD	5.81	1.60	1.51
1	K	28	GLU	CD-OE2	-5.74	1.19	1.25
2	V	44	GLU	CG-CD	5.73	1.60	1.51
1	W	237	GLN	CB-CG	-5.72	1.37	1.52
2	D	12	VAL	CB-CG1	5.67	1.64	1.52
1	G	21	LYS	CE-NZ	-5.61	1.35	1.49
1	C	253	GLU	CD-OE2	5.60	1.31	1.25
1	I	36	LYS	CD-CE	5.59	1.65	1.51
2	D	113	GLN	CD-OE1	-5.58	1.11	1.24
1	E	157	LYS	CB-CG	5.58	1.67	1.52
1	W	253	GLU	CD-OE1	5.55	1.31	1.25
2	X	43	LYS	CE-NZ	5.53	1.62	1.49
2	X	44	GLU	CD-OE2	-5.51	1.19	1.25
2	D	87	LYS	CB-CG	5.50	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	137	GLU	CG-CD	-5.48	1.43	1.51
2	B	107	LYS	CD-CE	5.45	1.64	1.51
2	F	89	GLU	CB-CG	-5.43	1.41	1.52
1	Y	275	GLU	CD-OE2	5.38	1.31	1.25
2	F	46	GLU	CB-CG	-5.37	1.42	1.52
1	E	234	LYS	CE-NZ	5.33	1.62	1.49
2	P	46	GLU	CB-CG	5.30	1.62	1.52
2	B	43	LYS	CE-NZ	5.26	1.62	1.49
1	G	21	LYS	CB-CG	5.23	1.66	1.52
1	E	187	LEU	CB-CG	5.23	1.67	1.52
1	Y	260	SER	CA-CB	5.20	1.60	1.52
1	I	131	ARG	CD-NE	5.17	1.55	1.46
1	I	234	LYS	CD-CE	5.12	1.64	1.51
1	A	27	LEU	CG-CD2	5.08	1.70	1.51
2	F	44	GLU	CG-CD	5.05	1.59	1.51
1	I	143	LYS	CG-CD	5.04	1.69	1.52

All (294) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	29	GLU	CG-CD-OE1	22.50	163.29	118.30
1	M	29	GLU	CG-CD-OE2	-20.57	77.16	118.30
1	M	29	GLU	OE1-CD-OE2	-19.80	99.54	123.30
1	U	173	LEU	CB-CG-CD2	18.87	143.08	111.00
1	I	173	LEU	CB-CG-CD1	18.14	141.83	111.00
2	N	107	LYS	CD-CE-NZ	-17.01	72.57	111.70
1	M	140	LYS	CD-CE-NZ	-16.82	73.03	111.70
1	I	131	ARG	CG-CD-NE	-15.94	78.33	111.80
2	B	43	LYS	CD-CE-NZ	-15.91	75.10	111.70
1	E	187	LEU	CB-CG-CD1	15.36	137.12	111.00
1	A	27	LEU	CB-CG-CD1	14.87	136.28	111.00
2	P	76	LYS	CD-CE-NZ	14.51	145.07	111.70
2	B	107	LYS	CG-CD-CE	13.29	151.76	111.90
2	F	113	GLN	CB-CA-C	-13.18	84.03	110.40
1	A	263	ILE	CG1-CB-CG2	13.10	140.21	111.40
1	E	187	LEU	CB-CG-CD2	-13.02	88.87	111.00
2	H	44	GLU	OE1-CD-OE2	12.87	138.74	123.30
1	O	143	LYS	CD-CE-NZ	-12.86	82.13	111.70
1	K	233	GLN	C-N-CA	12.35	152.57	121.70
1	G	34	GLU	OE1-CD-OE2	-12.31	108.53	123.30
2	R	113	GLN	CA-CB-CG	12.18	140.20	113.40
1	W	223	LYS	CA-CB-CG	12.17	140.17	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	282	LYS	CB-CG-CD	-12.13	80.06	111.60
2	F	113	GLN	N-CA-CB	12.06	132.31	110.60
1	K	293	VAL	CG1-CB-CG2	11.77	129.73	110.90
1	G	282	LYS	CD-CE-NZ	-11.76	84.66	111.70
1	A	248	LYS	CD-CE-NZ	11.52	138.19	111.70
1	I	271	GLU	OE1-CD-OE2	11.45	137.04	123.30
2	T	113	GLN	C-N-CA	-11.18	98.82	122.30
1	K	87	LYS	CD-CE-NZ	11.14	137.33	111.70
1	G	147	PRO	C-N-CA	11.14	149.54	121.70
2	D	13	GLN	CA-CB-CG	11.04	137.69	113.40
1	I	234	LYS	CA-CB-CG	-11.01	89.19	113.40
1	I	131	ARG	NE-CZ-NH2	-10.98	114.81	120.30
1	A	248	LYS	CB-CG-CD	10.78	139.63	111.60
1	I	133	LEU	CB-CG-CD1	-10.78	92.67	111.00
1	A	23	LEU	CB-CG-CD1	10.61	129.04	111.00
2	F	43	LYS	C-N-CA	-10.55	95.32	121.70
1	K	212	GLN	CB-CA-C	10.49	131.39	110.40
1	K	202	LEU	CB-CG-CD2	10.38	128.64	111.00
1	I	271	GLU	N-CA-CB	-10.31	92.04	110.60
1	W	223	LYS	N-CA-CB	10.28	129.10	110.60
1	U	173	LEU	CA-CB-CG	-10.25	91.73	115.30
2	B	12	VAL	CG1-CB-CG2	10.21	127.23	110.90
1	Q	193	MET	CB-CG-SD	10.14	142.83	112.40
1	O	234	LYS	CB-CA-C	10.09	130.57	110.40
1	Q	87	LYS	CA-CB-CG	10.03	135.48	113.40
1	A	234	LYS	CB-CA-C	10.03	130.45	110.40
1	C	148	ASN	CB-CA-C	9.91	130.22	110.40
1	A	27	LEU	CB-CG-CD2	-9.85	94.26	111.00
1	K	147	PRO	C-N-CA	9.84	146.30	121.70
1	C	147	PRO	C-N-CA	9.74	146.06	121.70
1	A	131	ARG	CG-CD-NE	-9.61	91.62	111.80
1	G	148	ASN	CB-CA-C	9.46	129.32	110.40
1	K	223	LYS	CD-CE-NZ	-9.33	90.25	111.70
2	L	45	ARG	CB-CG-CD	-9.32	87.37	111.60
2	V	76	LYS	CA-CB-CG	9.29	133.83	113.40
1	C	148	ASN	N-CA-CB	-9.27	93.91	110.60
2	L	45	ARG	CG-CD-NE	9.26	131.25	111.80
2	P	76	LYS	CB-CG-CD	9.24	135.62	111.60
1	G	27	LEU	CB-CG-CD2	-9.21	95.34	111.00
1	O	148	ASN	CB-CA-C	9.15	128.69	110.40
1	W	234	LYS	CD-CE-NZ	9.10	132.64	111.70
1	I	253	GLU	CA-CB-CG	9.09	133.40	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	200	LYS	CD-CE-NZ	9.07	132.57	111.70
1	A	140	LYS	CD-CE-NZ	-9.06	90.86	111.70
1	Y	275	GLU	CA-CB-CG	9.06	133.33	113.40
1	I	28	GLU	CG-CD-OE2	-9.03	100.24	118.30
1	K	87	LYS	CG-CD-CE	-9.02	84.86	111.90
2	H	44	GLU	CG-CD-OE2	-8.93	100.44	118.30
1	O	30	MET	CA-CB-CG	8.92	128.47	113.30
1	Y	202	LEU	CA-CB-CG	8.88	135.71	115.30
1	I	131	ARG	NE-CZ-NH1	8.87	124.73	120.30
1	K	28	GLU	OE1-CD-OE2	-8.86	112.67	123.30
1	C	278	GLN	N-CA-CB	-8.85	94.68	110.60
1	W	191	LYS	CD-CE-NZ	8.77	131.88	111.70
2	D	87	LYS	CB-CG-CD	-8.74	88.88	111.60
1	Y	87	LYS	CB-CG-CD	8.68	134.16	111.60
2	R	44	GLU	CG-CD-OE2	-8.63	101.05	118.30
1	M	180	VAL	CG1-CB-CG2	8.60	124.66	110.90
1	O	147	PRO	C-N-CA	8.55	143.07	121.70
1	O	234	LYS	CD-CE-NZ	8.44	131.11	111.70
1	K	173	LEU	CA-CB-CG	8.43	134.68	115.30
1	W	157	LYS	CB-CG-CD	8.39	133.42	111.60
2	R	113	GLN	N-CA-CB	8.31	125.55	110.60
1	U	259	LYS	CD-CE-NZ	-8.29	92.63	111.70
1	U	278	GLN	CA-CB-CG	-8.29	95.16	113.40
1	K	173	LEU	CB-CG-CD2	-8.29	96.92	111.00
1	G	148	ASN	N-CA-CB	-8.24	95.76	110.60
1	K	148	ASN	CB-CA-C	8.24	126.87	110.40
1	I	143	LYS	CD-CE-NZ	-8.21	92.81	111.70
1	E	259	LYS	CD-CE-NZ	8.14	130.44	111.70
1	I	271	GLU	CG-CD-OE2	-8.10	102.10	118.30
2	L	87	LYS	CA-CB-CG	8.10	131.21	113.40
1	O	140	LYS	CB-CG-CD	8.06	132.57	111.60
1	I	133	LEU	CB-CG-CD2	8.02	124.64	111.00
1	G	295	LYS	CB-CG-CD	8.01	132.43	111.60
1	K	234	LYS	CD-CE-NZ	8.01	130.12	111.70
2	H	12	VAL	C-N-CA	7.97	141.62	121.70
1	A	34	GLU	N-CA-CB	-7.95	96.29	110.60
1	U	143	LYS	CA-CB-CG	-7.89	96.05	113.40
1	Y	133	LEU	CA-CB-CG	7.88	133.43	115.30
2	F	44	GLU	N-CA-CB	7.87	124.76	110.60
1	K	223	LYS	N-CA-CB	-7.82	96.52	110.60
2	B	43	LYS	CG-CD-CE	7.70	135.00	111.90
1	I	271	GLU	CB-CA-C	7.66	125.71	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	113	GLN	C-N-CA	7.62	138.31	122.30
1	K	148	ASN	N-CA-CB	-7.62	96.89	110.60
1	O	282	LYS	CB-CA-C	-7.61	95.19	110.40
2	D	13	GLN	N-CA-CB	7.60	124.28	110.60
1	O	234	LYS	CG-CD-CE	7.58	134.65	111.90
1	K	234	LYS	CB-CG-CD	7.57	131.28	111.60
1	K	234	LYS	CA-CB-CG	7.52	129.94	113.40
1	K	245	GLN	N-CA-CB	7.52	124.13	110.60
2	D	13	GLN	CB-CA-C	-7.50	95.40	110.40
1	A	34	GLU	CB-CA-C	7.46	125.33	110.40
2	L	43	LYS	CB-CG-CD	7.42	130.89	111.60
1	K	200	LYS	CD-CE-NZ	-7.39	94.71	111.70
1	W	237	GLN	CA-CB-CG	7.36	129.59	113.40
1	W	259	LYS	CA-CB-CG	7.34	129.55	113.40
2	P	44	GLU	CG-CD-OE2	-7.27	103.76	118.30
1	Q	87	LYS	N-CA-CB	7.21	123.57	110.60
1	C	274	ARG	N-CA-CB	-7.19	97.66	110.60
1	O	140	LYS	CG-CD-CE	-7.19	90.33	111.90
1	C	254	LEU	CA-CB-CG	7.18	131.82	115.30
2	D	12	VAL	CG1-CB-CG2	7.18	122.38	110.90
1	C	140	LYS	CG-CD-CE	7.17	133.40	111.90
1	W	193	MET	CA-CB-CG	7.13	125.43	113.30
1	M	237	GLN	CB-CG-CD	7.13	130.14	111.60
1	C	278	GLN	CA-CB-CG	7.11	129.04	113.40
1	O	274	ARG	CG-CD-NE	7.07	126.65	111.80
1	G	234	LYS	CB-CG-CD	7.05	129.94	111.60
1	U	173	LEU	CB-CA-C	7.04	123.58	110.20
1	A	282	LYS	CD-CE-NZ	7.00	127.81	111.70
1	K	28	GLU	CB-CG-CD	-6.99	95.32	114.20
1	O	80	VAL	CA-CB-CG2	6.99	121.39	110.90
1	Y	275	GLU	N-CA-CB	6.98	123.16	110.60
2	D	3	GLN	CA-CB-CG	6.97	128.73	113.40
1	C	140	LYS	CD-CE-NZ	-6.95	95.72	111.70
1	W	259	LYS	CB-CG-CD	-6.92	93.60	111.60
1	E	234	LYS	CB-CG-CD	-6.90	93.65	111.60
2	V	75	ALA	C-N-CA	6.86	138.85	121.70
1	Q	143	LYS	CD-CE-NZ	-6.86	95.92	111.70
1	C	245	GLN	CA-CB-CG	-6.84	98.34	113.40
1	O	282	LYS	CG-CD-CE	6.83	132.39	111.90
1	I	143	LYS	CB-CG-CD	6.81	129.31	111.60
2	L	42	GLY	C-N-CA	6.79	138.69	121.70
1	A	133	LEU	CA-CB-CG	6.79	130.92	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	89	GLU	N-CA-CB	6.75	122.74	110.60
1	Y	87	LYS	CD-CE-NZ	6.74	127.20	111.70
1	G	27	LEU	CB-CG-CD1	6.74	122.45	111.00
1	O	148	ASN	N-CA-CB	-6.74	98.47	110.60
1	M	180	VAL	CA-CB-CG1	-6.73	100.80	110.90
2	P	76	LYS	CB-CA-C	-6.72	96.97	110.40
2	F	89	GLU	CA-CB-CG	6.71	128.17	113.40
2	P	44	GLU	OE1-CD-OE2	6.70	131.34	123.30
1	I	137	GLU	OE1-CD-OE2	6.69	131.32	123.30
1	Y	260	SER	N-CA-CB	6.67	120.50	110.50
1	I	28	GLU	OE1-CD-OE2	6.67	131.30	123.30
1	A	206	HIS	N-CA-CB	-6.66	98.61	110.60
1	W	223	LYS	CB-CA-C	-6.64	97.12	110.40
1	G	97	GLU	CG-CD-OE2	-6.63	105.03	118.30
2	P	113	GLN	C-N-CA	6.62	136.20	122.30
2	N	107	LYS	CG-CD-CE	-6.60	92.10	111.90
1	E	187	LEU	CD1-CG-CD2	6.58	130.24	110.50
1	O	274	ARG	CB-CG-CD	6.56	128.66	111.60
1	A	234	LYS	CD-CE-NZ	-6.54	96.66	111.70
2	F	44	GLU	CA-CB-CG	6.53	127.77	113.40
1	A	219	SER	N-CA-CB	6.52	120.28	110.50
1	O	142	LEU	CA-CB-CG	6.52	130.29	115.30
1	W	200	LYS	CB-CG-CD	6.52	128.55	111.60
2	R	12	VAL	CG1-CB-CG2	6.51	121.32	110.90
2	D	87	LYS	N-CA-CB	6.48	122.27	110.60
1	O	143	LYS	CG-CD-CE	6.48	131.35	111.90
2	J	13	GLN	CA-CB-CG	6.46	127.61	113.40
1	A	131	ARG	CB-CG-CD	6.46	128.39	111.60
1	G	239	VAL	CG1-CB-CG2	6.44	121.21	110.90
1	K	234	LYS	N-CA-CB	-6.44	99.02	110.60
2	H	13	GLN	N-CA-CB	-6.43	99.03	110.60
2	P	107	LYS	N-CA-CB	-6.42	99.04	110.60
2	F	45	ARG	CB-CG-CD	6.41	128.27	111.60
2	N	44	GLU	N-CA-CB	6.38	122.08	110.60
1	A	35	ILE	CG1-CB-CG2	-6.36	97.42	111.40
1	E	110	GLN	CA-CB-CG	6.34	127.34	113.40
1	O	234	LYS	CB-CG-CD	6.31	128.02	111.60
1	M	29	GLU	CB-CG-CD	-6.25	97.32	114.20
1	E	234	LYS	CD-CE-NZ	6.25	126.08	111.70
1	Y	275	GLU	CB-CA-C	-6.23	97.93	110.40
1	Q	110	GLN	N-CA-CB	6.22	121.81	110.60
1	W	293	VAL	CG1-CB-CG2	6.21	120.84	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	45	ARG	CG-CD-NE	-6.21	98.76	111.80
1	W	233	GLN	CA-CB-CG	6.17	126.98	113.40
1	K	35	ILE	CG1-CB-CG2	-6.17	97.83	111.40
1	I	245	GLN	N-CA-CB	6.17	121.70	110.60
1	K	212	GLN	CG-CD-NE2	-6.14	101.95	116.70
1	K	222	GLN	C-N-CA	6.12	136.99	121.70
2	F	45	ARG	CD-NE-CZ	-6.09	115.07	123.60
1	Y	234	LYS	CD-CE-NZ	-6.08	97.73	111.70
2	R	112	GLY	C-N-CA	-6.06	106.55	121.70
1	I	245	GLN	CA-CB-CG	-6.05	100.09	113.40
2	X	113	GLN	CA-CB-CG	6.05	126.71	113.40
2	N	44	GLU	CA-CB-CG	6.03	126.66	113.40
1	O	110	GLN	CG-CD-OE1	6.03	133.65	121.60
1	O	110	GLN	N-CA-CB	-6.01	99.78	110.60
1	A	234	LYS	N-CA-CB	-6.00	99.79	110.60
1	W	234	LYS	CG-CD-CE	-6.00	93.91	111.90
2	X	44	GLU	CG-CD-OE1	6.00	130.29	118.30
1	U	274	ARG	CA-CB-CG	-5.97	100.26	113.40
2	R	44	GLU	OE1-CD-OE2	5.97	130.46	123.30
1	I	244	THR	C-N-CA	-5.97	106.78	121.70
2	P	44	GLU	CB-CG-CD	5.96	130.30	114.20
2	F	113	GLN	CA-CB-CG	5.96	126.51	113.40
1	M	253	GLU	CG-CD-OE2	-5.96	106.38	118.30
1	I	173	LEU	CB-CG-CD2	-5.96	100.87	111.00
1	M	29	GLU	CA-CB-CG	5.95	126.48	113.40
1	I	28	GLU	CA-CB-CG	5.94	126.48	113.40
1	M	253	GLU	N-CA-CB	5.94	121.29	110.60
2	N	45	ARG	CG-CD-NE	5.93	124.25	111.80
1	E	255	VAL	CG1-CB-CG2	5.88	120.31	110.90
1	W	274	ARG	CG-CD-NE	-5.87	99.48	111.80
1	Y	32	GLN	CA-CB-CG	5.87	126.31	113.40
2	J	89	GLU	CA-CB-CG	5.86	126.30	113.40
2	N	43	LYS	CB-CA-C	-5.83	98.75	110.40
1	I	253	GLU	CG-CD-OE2	-5.82	106.66	118.30
2	P	113	GLN	CA-CB-CG	5.82	126.20	113.40
2	N	44	GLU	OE1-CD-OE2	5.81	130.28	123.30
2	P	76	LYS	CA-CB-CG	-5.80	100.63	113.40
2	T	44	GLU	CA-CB-CG	5.80	126.16	113.40
1	G	97	GLU	CG-CD-OE1	5.79	129.88	118.30
2	H	12	VAL	CA-CB-CG2	5.79	119.58	110.90
1	O	30	MET	CB-CG-SD	5.78	129.73	112.40
1	I	253	GLU	CB-CA-C	-5.77	98.86	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	237	GLN	N-CA-CB	5.75	120.95	110.60
1	K	212	GLN	N-CA-CB	-5.67	100.39	110.60
1	G	191	LYS	CD-CE-NZ	-5.67	98.67	111.70
2	L	43	LYS	CA-CB-CG	-5.63	101.01	113.40
1	A	270	LEU	CA-CB-CG	5.62	128.24	115.30
1	K	28	GLU	CG-CD-OE1	5.62	129.54	118.30
1	E	288	ILE	CG1-CB-CG2	-5.58	99.13	111.40
2	L	87	LYS	N-CA-CB	5.58	120.64	110.60
1	K	110	GLN	CA-CB-CG	5.56	125.63	113.40
1	I	200	LYS	CB-CG-CD	-5.55	97.17	111.60
2	N	107	LYS	CA-CB-CG	-5.53	101.24	113.40
1	U	143	LYS	N-CA-CB	-5.53	100.65	110.60
1	G	87	LYS	CA-CB-CG	5.52	125.54	113.40
2	L	45	ARG	CB-CA-C	-5.52	99.37	110.40
2	B	19	ARG	CG-CD-NE	-5.50	100.24	111.80
1	K	223	LYS	CA-CB-CG	5.48	125.46	113.40
1	G	140	LYS	CD-CE-NZ	5.47	124.28	111.70
2	H	43	LYS	C-N-CA	5.45	135.33	121.70
1	M	253	GLU	CB-CA-C	-5.45	99.50	110.40
2	L	45	ARG	CD-NE-CZ	-5.44	115.98	123.60
1	Q	193	MET	CG-SD-CE	-5.40	91.56	100.20
1	W	237	GLN	N-CA-CB	5.40	120.32	110.60
1	A	248	LYS	CA-CB-CG	-5.38	101.57	113.40
1	W	253	GLU	CA-CB-CG	5.37	125.22	113.40
2	H	11	LEU	CB-CG-CD1	5.37	120.13	111.00
1	A	158	LEU	CA-CB-CG	-5.36	102.98	115.30
1	K	245	GLN	CB-CA-C	-5.36	99.69	110.40
1	K	200	LYS	CB-CG-CD	-5.35	97.70	111.60
1	G	259	LYS	CG-CD-CE	-5.35	95.86	111.90
1	K	87	LYS	CB-CA-C	-5.34	99.72	110.40
1	I	143	LYS	CG-CD-CE	-5.32	95.94	111.90
1	U	259	LYS	CB-CG-CD	-5.29	97.84	111.60
1	Y	202	LEU	CD1-CG-CD2	5.28	126.35	110.50
1	A	233	GLN	CA-CB-CG	5.27	125.00	113.40
2	V	76	LYS	CG-CD-CE	5.27	127.71	111.90
1	Y	87	LYS	CG-CD-CE	-5.27	96.10	111.90
1	Q	193	MET	CA-CB-CG	5.24	122.21	113.30
1	G	102	GLN	CB-CG-CD	5.23	125.20	111.60
2	F	89	GLU	CB-CA-C	-5.23	99.95	110.40
1	U	174	ALA	N-CA-CB	-5.20	102.83	110.10
1	U	142	LEU	C-N-CA	5.18	134.66	121.70
1	C	254	LEU	CD1-CG-CD2	5.18	126.04	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	213	MET	CA-CB-CG	5.17	122.10	113.30
2	J	89	GLU	N-CA-CB	5.17	119.91	110.60
1	K	234	LYS	CB-CA-C	5.16	120.72	110.40
1	O	234	LYS	CA-CB-CG	-5.16	102.06	113.40
1	G	295	LYS	CG-CD-CE	-5.14	96.47	111.90
1	O	148	ASN	C-N-CA	5.14	134.55	121.70
1	E	157	LYS	CD-CE-NZ	-5.14	99.89	111.70
1	C	81	MET	CA-CB-CG	5.13	122.03	113.30
2	R	113	GLN	C-N-CA	-5.13	111.52	122.30
1	E	287	ASN	C-N-CA	-5.13	108.88	121.70
1	A	140	LYS	CA-CB-CG	5.11	124.65	113.40
2	J	113	GLN	CB-CA-C	-5.09	100.21	110.40
2	H	107	LYS	CB-CA-C	-5.09	100.21	110.40
1	O	234	LYS	N-CA-CB	-5.09	101.43	110.60
1	G	27	LEU	CA-CB-CG	-5.09	103.59	115.30
1	K	87	LYS	N-CA-CB	5.09	119.76	110.60
1	E	259	LYS	CA-CB-CG	-5.08	102.22	113.40
2	F	45	ARG	CA-CB-CG	5.05	124.51	113.40
2	D	107	LYS	CB-CG-CD	-5.04	98.49	111.60
1	Q	109	LEU	C-N-CA	-5.03	109.12	121.70

There are no chirality outliers.

