



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:19 PM UTC

PDB ID : 9FVE / pdb_00009fve
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:

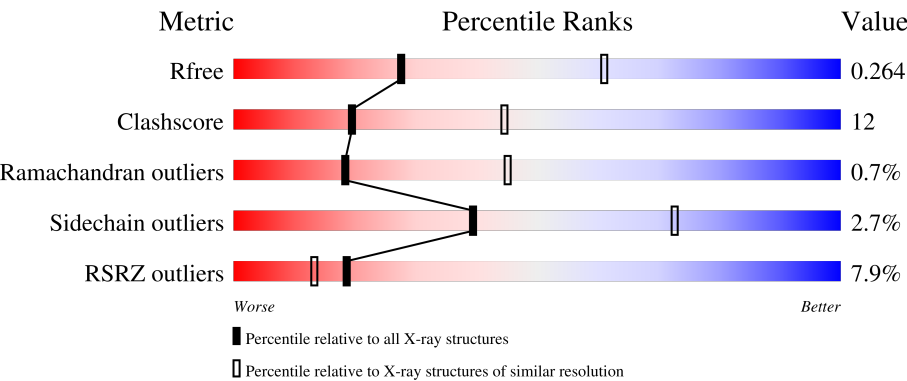
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance 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}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	303	47% 49% 41% 7% ..
1	C	303	8% 75% 20% ..
1	E	303	3% 82% 14% ..
1	G	303	6% 76% 18% ..
1	I	303	5% 76% 18% ..

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Mol	Chain	Length	Quality of chain
1	K	303	
1	M	303	
1	O	303	
1	Q	303	
1	U	303	
1	W	303	
1	Y	303	
2	B	123	
2	D	123	
2	F	123	
2	H	123	
2	J	123	
2	L	123	
2	N	123	
2	P	123	
2	R	123	
2	T	123	
2	V	123	
2	X	123	

2 Entry composition

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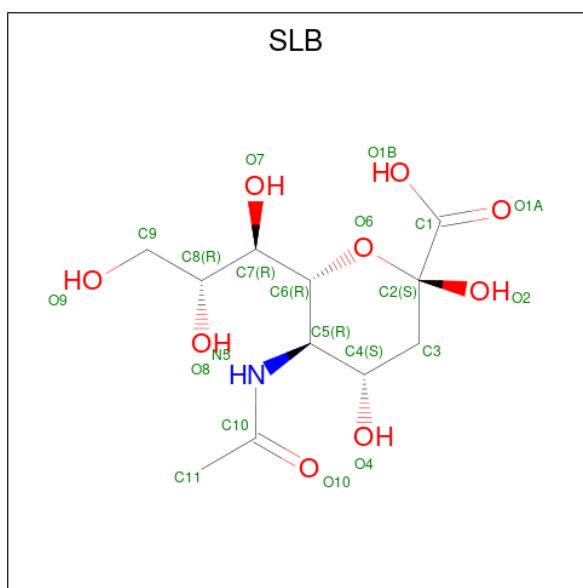
Chain	Residue	Modelled	Actual	Comment	Reference
U	-1	MET	-	expression tag	UNP Q9KR64
U	0	GLY	ALA	conflict	UNP Q9KR64
U	73	ALA	TRP	engineered mutation	UNP Q9KR64
W	-3	GLY	-	expression tag	UNP Q9KR64
W	-2	ALA	-	expression tag	UNP Q9KR64
W	-1	MET	-	expression tag	UNP Q9KR64
W	0	GLY	ALA	conflict	UNP Q9KR64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

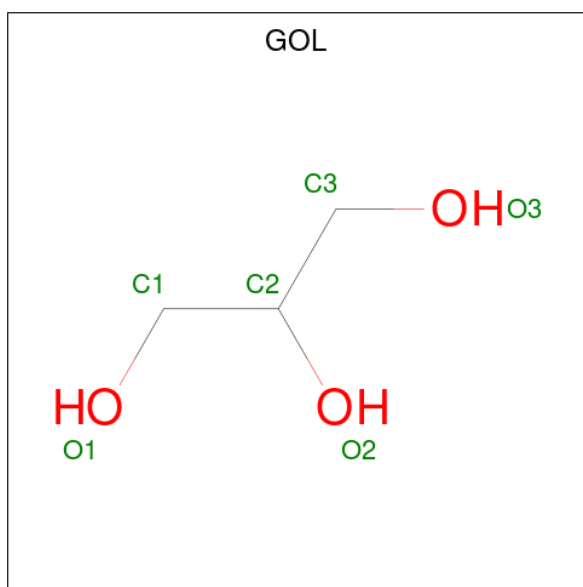
- Molecule 3 is N-acetyl-beta-neuraminic acid (CCD ID: SLB) (formula: C₁₁H₁₉NO₉) (labeled

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 (CCD ID: GOL) (formula: C₃H₈O₃).