All (57) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	ARG	Sidechain
1	A	159	SER	Mainchain
1	A	219	SER	Mainchain
1	A	274	ARG	Sidechain
1	A	33	GLY	Peptide
2	B	113	GLN	Peptide
1	C	148	ASN	Sidechain
1	C	274	ARG	Sidechain
1	C	278	GLN	Sidechain
2	D	113	GLN	Sidechain
2	D	86	LEU	Mainchain
2	D	87	LYS	Mainchain
1	E	275	GLU	Peptide
1	E	287	ASN	Peptide
1	G	148	ASN	Sidechain
1	G	271	GLU	Sidechain
2	H	44	GLU	Sidechain

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Mol	Chain	Res	Type	Group
1	I	245	GLN	Sidechain
1	I	271	GLU	Sidechain
2	J	106	ARG	Peptide
2	J	13	GLN	Peptide
1	K	148	ASN	Sidechain
1	K	212	GLN	Sidechain
1	K	245	GLN	Mainchain
2	L	107	LYS	Peptide
2	L	43	LYS	Mainchain
2	L	45	ARG	Sidechain
1	M	178	ASN	Peptide
1	M	236	VAL	Peptide
1	M	237	GLN	Peptide
1	M	28	GLU	Peptide
1	M	29	GLU	Sidechain
2	N	12	VAL	Peptide
1	O	139	PHE	Peptide
1	O	148	ASN	Sidechain
1	O	233	GLN	Peptide
1	O	234	LYS	Peptide,Mainchain
1	O	274	ARG	Sidechain
2	P	112	GLY	Peptide
2	P	44	GLU	Peptide,Sidechain
2	R	113	GLN	Sidechain
2	R	43	LYS	Peptide
2	R	45	ARG	Sidechain
2	T	112	GLY	Peptide
1	U	159	SER	Peptide
1	U	173	LEU	Mainchain
1	U	274	ARG	Sidechain
1	W	109	LEU	Peptide
1	W	159	SER	Peptide
1	W	237	GLN	Sidechain
1	W	274	ARG	Sidechain
1	W	93	ARG	Sidechain
1	Y	131	ARG	Sidechain
1	Y	260	SER	Mainchain
1	Y	275	GLU	Peptide

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	2360	2341	2342	146	4
1	C	2360	2336	2342	48	0
1	E	2369	2348	2347	50	1
1	G	2360	2340	2341	64	0
1	I	2360	2342	2342	52	1
1	K	2360	2341	2342	68	0
1	M	2360	2341	2342	44	0
1	O	2360	2340	2342	81	3
1	Q	2360	2341	2342	20	0
1	U	2360	2341	2342	40	2
1	W	2360	2340	2342	46	1
1	Y	2360	2340	2342	36	1
2	B	945	891	893	19	0
2	D	939	887	888	22	2
2	F	949	896	896	10	0
2	H	949	896	895	10	0
2	J	949	896	896	11	3
2	L	949	898	896	19	1
2	N	949	896	896	34	2
2	P	949	897	896	9	0
2	R	949	896	896	13	0
2	T	949	896	896	10	3
2	V	949	896	896	10	0
2	X	949	896	896	4	0
3	A	20	17	17	0	0
3	C	20	17	17	2	0
3	E	20	17	17	0	0
3	G	20	17	17	0	0
3	I	20	17	17	0	0
3	K	20	17	17	0	0
3	M	20	17	17	0	0
3	O	20	17	17	0	0
3	Q	20	17	17	1	0
3	U	20	17	17	0	0
3	W	20	17	17	1	0
3	Y	20	17	17	0	0
4	E	6	8	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	6	8	8	0	0
4	Q	6	8	7	1	0
4	U	18	24	24	0	0
All	All	39979	39084	39099	845	12

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (845) 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:I:131:ARG:CG	1:I:131:ARG:CB	1.74	1.64
1:G:191:LYS:CE	1:G:191:LYS:CD	1.75	1.63
2:L:43:LYS:CB	2:L:43:LYS:CG	1.75	1.62
1:K:234:LYS:CD	1:K:234:LYS:CG	1.76	1.61
1:O:263:ILE:CD1	1:O:263:ILE:CG1	1.75	1.59
2:B:43:LYS:CD	2:B:43:LYS:CG	1.81	1.59
2:B:43:LYS:CD	2:B:43:LYS:CE	1.79	1.58
1:M:180:VAL:CG2	1:M:180:VAL:CB	1.78	1.57
1:C:295:LYS:CE	1:C:295:LYS:NZ	1.68	1.57
1:K:212:GLN:CG	1:K:212:GLN:CB	1.80	1.56
1:G:239:VAL:CG1	1:G:239:VAL:CB	1.74	1.56
1:A:234:LYS:CB	1:A:234:LYS:CG	1.76	1.56
1:G:140:LYS:CD	1:G:140:LYS:CG	1.84	1.56
1:O:282:LYS:CD	1:O:282:LYS:CG	1.82	1.56
1:K:293:VAL:CG2	1:K:293:VAL:CB	1.78	1.55
1:M:140:LYS:CE	1:M:140:LYS:CD	1.80	1.55
1:O:143:LYS:CE	1:O:143:LYS:NZ	1.69	1.55
1:A:248:LYS:NZ	1:A:248:LYS:CE	1.68	1.52
1:A:263:ILE:CD1	1:A:263:ILE:CG1	1.82	1.52
1:E:238:LYS:CE	1:E:238:LYS:NZ	1.68	1.52
1:Y:202:LEU:CD2	1:Y:202:LEU:CG	1.88	1.52
1:Q:288:ILE:CG1	1:Q:288:ILE:CD1	1.83	1.51
2:N:107:LYS:CG	2:N:107:LYS:CB	1.86	1.51
1:O:282:LYS:NZ	1:O:282:LYS:CE	1.73	1.49
1:K:234:LYS:CD	1:K:234:LYS:CE	1.89	1.49
1:E:187:LEU:CG	1:E:187:LEU:CD2	1.91	1.49
1:I:36:LYS:CE	1:I:36:LYS:NZ	1.72	1.49
1:G:259:LYS:CE	1:G:259:LYS:NZ	1.76	1.48
2:N:107:LYS:CG	2:N:107:LYS:CD	1.90	1.47
1:E:187:LEU:CD1	1:E:187:LEU:HG	1.45	1.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:87:LYS:CE	2:L:87:LYS:NZ	1.76	1.46
2:N:107:LYS:CD	2:N:107:LYS:CE	1.93	1.46
1:A:140:LYS:CE	1:A:140:LYS:NZ	1.78	1.46
1:U:173:LEU:CG	1:U:173:LEU:CD2	1.95	1.45
1:E:187:LEU:CG	1:E:187:LEU:CD1	1.97	1.43
1:G:234:LYS:CE	1:G:234:LYS:NZ	1.79	1.41
1:G:191:LYS:CE	1:G:191:LYS:NZ	1.82	1.41
1:O:200:LYS:CE	1:O:200:LYS:NZ	1.86	1.37
1:U:173:LEU:CG	1:U:173:LEU:CD1	2.02	1.36
2:N:45:ARG:HD2	2:N:107:LYS:NZ	1.47	1.27
1:O:282:LYS:CD	1:O:282:LYS:CB	2.13	1.26
1:M:140:LYS:CD	1:M:140:LYS:NZ	2.03	1.21
1:O:143:LYS:NZ	1:O:143:LYS:CD	2.08	1.15
2:N:107:LYS:CD	2:N:107:LYS:NZ	2.10	1.14
2:B:43:LYS:CD	2:B:43:LYS:NZ	2.08	1.13
1:E:187:LEU:CD2	1:E:187:LEU:HA	1.81	1.09
1:E:187:LEU:CD2	1:E:187:LEU:CA	2.35	1.04
2:B:107:LYS:NZ	2:B:107:LYS:CE	2.22	1.01
1:U:173:LEU:CD2	1:U:173:LEU:HG	1.87	1.01
2:L:43:LYS:H	2:L:43:LYS:HG3	1.26	0.98
1:M:140:LYS:NZ	1:M:140:LYS:HD3	1.80	0.97
1:E:187:LEU:CA	1:E:187:LEU:HD23	1.94	0.97
1:O:282:LYS:CD	1:O:282:LYS:HB2	1.96	0.95
1:I:250:GLN:OE1	1:I:253:GLU:HG3	1.66	0.95
1:W:128:THR:OG1	1:W:199:GLN:OE1	1.83	0.94
1:A:140:LYS:NZ	1:A:140:LYS:CD	2.29	0.94
1:A:15:VAL:HG11	1:A:247:VAL:HG22	1.50	0.93
1:G:31:SER:HB2	1:G:34:GLU:HB2	1.49	0.92
1:O:131:ARG:NH2	1:O:138:ASP:O	2.02	0.92
2:B:43:LYS:NZ	2:B:43:LYS:HD3	1.84	0.91
1:M:234:LYS:O	1:M:237:GLN:HB3	1.69	0.90
2:N:45:ARG:CD	2:N:107:LYS:NZ	2.35	0.89
2:N:45:ARG:HD2	2:N:107:LYS:HZ2	1.37	0.89
1:K:35:ILE:HD11	1:K:228:ASP:HB3	1.53	0.88
1:E:187:LEU:CD2	1:E:187:LEU:CB	2.51	0.88
1:I:275:GLU:OE2	1:I:278:GLN:NE2	2.06	0.87
2:D:43:LYS:HE3	1:G:282:LYS:NZ	1.90	0.87
1:A:187:LEU:HA	1:A:190:ILE:HD12	1.57	0.87
2:V:73:ASP:HB3	2:V:76:LYS:HG3	1.55	0.86
1:W:156:ALA:O	1:W:159:SER:HB2	1.76	0.86
2:L:43:LYS:CG	2:L:43:LYS:CA	2.54	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:230:ASP:O	1:O:234:LYS:HB2	1.76	0.85
1:A:233:GLN:O	1:A:236:VAL:N	2.10	0.85
1:W:237:GLN:O	1:W:240:GLY:N	2.10	0.84
1:M:180:VAL:CG2	1:M:180:VAL:HB	2.06	0.84
1:E:187:LEU:HA	1:E:187:LEU:HD22	1.59	0.83
1:O:282:LYS:CA	1:O:282:LYS:HD2	2.08	0.83
1:O:143:LYS:NZ	1:O:143:LYS:HD2	1.94	0.83
1:O:93:ARG:NH1	1:O:97:GLU:OE1	2.12	0.83
2:N:45:ARG:HD2	2:N:107:LYS:HZ3	1.41	0.83
2:D:43:LYS:HE3	1:G:282:LYS:HZ1	1.40	0.82
1:K:293:VAL:CG2	1:K:293:VAL:HB	2.05	0.82
1:I:55:LEU:CD2	1:I:215:ILE:HG22	2.09	0.82
2:N:12:VAL:O	2:N:119:VAL:HA	1.78	0.82
1:M:237:GLN:NE2	1:M:241:ASP:OD2	2.13	0.82
2:L:45:ARG:NH1	2:L:111:TRP:CZ2	2.47	0.82
2:N:107:LYS:CD	2:N:107:LYS:HZ3	1.91	0.81
1:E:187:LEU:HA	1:E:187:LEU:HD23	1.54	0.80
1:K:174:ALA:HB1	1:K:180:VAL:HG22	1.61	0.80
1:O:282:LYS:CB	1:O:282:LYS:HD2	2.08	0.80
1:E:187:LEU:HD23	1:E:187:LEU:N	1.96	0.80
1:K:172:TYR:OH	1:K:197:GLU:OE1	1.99	0.80
1:E:187:LEU:HB2	1:E:251:GLU:HG2	1.64	0.79
1:M:140:LYS:CD	1:M:140:LYS:HZ2	1.93	0.79
1:I:14:SER:OG	1:I:16:GLU:OE1	2.01	0.78
1:E:272:PRO:O	1:E:275:GLU:HG2	1.83	0.78
2:L:43:LYS:CG	2:L:43:LYS:H	1.97	0.77
2:N:107:LYS:HZ3	2:N:107:LYS:HD3	1.47	0.77
1:Y:68:GLY:HA3	1:Y:81:MET:HG3	1.67	0.77
2:N:107:LYS:NZ	2:N:107:LYS:HD3	2.00	0.77
1:K:250:GLN:HB3	1:K:254:LEU:HD11	1.67	0.76
1:G:23:LEU:HG	1:G:27:LEU:CD1	2.16	0.76
1:A:281:TYR:HB3	1:A:293:VAL:HG11	1.67	0.76
1:O:282:LYS:HB2	1:O:282:LYS:HD3	1.68	0.76
1:O:200:LYS:HD2	1:O:263:ILE:CD1	2.16	0.76
1:U:156:ALA:O	1:U:159:SER:HB2	1.86	0.75
1:M:236:VAL:O	1:M:237:GLN:O	2.03	0.75
1:G:93:ARG:O	1:G:97:GLU:HG3	1.87	0.75
2:N:107:LYS:CG	2:N:107:LYS:CA	2.64	0.75
1:G:23:LEU:HG	1:G:27:LEU:HD11	1.69	0.75
2:L:45:ARG:HH12	2:L:107:LYS:HG3	1.52	0.75
1:A:23:LEU:HD12	1:A:235:ALA:HB1	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:239:VAL:CG1	1:G:239:VAL:CA	2.64	0.74
1:A:31:SER:O	1:A:34:GLU:OE1	2.04	0.74
2:L:43:LYS:HG3	2:L:43:LYS:N	2.03	0.73
1:O:200:LYS:HD2	1:O:263:ILE:HD12	1.71	0.73
1:G:31:SER:CB	1:G:34:GLU:HB2	2.18	0.73
1:A:101:GLY:O	1:A:104:VAL:HG22	1.89	0.73
2:B:43:LYS:HD3	2:B:43:LYS:HZ3	1.53	0.72
1:A:23:LEU:HD12	1:A:239:VAL:HG21	1.70	0.72
1:K:220:THR:O	1:K:223:LYS:HB2	1.90	0.71
1:A:281:TYR:CG	1:A:293:VAL:HG21	2.26	0.71
1:I:55:LEU:HD23	1:I:215:ILE:HG22	1.72	0.71
1:A:242:ALA:O	1:A:246:THR:OG1	2.08	0.70
2:J:12:VAL:HG22	2:J:13:GLN:N	2.06	0.70
1:W:183:GLN:HG2	1:W:184:GLU:H	1.55	0.70
1:M:194:LYS:HD3	1:M:197:GLU:OE2	1.90	0.70
1:K:115:ARG:O	1:K:215:ILE:HA	1.92	0.70
1:O:77:ALA:O	1:O:80:VAL:HG23	1.91	0.70
1:O:262:GLY:O	1:O:263:ILE:O	2.10	0.70
1:M:140:LYS:HD3	1:M:140:LYS:HZ3	1.57	0.69
2:H:106:ARG:NH1	2:H:107:LYS:O	2.26	0.69
1:I:131:ARG:CG	1:I:131:ARG:CA	2.68	0.69
2:B:43:LYS:CD	2:B:43:LYS:HZ2	2.05	0.69
1:A:128:THR:OG1	1:A:199:GLN:HG3	1.92	0.69
1:Q:288:ILE:CD1	1:Q:288:ILE:CB	2.71	0.69
1:A:175:LEU:HD23	1:A:180:VAL:HG23	1.74	0.69
1:G:259:LYS:NZ	1:G:265:VAL:HB	2.08	0.69
2:T:6:GLU:CD	2:T:114:GLY:H	1.95	0.69
1:Y:133:LEU:HD22	1:Y:139:PHE:CD1	2.28	0.69
1:A:235:ALA:C	1:A:239:VAL:HG23	2.12	0.69
1:G:22:MET:SD	1:G:239:VAL:HG12	2.33	0.68
1:K:142:LEU:O	1:K:161:ALA:HB1	1.92	0.68
1:O:80:VAL:HG12	1:O:92:LEU:CD1	2.23	0.68
1:W:193:MET:O	1:W:194:LYS:HG2	1.92	0.68
1:Y:259:LYS:O	1:Y:262:GLY:N	2.26	0.68
1:K:282:LYS:NZ	1:K:283:GLU:OE2	2.26	0.68
1:M:237:GLN:O	1:M:239:VAL:N	2.26	0.68
2:L:45:ARG:NH1	2:L:107:LYS:HG3	2.09	0.68
1:O:263:ILE:CD1	1:O:263:ILE:CB	2.71	0.68
1:G:95:MET:CE	1:G:296:LEU:HB3	2.25	0.67
1:W:183:GLN:HG2	1:W:184:GLU:N	2.09	0.67
1:E:187:LEU:HG	1:E:187:LEU:HD12	1.68	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:131:ARG:CB	1:I:131:ARG:CD	2.67	0.67
1:A:83:PRO:HB2	1:A:277:MET:HG3	1.76	0.67
1:O:143:LYS:CD	1:O:143:LYS:HZ3	2.04	0.67
1:Y:202:LEU:CD2	1:Y:202:LEU:HG	2.16	0.66
1:O:282:LYS:CD	1:O:282:LYS:CA	2.71	0.66
1:K:250:GLN:O	1:K:254:LEU:HG	1.95	0.66
2:B:91:THR:HG23	2:B:118:THR:HA	1.77	0.66
2:J:12:VAL:HG22	2:J:13:GLN:H	1.62	0.65
1:K:109:LEU:HD23	1:K:110:GLN:HB2	1.78	0.65
1:G:95:MET:HE3	1:G:296:LEU:HB3	1.79	0.65
1:W:61:ASP:O	1:W:62:ILE:HD13	1.97	0.65
1:O:71:GLY:HA3	1:O:78:GLU:HG3	1.77	0.65
2:J:85:SER:O	2:J:85:SER:OG	2.13	0.64
2:F:10:ARG:HG3	2:F:10:ARG:HH11	1.62	0.64
1:C:295:LYS:NZ	1:C:295:LYS:CD	2.59	0.64
1:E:275:GLU:HB2	1:E:276:ALA:HB2	1.80	0.64
2:T:44:GLU:CD	2:T:44:GLU:H	2.00	0.64
1:G:191:LYS:CE	1:G:191:LYS:CG	2.72	0.64
1:K:219:SER:O	1:K:223:LYS:HG3	1.98	0.64
1:A:234:LYS:O	1:A:238:LYS:HB2	1.97	0.64
2:N:107:LYS:CG	2:N:107:LYS:CE	2.76	0.64
1:K:134:ASN:N	1:K:138:ASP:OD1	2.31	0.63
1:I:250:GLN:HA	1:I:253:GLU:CG	2.28	0.63
1:K:293:VAL:CG2	1:K:293:VAL:CA	2.74	0.63
1:A:29:GLU:HG2	1:A:30:MET:SD	2.39	0.63
1:A:244:THR:O	1:A:248:LYS:HD2	1.99	0.63
1:O:173:LEU:O	1:O:177:THR:HG23	1.98	0.63
1:E:187:LEU:HB2	1:E:188:PRO:HD3	1.78	0.63
1:I:55:LEU:CD2	1:I:215:ILE:CG2	2.77	0.63
1:W:274:ARG:HB3	1:W:274:ARG:CZ	2.28	0.63
1:U:125:ARG:NE	1:U:184:GLU:OE2	2.30	0.62
1:A:296:LEU:HA	1:A:299:MET:HG3	1.81	0.62
1:I:245:GLN:CG	1:I:249:THR:HG23	2.29	0.62
1:U:142:LEU:HD12	1:U:181:ASP:HB2	1.81	0.62
1:E:274:ARG:O	1:E:275:GLU:C	2.38	0.62
1:W:188:PRO:O	1:W:192:THR:OG1	2.11	0.62
2:H:12:VAL:CG2	2:H:13:GLN:N	2.63	0.62
1:O:143:LYS:NZ	1:O:143:LYS:HD3	2.10	0.62
1:A:255:VAL:HG12	1:A:259:LYS:NZ	2.14	0.62
1:Y:128:THR:HG22	1:Y:202:LEU:HD23	1.81	0.62
2:H:39:GLN:NE2	2:H:43:LYS:O	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:6:GLU:CD	2:R:114:GLY:H	2.02	0.62
1:W:132:PRO:HA	1:W:201:ASN:HD22	1.63	0.62
1:M:79:ALA:HA	1:M:82:LEU:HD12	1.80	0.62
1:O:233:GLN:C	1:O:236:VAL:HG22	2.20	0.62
2:D:83:MET:HB3	2:D:86:LEU:HD21	1.82	0.61
1:A:35:ILE:HD11	1:A:228:ASP:CG	2.20	0.61
1:E:172:TYR:OH	1:E:197:GLU:OE2	2.11	0.61
1:K:71:GLY:HA3	1:K:78:GLU:HG3	1.82	0.61
1:W:61:ASP:C	1:W:62:ILE:HD13	2.20	0.61
1:A:255:VAL:O	1:A:259:LYS:HG3	2.00	0.61
1:I:79:ALA:HA	1:I:82:LEU:HD12	1.81	0.61
1:I:28:GLU:HG2	2:P:1:GLN:OE1	2.01	0.61
1:Y:93:ARG:O	1:Y:97:GLU:HG3	2.01	0.61
1:G:199:GLN:O	1:G:263:ILE:HD11	2.00	0.61
1:A:129:SER:N	1:A:199:GLN:OE1	2.34	0.61
1:A:235:ALA:O	1:A:238:LYS:N	2.34	0.61
2:L:43:LYS:CG	2:L:43:LYS:N	2.61	0.61
1:Y:133:LEU:CD2	1:Y:139:PHE:HA	2.31	0.61
1:C:136:ILE:HD12	1:C:272:PRO:HB2	1.82	0.61
1:K:121:TYR:HB3	1:K:244:THR:HG23	1.83	0.60
1:I:245:GLN:O	1:I:248:LYS:N	2.34	0.60
2:N:45:ARG:HD2	2:N:107:LYS:HZ1	1.55	0.60
1:A:15:VAL:CG1	1:A:247:VAL:HG22	2.28	0.60
1:A:32:GLN:O	1:A:34:GLU:HG3	2.00	0.60
1:G:79:ALA:HA	1:G:82:LEU:HD12	1.84	0.60
2:D:87:LYS:HB3	2:D:88:PRO:HD2	1.83	0.60
1:I:250:GLN:HA	1:I:253:GLU:HG2	1.83	0.60
2:T:12:VAL:HG12	2:T:13:GLN:H	1.65	0.60
1:A:263:ILE:CD1	1:A:263:ILE:CB	2.76	0.60
1:K:142:LEU:HD12	1:K:181:ASP:HB2	1.83	0.60
1:O:200:LYS:CD	1:O:263:ILE:CD1	2.80	0.60
2:D:87:LYS:HB3	2:D:88:PRO:CD	2.32	0.59
1:G:23:LEU:C	1:G:27:LEU:HD12	2.23	0.59
1:W:193:MET:C	1:W:194:LYS:HG2	2.22	0.59
1:A:23:LEU:HD23	1:A:37:LEU:CD2	2.33	0.59
1:W:237:GLN:O	1:W:238:LYS:C	2.39	0.59
1:I:16:GLU:HG2	1:I:212:GLN:HE22	1.66	0.59
2:H:20:LEU:HG	2:H:83:MET:HE2	1.85	0.59
1:O:250:GLN:O	1:O:254:LEU:HG	2.03	0.59
1:U:288:ILE:HG22	1:U:290:GLN:H	1.66	0.59
1:A:296:LEU:HA	1:A:299:MET:HE2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:79:ALA:HB2	1:Q:284:PHE:CE1	2.38	0.59
1:C:23:LEU:O	1:C:27:LEU:HG	2.02	0.59
1:I:55:LEU:HD23	1:I:215:ILE:CG2	2.33	0.59
1:G:136:ILE:HG21	1:G:272:PRO:HB2	1.83	0.58
1:E:194:LYS:HB3	1:E:197:GLU:HG3	1.84	0.58
1:K:293:VAL:CG1	2:R:41:PRO:HG3	2.33	0.58
2:V:73:ASP:HB3	2:V:76:LYS:CG	2.29	0.58
1:Y:55:LEU:HD11	1:Y:63:THR:HG22	1.85	0.58
1:A:142:LEU:O	1:A:161:ALA:HB1	2.03	0.58
1:C:269:ASP:O	1:C:272:PRO:HD2	2.04	0.58
2:D:91:THR:HG23	2:D:118:THR:HA	1.86	0.58
1:E:140:LYS:HD2	1:E:160:GLY:HA3	1.86	0.58
1:K:234:LYS:CG	1:K:234:LYS:CE	2.81	0.58
1:C:80:VAL:CG1	1:C:92:LEU:CD1	2.81	0.58
1:W:193:MET:O	1:W:194:LYS:CG	2.52	0.58
1:I:245:GLN:HG2	1:I:249:THR:HG23	1.85	0.58
1:A:256:SER:O	1:A:259:LYS:N	2.36	0.58
1:I:157:LYS:HD2	1:I:163:PRO:HG2	1.85	0.58
1:I:268:PRO:O	1:I:270:LEU:HD12	2.04	0.58
1:A:93:ARG:O	1:A:97:GLU:HG2	2.03	0.58
1:A:102:GLN:OE1	1:A:105:ARG:NH1	2.37	0.58
2:D:10:ARG:HG3	2:D:10:ARG:HH11	1.69	0.58
1:A:102:GLN:HA	1:A:105:ARG:HG3	1.86	0.57
1:I:24:ALA:O	1:I:28:GLU:HB2	2.04	0.57
1:C:271:GLU:HB3	1:C:272:PRO:HD3	1.86	0.57
2:L:87:LYS:NZ	2:L:87:LYS:CD	2.65	0.57
1:Y:201:ASN:HD22	1:Y:264:ASN:HB3	1.69	0.57
1:A:127:THR:H	1:A:203:ALA:HB3	1.69	0.57
1:A:133:LEU:CD1	1:A:203:ALA:HB2	2.35	0.57
2:D:3:GLN:N	2:D:3:GLN:OE1	2.36	0.57
1:O:262:GLY:O	1:O:263:ILE:C	2.42	0.57
1:A:271:GLU:HA	1:A:274:ARG:HB2	1.87	0.57
1:O:271:GLU:HA	1:O:274:ARG:HG3	1.87	0.57
1:C:65:ALA:O	1:C:213:MET:N	2.36	0.56
1:K:282:LYS:HE3	1:K:283:GLU:HG2	1.87	0.56
2:L:44:GLU:O	2:L:45:ARG:C	2.41	0.56
1:A:126:GLU:OE1	1:A:205:THR:N	2.38	0.56
1:M:176:GLN:HG2	1:Q:227:THR:HG21	1.86	0.56
2:N:45:ARG:HB2	2:N:107:LYS:HZ1	1.71	0.56
1:A:272:PRO:HA	1:A:275:GLU:HG2	1.87	0.56
1:O:200:LYS:CD	1:O:263:ILE:HD13	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:250:GLN:HA	1:W:253:GLU:HG3	1.87	0.56
1:A:65:ALA:O	1:A:213:MET:N	2.36	0.55
1:A:157:LYS:O	1:A:160:GLY:N	2.39	0.55
1:C:84:TYR:CD1	1:C:274:ARG:NH2	2.74	0.55
1:K:119:THR:HA	1:K:213:MET:HA	1.88	0.55
1:O:200:LYS:HD2	1:O:263:ILE:HD13	1.87	0.55
1:O:230:ASP:O	1:O:234:LYS:CB	2.50	0.55
1:C:84:TYR:HD1	1:C:274:ARG:NH2	2.05	0.55
1:K:186:PRO:HG2	1:K:189:THR:HG22	1.87	0.55
1:U:250:GLN:HB3	1:U:254:LEU:HD23	1.89	0.55
1:A:27:LEU:HD11	1:A:232:ILE:HA	1.89	0.55
1:A:234:LYS:CG	1:A:234:LYS:CA	2.77	0.55
2:D:86:LEU:O	2:D:87:LYS:CG	2.55	0.55
1:K:187:LEU:HD23	1:K:190:ILE:HD12	1.86	0.55
1:A:121:TYR:CZ	1:A:123:GLY:HA2	2.41	0.55
2:H:20:LEU:HD11	2:H:83:MET:HE1	1.89	0.55
1:U:250:GLN:HB3	1:U:254:LEU:CD2	2.37	0.55
1:A:23:LEU:CD1	1:A:239:VAL:HG21	2.37	0.55
1:A:133:LEU:HD23	1:A:139:PHE:CZ	2.41	0.55
2:J:6:GLU:CD	2:J:114:GLY:H	2.10	0.55
1:Y:83:PRO:HB2	1:Y:277:MET:HG3	1.88	0.55
1:A:273:PHE:O	1:A:276:ALA:N	2.39	0.55
1:K:121:TYR:CB	1:K:244:THR:HG23	2.37	0.55
1:A:235:ALA:O	1:A:239:VAL:HG23	2.07	0.55
1:O:125:ARG:NE	1:O:184:GLU:OE2	2.36	0.55
1:O:143:LYS:O	1:O:180:VAL:HG22	2.07	0.55
1:Y:133:LEU:HD22	1:Y:139:PHE:CG	2.42	0.55
1:C:140:LYS:HE2	1:C:160:GLY:CA	2.37	0.55
2:H:12:VAL:HG22	2:H:13:GLN:N	2.22	0.55
1:K:174:ALA:CB	1:K:180:VAL:HG22	2.33	0.55
1:U:143:LYS:O	1:U:181:ASP:N	2.40	0.54
1:A:266:THR:HG22	1:A:268:PRO:HD3	1.88	0.54
2:B:44:GLU:OE1	2:B:44:GLU:HA	2.07	0.54
1:G:71:GLY:HA3	1:G:78:GLU:HG3	1.89	0.54
1:K:27:LEU:HD21	1:K:232:ILE:HA	1.89	0.54
1:A:92:LEU:CD2	1:A:211:ASP:HB3	2.36	0.54
1:K:203:ALA:O	1:K:205:THR:N	2.40	0.54
2:F:39:GLN:HG3	2:F:45:ARG:HA	1.90	0.54
2:V:73:ASP:O	2:V:76:LYS:HB2	2.07	0.54
1:W:202:LEU:HD22	1:W:265:VAL:HG13	1.88	0.54
1:W:237:GLN:O	1:W:239:VAL:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:133:LEU:HD21	1:Y:142:LEU:HD22	1.90	0.54
2:R:17:SER:HB2	2:V:58:SER:HB2	1.89	0.54
1:C:249:THR:O	1:C:253:GLU:HG2	2.08	0.54
1:G:31:SER:O	1:G:34:GLU:HG2	2.08	0.54
1:G:191:LYS:CD	1:G:191:LYS:NZ	2.71	0.54
1:K:133:LEU:HD21	1:K:142:LEU:HD22	1.90	0.54
1:Q:93:ARG:NH1	1:Q:97:GLU:OE1	2.40	0.54
1:Q:212:GLN:OE1	3:Q:301:SLB:H113	2.08	0.54
1:Y:121:TYR:HB3	1:Y:244:THR:HG23	1.90	0.54
1:A:124:THR:HG22	1:A:206:HIS:HA	1.89	0.54
2:N:45:ARG:CD	2:N:107:LYS:HZ1	2.15	0.54
1:E:272:PRO:HA	1:E:275:GLU:HG2	1.90	0.53
2:P:52:SER:HB3	2:P:57:ASN:HB2	1.90	0.53
2:N:12:VAL:C	2:N:13:GLN:HG2	2.28	0.53
2:V:73:ASP:CB	2:V:76:LYS:HG3	2.33	0.53
1:G:259:LYS:HZ2	1:G:265:VAL:HB	1.72	0.53
1:Y:203:ALA:O	1:Y:205:THR:N	2.42	0.53
2:D:40:ALA:HB1	2:D:41:PRO:HD2	1.89	0.53
1:O:184:GLU:HG3	1:O:207:HIS:NE2	2.24	0.53
1:A:82:LEU:HD22	1:A:281:TYR:HD1	1.74	0.53
1:W:34:GLU:C	1:W:35:ILE:HD13	2.28	0.53
1:K:35:ILE:HD13	1:K:232:ILE:HD11	1.90	0.53
1:M:113:ASN:OD1	1:M:218:GLU:HB3	2.09	0.53
2:N:45:ARG:HB2	2:N:107:LYS:NZ	2.24	0.53
1:A:128:THR:C	1:A:199:GLN:OE1	2.47	0.53
1:G:213:MET:HE2	1:G:215:ILE:HD11	1.90	0.53
1:M:180:VAL:CG2	1:M:180:VAL:CA	2.79	0.53
1:A:15:VAL:HG21	1:A:188:PRO:CB	2.39	0.53
1:C:131:ARG:NH2	1:C:138:ASP:O	2.42	0.53
1:W:207:HIS:CD2	1:W:208:ILE:HD12	2.44	0.53
1:G:184:GLU:HG3	1:G:207:HIS:NE2	2.23	0.52
2:V:6:GLU:HB2	2:V:115:THR:HG23	1.92	0.52
1:A:175:LEU:CD2	1:A:180:VAL:HG23	2.39	0.52
1:C:84:TYR:CB	1:C:274:ARG:HG2	2.39	0.52
2:D:10:ARG:HH11	2:D:10:ARG:CG	2.22	0.52
1:A:101:GLY:O	1:A:104:VAL:CG2	2.57	0.52
1:G:69:ARG:NH1	1:G:148:ASN:O	2.35	0.52
2:N:45:ARG:CB	2:N:107:LYS:HZ1	2.21	0.52
1:A:133:LEU:HD11	1:A:203:ALA:HB2	1.91	0.52
2:N:108:TYR:HB2	2:N:111:TRP:CZ2	2.45	0.52
1:A:27:LEU:HD23	1:A:35:ILE:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:34:GLU:OE2	1:U:34:GLU:HA	2.10	0.52
1:U:173:LEU:CD1	1:U:173:LEU:HA	2.39	0.52
1:A:89:PHE:HB2	1:A:121:TYR:CD1	2.45	0.52
1:G:71:GLY:HA3	1:G:78:GLU:CG	2.40	0.52
1:I:213:MET:HE3	1:I:215:ILE:HD11	1.92	0.52
1:O:233:GLN:CA	1:O:236:VAL:HG22	2.40	0.52
2:D:43:LYS:HE3	1:G:282:LYS:HZ3	1.73	0.52
1:O:200:LYS:HD2	1:O:263:ILE:HA	1.91	0.52
1:Q:183:GLN:OE1	1:Q:185:ASN:HB2	2.09	0.52
1:I:133:LEU:HD23	1:I:139:PHE:CD1	2.45	0.52
1:A:133:LEU:HD13	1:A:203:ALA:HA	1.92	0.52
1:G:259:LYS:HZ1	1:G:265:VAL:HB	1.73	0.52
1:I:263:ILE:N	1:I:263:ILE:HD13	2.25	0.52
1:Y:275:GLU:O	1:Y:278:GLN:HG2	2.10	0.52
2:F:45:ARG:HD3	2:F:111:TRP:CH2	2.45	0.51
2:L:88:PRO:HA	2:L:119:VAL:HB	1.92	0.51
1:E:272:PRO:HA	1:E:275:GLU:CD	2.31	0.51
1:O:109:LEU:HA	1:O:114:TRP:O	2.09	0.51
1:C:184:GLU:O	1:C:185:ASN:OD1	2.27	0.51
1:O:203:ALA:O	1:O:205:THR:N	2.44	0.51
1:A:271:GLU:O	1:A:275:GLU:HB3	2.10	0.51
1:K:63:THR:HG23	1:K:64:TYR:O	2.11	0.51
1:C:182:GLY:HA2	1:C:199:GLN:NE2	2.25	0.51
1:W:27:LEU:HD12	1:W:231:ILE:HG22	1.93	0.51
1:Y:55:LEU:HD23	1:Y:60:LEU:HB3	1.93	0.51
1:K:121:TYR:CZ	1:K:123:GLY:HA2	2.46	0.51
1:Y:275:GLU:HB2	1:Y:276:ALA:CA	2.40	0.51
1:M:114:TRP:HB3	1:M:215:ILE:HG21	1.92	0.51
1:Y:274:ARG:O	1:Y:275:GLU:C	2.45	0.51
1:A:95:MET:SD	1:A:296:LEU:HD22	2.51	0.51
2:D:113:GLN:NE2	2:D:113:GLN:CA	2.74	0.51
1:G:213:MET:CE	1:G:215:ILE:HD11	2.40	0.51
1:G:239:VAL:CG1	1:G:239:VAL:HB	2.19	0.51
1:O:232:ILE:O	1:O:234:LYS:N	2.44	0.51
1:A:64:TYR:HD1	1:A:212:GLN:HG3	1.75	0.51
1:I:15:VAL:CG2	1:I:16:GLU:N	2.74	0.50
1:K:191:LYS:O	1:K:194:LYS:N	2.34	0.50
2:B:17:SER:HB2	2:L:58:SER:HB2	1.93	0.50
1:C:134:ASN:O	1:C:268:PRO:HB3	2.11	0.50
2:N:58:SER:HB2	2:X:17:SER:HB2	1.94	0.50
1:O:143:LYS:HZ3	1:O:143:LYS:HD3	1.69	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:233:GLN:HA	1:O:236:VAL:CG2	2.41	0.50
1:W:182:GLY:HA2	1:W:199:GLN:HE22	1.77	0.50
1:K:63:THR:HG23	1:K:64:TYR:N	2.25	0.50
2:P:17:SER:HB2	2:T:58:SER:HB2	1.93	0.50
1:Y:128:THR:CG2	1:Y:202:LEU:HD23	2.41	0.50
1:A:185:ASN:O	1:A:190:ILE:HD11	2.12	0.50
1:U:145:ARG:CG	1:U:166:MET:HG2	2.42	0.50
2:J:12:VAL:CG2	2:J:13:GLN:H	2.22	0.50
2:N:13:GLN:O	2:N:14:THR:C	2.50	0.50
1:U:143:LYS:HB2	1:U:181:ASP:CG	2.32	0.50
1:A:94:ARG:O	1:A:98:SER:N	2.45	0.50
1:C:140:LYS:HE2	1:C:160:GLY:HA3	1.94	0.50
1:G:184:GLU:HG3	1:G:207:HIS:CE1	2.47	0.50
1:O:67:PHE:HD2	1:O:80:VAL:HG11	1.77	0.50
1:O:71:GLY:HA3	1:O:78:GLU:CG	2.40	0.50
1:W:194:LYS:HA	1:W:196:TYR:CE1	2.47	0.50
2:L:48:VAL:HG22	2:L:49:ALA:N	2.27	0.50
1:G:259:LYS:NZ	1:G:259:LYS:HG3	2.27	0.49
1:A:140:LYS:NZ	1:A:140:LYS:HD2	2.21	0.49
1:K:142:LEU:CD1	1:K:181:ASP:HB2	2.41	0.49
1:A:234:LYS:CB	1:A:234:LYS:CD	2.80	0.49
1:A:81:MET:CG	1:A:81:MET:O	2.61	0.49
1:C:288:ILE:N	1:C:288:ILE:HD12	2.27	0.49
2:T:12:VAL:HG12	2:T:13:GLN:N	2.27	0.49
2:D:86:LEU:O	2:D:87:LYS:HG3	2.12	0.49
1:W:212:GLN:NE2	3:W:301:SLB:H113	2.28	0.49
1:C:31:SER:HB2	1:C:35:ILE:HG12	1.94	0.49
1:W:34:GLU:O	1:W:35:ILE:HD13	2.12	0.49
1:A:140:LYS:NZ	1:A:140:LYS:CG	2.76	0.49
1:C:6:MET:HG3	1:C:62:ILE:HB	1.94	0.49
1:G:140:LYS:CG	1:G:140:LYS:CE	2.88	0.49
1:W:183:GLN:NE2	1:W:185:ASN:HB2	2.27	0.49
1:C:175:LEU:HD22	1:C:199:GLN:NE2	2.28	0.49
1:I:245:GLN:HG3	1:I:249:THR:HG23	1.95	0.49
1:M:92:LEU:CD2	1:M:211:ASP:HB3	2.43	0.49
2:H:39:GLN:HG3	2:H:43:LYS:O	2.13	0.49
1:O:232:ILE:O	1:O:236:VAL:HG22	2.13	0.49
1:O:263:ILE:CD1	1:O:263:ILE:CA	2.90	0.49
1:A:218:GLU:O	1:A:221:TRP:HB3	2.12	0.48
1:K:282:LYS:CE	1:K:283:GLU:HG2	2.42	0.48
2:H:67:ARG:NH1	2:H:85:SER:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:266:THR:O	1:M:268:PRO:HD3	2.13	0.48
2:N:67:ARG:HG2	2:N:85:SER:OG	2.13	0.48
1:W:55:LEU:HD11	1:W:63:THR:HG22	1.95	0.48
1:C:182:GLY:HA2	1:C:199:GLN:HE22	1.78	0.48
2:F:10:ARG:HH11	2:F:10:ARG:CG	2.26	0.48
1:I:16:GLU:HG2	1:I:212:GLN:NE2	2.27	0.48
1:K:70:MET:HG3	1:K:108:MET:SD	2.54	0.48
1:O:184:GLU:CG	1:O:207:HIS:HE2	2.26	0.48
1:Y:233:GLN:O	1:Y:236:VAL:HG22	2.12	0.48
1:K:212:GLN:CB	1:K:212:GLN:CD	2.76	0.48
2:T:52:SER:HB3	2:T:57:ASN:HB2	1.94	0.48
1:U:84:TYR:CE1	1:U:207:HIS:HA	2.48	0.48
1:Y:143:LYS:O	1:Y:180:VAL:HG22	2.12	0.48
1:A:272:PRO:O	1:A:275:GLU:HG2	2.14	0.48
2:J:12:VAL:CG2	2:J:13:GLN:N	2.73	0.48
1:M:82:LEU:HD22	1:M:281:TYR:HD1	1.77	0.48
1:W:202:LEU:O	1:W:266:THR:HG22	2.13	0.48
1:A:255:VAL:HG12	1:A:259:LYS:HZ2	1.75	0.48
1:E:272:PRO:CA	1:E:275:GLU:HG2	2.43	0.48
1:K:153:LEU:HD21	1:K:165:PRO:HG3	1.94	0.48
1:Q:203:ALA:O	1:Q:205:THR:N	2.47	0.48
1:Y:281:TYR:HB3	1:Y:293:VAL:HG11	1.95	0.48
1:E:3:THR:HG23	1:E:3:THR:O	2.12	0.48
1:O:279:PRO:HA	1:O:282:LYS:HD3	1.94	0.48
1:I:245:GLN:HG2	1:I:249:THR:CG2	2.43	0.48
1:O:3:THR:HG23	1:O:3:THR:O	2.14	0.48
1:U:22:MET:O	1:U:26:THR:HG23	2.12	0.48
1:U:278:GLN:OE1	1:U:281:TYR:CD2	2.67	0.48
1:A:205:THR:O	1:A:206:HIS:C	2.49	0.48
1:G:266:THR:O	1:G:268:PRO:HD3	2.13	0.48
1:O:233:GLN:HA	1:O:236:VAL:HG22	1.95	0.48
1:U:278:GLN:OE1	1:U:281:TYR:HD2	1.97	0.48
1:Y:133:LEU:HD23	1:Y:138:ASP:C	2.34	0.48
1:A:244:THR:C	1:A:248:LYS:HD2	2.35	0.48
1:G:184:GLU:CG	1:G:207:HIS:HE2	2.27	0.48
1:A:285:ASP:OD2	1:A:293:VAL:HG12	2.14	0.47
1:C:221:TRP:CE2	1:C:229:LYS:HD3	2.49	0.47
1:E:82:LEU:HD23	1:E:151:GLN:OE1	2.14	0.47
1:I:25:ASP:O	1:I:28:GLU:HB3	2.15	0.47
1:M:92:LEU:HD23	1:M:211:ASP:HB3	1.95	0.47
2:N:67:ARG:CZ	2:N:87:LYS:HE2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:292:ILE:HD13	4:Q:302:GOL:H2	1.95	0.47
1:A:158:LEU:HB3	1:A:276:ALA:HB1	1.96	0.47
1:W:183:GLN:CG	1:W:184:GLU:N	2.76	0.47
1:A:154:ASN:O	1:A:158:LEU:HG	2.14	0.47
1:A:79:ALA:HA	1:A:82:LEU:HD12	1.96	0.47
2:F:45:ARG:HD2	2:F:107:LYS:NZ	2.29	0.47
2:N:107:LYS:HG2	2:N:111:TRP:HZ2	1.80	0.47
1:U:173:LEU:O	1:U:177:THR:N	2.40	0.47
2:V:87:LYS:HG3	2:V:89:GLU:HG2	1.95	0.47
1:I:200:LYS:HA	1:I:200:LYS:HD3	1.44	0.47
1:K:136:ILE:HD13	1:K:273:PHE:CD2	2.49	0.47
1:K:189:THR:HA	1:K:192:THR:OG1	2.15	0.47
1:O:227:THR:O	1:O:231:ILE:HG13	2.15	0.47
1:A:33:GLY:CA	1:A:34:GLU:HG3	2.45	0.47
1:A:226:ASP:O	1:A:230:ASP:OD2	2.33	0.47
2:D:113:GLN:NE2	2:D:113:GLN:HA	2.30	0.47
1:M:73:ALA:HB1	1:M:112:PHE:CZ	2.50	0.47
1:O:105:ARG:HG3	1:O:105:ARG:HH11	1.80	0.47
1:O:232:ILE:C	1:O:234:LYS:N	2.68	0.47
2:P:6:GLU:OE2	2:P:112:GLY:HA3	2.14	0.47
2:X:52:SER:HB3	2:X:57:ASN:HB2	1.96	0.47
1:C:80:VAL:HG11	1:C:92:LEU:CD1	2.45	0.47
1:E:272:PRO:HA	1:E:275:GLU:CG	2.44	0.47
1:G:3:THR:O	1:G:3:THR:HG23	2.15	0.47
1:O:21:LYS:NZ	1:O:25:ASP:OD1	2.45	0.47
1:A:143:LYS:O	1:A:181:ASP:N	2.46	0.47
1:C:55:LEU:HD11	1:C:63:THR:HG22	1.97	0.47
2:P:39:GLN:HG3	2:P:44:GLU:O	2.14	0.47
1:U:173:LEU:HA	1:U:173:LEU:HD12	1.97	0.47
1:C:3:THR:HG23	1:C:3:THR:O	2.14	0.47
1:K:6:MET:CE	1:K:37:LEU:HD21	2.45	0.47
2:N:67:ARG:NH1	2:N:90:ASP:OD2	2.34	0.47
1:W:125:ARG:HD3	1:W:210:ASN:OD1	2.15	0.47
1:I:270:LEU:HA	1:I:273:PHE:HD1	1.79	0.46
2:J:52:SER:HB3	2:J:57:ASN:HB2	1.96	0.46
1:A:67:PHE:CZ	1:A:104:VAL:HG21	2.50	0.46
1:A:84:TYR:CE2	1:A:273:PHE:HB3	2.49	0.46
1:A:145:ARG:HG2	1:A:166:MET:HG2	1.96	0.46
2:B:83:MET:HE2	2:B:86:LEU:HD11	1.96	0.46
1:G:284:PHE:O	1:G:288:ILE:HG12	2.15	0.46
1:K:243:HIS:O	1:K:244:THR:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ASP:OD1	1:C:48:ASP:N	2.49	0.46
1:I:187:LEU:N	1:I:188:PRO:HD2	2.30	0.46
1:I:266:THR:O	1:I:268:PRO:HD3	2.15	0.46
1:K:200:LYS:HA	1:K:200:LYS:HD3	1.75	0.46
2:L:48:VAL:CG2	2:L:49:ALA:N	2.78	0.46
1:U:184:GLU:HG3	1:U:207:HIS:NE2	2.30	0.46
1:Y:273:PHE:HD1	1:Y:273:PHE:H	1.63	0.46
1:A:187:LEU:HD12	1:A:202:LEU:HD11	1.97	0.46
2:B:33:VAL:CG2	2:B:101:PHE:HA	2.46	0.46
1:E:272:PRO:O	1:E:275:GLU:CG	2.59	0.46
1:G:143:LYS:O	1:G:180:VAL:HG13	2.15	0.46
1:I:244:THR:O	1:I:245:GLN:C	2.50	0.46
2:J:42:GLY:C	2:J:43:LYS:HG2	2.35	0.46
1:K:71:GLY:HA3	1:K:78:GLU:CG	2.46	0.46
2:N:107:LYS:HG2	2:N:111:TRP:CZ2	2.51	0.46
2:R:89:GLU:OE2	2:R:89:GLU:N	2.47	0.46
1:A:128:THR:OG1	1:A:199:GLN:CG	2.63	0.46
1:C:84:TYR:HD1	1:C:274:ARG:HH21	1.59	0.46
1:G:23:LEU:O	1:G:27:LEU:HD12	2.16	0.46
1:W:207:HIS:HD2	1:W:208:ILE:HD12	1.78	0.46
1:A:35:ILE:CD1	1:A:228:ASP:HB3	2.45	0.46
1:E:65:ALA:HB3	1:E:215:ILE:CD1	2.46	0.46
1:E:155:TYR:O	1:E:159:SER:OG	2.34	0.46
1:E:172:TYR:HD1	1:E:173:LEU:HD12	1.81	0.46
1:M:79:ALA:HA	1:M:82:LEU:CD1	2.43	0.46
2:P:12:VAL:HG12	2:P:13:GLN:N	2.31	0.46
1:C:77:ALA:O	1:C:80:VAL:HG23	2.16	0.46
1:G:95:MET:HE2	1:G:296:LEU:HB3	1.95	0.46
1:G:129:SER:HB3	1:G:133:LEU:HD11	1.98	0.46
1:G:271:GLU:N	1:G:272:PRO:HD2	2.31	0.46
2:J:36:TRP:HD1	2:J:70:ILE:HD12	1.81	0.46
1:M:81:MET:O	1:M:81:MET:HG2	2.16	0.46
2:N:12:VAL:C	2:N:13:GLN:CG	2.85	0.46
1:O:143:LYS:NZ	1:O:181:ASP:OD1	2.49	0.46
1:O:184:GLU:HG3	1:O:207:HIS:CE1	2.51	0.46
1:A:84:TYR:HE2	1:A:273:PHE:HB3	1.82	0.45
1:A:187:LEU:CD1	1:A:202:LEU:HD11	2.46	0.45
1:A:281:TYR:HB3	1:A:293:VAL:HG21	1.99	0.45
1:C:271:GLU:CB	1:C:272:PRO:HD3	2.45	0.45
1:I:270:LEU:HA	1:I:273:PHE:CD1	2.52	0.45
1:U:191:LYS:HD3	1:U:254:LEU:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ILE:HG12	1:A:216:ILE:HG13	1.98	0.45
1:A:225:SER:O	1:A:229:LYS:HG3	2.17	0.45
1:G:232:ILE:O	1:G:236:VAL:HG13	2.16	0.45
1:G:292:ILE:O	1:G:295:LYS:HB3	2.16	0.45
1:M:180:VAL:CG1	1:M:181:ASP:N	2.78	0.45
1:O:232:ILE:C	1:O:234:LYS:H	2.20	0.45
2:R:39:GLN:CD	2:R:45:ARG:HG3	2.36	0.45
1:E:95:MET:HG2	1:E:296:LEU:HD22	1.98	0.45
2:H:45:ARG:HE	2:H:45:ARG:HB2	1.61	0.45
1:K:83:PRO:HG2	1:K:277:MET:HE3	1.97	0.45
1:O:120:TRP:O	1:O:212:GLN:N	2.49	0.45
1:A:256:SER:O	1:A:259:LYS:HB2	2.16	0.45
1:G:184:GLU:HG3	1:G:207:HIS:HE2	1.81	0.45
1:O:270:LEU:O	1:O:274:ARG:HG2	2.16	0.45
1:W:126:GLU:O	1:W:184:GLU:HA	2.17	0.45
1:C:55:LEU:HD23	1:C:217:SER:HB2	1.97	0.45
2:D:87:LYS:CB	2:D:88:PRO:CD	2.94	0.45
1:G:23:LEU:CG	1:G:27:LEU:HD11	2.45	0.45
1:G:125:ARG:HE	1:G:184:GLU:CD	2.20	0.45
1:K:224:LEU:HD13	1:K:232:ILE:HD12	1.97	0.45
1:U:184:GLU:HG3	1:U:207:HIS:CE1	2.51	0.45
1:A:145:ARG:CG	1:A:166:MET:HG2	2.47	0.45
1:O:175:LEU:HD11	1:O:183:GLN:HG2	1.99	0.45
1:A:33:GLY:C	1:A:34:GLU:HG3	2.38	0.45
2:J:91:THR:HG23	2:J:118:THR:HA	1.99	0.45
1:U:69:ARG:O	1:U:69:ARG:HG3	2.17	0.45
2:V:52:SER:HB3	2:V:57:ASN:HB2	1.98	0.45
1:E:271:GLU:N	1:E:272:PRO:HD2	2.32	0.45
1:O:228:ASP:HA	1:O:231:ILE:HD12	1.97	0.45
1:W:132:PRO:CA	1:W:201:ASN:HD22	2.30	0.45
1:C:147:PRO:HD2	1:C:184:GLU:OE2	2.17	0.45
1:C:245:GLN:OE1	1:O:245:GLN:HG3	2.16	0.45
2:D:14:THR:HG23	2:D:87:LYS:HG2	1.98	0.45
1:I:101:GLY:O	1:I:104:VAL:HG22	2.17	0.45
1:I:200:LYS:HB2	1:I:200:LYS:HE2	1.77	0.45
1:E:134:ASN:O	1:E:268:PRO:HB3	2.17	0.44
1:K:293:VAL:HG11	2:R:41:PRO:HG3	1.98	0.44
1:M:180:VAL:HG13	1:M:182:GLY:H	1.81	0.44
1:O:184:GLU:O	1:O:185:ASN:ND2	2.50	0.44
1:U:186:PRO:O	1:U:190:ILE:HG13	2.17	0.44
1:Y:55:LEU:HD22	1:Y:60:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:255:VAL:HG13	1:E:259:LYS:HD2	1.98	0.44
1:G:82:LEU:HD23	1:G:280:LEU:HD21	1.99	0.44
1:O:184:GLU:HG3	1:O:207:HIS:HE2	1.81	0.44
2:P:29:PHE:CD1	2:P:77:ASN:HA	2.52	0.44
1:Q:5:LYS:HD3	1:Q:40:TYR:OH	2.17	0.44
2:B:13:GLN:HA	2:B:120:SER:O	2.17	0.44
2:B:96:CYS:O	2:B:112:GLY:N	2.40	0.44
1:C:104:VAL:O	1:C:108:MET:HG3	2.18	0.44
1:C:271:GLU:HB3	1:C:272:PRO:CD	2.46	0.44
1:E:272:PRO:HA	1:E:275:GLU:OE2	2.16	0.44
1:A:234:LYS:O	1:A:238:LYS:CB	2.66	0.44
1:A:255:VAL:HG12	1:A:259:LYS:HZ1	1.82	0.44
1:I:201:ASN:HA	1:I:264:ASN:O	2.18	0.44
1:A:27:LEU:CD1	1:A:232:ILE:HA	2.47	0.44
1:A:67:PHE:HA	1:A:213:MET:SD	2.57	0.44
1:I:128:THR:HB	1:I:199:GLN:HB3	1.99	0.44
1:M:67:PHE:HA	1:M:213:MET:SD	2.58	0.44
1:M:203:ALA:O	1:M:205:THR:N	2.51	0.44
1:O:282:LYS:HD2	1:O:282:LYS:N	2.32	0.44
1:A:64:TYR:HD1	1:A:212:GLN:CG	2.31	0.44
2:F:107:LYS:HD2	2:F:107:LYS:HA	1.77	0.44
1:U:266:THR:O	1:U:268:PRO:HD3	2.18	0.44
1:Y:273:PHE:N	1:Y:273:PHE:CD1	2.85	0.44
1:A:120:TRP:CZ2	1:A:214:VAL:HG21	2.53	0.44
1:I:235:ALA:O	1:I:239:VAL:HG23	2.18	0.44
2:J:29:PHE:HZ	2:J:79:VAL:HG22	1.82	0.44
1:G:3:THR:O	1:G:3:THR:CG2	2.66	0.44
1:I:261:GLU:O	1:I:263:ILE:HD13	2.17	0.44
1:K:69:ARG:NH1	1:K:148:ASN:O	2.40	0.44
2:N:12:VAL:HA	2:N:13:GLN:HG3	1.99	0.44
1:G:233:GLN:O	1:G:237:GLN:HG3	2.18	0.44
1:I:121:TYR:HB3	1:I:244:THR:HG23	1.99	0.44
1:M:213:MET:HE2	1:M:215:ILE:HD11	1.98	0.44
1:A:53:GLN:OE1	2:B:101:PHE:HB2	2.18	0.43
1:A:120:TRP:CE2	1:A:240:GLY:HA3	2.53	0.43
1:C:95:MET:SD	1:C:296:LEU:HB3	2.58	0.43
2:D:20:LEU:HG	2:D:83:MET:HE2	2.00	0.43
1:E:194:LYS:O	1:E:197:GLU:HG3	2.17	0.43
1:K:187:LEU:CD2	1:K:202:LEU:HD11	2.47	0.43
1:Q:62:ILE:HD13	1:Q:216:ILE:HA	2.00	0.43
2:R:10:ARG:NE	2:V:57:ASN:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:250:GLN:C	1:U:254:LEU:HD23	2.38	0.43
1:W:55:LEU:HD23	1:W:60:LEU:O	2.17	0.43
1:Y:270:LEU:O	1:Y:273:PHE:HB2	2.18	0.43
1:M:200:LYS:N	1:M:200:LYS:HE2	2.33	0.43
1:C:55:LEU:CD1	1:C:63:THR:HG22	2.48	0.43
1:M:237:GLN:CG	1:M:238:LYS:N	2.79	0.43
2:P:87:LYS:HB3	2:P:89:GLU:OE1	2.18	0.43
1:W:183:GLN:HE21	1:W:185:ASN:HD22	1.66	0.43
1:W:249:THR:O	1:W:253:GLU:HG3	2.18	0.43
1:A:69:ARG:O	1:A:69:ARG:HG3	2.18	0.43
1:A:112:PHE:CD1	2:B:101:PHE:CZ	3.06	0.43
1:K:187:LEU:HD21	1:K:202:LEU:HD11	1.99	0.43
1:O:278:GLN:N	1:O:279:PRO:HD2	2.34	0.43
1:Q:288:ILE:CD1	1:Q:288:ILE:CA	2.96	0.43
1:U:93:ARG:NH2	1:U:118:ASP:OD1	2.51	0.43
1:A:25:ASP:O	1:A:29:GLU:N	2.44	0.43
1:A:259:LYS:C	1:A:261:GLU:H	2.22	0.43
1:C:194:LYS:HB3	1:C:197:GLU:HG3	2.01	0.43
2:D:10:ARG:CG	2:D:10:ARG:NH1	2.81	0.43
2:F:41:PRO:HB2	1:I:293:VAL:HG12	2.00	0.43
1:I:245:GLN:O	1:I:246:THR:C	2.57	0.43
1:K:150:LYS:HA	1:K:153:LEU:HD12	2.00	0.43
2:N:45:ARG:CD	2:N:107:LYS:HZ2	2.17	0.43
2:D:10:ARG:HD2	2:D:18:LEU:HD11	2.01	0.43
1:G:129:SER:CB	1:G:133:LEU:HD11	2.49	0.43
1:K:4:LEU:CD1	1:K:4:LEU:N	2.81	0.43
1:K:35:ILE:HD13	1:K:35:ILE:HG21	1.79	0.43
1:M:166:MET:HE3	1:M:180:VAL:HG21	1.99	0.43
1:U:175:LEU:HD23	1:U:199:GLN:HG2	2.00	0.43
1:W:235:ALA:O	1:W:236:VAL:C	2.56	0.43
1:A:30:MET:CE	1:A:238:LYS:NZ	2.82	0.43
1:M:178:ASN:N	1:M:178:ASN:HD22	2.14	0.43
1:M:180:VAL:HG13	1:M:181:ASP:N	2.33	0.43
1:U:255:VAL:O	1:U:259:LYS:HG3	2.19	0.43
1:W:131:ARG:HB2	1:W:132:PRO:CD	2.48	0.43
1:W:250:GLN:O	1:W:254:LEU:HG	2.19	0.43
1:A:48:ASP:OD2	1:A:48:ASP:N	2.50	0.43
1:A:70:MET:HE2	1:A:70:MET:HA	2.01	0.43
1:A:101:GLY:O	1:A:105:ARG:CG	2.67	0.43
1:A:203:ALA:HB1	1:A:205:THR:HG23	2.00	0.43
1:A:224:LEU:HD13	1:A:232:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:GLN:O	1:A:254:LEU:N	2.44	0.43
2:F:45:ARG:HD2	2:F:107:LYS:CE	2.48	0.43
2:F:45:ARG:HD2	2:F:45:ARG:HH11	1.47	0.43
1:I:270:LEU:HD12	1:I:270:LEU:N	2.34	0.43
1:M:237:GLN:O	1:M:240:GLY:N	2.37	0.43
1:Q:121:TYR:HB3	1:Q:244:THR:HG23	2.01	0.43
2:T:6:GLU:CD	2:T:114:GLY:N	2.68	0.43
1:A:191:LYS:HG3	1:A:257:PHE:CD2	2.54	0.43
1:I:76:ARG:HA	1:I:288:ILE:HD11	2.00	0.43
1:M:8:MET:HG2	1:M:41:PRO:HA	2.01	0.43
1:M:236:VAL:C	1:M:237:GLN:O	2.58	0.43
2:N:11:LEU:HG	2:N:13:GLN:HE21	1.83	0.43
1:A:92:LEU:HD23	1:A:211:ASP:HB3	2.01	0.43
1:A:203:ALA:O	1:A:268:PRO:HD2	2.18	0.43
1:A:293:VAL:HG13	1:A:294:SER:N	2.34	0.43
1:G:191:LYS:CD	1:G:254:LEU:HD21	2.49	0.43
1:Q:244:THR:HG22	1:Q:248:LYS:HE2	2.01	0.43
1:U:267:TYR:N	1:U:267:TYR:CD1	2.86	0.43
1:E:175:LEU:HD11	1:E:183:GLN:HG2	2.00	0.42
1:K:48:ASP:N	1:K:48:ASP:OD1	2.52	0.42
2:R:6:GLU:OE1	2:R:114:GLY:N	2.45	0.42
1:U:145:ARG:HG2	1:U:166:MET:HG2	2.00	0.42
1:W:190:ILE:HA	1:W:195:PHE:CD2	2.54	0.42
1:M:78:GLU:HG3	1:M:81:MET:HE3	2.01	0.42
1:U:92:LEU:HD23	1:U:211:ASP:HB3	2.00	0.42
1:W:27:LEU:HD11	1:W:232:ILE:HA	2.00	0.42
1:W:137:GLU:N	1:W:137:GLU:OE1	2.51	0.42
1:W:183:GLN:NE2	1:W:185:ASN:HD22	2.16	0.42
1:K:34:GLU:OE2	1:K:34:GLU:N	2.52	0.42
1:K:293:VAL:CG1	2:R:41:PRO:CG	2.97	0.42
2:T:113:GLN:O	2:T:114:GLY:O	2.37	0.42
1:A:15:VAL:HG21	1:A:188:PRO:HB3	2.02	0.42
2:D:37:PHE:HA	2:D:48:VAL:HG23	2.01	0.42
1:E:48:ASP:OD1	1:E:48:ASP:N	2.52	0.42
1:E:166:MET:CE	1:E:174:ALA:CB	2.98	0.42
1:I:49:ARG:HG3	1:I:72:LEU:HD13	2.02	0.42
2:L:39:GLN:HG3	2:L:43:LYS:O	2.20	0.42
1:U:176:GLN:HB2	1:U:198:VAL:HG11	2.01	0.42
1:A:124:THR:CG2	1:A:206:HIS:HA	2.48	0.42
1:A:281:TYR:CB	1:A:293:VAL:HG21	2.49	0.42
2:D:89:GLU:OE2	2:D:89:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22:MET:HA	1:E:25:ASP:HB2	2.01	0.42
1:E:272:PRO:C	1:E:275:GLU:H	2.23	0.42
1:E:288:ILE:HG21	1:E:288:ILE:HD12	1.74	0.42
1:M:153:LEU:HD23	1:M:163:PRO:HB2	2.02	0.42
1:A:67:PHE:HB2	1:A:211:ASP:OD2	2.20	0.42
1:C:87:LYS:HD2	1:C:87:LYS:N	2.35	0.42
1:C:272:PRO:HA	1:C:275:GLU:HG2	2.02	0.42
1:G:119:THR:HA	1:G:213:MET:HA	2.02	0.42
1:G:173:LEU:HD23	1:G:177:THR:HG23	2.02	0.42
1:K:128:THR:HB	1:K:199:GLN:HG3	2.00	0.42
1:O:80:VAL:HG13	1:O:95:MET:HE3	2.01	0.42
1:C:125:ARG:HH22	3:C:301:SLB:C2	2.33	0.42
1:C:271:GLU:N	1:C:272:PRO:CD	2.82	0.42
1:K:293:VAL:CG1	2:R:41:PRO:CB	2.97	0.42
1:O:115:ARG:NH1	1:O:218:GLU:OE2	2.51	0.42
2:V:38:ARG:NE	2:V:46:GLU:OE1	2.44	0.42
1:Y:48:ASP:OD1	1:Y:48:ASP:N	2.53	0.42
1:E:34:GLU:HG3	1:G:177:THR:HG22	2.02	0.42
1:K:73:ALA:HB1	1:K:112:PHE:CZ	2.54	0.42
1:Q:278:GLN:N	1:Q:279:PRO:HD2	2.33	0.42
2:R:12:VAL:O	2:R:119:VAL:HA	2.19	0.42
1:U:156:ALA:HA	1:U:159:SER:OG	2.20	0.42
1:Y:65:ALA:HB3	1:Y:215:ILE:HD11	2.01	0.42
1:A:64:TYR:CD1	1:A:212:GLN:CG	3.03	0.42
1:A:273:PHE:O	1:A:274:ARG:C	2.59	0.42
1:K:85:VAL:CG1	1:K:86:ALA:N	2.83	0.42
1:M:130:ASN:ND2	1:M:181:ASP:HA	2.34	0.42
2:N:68:PHE:N	2:N:68:PHE:CD1	2.88	0.42
2:X:33:VAL:N	2:X:99:ASP:O	2.52	0.42
1:A:114:TRP:CZ2	2:B:101:PHE:CZ	3.08	0.41
1:A:116:ALA:HB2	1:A:213:MET:CE	2.49	0.41
1:A:120:TRP:CE2	1:A:240:GLY:CA	3.03	0.41
1:A:196:TYR:HD2	1:A:258:PHE:HE1	1.67	0.41
1:G:187:LEU:HD23	1:G:190:ILE:HD12	2.01	0.41
1:O:44:GLN:HE21	1:O:44:GLN:HB3	1.69	0.41
1:O:125:ARG:HE	1:O:184:GLU:CD	2.21	0.41
1:O:136:ILE:O	1:O:139:PHE:HB2	2.19	0.41
1:E:213:MET:HE3	1:E:215:ILE:HD11	2.02	0.41
1:G:96:PHE:CE1	1:G:105:ARG:HD2	2.56	0.41
1:O:35:ILE:HD11	1:O:228:ASP:CG	2.40	0.41
1:U:280:LEU:O	1:U:283:GLU:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:14:SER:HA	1:W:192:THR:HG21	2.03	0.41
1:W:128:THR:CG2	1:W:190:ILE:HD13	2.50	0.41
1:Y:203:ALA:O	1:Y:205:THR:HG23	2.19	0.41
1:A:277:MET:O	1:A:280:LEU:HB3	2.20	0.41
1:C:69:ARG:HD3	3:C:301:SLB:O9	2.20	0.41
1:C:151:GLN:OE1	1:C:280:LEU:HD21	2.20	0.41
1:E:22:MET:O	1:E:26:THR:N	2.46	0.41
1:G:191:LYS:HD2	1:G:254:LEU:HD21	2.02	0.41
1:I:173:LEU:O	1:I:176:GLN:N	2.53	0.41
1:Q:175:LEU:HD23	1:Q:180:VAL:HG23	2.02	0.41
1:Y:259:LYS:HB2	1:Y:259:LYS:HE2	1.79	0.41
2:L:44:GLU:H	2:L:44:GLU:HG2	1.43	0.41
1:M:199:GLN:C	1:M:200:LYS:HE2	2.41	0.41
1:U:68:GLY:HA3	1:U:81:MET:HB2	2.01	0.41
1:U:145:ARG:HG3	1:U:166:MET:HG2	2.01	0.41
1:Y:278:GLN:N	1:Y:279:PRO:HD2	2.35	0.41
1:A:82:LEU:HD22	1:A:281:TYR:CD1	2.54	0.41
1:A:101:GLY:O	1:A:105:ARG:HG3	2.20	0.41
1:A:120:TRP:NE1	1:A:240:GLY:HA3	2.36	0.41
1:Q:288:ILE:CD1	1:Q:288:ILE:HA	2.50	0.41
1:K:4:LEU:N	1:K:4:LEU:HD12	2.36	0.41
1:M:79:ALA:CA	1:M:82:LEU:HD12	2.49	0.41
1:Q:143:LYS:HB3	1:Q:181:ASP:H	1.85	0.41
2:N:52:SER:HB3	2:N:57:ASN:HB2	2.03	0.41
1:Q:77:ALA:O	1:Q:80:VAL:HG22	2.21	0.41
2:B:83:MET:HB2	2:B:86:LEU:HD21	2.02	0.41
1:C:80:VAL:HG12	1:C:92:LEU:CD1	2.50	0.41
1:E:120:TRP:O	1:E:212:GLN:N	2.54	0.41
2:L:52:SER:HB3	2:L:57:ASN:HB2	2.01	0.41
1:O:228:ASP:O	1:O:232:ILE:HG13	2.21	0.41
2:T:12:VAL:CG1	2:T:13:GLN:H	2.30	0.41
2:X:83:MET:HB3	2:X:86:LEU:HD21	2.03	0.41
1:A:15:VAL:HG21	1:A:188:PRO:HB2	2.02	0.41
1:A:94:ARG:HA	1:A:97:GLU:HB2	2.02	0.41
1:A:144:LEU:O	1:A:163:PRO:HA	2.20	0.41
1:E:166:MET:HE3	1:E:174:ALA:CB	2.51	0.41
1:E:187:LEU:N	1:E:188:PRO:CD	2.83	0.41
2:F:33:VAL:HG13	2:F:51:ILE:O	2.21	0.41
1:G:48:ASP:OD1	1:G:48:ASP:N	2.54	0.41
1:I:26:THR:O	1:I:30:MET:HG2	2.21	0.41
1:I:44:GLN:HG3	1:I:45:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:80:VAL:CG1	1:O:92:LEU:CD1	2.97	0.41
1:O:135:SER:N	1:O:138:ASP:OD2	2.43	0.41
1:A:112:PHE:CD1	2:B:101:PHE:CE2	3.09	0.41
1:E:272:PRO:O	1:E:275:GLU:CB	2.68	0.41
2:H:10:ARG:HH11	2:H:10:ARG:HG3	1.85	0.41
1:K:243:HIS:C	1:K:245:GLN:N	2.72	0.41
2:T:113:GLN:O	2:T:114:GLY:C	2.55	0.41
1:U:173:LEU:O	1:U:177:THR:HG23	2.20	0.41
1:W:202:LEU:HD21	1:W:204:MET:SD	2.61	0.41
1:A:125:ARG:HD3	1:A:184:GLU:OE1	2.21	0.40
1:A:263:ILE:CD1	1:A:263:ILE:CA	2.99	0.40
1:C:270:LEU:O	1:C:271:GLU:C	2.59	0.40
1:K:132:PRO:HA	1:K:201:ASN:OD1	2.21	0.40
1:O:281:TYR:O	1:O:282:LYS:C	2.60	0.40
1:U:156:ALA:O	1:U:157:LYS:C	2.59	0.40
1:W:183:GLN:HE21	1:W:185:ASN:ND2	2.19	0.40
1:A:79:ALA:O	1:A:82:LEU:HD12	2.20	0.40
1:K:257:PHE:CD2	1:K:257:PHE:C	2.93	0.40
1:M:30:MET:CE	1:M:30:MET:HA	2.51	0.40
1:M:126:GLU:HG3	1:M:187:LEU:CD1	2.51	0.40
1:O:263:ILE:CD1	1:O:263:ILE:HA	2.51	0.40
2:P:44:GLU:HG2	2:P:45:ARG:O	2.21	0.40
1:Y:65:ALA:HB3	1:Y:215:ILE:CD1	2.51	0.40
1:A:104:VAL:HG23	1:A:105:ARG:N	2.37	0.40
1:A:232:ILE:O	1:A:233:GLN:C	2.55	0.40
1:C:275:GLU:HA	1:C:278:GLN:HE21	1.85	0.40
1:I:55:LEU:HD21	1:I:215:ILE:HG22	1.98	0.40
1:O:213:MET:HE3	1:O:215:ILE:HD11	2.03	0.40
2:R:39:GLN:NE2	2:R:45:ARG:HG3	2.36	0.40
1:A:126:GLU:OE1	1:A:206:HIS:N	2.54	0.40
1:E:28:GLU:HB3	1:E:35:ILE:O	2.21	0.40
1:O:143:LYS:HD2	1:O:143:LYS:HZ2	1.84	0.40
2:R:40:ALA:HB1	2:R:41:PRO:HD2	2.03	0.40
1:Y:274:ARG:O	1:Y:275:GLU:O	2.39	0.40
1:Q:79:ALA:HB2	1:Q:284:PHE:HE1	1.86	0.40
1:Y:236:VAL:HG23	1:Y:237:GLN:N	2.37	0.40