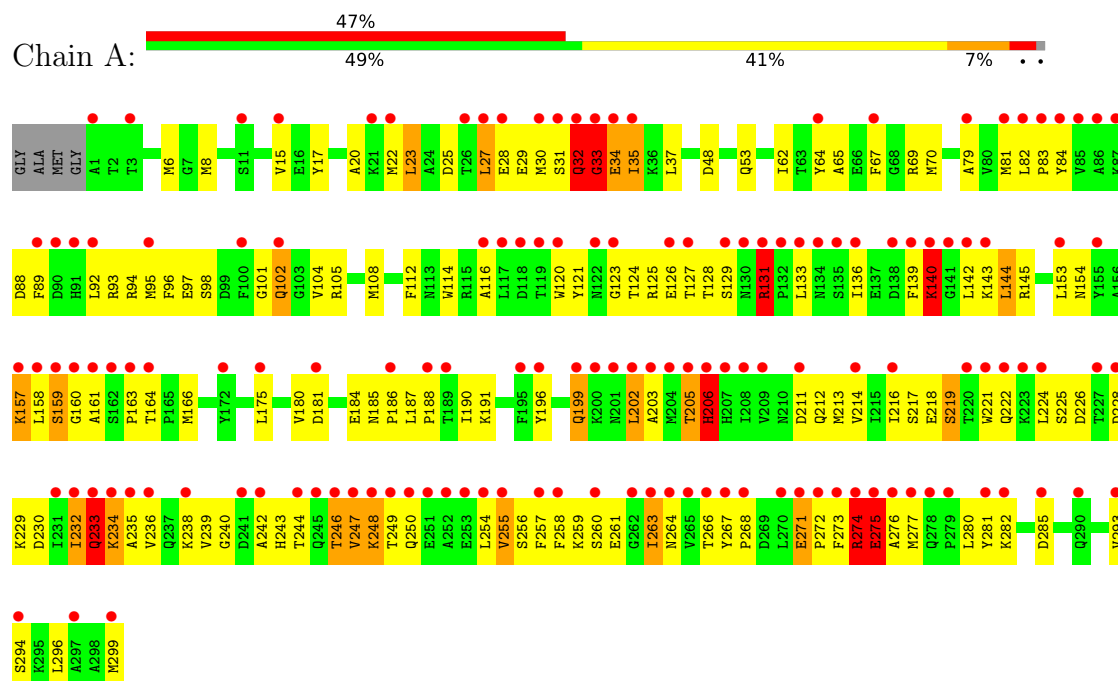


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	H	O	0	0
			14	3	8	3		
4	G	1	Total	C	H	O	0	0
			14	3	8	3		
4	Q	1	Total	C	H	O	0	0
			14	3	8	3		
4	U	1	Total	C	H	O	0	0
			14	3	8	3		
4	U	1	Total	C	H	O	0	0
			14	3	8	3		
4	U	1	Total	C	H	O	0	0
			14	3	8	3		

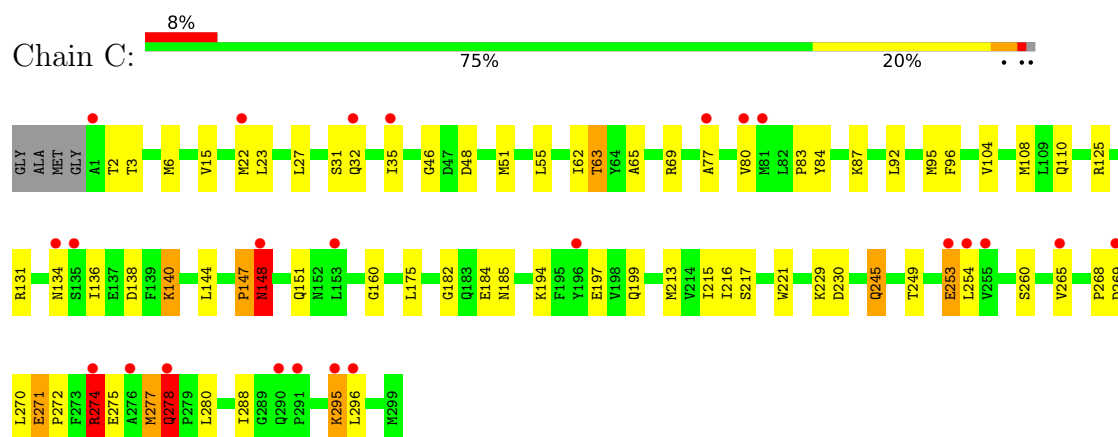
3 Residue-property plots [i](#)

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.