All (12) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:LYS:NZ	2:J:44:GLU:OE1[4_446]	1.62	0.58
1:O:275:GLU:HG3	2:T:43:LYS:HZ1[4_456]	1.18	0.42
1:O:274:ARG:HH11	2:T:42:GLY:O[4_456]	1.22	0.38
1:A:17:TYR:OH	1:I:290:GLN:OE1[3_445]	1.90	0.30
1:O:274:ARG:NH1	2:T:42:GLY:O[4_456]	1.90	0.30
1:A:282:LYS:HZ2	2:J:44:GLU:OE1[4_446]	1.32	0.28
2:D:13:GLN:HE22	1:W:59:ASP:OD2[3_455]	1.44	0.16
1:E:17:TYR:OH	1:U:290:GLN:HE22[4_455]	1.47	0.13
2:N:43:LYS:HZ2	1:Y:271:GLU:OE2[2_556]	1.47	0.13
2:L:42:GLY:O	1:U:87:LYS:NZ[2_455]	2.13	0.07
2:D:57:ASN:OD1	2:N:10:ARG:HE[3_455]	1.58	0.02
1:A:282:LYS:HZ3	2:J:44:GLU:OE1[4_446]	1.60	0.00

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	297/303 (98%)	286 (96%)	9 (3%)	2 (1%)	19	46
1	C	297/303 (98%)	290 (98%)	6 (2%)	1 (0%)	37	65
1	E	299/303 (99%)	289 (97%)	9 (3%)	1 (0%)	37	65
1	G	297/303 (98%)	286 (96%)	9 (3%)	2 (1%)	19	46
1	I	297/303 (98%)	290 (98%)	5 (2%)	2 (1%)	19	46
1	K	297/303 (98%)	286 (96%)	8 (3%)	3 (1%)	13	37
1	M	297/303 (98%)	288 (97%)	4 (1%)	5 (2%)	7	24
1	O	297/303 (98%)	285 (96%)	8 (3%)	4 (1%)	10	30
1	Q	297/303 (98%)	292 (98%)	4 (1%)	1 (0%)	37	65
1	U	297/303 (98%)	289 (97%)	5 (2%)	3 (1%)	13	37
1	W	297/303 (98%)	290 (98%)	5 (2%)	2 (1%)	19	46
1	Y	297/303 (98%)	292 (98%)	3 (1%)	2 (1%)	19	46
2	B	120/123 (98%)	120 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	119/123 (97%)	117 (98%)	2 (2%)	0	100	100
2	F	121/123 (98%)	121 (100%)	0	0	100	100
2	H	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
2	J	121/123 (98%)	119 (98%)	1 (1%)	1 (1%)	16	42
2	L	121/123 (98%)	117 (97%)	3 (2%)	1 (1%)	16	42
2	N	121/123 (98%)	121 (100%)	0	0	100	100
2	P	121/123 (98%)	115 (95%)	5 (4%)	1 (1%)	16	42
2	R	121/123 (98%)	119 (98%)	1 (1%)	1 (1%)	16	42
2	T	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
2	V	121/123 (98%)	119 (98%)	1 (1%)	1 (1%)	16	42
2	X	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
All	All	5015/5112 (98%)	4888 (98%)	94 (2%)	33 (1%)	19	46

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	204	MET
1	G	267	TYR
1	I	204	MET
1	I	267	TYR
1	K	204	MET
2	L	43	LYS
1	M	204	MET
1	M	237	GLN
1	O	204	MET
1	Q	204	MET
2	R	44	GLU
1	U	204	MET
1	W	204	MET
1	Y	204	MET
1	G	204	MET
2	J	107	LYS
1	K	293	VAL
1	M	29	GLU
1	O	263	ILE
1	O	267	TYR
1	U	267	TYR
1	U	283	GLU

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Mol	Chain	Res	Type
2	V	89	GLU
1	A	260	SER
1	K	267	TYR
1	M	238	LYS
1	O	233	GLN
1	Y	267	TYR
2	P	27	ASP
1	W	110	GLN
1	A	267	TYR
1	C	148	ASN
1	M	267	TYR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	258/259 (100%)	236 (92%)	22 (8%)	8 26
1	C	258/259 (100%)	249 (96%)	9 (4%)	31 63
1	E	258/259 (100%)	254 (98%)	4 (2%)	58 84
1	G	258/259 (100%)	251 (97%)	7 (3%)	40 72
1	I	258/259 (100%)	253 (98%)	5 (2%)	52 81
1	K	258/259 (100%)	250 (97%)	8 (3%)	35 68
1	M	258/259 (100%)	253 (98%)	5 (2%)	52 81
1	O	258/259 (100%)	250 (97%)	8 (3%)	35 68
1	Q	258/259 (100%)	249 (96%)	9 (4%)	31 63
1	U	258/259 (100%)	254 (98%)	4 (2%)	58 84
1	W	258/259 (100%)	251 (97%)	7 (3%)	40 72
1	Y	258/259 (100%)	252 (98%)	6 (2%)	45 77
2	B	98/98 (100%)	93 (95%)	5 (5%)	20 49
2	D	97/98 (99%)	96 (99%)	1 (1%)	73 91
2	F	98/98 (100%)	96 (98%)	2 (2%)	50 80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	98/98 (100%)	93 (95%)	5 (5%)	20 49
2	J	98/98 (100%)	94 (96%)	4 (4%)	26 57
2	L	98/98 (100%)	94 (96%)	4 (4%)	26 57
2	N	98/98 (100%)	93 (95%)	5 (5%)	20 49
2	P	98/98 (100%)	95 (97%)	3 (3%)	35 68
2	R	98/98 (100%)	96 (98%)	2 (2%)	50 80
2	T	98/98 (100%)	95 (97%)	3 (3%)	35 68
2	V	98/98 (100%)	96 (98%)	2 (2%)	50 80
2	X	98/98 (100%)	96 (98%)	2 (2%)	50 80
All	All	4271/4284 (100%)	4139 (97%)	132 (3%)	35 68

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	MET
1	A	32	GLN
1	A	82	LEU
1	A	90	ASP
1	A	93	ARG
1	A	131	ARG
1	A	140	LYS
1	A	144	LEU
1	A	153	LEU
1	A	157	LYS
1	A	196	TYR
1	A	202	LEU
1	A	206	HIS
1	A	217	SER
1	A	233	GLN
1	A	246	THR
1	A	251	GLU
1	A	264	ASN
1	A	271	GLU
1	A	274	ARG
1	A	275	GLU
1	A	286	SER
2	B	19	ARG
2	B	44	GLU
2	B	52	SER

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Mol	Chain	Res	Type
2	B	113	GLN
2	B	120	SER
1	C	2	THR
1	C	15	VAL
1	C	21	LYS
1	C	32	GLN
1	C	110	GLN
1	C	226	ASP
1	C	230	ASP
1	C	260	SER
1	C	283	GLU
2	D	107	LYS
1	E	81	MET
1	E	159	SER
1	E	200	LYS
1	E	255	VAL
2	F	3	GLN
2	F	113	GLN
1	G	93	ARG
1	G	148	ASN
1	G	184	GLU
1	G	217	SER
1	G	234	LYS
1	G	275	GLU
1	G	282	LYS
2	H	13	GLN
2	H	44	GLU
2	H	63	SER
2	H	113	GLN
2	H	121	SER
1	I	28	GLU
1	I	36	LYS
1	I	137	GLU
1	I	200	LYS
1	I	217	SER
2	J	44	GLU
2	J	85	SER
2	J	107	LYS
2	J	113	GLN
1	K	63	THR
1	K	85	VAL
1	K	110	GLN

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Mol	Chain	Res	Type
1	K	148	ASN
1	K	159	SER
1	K	166	MET
1	K	227	THR
1	K	234	LYS
2	L	44	GLU
2	L	87	LYS
2	L	107	LYS
2	L	116	GLN
1	M	81	MET
1	M	82	LEU
1	M	93	ARG
1	M	176	GLN
1	M	217	SER
2	N	1	GLN
2	N	12	VAL
2	N	44	GLU
2	N	87	LYS
2	N	116	GLN
1	O	32	GLN
1	O	143	LYS
1	O	148	ASN
1	O	184	GLU
1	O	200	LYS
1	O	217	SER
1	O	260	SER
1	O	282	LYS
2	P	67	ARG
2	P	76	LYS
2	P	116	GLN
1	Q	90	ASP
1	Q	93	ARG
1	Q	143	LYS
1	Q	157	LYS
1	Q	183	GLN
1	Q	191	LYS
1	Q	212	GLN
1	Q	236	VAL
1	Q	260	SER
2	R	44	GLU
2	R	113	GLN
2	T	0	SER

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Mol	Chain	Res	Type
2	T	43	LYS
2	T	44	GLU
1	U	21	LYS
1	U	93	ARG
1	U	184	GLU
1	U	255	VAL
2	V	63	SER
2	V	87	LYS
1	W	14	SER
1	W	153	LEU
1	W	162	SER
1	W	183	GLN
1	W	266	THR
1	W	274	ARG
1	W	282	LYS
2	X	87	LYS
2	X	113	GLN
1	Y	93	ARG
1	Y	140	LYS
1	Y	202	LEU
1	Y	217	SER
1	Y	256	SER
1	Y	273	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	GLN
1	C	183	GLN
1	C	278	GLN
2	D	113	GLN
1	G	102	GLN
2	H	113	GLN
1	I	212	GLN
1	K	110	GLN
1	K	212	GLN
1	M	178	ASN
2	N	13	GLN
1	O	110	GLN
1	O	278	GLN
1	U	148	ASN
1	W	102	GLN

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Mol	Chain	Res	Type
1	W	183	GLN
1	W	212	GLN
1	W	233	GLN
1	W	237	GLN
2	X	102	HIS
1	Y	201	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

18 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	$\#\|Z\| > 2$
3	SLB	G	301	-	20,20,21	1.36	3 (15%)	24,28,31	1.40	3 (12%)
3	SLB	U	301	-	20,20,21	1.43	3 (15%)	24,28,31	1.22	3 (12%)
3	SLB	E	301	-	20,20,21	1.41	3 (15%)	24,28,31	1.25	2 (8%)
3	SLB	Y	301	-	20,20,21	1.35	3 (15%)	24,28,31	1.25	3 (12%)
3	SLB	Q	301	-	20,20,21	1.36	3 (15%)	24,28,31	1.17	3 (12%)
3	SLB	W	301	-	20,20,21	1.43	3 (15%)	24,28,31	1.19	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	E	302	-	5,5,5	0.92	0	5,5,5	0.99	0
3	SLB	O	301	-	20,20,21	1.37	3 (15%)	24,28,31	1.31	5 (20%)
3	SLB	I	301	-	20,20,21	1.33	3 (15%)	24,28,31	1.23	5 (20%)
4	GOL	U	302	-	5,5,5	0.86	0	5,5,5	0.98	0
3	SLB	A	301	-	20,20,21	1.45	3 (15%)	24,28,31	1.43	4 (16%)
3	SLB	M	301	-	20,20,21	1.37	3 (15%)	24,28,31	1.36	3 (12%)
4	GOL	G	302	-	5,5,5	1.19	1 (20%)	5,5,5	1.42	1 (20%)
4	GOL	U	303	-	5,5,5	0.88	0	5,5,5	1.08	0
4	GOL	U	304	-	5,5,5	0.83	0	5,5,5	1.06	0
4	GOL	Q	302	-	5,5,5	1.30	1 (20%)	5,5,5	1.35	1 (20%)
3	SLB	K	301	-	20,20,21	1.37	2 (10%)	24,28,31	1.31	4 (16%)
3	SLB	C	301	-	20,20,21	1.37	3 (15%)	24,28,31	1.37	4 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SLB	G	301	-	-	3/18/34/38	0/1/1/1
3	SLB	U	301	-	-	7/18/34/38	0/1/1/1
3	SLB	E	301	-	-	2/18/34/38	0/1/1/1
3	SLB	Y	301	-	-	1/18/34/38	0/1/1/1
3	SLB	Q	301	-	-	1/18/34/38	0/1/1/1
3	SLB	W	301	-	-	2/18/34/38	0/1/1/1
4	GOL	E	302	-	-	2/4/4/4	-
3	SLB	O	301	-	-	1/18/34/38	0/1/1/1
3	SLB	I	301	-	-	3/18/34/38	0/1/1/1
4	GOL	U	302	-	-	0/4/4/4	-
3	SLB	A	301	-	-	6/18/34/38	0/1/1/1
3	SLB	M	301	-	-	1/18/34/38	0/1/1/1
4	GOL	G	302	-	-	0/4/4/4	-
4	GOL	U	303	-	-	0/4/4/4	-
4	GOL	U	304	-	-	0/4/4/4	-
4	GOL	Q	302	-	-	2/4/4/4	-
3	SLB	K	301	-	-	1/18/34/38	0/1/1/1
3	SLB	C	301	-	-	3/18/34/38	0/1/1/1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	301	SLB	C10-N5	3.47	1.46	1.34
3	A	301	SLB	C10-N5	3.41	1.46	1.34
3	E	301	SLB	C10-N5	3.31	1.45	1.34
3	W	301	SLB	C10-N5	3.31	1.45	1.34
3	M	301	SLB	C10-N5	3.30	1.45	1.34
3	Q	301	SLB	C10-N5	3.30	1.45	1.34
3	I	301	SLB	C10-N5	3.29	1.45	1.34
3	O	301	SLB	C10-N5	3.29	1.45	1.34
3	K	301	SLB	C10-N5	3.26	1.45	1.34
3	Y	301	SLB	C10-N5	3.24	1.45	1.34
3	C	301	SLB	C10-N5	3.24	1.45	1.34
3	G	301	SLB	C10-N5	3.18	1.45	1.34
3	A	301	SLB	O6-C6	-2.76	1.39	1.44
3	W	301	SLB	O6-C2	-2.74	1.40	1.43
3	U	301	SLB	O6-C6	-2.71	1.39	1.44
3	U	301	SLB	O6-C2	-2.61	1.40	1.43
3	W	301	SLB	O6-C6	-2.60	1.39	1.44
3	E	301	SLB	O6-C6	-2.58	1.39	1.44
3	A	301	SLB	O6-C2	-2.58	1.40	1.43
4	Q	302	GOL	O2-C2	-2.43	1.36	1.43
3	O	301	SLB	O6-C2	-2.42	1.40	1.43
3	C	301	SLB	O6-C2	-2.36	1.40	1.43
3	G	301	SLB	O6-C2	-2.36	1.40	1.43
3	M	301	SLB	O6-C2	-2.34	1.40	1.43
3	E	301	SLB	O6-C2	-2.34	1.40	1.43
3	Q	301	SLB	O6-C2	-2.33	1.40	1.43
3	K	301	SLB	O6-C2	-2.33	1.40	1.43
3	M	301	SLB	O6-C6	-2.25	1.40	1.44
3	Y	301	SLB	O6-C2	-2.21	1.40	1.43
3	Q	301	SLB	O6-C6	-2.18	1.40	1.44
3	G	301	SLB	O6-C6	-2.17	1.40	1.44
4	G	302	GOL	O2-C2	-2.14	1.37	1.43
3	I	301	SLB	O6-C2	-2.11	1.40	1.43
3	Y	301	SLB	O6-C6	-2.10	1.40	1.44
3	O	301	SLB	O6-C6	-2.09	1.40	1.44
3	C	301	SLB	O6-C6	-2.04	1.40	1.44
3	I	301	SLB	O6-C6	-2.00	1.40	1.44

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	301	SLB	C6-O6-C2	3.74	119.33	111.34
3	G	301	SLB	C6-O6-C2	3.72	119.29	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	301	SLB	C9-C8-C7	-3.56	104.69	112.41
3	K	301	SLB	C6-O6-C2	3.23	118.26	111.34
3	C	301	SLB	C6-O6-C2	3.21	118.21	111.34
3	E	301	SLB	C6-O6-C2	3.20	118.19	111.34
3	O	301	SLB	C6-O6-C2	3.18	118.14	111.34
3	Y	301	SLB	C6-O6-C2	3.04	117.84	111.34
3	A	301	SLB	C6-O6-C2	2.98	117.71	111.34
3	Q	301	SLB	C6-O6-C2	2.86	117.46	111.34
4	G	302	GOL	C3-C2-C1	-2.85	100.63	111.70
3	I	301	SLB	C6-O6-C2	2.84	117.42	111.34
3	U	301	SLB	C9-C8-C7	-2.78	106.39	112.41
3	W	301	SLB	C9-C8-C7	-2.66	106.65	112.41
3	C	301	SLB	C8-C7-C6	-2.58	108.14	113.03
4	Q	302	GOL	C3-C2-C1	-2.53	101.85	111.70
3	I	301	SLB	O1B-C1-C2	2.50	120.18	113.03
3	M	301	SLB	O1B-C1-C2	2.48	120.12	113.03
3	C	301	SLB	O1B-C1-C2	2.48	120.10	113.03
3	O	301	SLB	O1B-C1-C2	2.47	120.08	113.03
3	K	301	SLB	O1B-C1-C2	2.42	119.94	113.03
3	U	301	SLB	O1B-C1-C2	2.39	119.85	113.03
3	A	301	SLB	O1B-C1-C2	2.39	119.84	113.03
3	I	301	SLB	C8-C7-C6	-2.37	108.53	113.03
3	E	301	SLB	O1B-C1-C2	2.37	119.80	113.03
3	Q	301	SLB	O1B-C1-C2	2.36	119.77	113.03
3	G	301	SLB	O1B-C1-C2	2.36	119.77	113.03
3	Y	301	SLB	O1B-C1-C2	2.35	119.75	113.03
3	U	301	SLB	C6-O6-C2	2.30	116.26	111.34
3	W	301	SLB	O1B-C1-C2	2.29	119.58	113.03
3	A	301	SLB	C11-C10-N5	2.29	119.98	116.10
3	C	301	SLB	C11-C10-N5	2.27	119.94	116.10
3	G	301	SLB	C8-C7-C6	-2.22	108.81	113.03
3	W	301	SLB	C6-O6-C2	2.18	116.01	111.34
3	K	301	SLB	C11-C10-N5	2.17	119.77	116.10
3	O	301	SLB	C11-C10-N5	2.12	119.69	116.10
3	O	301	SLB	C8-C7-C6	-2.12	109.02	113.03
3	M	301	SLB	C11-C10-N5	2.10	119.66	116.10
3	W	301	SLB	C11-C10-N5	2.09	119.63	116.10
3	Y	301	SLB	C11-C10-N5	2.08	119.63	116.10
3	K	301	SLB	O1B-C1-O1A	-2.07	119.40	124.09
3	I	301	SLB	C11-C10-N5	2.05	119.57	116.10
3	O	301	SLB	O1B-C1-O1A	-2.04	119.45	124.09
3	Q	301	SLB	C11-C10-N5	2.03	119.54	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	301	SLB	O1B-C1-O1A	-2.02	119.51	124.09

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	SLB	O1A-C1-C2-O6
3	A	301	SLB	C6-C7-C8-C9
3	A	301	SLB	O7-C7-C8-C9
3	E	301	SLB	O1A-C1-C2-O6
3	K	301	SLB	O1A-C1-C2-O6
3	A	301	SLB	O7-C7-C8-O8
3	A	301	SLB	C6-C7-C8-O8
3	C	301	SLB	O1A-C1-C2-O6
3	G	301	SLB	O1A-C1-C2-O6
3	I	301	SLB	O1A-C1-C2-O6
3	M	301	SLB	O1A-C1-C2-O6
3	O	301	SLB	O1A-C1-C2-O6
3	Q	301	SLB	O1A-C1-C2-O6
3	U	301	SLB	O1A-C1-C2-O6
3	W	301	SLB	O1A-C1-C2-O6
3	Y	301	SLB	O1A-C1-C2-O6
3	U	301	SLB	C6-C7-C8-O8
4	E	302	GOL	O2-C2-C3-O3
3	U	301	SLB	C6-C7-C8-C9
4	Q	302	GOL	O2-C2-C3-O3
4	E	302	GOL	C1-C2-C3-O3
4	Q	302	GOL	C1-C2-C3-O3
3	U	301	SLB	O7-C7-C8-C9
3	W	301	SLB	O8-C8-C9-O9
3	U	301	SLB	O7-C7-C8-O8
3	A	301	SLB	O1B-C1-C2-C3
3	C	301	SLB	O1A-C1-C2-C3
3	C	301	SLB	O1B-C1-C2-C3
3	E	301	SLB	O1B-C1-C2-C3
3	G	301	SLB	O1A-C1-C2-C3
3	G	301	SLB	O1B-C1-C2-C3
3	I	301	SLB	O1A-C1-C2-C3
3	I	301	SLB	O1B-C1-C2-C3
3	U	301	SLB	O1A-C1-C2-C3
3	U	301	SLB	O1B-C1-C2-C3

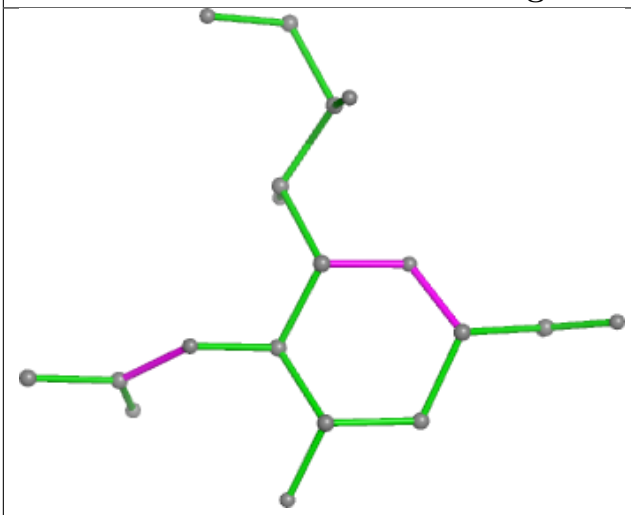
There are no ring outliers.

4 monomers are involved in 5 short contacts:

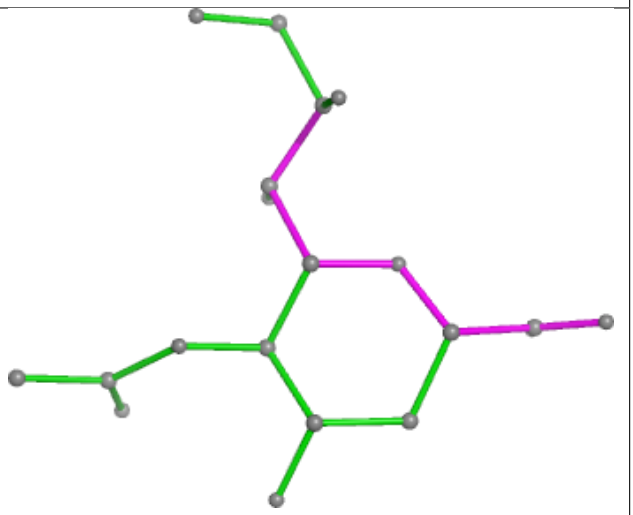
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Q	301	SLB	1	0
3	W	301	SLB	1	0
4	Q	302	GOL	1	0
3	C	301	SLB	2	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

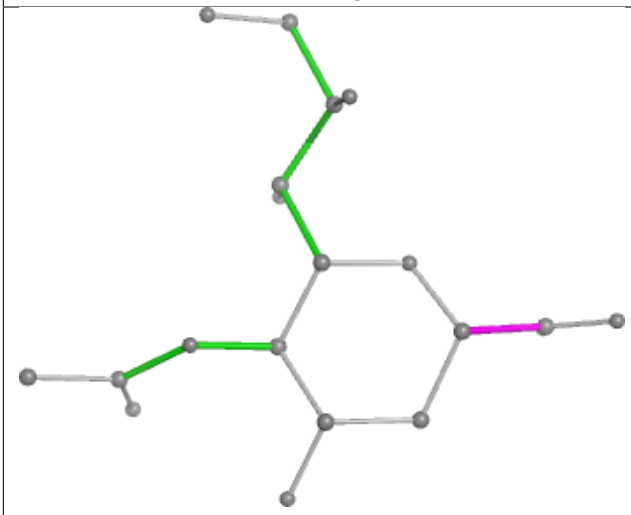
Ligand SLB G 301



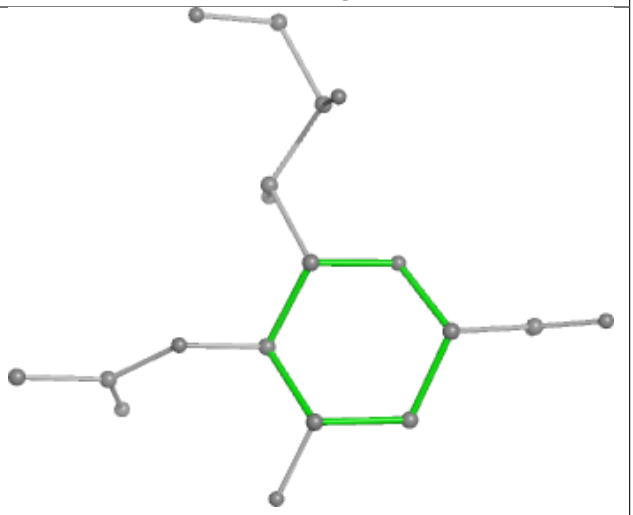
Bond lengths



Bond angles

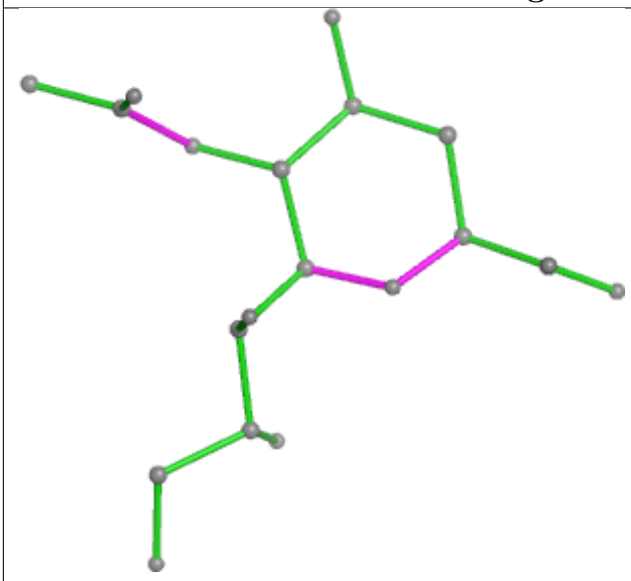


Torsions

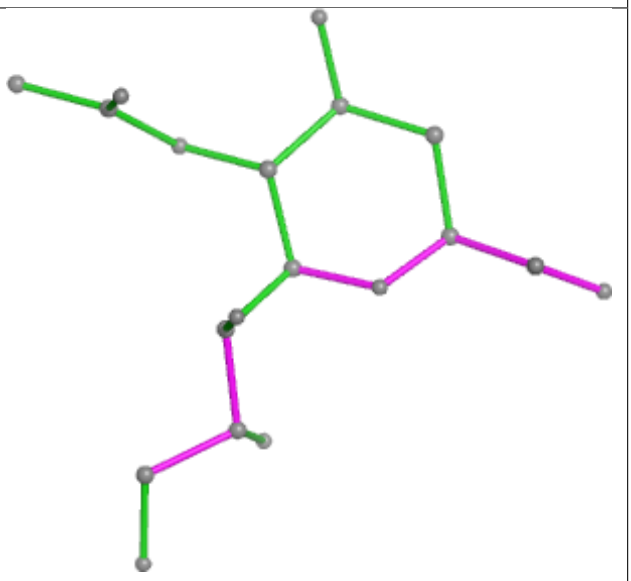


Rings

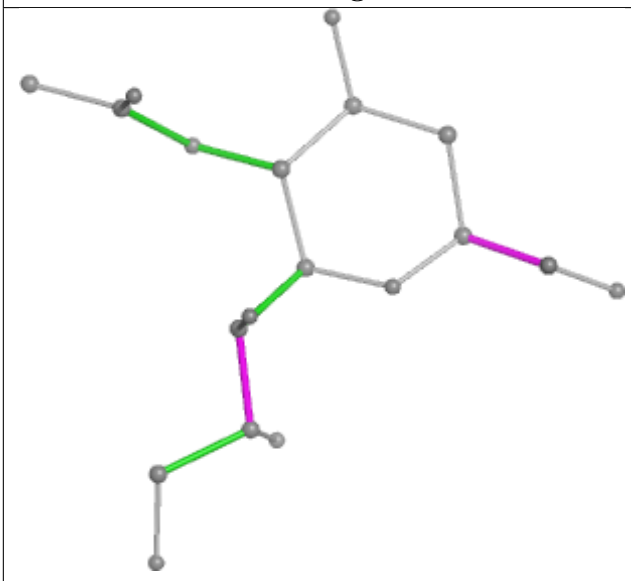
Ligand SLB U 301



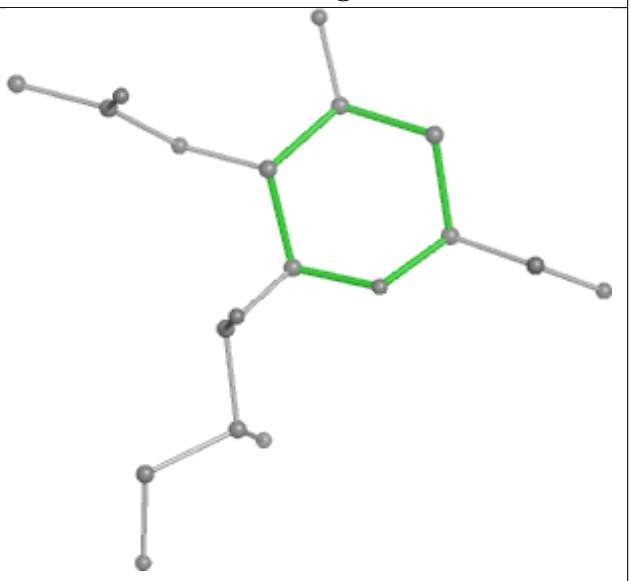
Bond lengths



Bond angles

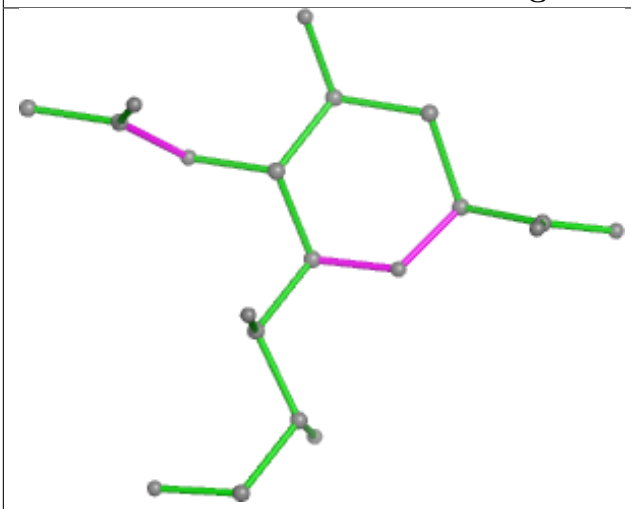


Torsions

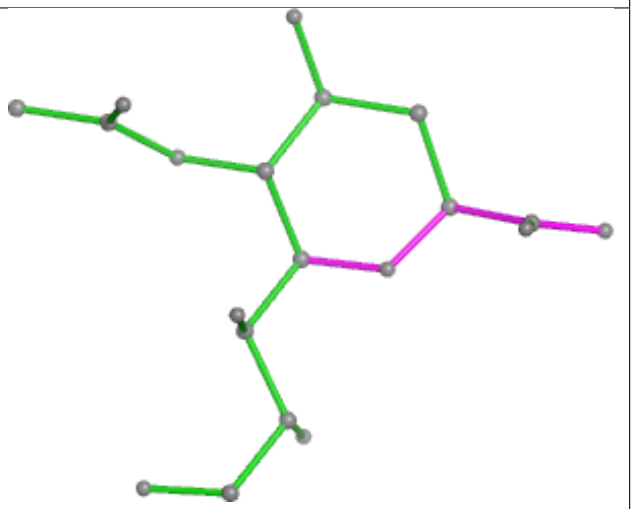


Rings

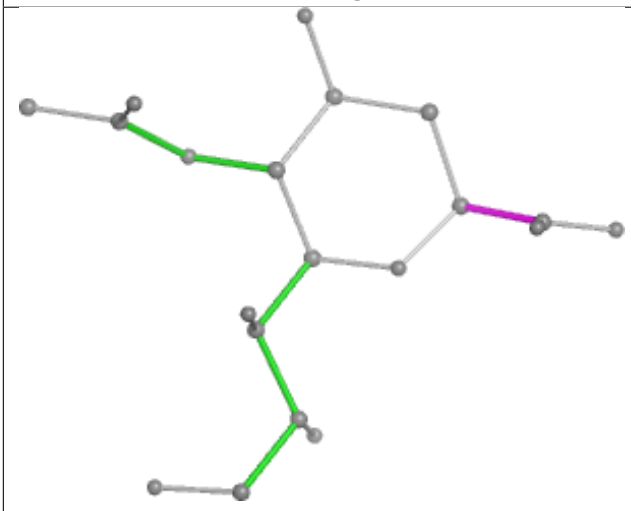
Ligand SLB E 301



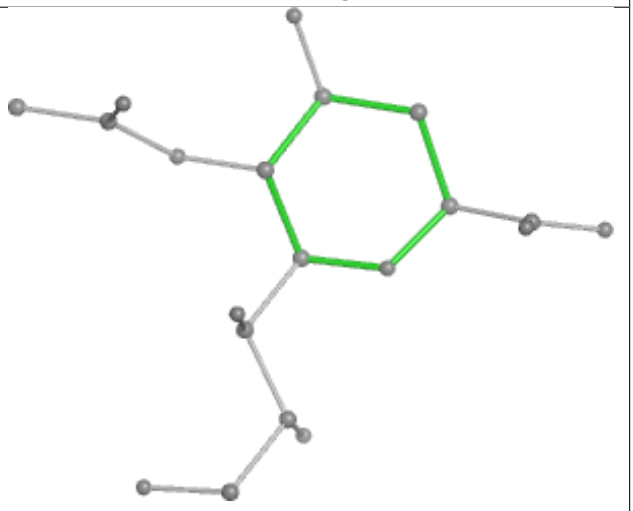
Bond lengths



Bond angles

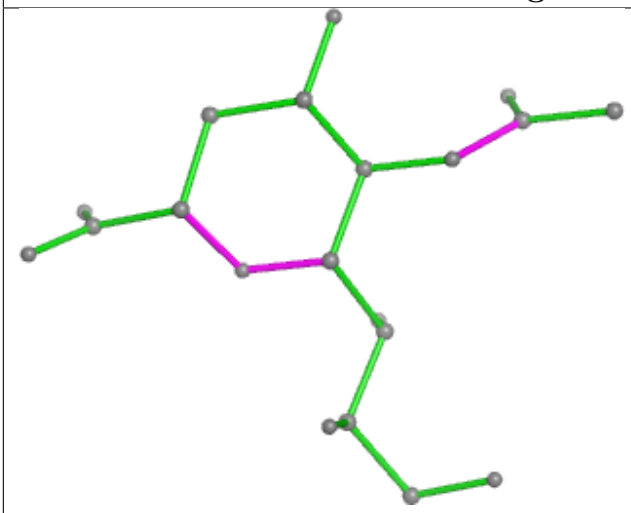


Torsions

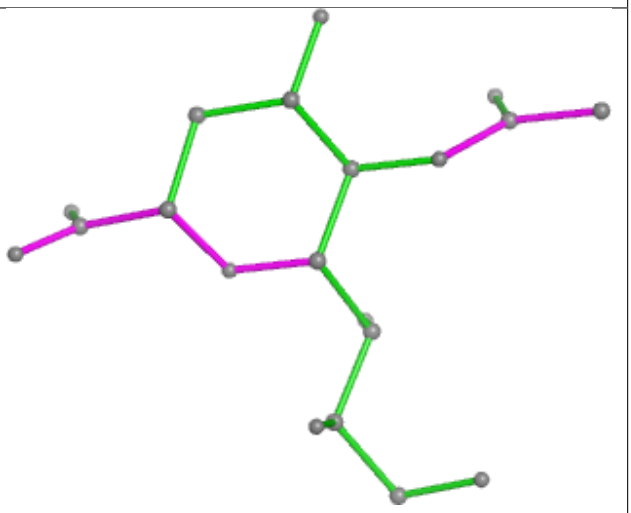


Rings

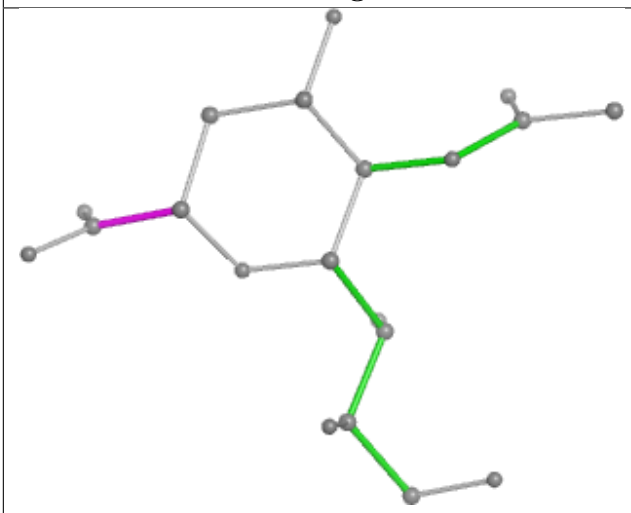
Ligand SLB Y 301



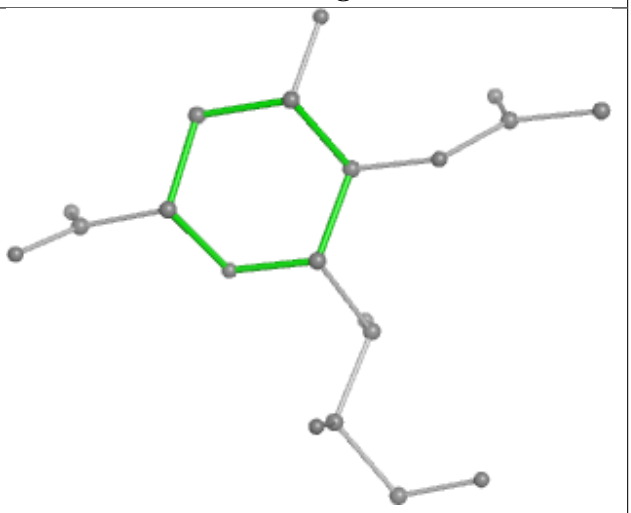
Bond lengths



Bond angles

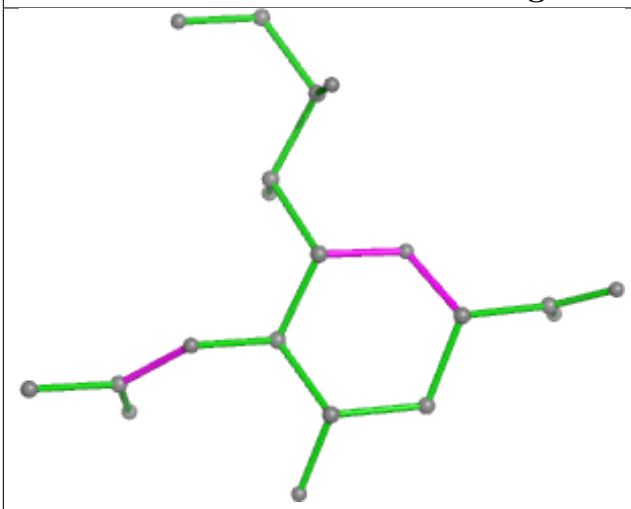


Torsions

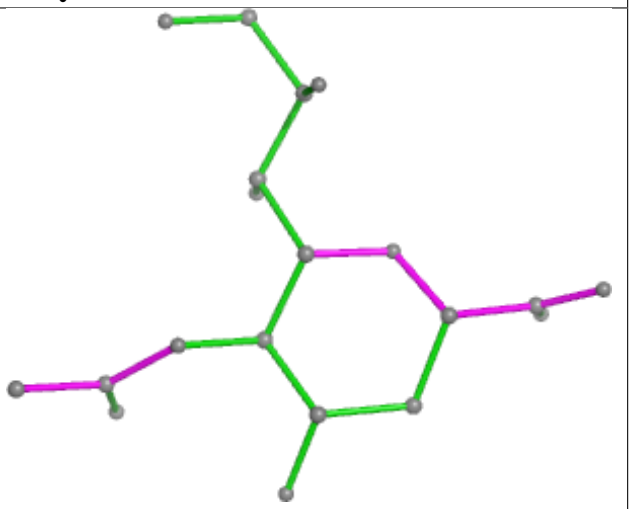


Rings

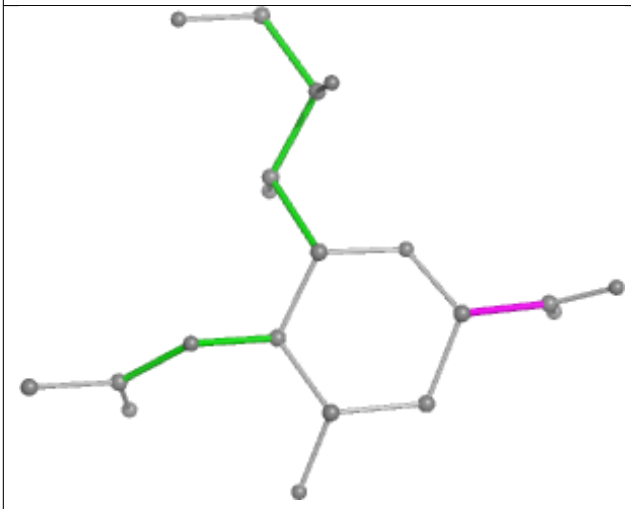
Ligand SLB Q 301



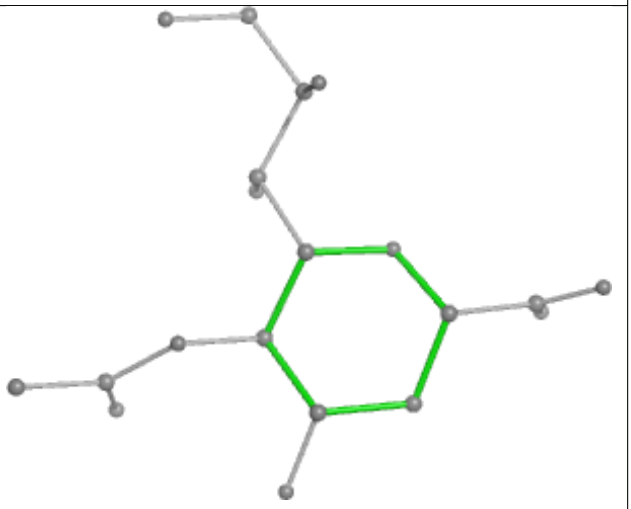
Bond lengths



Bond angles

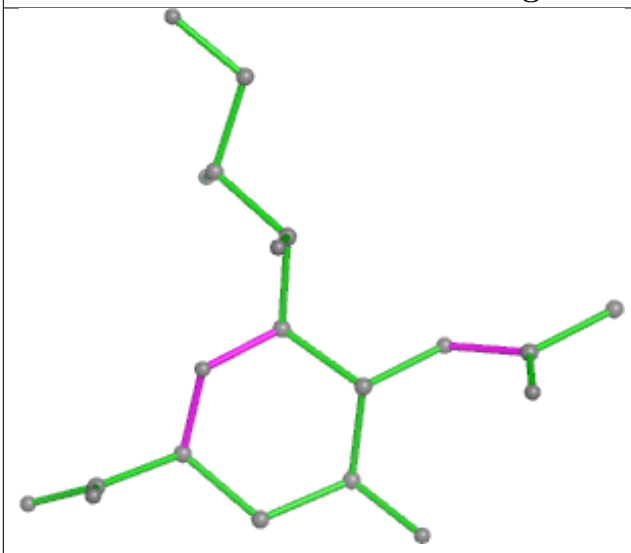


Torsions

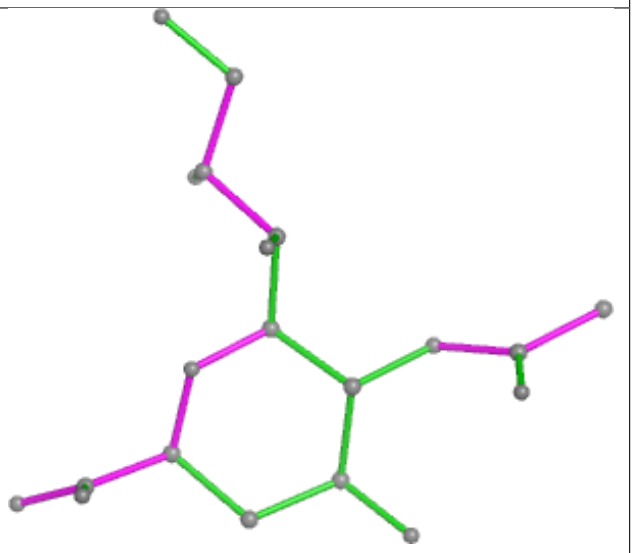


Rings

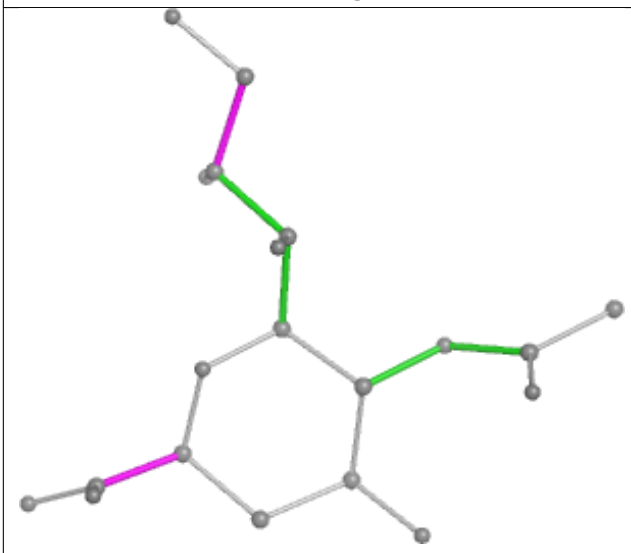
Ligand SLB W 301



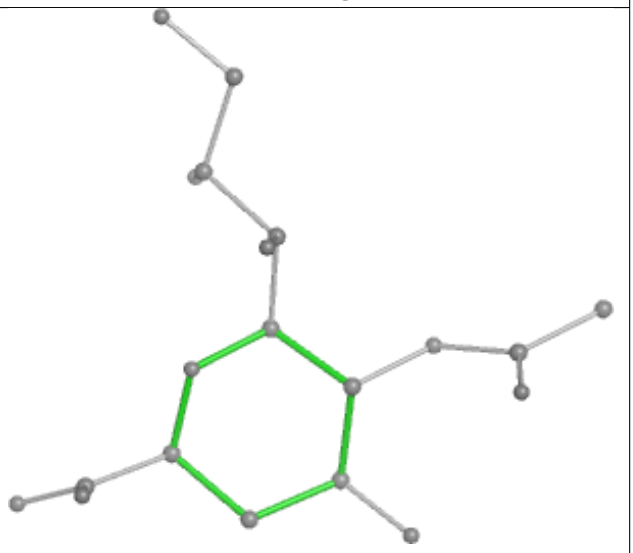
Bond lengths



Bond angles

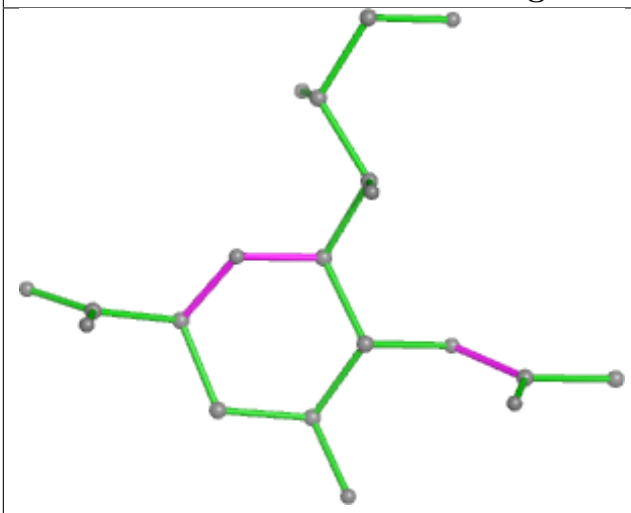


Torsions

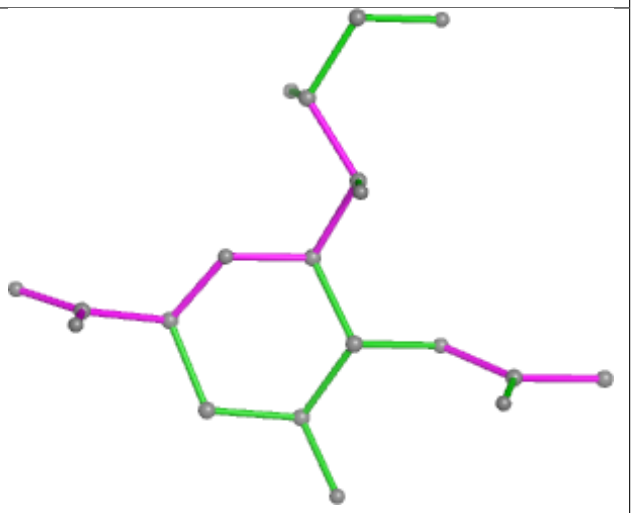


Rings

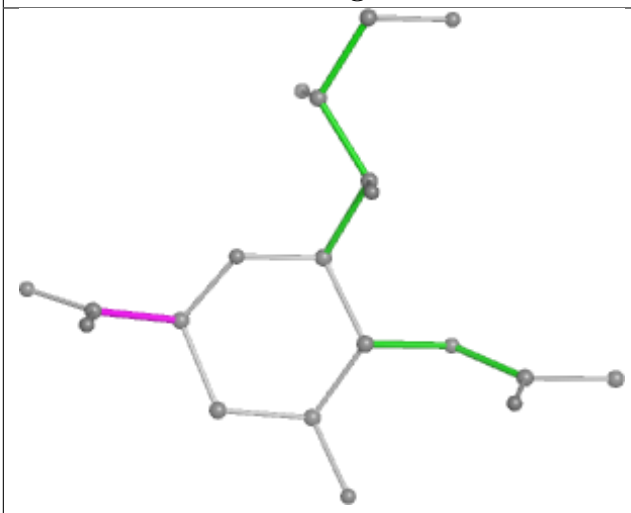
Ligand SLB O 301



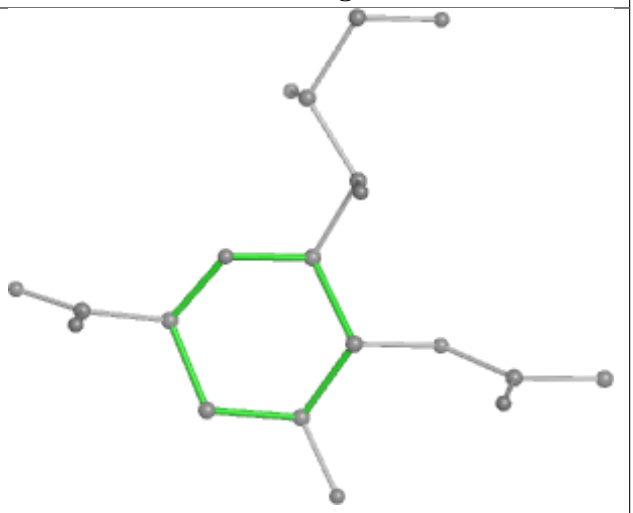
Bond lengths



Bond angles

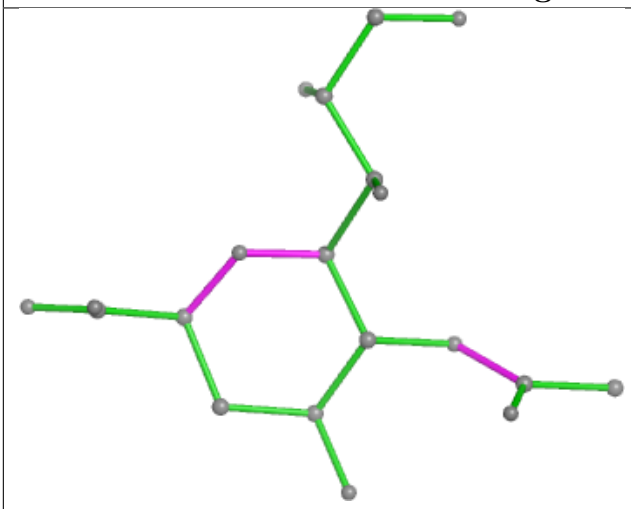


Torsions

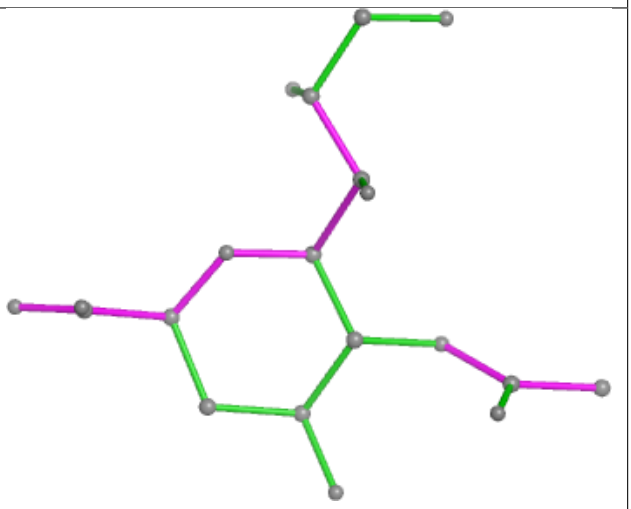


Rings

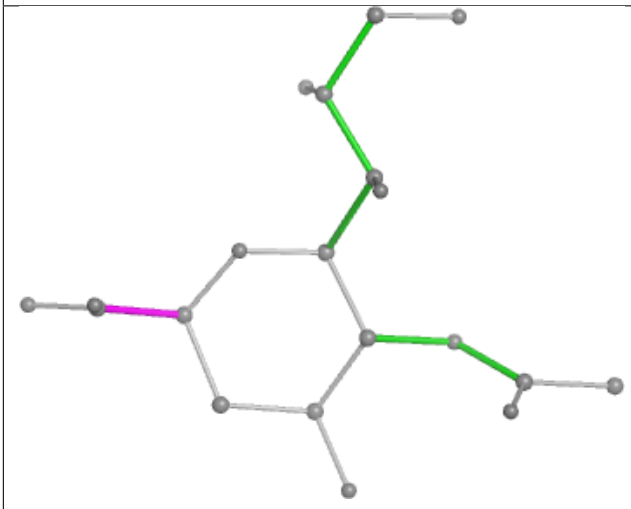
Ligand SLB I 301



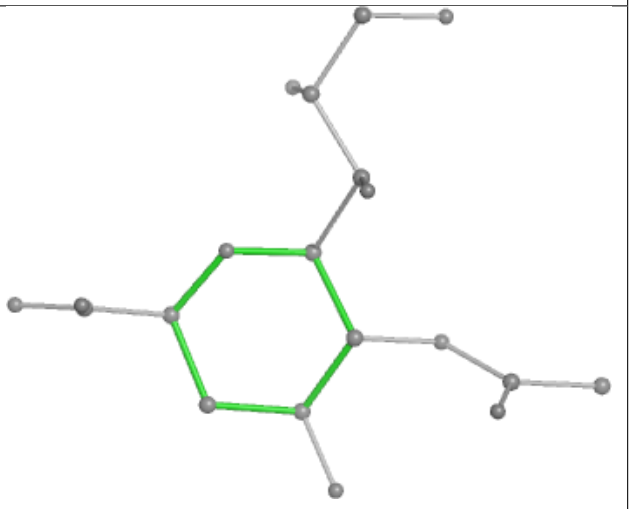
Bond lengths



Bond angles

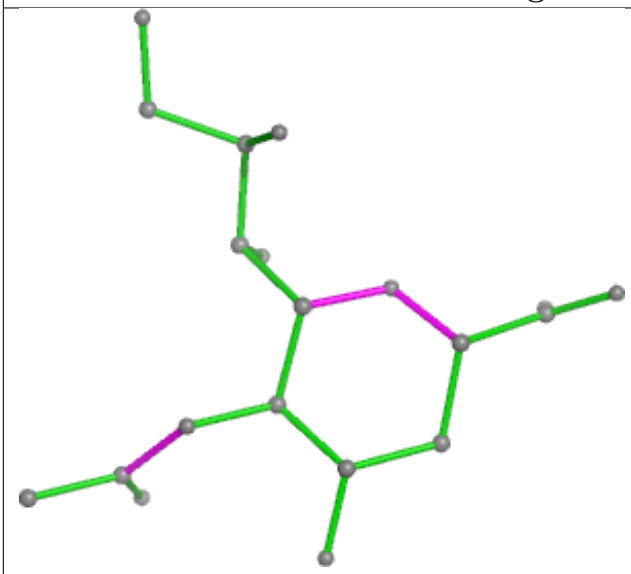


Torsions

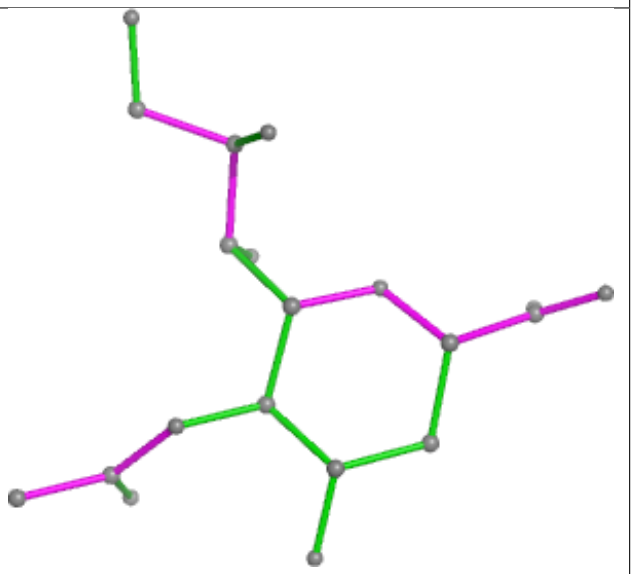


Rings

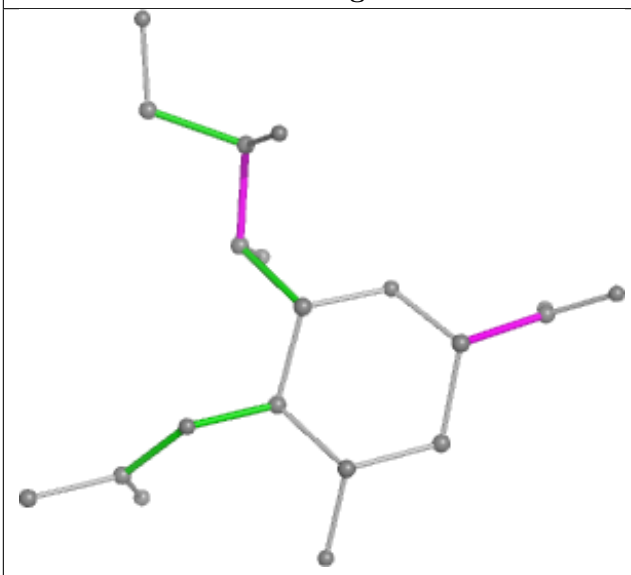
Ligand SLB A 301



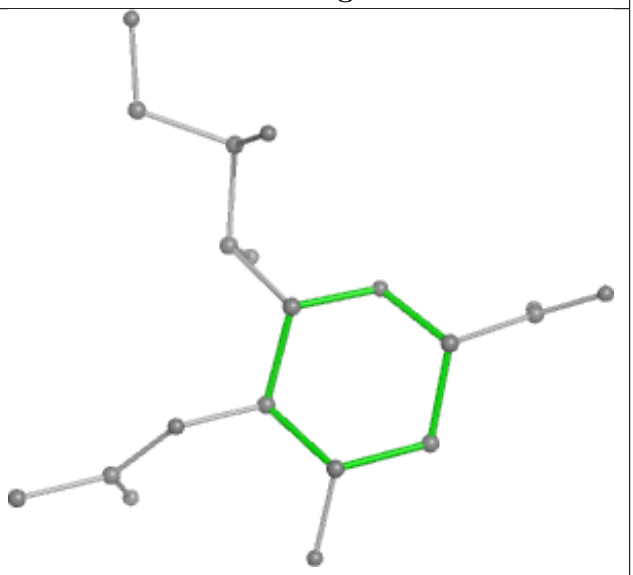
Bond lengths



Bond angles

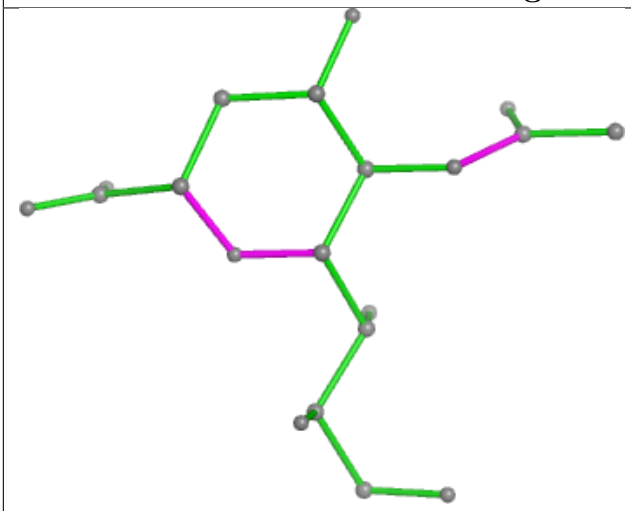


Torsions

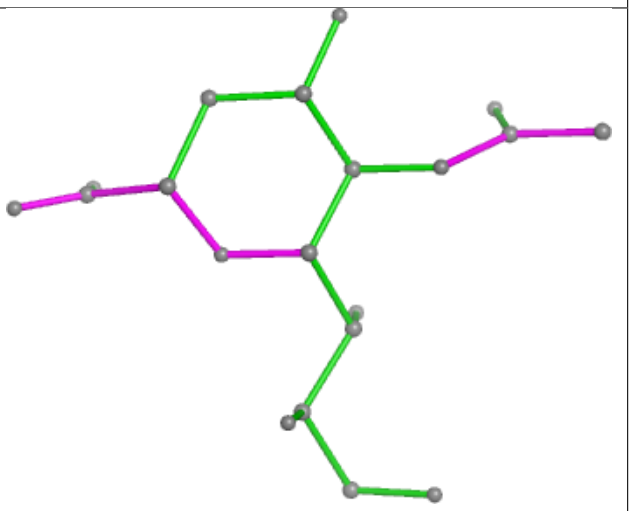


Rings

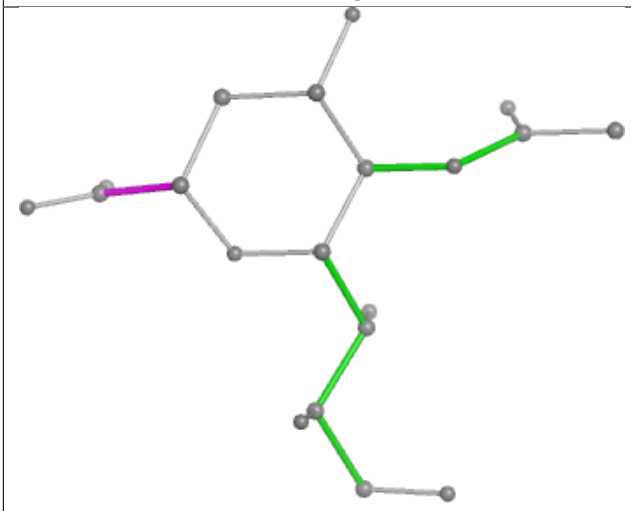
Ligand SLB M 301



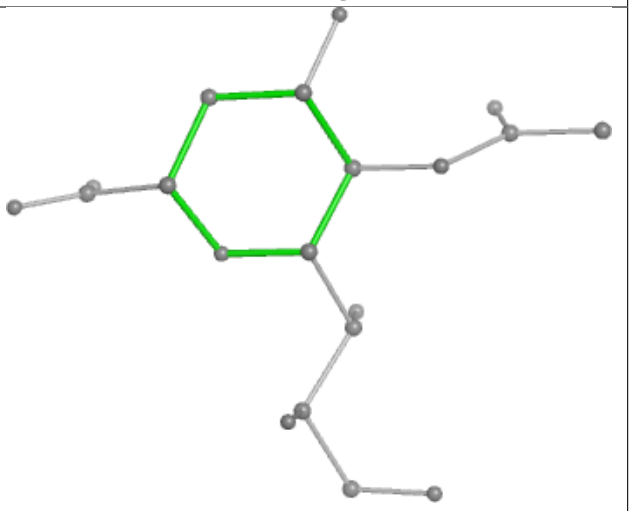
Bond lengths



Bond angles

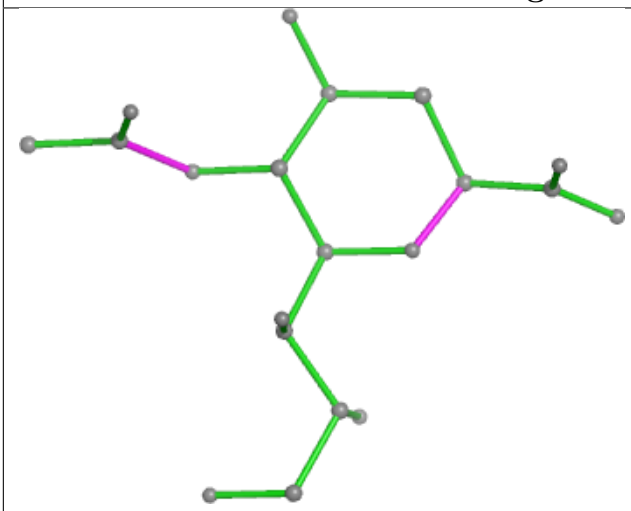


Torsions

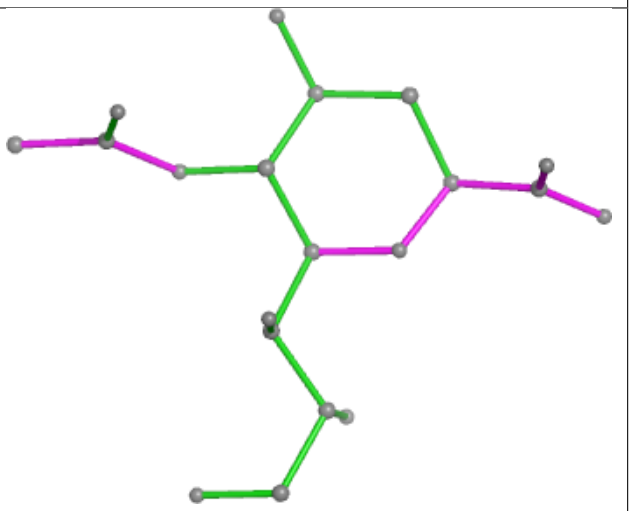


Rings

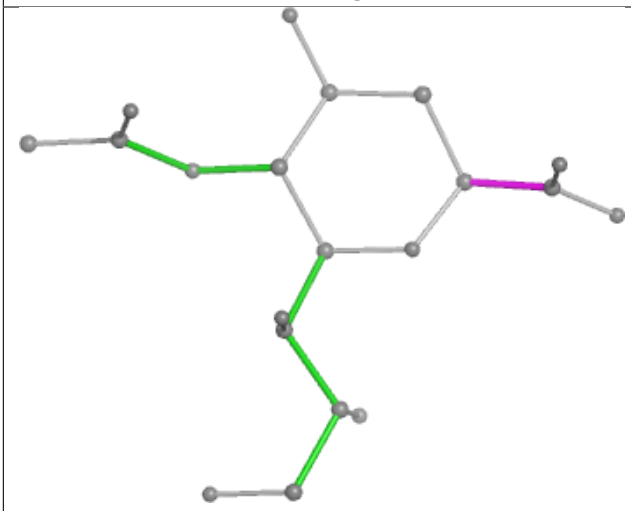
Ligand SLB K 301



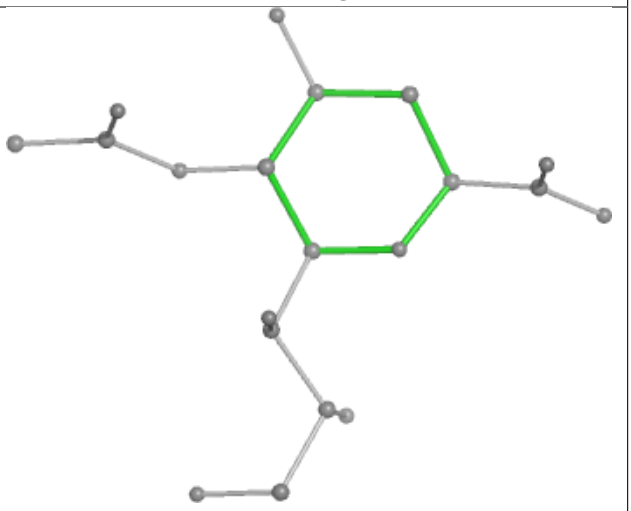
Bond lengths



Bond angles

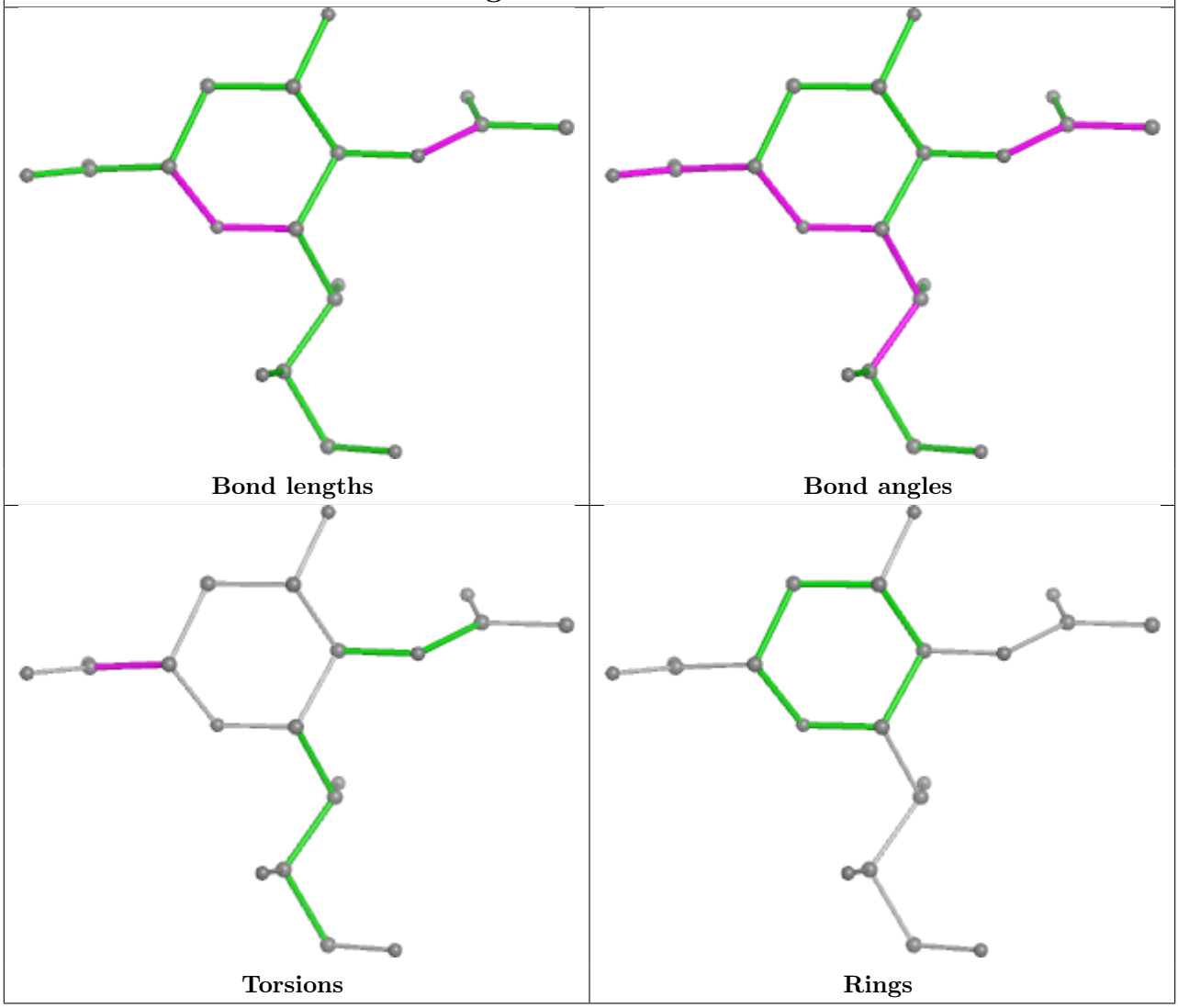


Torsions



Rings

Ligand SLB C 301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	299/303 (98%)	1.85	132 (44%) 1 1	37, 82, 117, 133	0
1	C	299/303 (98%)	0.69	18 (6%) 29 22	33, 60, 81, 93	0
1	E	301/303 (99%)	0.04	7 (2%) 61 53	24, 42, 62, 98	0
1	G	299/303 (98%)	0.45	13 (4%) 40 33	27, 56, 81, 93	0
1	I	299/303 (98%)	0.49	12 (4%) 43 35	32, 55, 82, 100	0
1	K	299/303 (98%)	0.86	28 (9%) 15 12	30, 63, 85, 96	0
1	M	299/303 (98%)	-0.03	6 (2%) 64 57	26, 42, 58, 77	0
1	O	299/303 (98%)	0.43	15 (5%) 35 28	29, 54, 79, 92	0
1	Q	299/303 (98%)	-0.08	2 (0%) 84 79	26, 42, 63, 78	0
1	U	299/303 (98%)	0.11	6 (2%) 64 57	23, 44, 68, 81	0
1	W	299/303 (98%)	0.66	29 (9%) 15 11	32, 61, 88, 103	0
1	Y	299/303 (98%)	0.13	8 (2%) 56 48	23, 45, 70, 91	0
2	B	122/123 (99%)	0.41	7 (5%) 30 24	30, 45, 72, 94	0
2	D	121/123 (98%)	0.38	7 (5%) 30 23	34, 48, 76, 97	0
2	F	123/123 (100%)	0.13	7 (5%) 30 24	25, 40, 74, 92	0
2	H	123/123 (100%)	0.02	7 (5%) 30 24	25, 35, 70, 86	0
2	J	123/123 (100%)	0.34	9 (7%) 22 17	27, 42, 76, 93	0
2	L	123/123 (100%)	0.07	5 (4%) 42 34	28, 38, 67, 83	0
2	N	123/123 (100%)	0.29	12 (9%) 14 11	26, 39, 70, 92	0
2	P	123/123 (100%)	-0.02	2 (1%) 70 63	25, 34, 55, 78	0
2	R	123/123 (100%)	-0.19	2 (1%) 70 63	22, 32, 59, 90	0
2	T	123/123 (100%)	-0.11	6 (4%) 36 28	23, 34, 59, 92	0
2	V	123/123 (100%)	-0.09	6 (4%) 36 28	23, 32, 56, 70	0
2	X	123/123 (100%)	-0.09	3 (2%) 59 52	28, 38, 57, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	5063/5112 (99%)	0.36	349 (6%)	24	18	22, 48, 84, 133	0

All (349) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	V	0	SER	8.2
2	L	43	LYS	5.9
2	H	42	GLY	5.8
1	E	187	LEU	5.7
2	B	0	SER	5.4
1	A	118	ASP	5.4
1	A	273	PHE	5.2
1	A	34	GLU	5.1
2	J	13	GLN	5.1
1	A	206	HIS	5.1
1	A	265	VAL	5.1
1	A	136	ILE	5.0
1	A	133	LEU	4.8
1	A	158	LEU	4.7
1	A	266	THR	4.7
1	A	202	LEU	4.7
1	A	254	LEU	4.6
1	A	134	ASN	4.5
1	W	2	THR	4.5
2	B	101	PHE	4.4
1	A	32	GLN	4.4
1	A	84	TYR	4.3
1	G	1	ALA	4.3
1	A	258	PHE	4.2
1	A	211	ASP	4.1
2	L	42	GLY	4.1
1	A	159	SER	4.0
1	A	281	TYR	4.0
2	F	113	GLN	4.0
2	R	-1	GLY	4.0
1	K	28	GLU	4.0
1	A	260	SER	4.0
1	A	27	LEU	4.0
1	A	285	ASP	4.0
1	A	205	THR	3.9
1	A	132	PRO	3.9
1	A	246	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	O	263	ILE	3.9
1	A	1	ALA	3.8
2	H	107	LYS	3.8
2	N	12	VAL	3.8
1	W	195	PHE	3.8
1	Y	133	LEU	3.8
1	A	116	ALA	3.8
2	J	107	LYS	3.7
2	L	45	ARG	3.7
1	E	-1	MET	3.7
1	A	238	LYS	3.7
1	A	35	ILE	3.7
2	V	-1	GLY	3.7
1	A	270	LEU	3.7
1	A	282	LYS	3.7
1	C	81	MET	3.7
1	W	1	ALA	3.7
1	A	201	ASN	3.7
1	A	87	LYS	3.7
2	N	40	ALA	3.7
1	A	138	ASP	3.6
1	W	237	GLN	3.6
1	C	274	ARG	3.6
1	U	159	SER	3.6
1	A	26	THR	3.6
1	A	255	VAL	3.5
1	A	263	ILE	3.5
1	W	159	SER	3.5
1	E	275	GLU	3.5
1	W	3	THR	3.5
2	H	-1	GLY	3.5
1	A	22	MET	3.5
1	I	28	GLU	3.5
1	O	262	GLY	3.5
1	A	139	PHE	3.4
1	A	272	PRO	3.4
1	K	148	ASN	3.4
1	A	155	TYR	3.4
1	A	161	ALA	3.4
1	G	148	ASN	3.4
1	Y	113	ASN	3.4
1	A	251	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	K	182	GLY	3.4
1	A	86	ALA	3.4
1	A	127	THR	3.4
1	K	203	ALA	3.4
2	F	41	PRO	3.4
1	A	248	LYS	3.4
1	W	128	THR	3.3
1	A	120	TRP	3.3
1	A	92	LEU	3.3
1	K	245	GLN	3.3
1	K	35	ILE	3.3
1	O	182	GLY	3.3
2	P	-1	GLY	3.3
2	J	41	PRO	3.3
2	T	13	GLN	3.2
1	C	254	LEU	3.2
1	A	203	ALA	3.2
1	O	1	ALA	3.2
2	D	121	SER	3.2
1	A	277	MET	3.2
2	R	113	GLN	3.2
1	A	264	ASN	3.2
1	A	204	MET	3.2
1	W	193	MET	3.2
2	B	121	SER	3.2
1	A	181	ASP	3.2
1	A	297	ALA	3.1
2	N	43	LYS	3.1
1	A	130	ASN	3.1
1	C	291	PRO	3.1
1	A	15	VAL	3.1
2	B	13	GLN	3.1
1	A	252	ALA	3.1
1	M	215	ILE	3.1
1	A	245	GLN	3.0
2	X	113	GLN	3.0
1	C	77	ALA	3.0
2	L	44	GLU	3.0
1	A	231	ILE	3.0
1	W	234	LYS	3.0
1	A	141	GLY	3.0
1	C	32	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	I	245	GLN	3.0
2	N	42	GLY	3.0
1	A	119	THR	3.0
1	A	129	SER	3.0
1	A	85	VAL	3.0
1	A	199	GLN	3.0
2	D	13	GLN	3.0
2	F	-1	GLY	2.9
1	A	290	GLN	2.9
1	A	247	VAL	2.9
1	Q	193	MET	2.9
1	K	212	GLN	2.9
1	M	29	GLU	2.9
1	A	275	GLU	2.9
1	A	257	PHE	2.9
1	A	90	ASP	2.9
1	M	238	LYS	2.9
1	W	200	LYS	2.9
2	D	41	PRO	2.9
2	N	41	PRO	2.9
1	A	79	ALA	2.9
1	A	189	THR	2.9
1	E	197	GLU	2.9
1	A	31	SER	2.8
1	Q	87	LYS	2.8
1	A	102	GLN	2.8
1	A	278	GLN	2.8
2	V	65	ALA	2.8
1	C	148	ASN	2.8
2	N	0	SER	2.8
1	C	290	GLN	2.8
1	C	276	ALA	2.8
2	N	54	THR	2.8
2	D	42	GLY	2.8
1	A	222	GLN	2.8
1	A	236	VAL	2.8
1	E	97	GLU	2.8
1	U	274	ARG	2.8
1	A	200	LYS	2.8
1	Y	275	GLU	2.8
1	A	82	LEU	2.8
1	E	0	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	M	180	VAL	2.7
1	A	81	MET	2.7
1	A	157	LYS	2.7
1	A	126	GLU	2.7
1	K	1	ALA	2.7
1	K	161	ALA	2.7
1	A	21	LYS	2.7
1	O	32	GLN	2.7
2	B	25	SER	2.7
1	A	207	HIS	2.7
2	J	42	GLY	2.7
2	N	13	GLN	2.7
2	J	-1	GLY	2.7
1	I	174	ALA	2.6
2	D	113	GLN	2.6
1	C	296	LEU	2.6
1	A	83	PRO	2.6
1	A	249	THR	2.6
1	W	255	VAL	2.6
1	A	235	ALA	2.6
1	K	233	GLN	2.6
1	W	264	ASN	2.6
2	V	44	GLU	2.6
1	C	135	SER	2.6
1	O	31	SER	2.6
2	F	40	ALA	2.6
1	A	142	LEU	2.6
2	L	107	LYS	2.6
1	A	162	SER	2.6
1	A	293	VAL	2.6
1	O	180	VAL	2.6
1	A	140	LYS	2.5
1	A	143	LYS	2.5
1	G	87	LYS	2.5
2	H	43	LYS	2.5
1	A	186	PRO	2.5
2	N	45	ARG	2.5
1	I	289	GLY	2.5
2	F	121	SER	2.5
1	A	262	GLY	2.5
1	G	34	GLU	2.5
1	G	134	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
2	P	44	GLU	2.5
1	K	159	SER	2.5
1	C	295	LYS	2.5
1	O	110	GLN	2.5
1	M	197	GLU	2.5
1	A	220	THR	2.5
1	A	208	ILE	2.5
1	O	35	ILE	2.5
1	A	221	TRP	2.5
1	O	30	MET	2.5
1	A	223	LYS	2.4
1	M	237	GLN	2.4
1	A	33	GLY	2.4
2	T	112	GLY	2.4
1	G	275	GLU	2.4
2	B	44	GLU	2.4
1	I	30	MET	2.4
2	V	76	LYS	2.4
1	W	196	TYR	2.4
2	H	13	GLN	2.4
2	H	121	SER	2.4
1	U	283	GLU	2.4
2	J	89	GLU	2.4
1	G	259	LYS	2.4
1	A	67	PHE	2.4
1	A	274	ARG	2.4
1	C	255	VAL	2.4
1	A	276	ALA	2.4
1	W	148	ASN	2.4
1	A	153	LEU	2.4
1	G	135	SER	2.4
1	W	253	GLU	2.4
1	G	102	GLN	2.3
1	K	202	LEU	2.3
1	A	209	VAL	2.3
2	N	107	LYS	2.3
2	V	121	SER	2.3
1	I	271	GLU	2.3
1	C	1	ALA	2.3
1	K	122	ASN	2.3
1	K	4	LEU	2.3
2	J	113	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
2	T	113	GLN	2.3
1	O	282	LYS	2.3
1	C	269	ASP	2.3
1	I	211	ASP	2.3
1	W	258	PHE	2.3
1	W	274	ARG	2.3
1	K	2	THR	2.3
1	C	134	ASN	2.3
1	I	234	LYS	2.3
1	W	259	LYS	2.3
2	X	43	LYS	2.3
1	K	12	VAL	2.3
1	W	58	GLY	2.3
1	A	163	PRO	2.3
1	I	178	ASN	2.3
1	K	191	LYS	2.3
2	F	43	LYS	2.3
1	A	123	GLY	2.3
1	A	135	SER	2.3
1	K	27	LEU	2.3
1	Y	202	LEU	2.3
1	O	140	LYS	2.3
1	W	192	THR	2.3
2	J	43	LYS	2.3
2	B	65	ALA	2.2
2	J	120	SER	2.2
1	W	189	THR	2.2
1	A	64	TYR	2.2
1	A	233	GLN	2.2
1	A	242	ALA	2.2
1	K	116	ALA	2.2
1	A	294	SER	2.2
1	K	244	THR	2.2
1	G	265	VAL	2.2
1	W	13	GLY	2.2
2	N	-1	GLY	2.2
2	T	114	GLY	2.2
1	A	267	TYR	2.2
1	W	201	ASN	2.2
1	A	30	MET	2.2
2	H	44	GLU	2.2
1	W	173	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	272	PRO	2.2
1	A	28	GLU	2.2
1	A	234	LYS	2.2
1	K	137	GLU	2.2
2	F	44	GLU	2.2
1	A	228	ASP	2.2
1	A	3	THR	2.1
1	I	131	ARG	2.1
1	A	175	LEU	2.1
1	A	271	GLU	2.1
1	I	215	ILE	2.1
2	T	42	GLY	2.1
1	E	166	MET	2.1
1	K	32	GLN	2.1
1	K	257	PHE	2.1
1	O	202	LEU	2.1
1	A	268	PRO	2.1
1	O	80	VAL	2.1
1	A	241	ASP	2.1
1	A	11	SER	2.1
1	A	164	THR	2.1
1	A	224	LEU	2.1
1	A	172	TYR	2.1
1	K	253	GLU	2.1
2	X	44	GLU	2.1
1	A	188	PRO	2.1
1	W	293	VAL	2.1
1	W	93	ARG	2.1
2	T	-1	GLY	2.1
1	A	91	HIS	2.1
1	I	176	GLN	2.1
1	K	187	LEU	2.1
1	U	196	TYR	2.1
1	C	253	GLU	2.1
1	Y	137	GLU	2.1
1	A	95	MET	2.1
1	C	22	MET	2.1
1	K	33	GLY	2.1
2	D	112	GLY	2.1
2	N	66	GLY	2.1
1	A	89	PHE	2.1
1	W	202	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	W	32	GLN	2.0
1	Y	1	ALA	2.0
1	A	253	GLU	2.0
1	A	279	PRO	2.0
1	O	274	ARG	2.0
1	Y	255	VAL	2.0
1	G	295	LYS	2.0
1	A	117	LEU	2.0
1	U	173	LEU	2.0
1	K	64	TYR	2.0
1	A	232	ILE	2.0
1	G	288	ILE	2.0
1	A	122	ASN	2.0
1	U	178	ASN	2.0
1	W	30	MET	2.0
1	K	293	VAL	2.0
1	Y	131	ARG	2.0
2	D	107	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	U	303	6/6	0.14	0.24	100,121,134,136	0
4	GOL	U	302	6/6	0.39	0.27	81,102,117,123	0
4	GOL	Q	302	6/6	0.78	0.18	34,43,52,59	0
4	GOL	U	304	6/6	0.78	0.17	50,60,68,80	0
4	GOL	E	302	6/6	0.79	0.20	27,44,53,63	0

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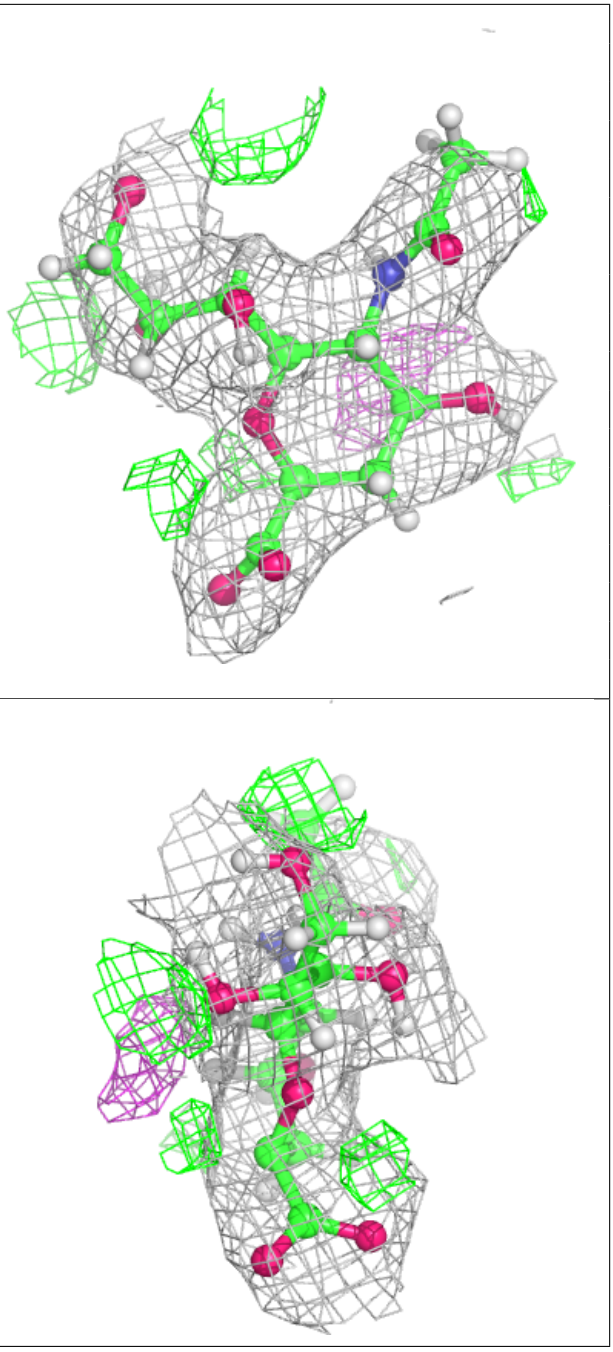
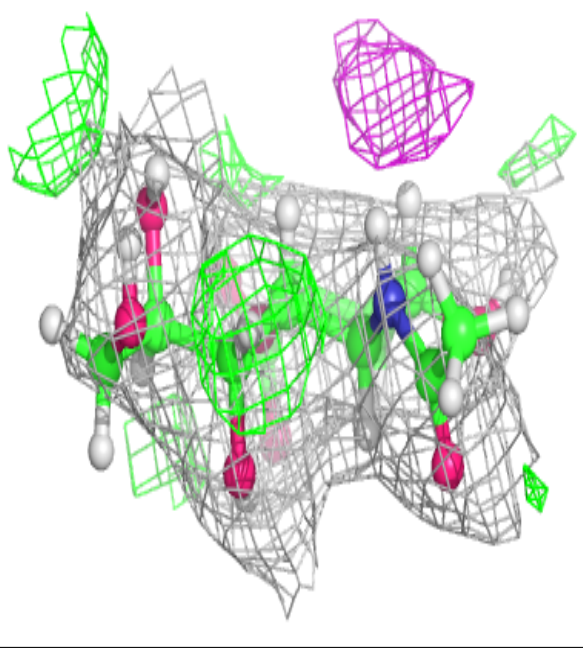
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	G	302	6/6	0.79	0.25	75,90,98,103	0
3	SLB	K	301	20/21	0.86	0.14	39,53,62,66	0
3	SLB	W	301	20/21	0.88	0.15	41,51,63,74	0
3	SLB	A	301	20/21	0.89	0.13	42,53,69,75	0
3	SLB	U	301	20/21	0.89	0.11	21,31,39,44	0
3	SLB	E	301	20/21	0.89	0.10	23,35,46,53	0
3	SLB	M	301	20/21	0.90	0.11	24,32,42,46	0
3	SLB	I	301	20/21	0.90	0.12	29,36,44,47	0
3	SLB	C	301	20/21	0.90	0.12	31,43,56,58	0
3	SLB	G	301	20/21	0.92	0.12	25,33,44,52	0
3	SLB	Q	301	20/21	0.92	0.11	28,35,42,46	0
3	SLB	O	301	20/21	0.93	0.12	30,40,48,53	0
3	SLB	Y	301	20/21	0.93	0.09	26,34,47,47	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 SLB K 301:

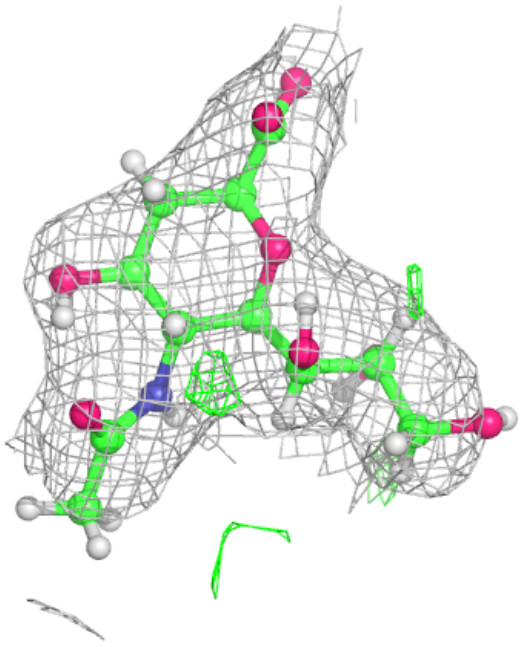
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

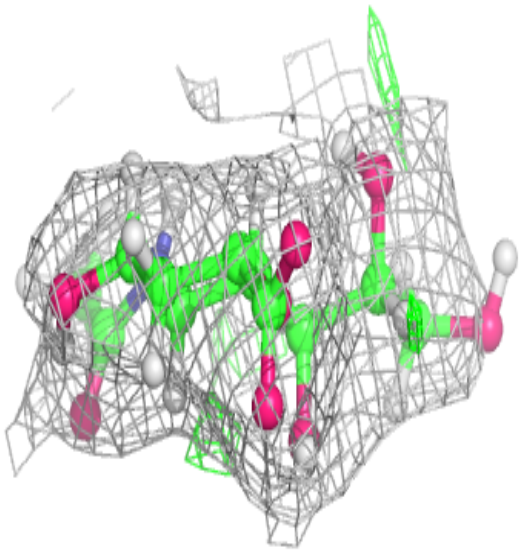




Electron density around SLB W 301:

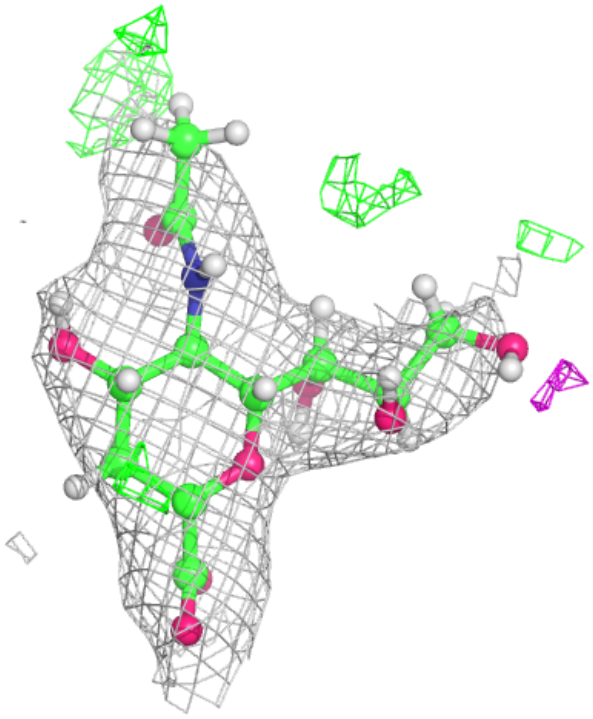
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

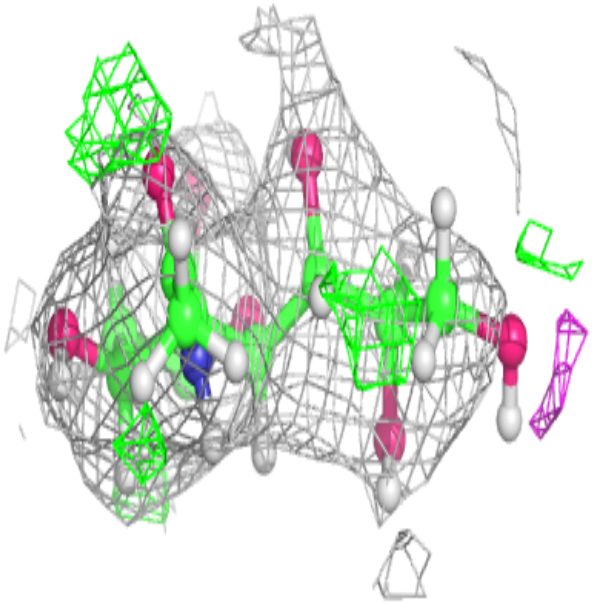


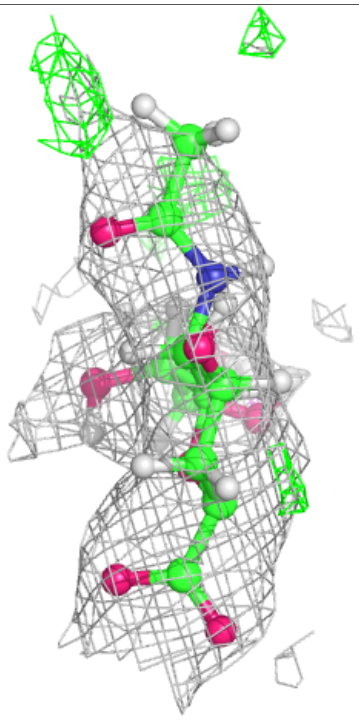


Electron density around SLB A 301:

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

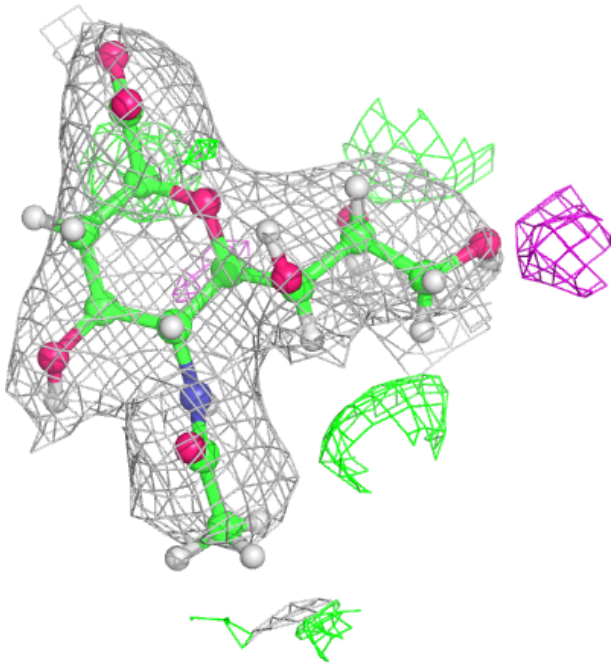


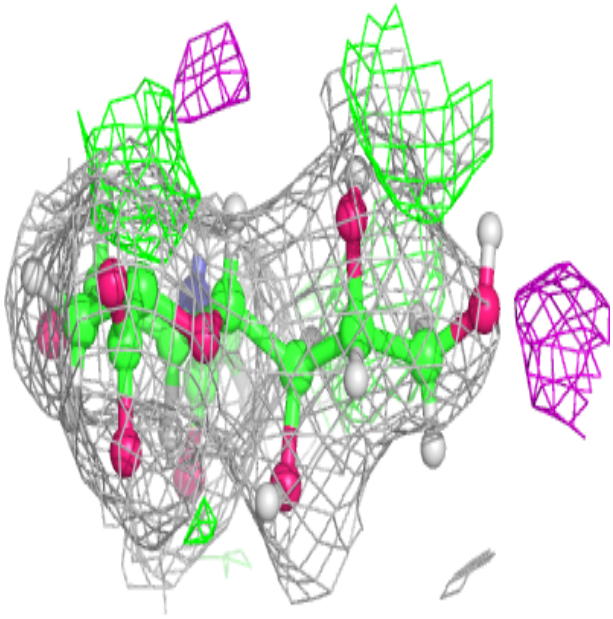




Electron density around SLB U 301:

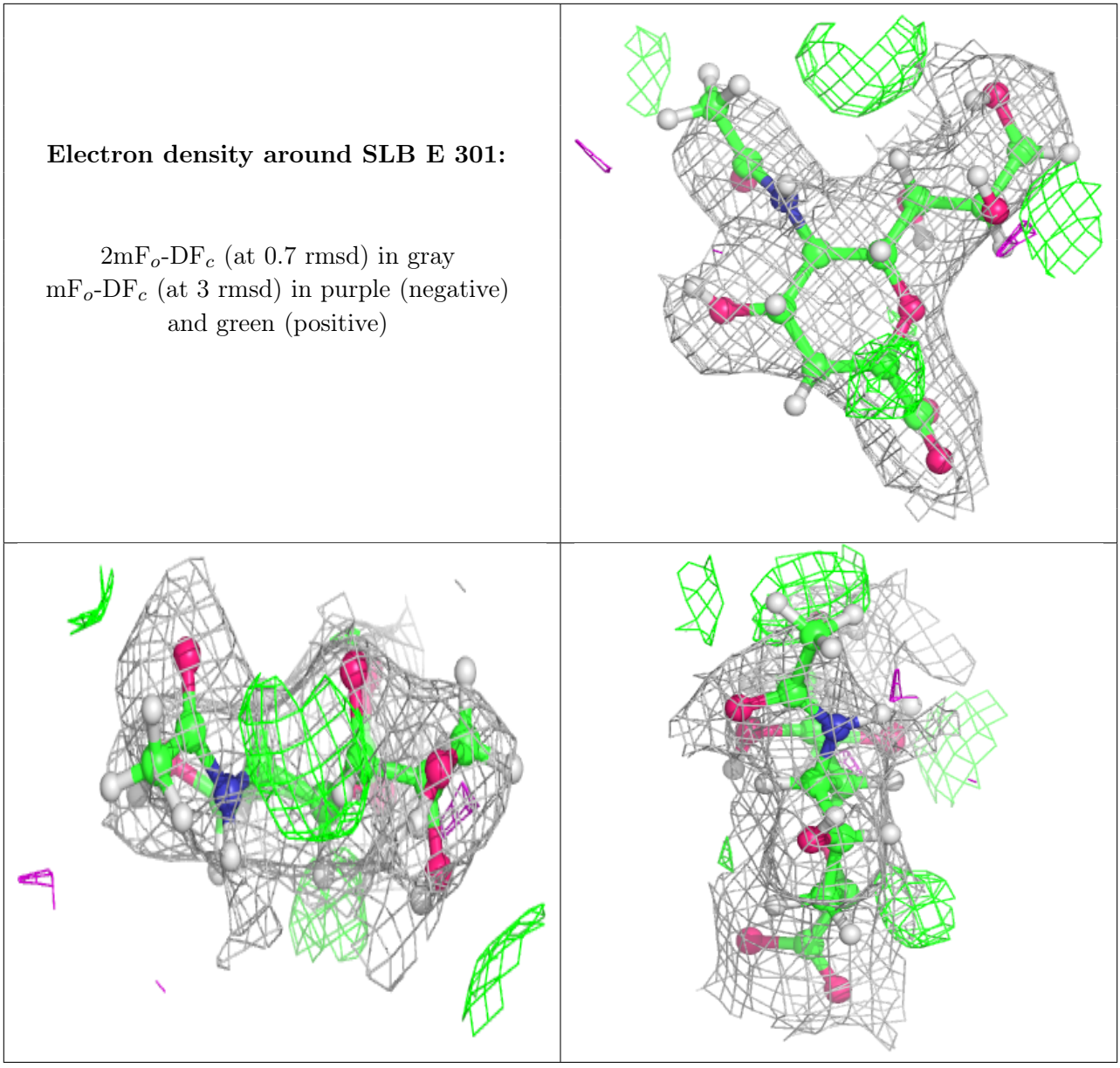
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





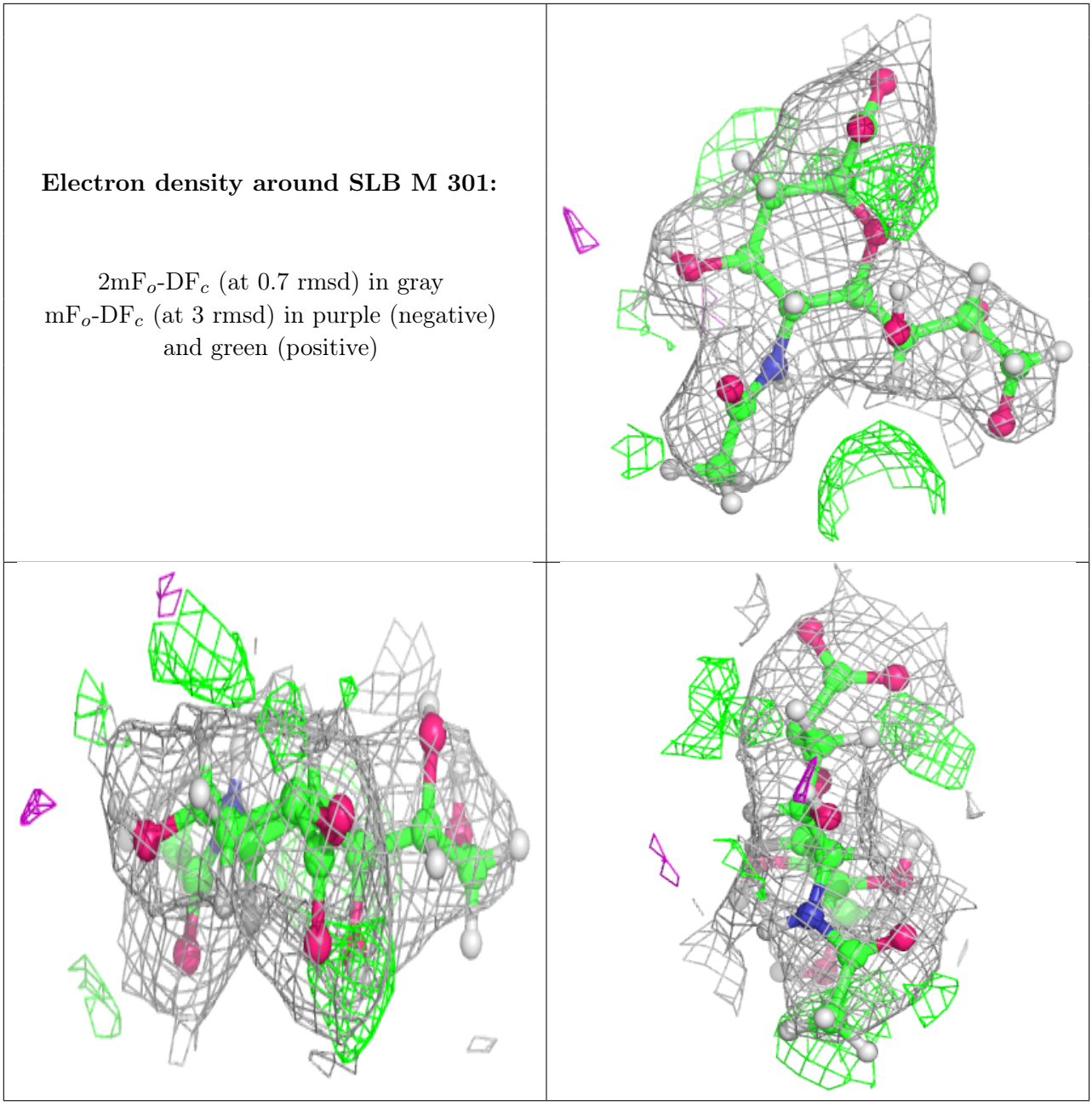
Electron density around SLB E 301:

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



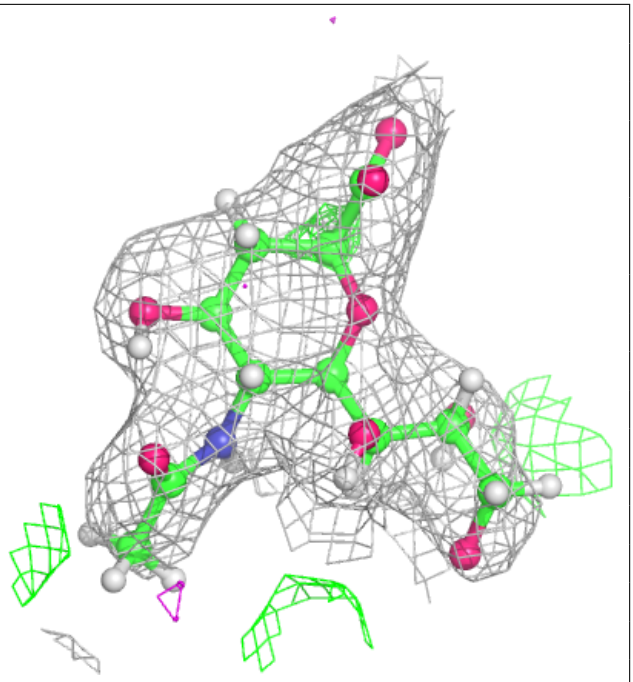
Electron density around SLB M 301:

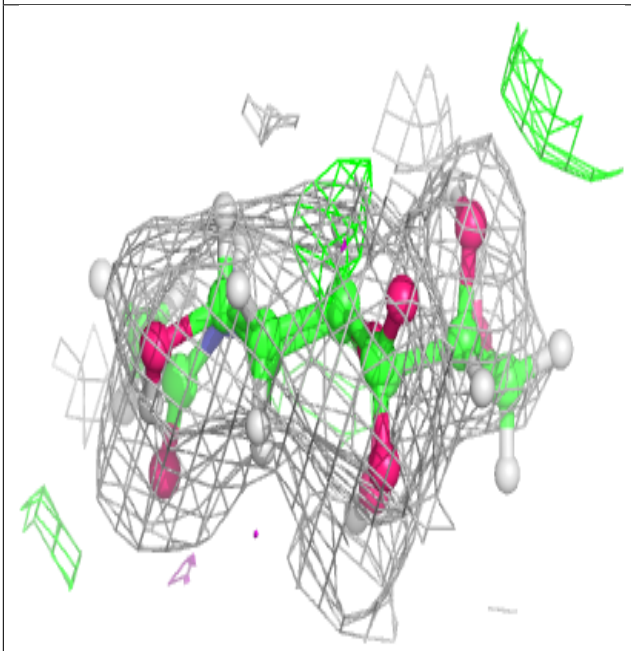
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

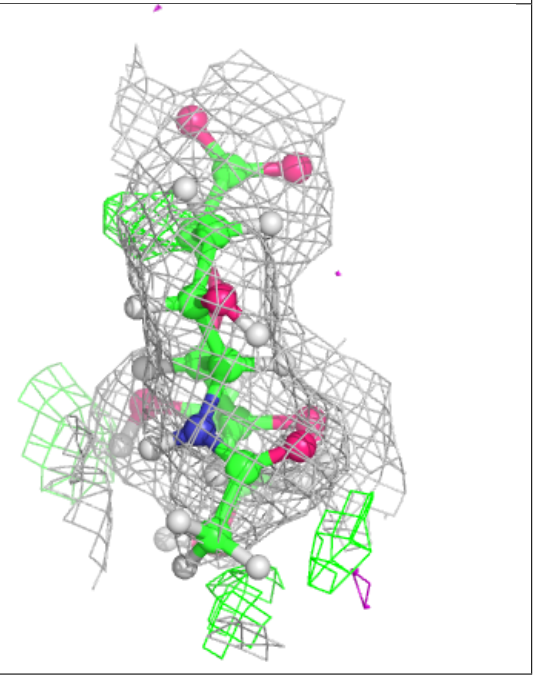


Electron density around SLB I 301:

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

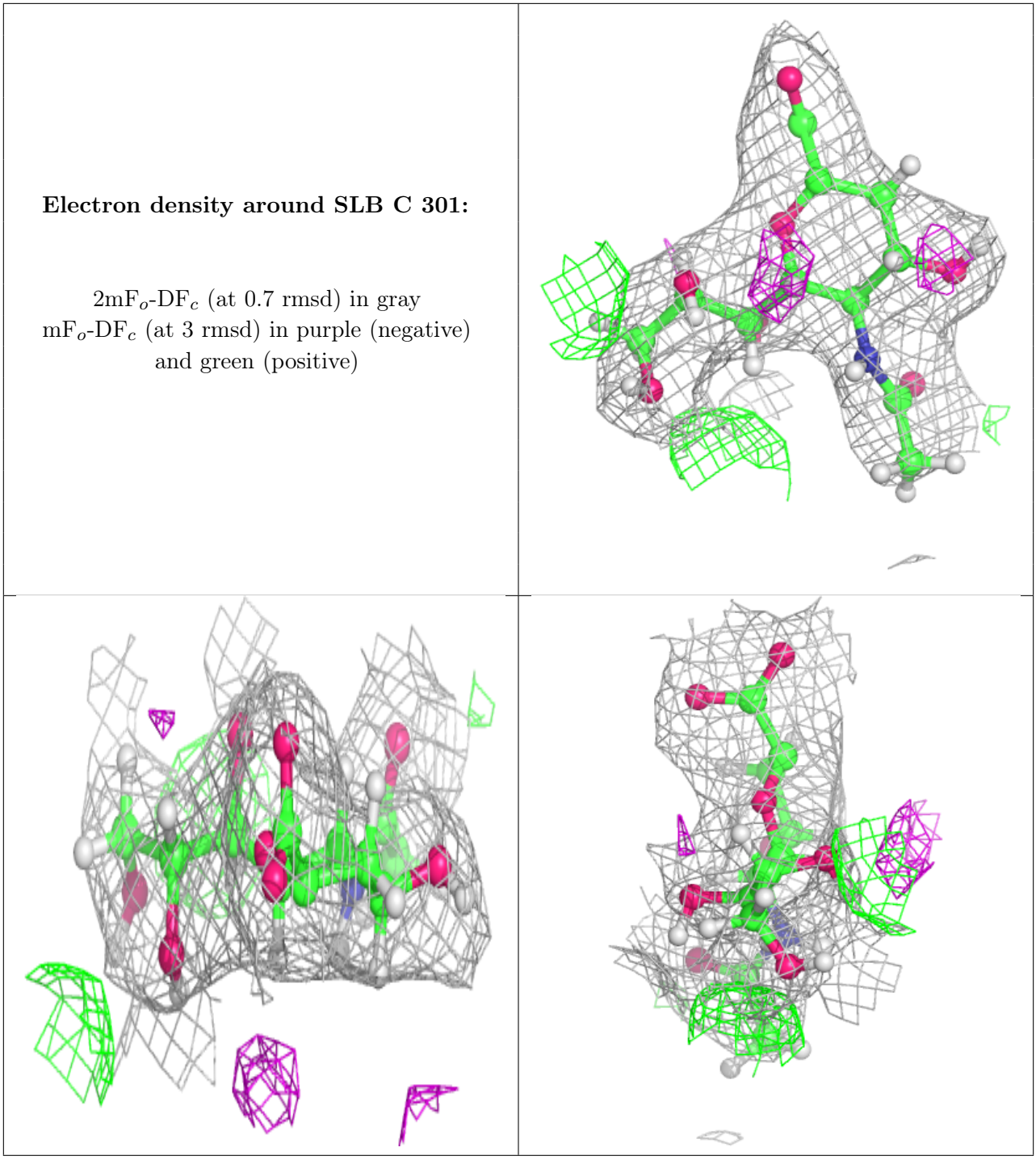






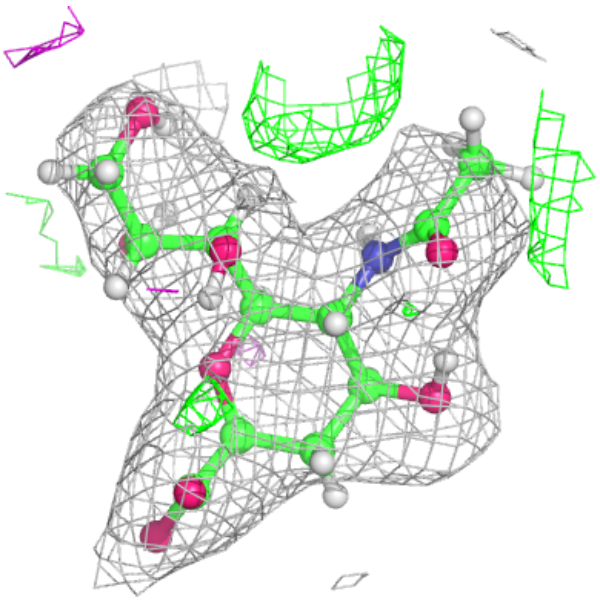
Electron density around SLB C 301:

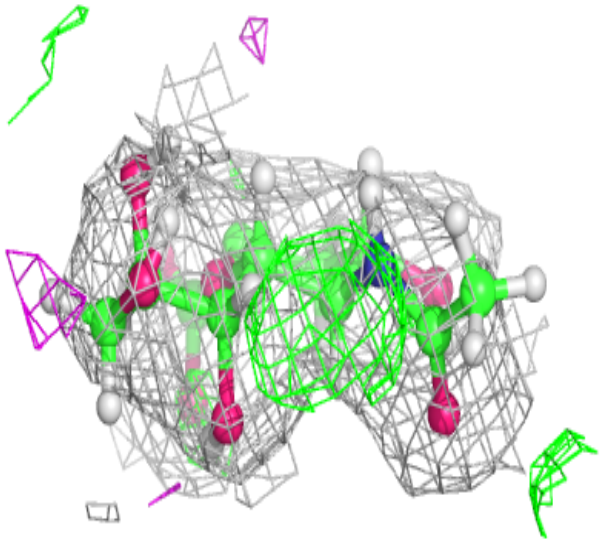
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

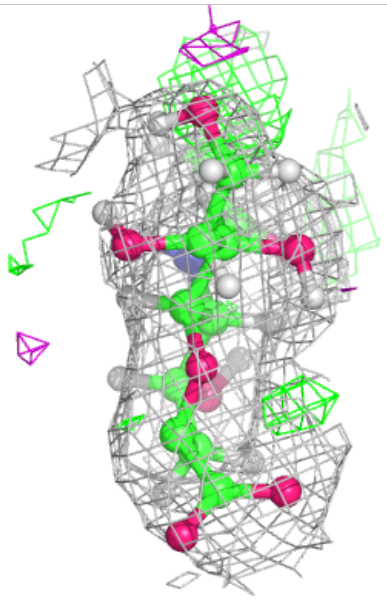


Electron density around SLB G 301:

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

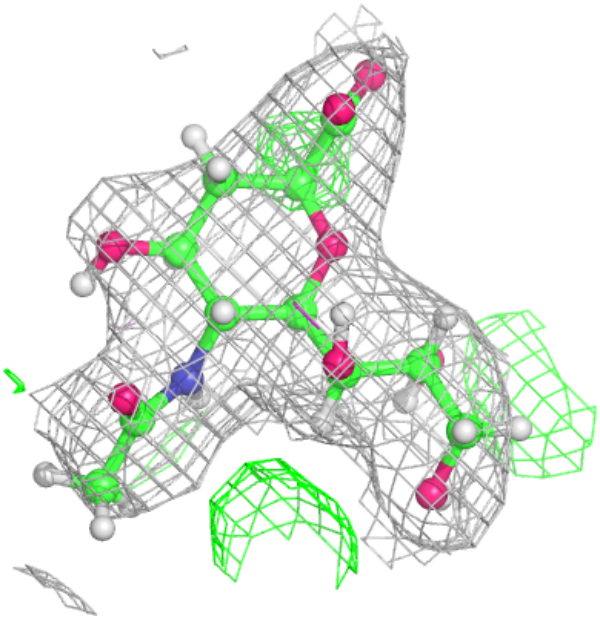


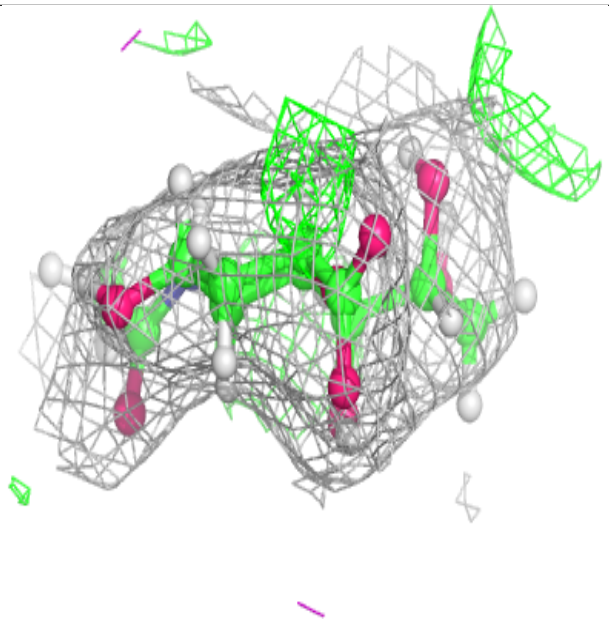


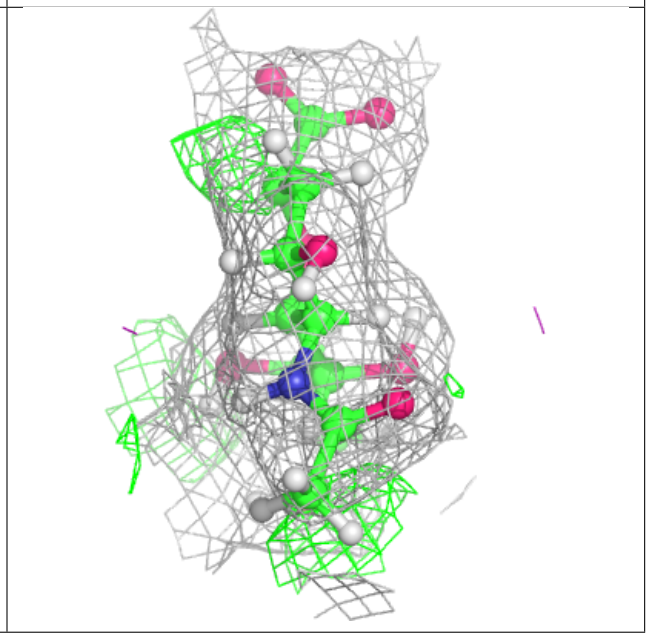


Electron density around SLB Q 301:

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

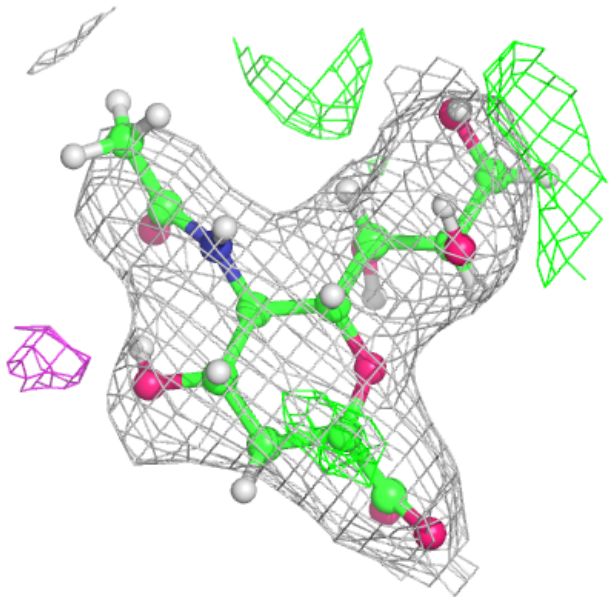


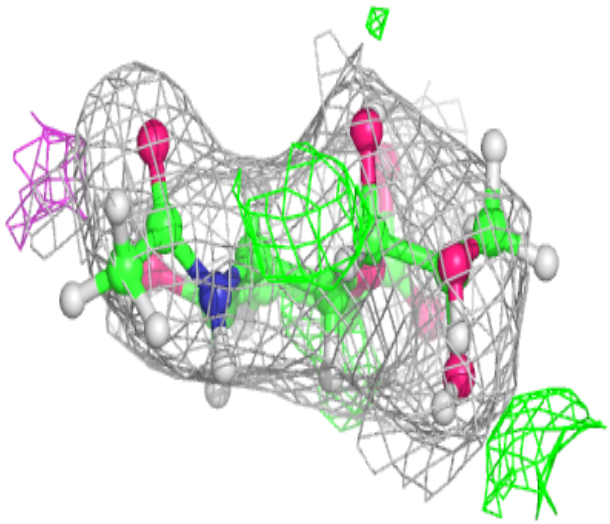


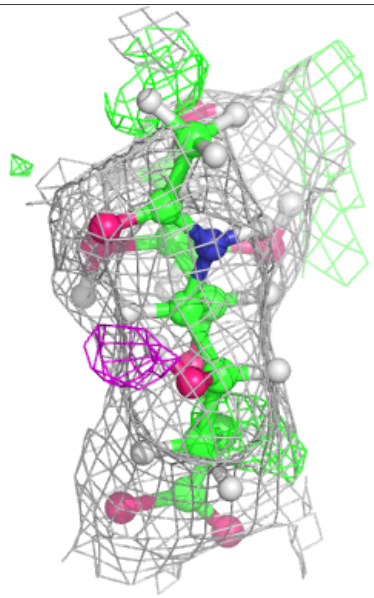


Electron density around SLB O 301:

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

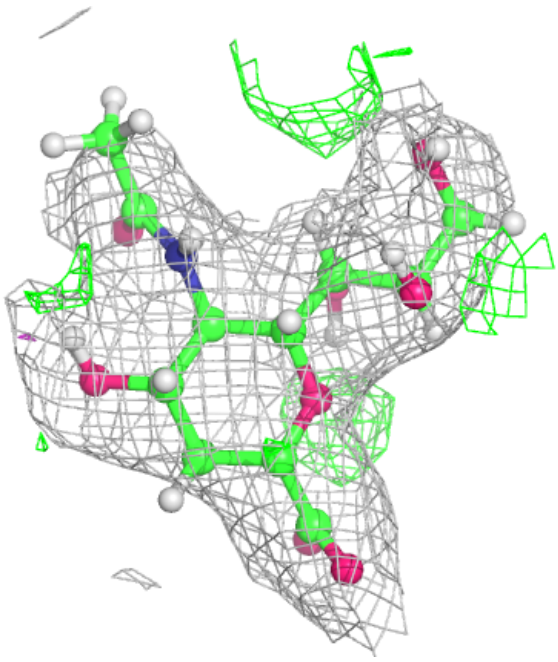


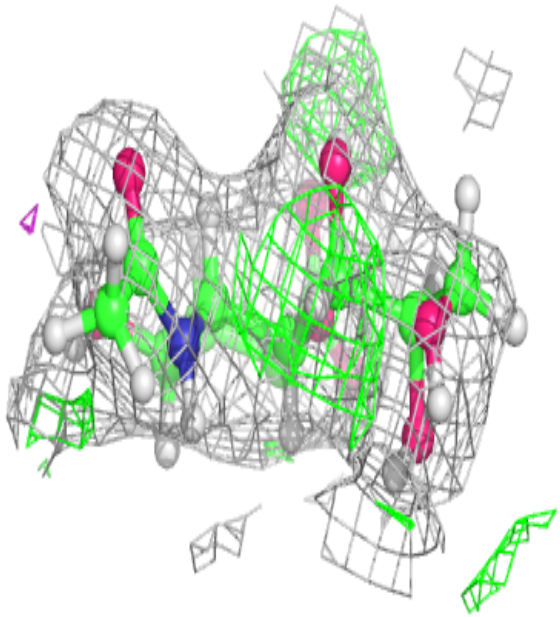


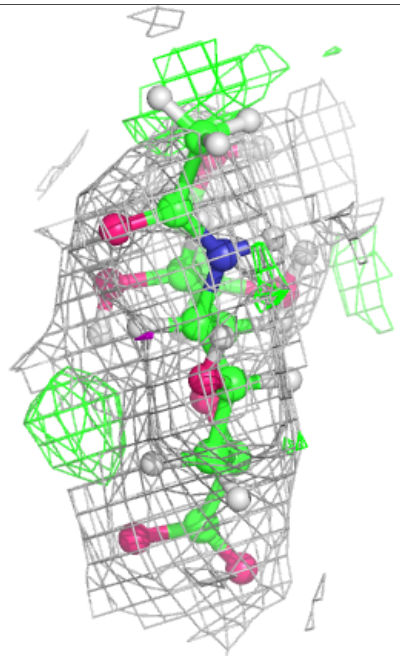


Electron density around SLB Y 301:

$2mF_o$-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

There are no such residues in this entry.