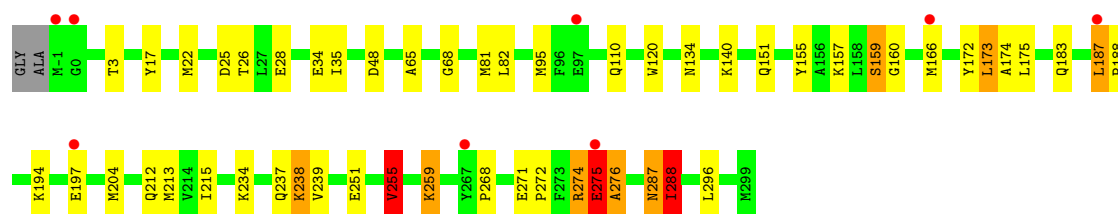
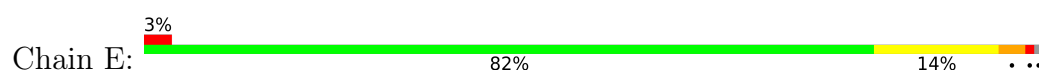
- Molecule 1: Sialic acid-binding periplasmic protein SiaP



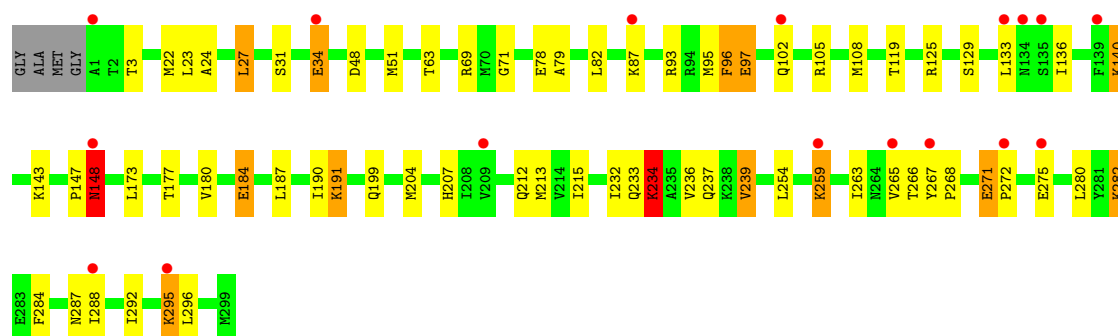
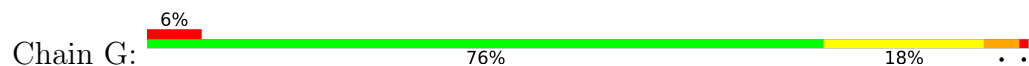
- Molecule 1: Sialic acid-binding periplasmic protein SiaP



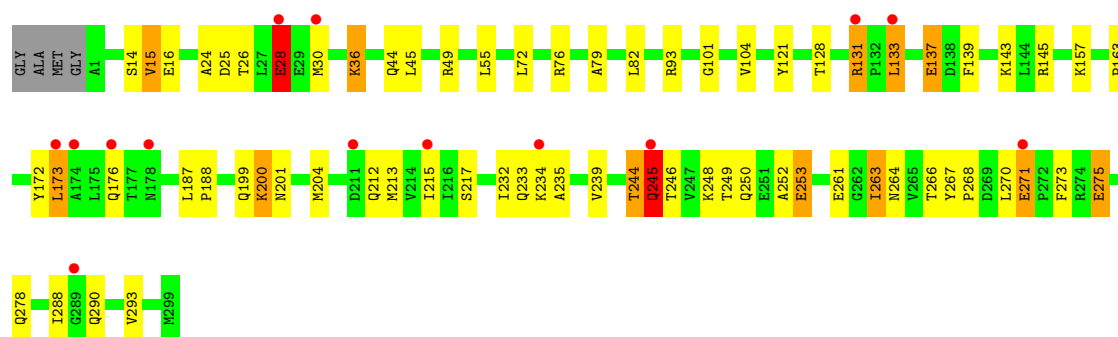
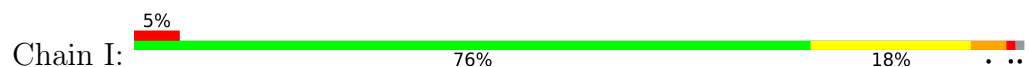
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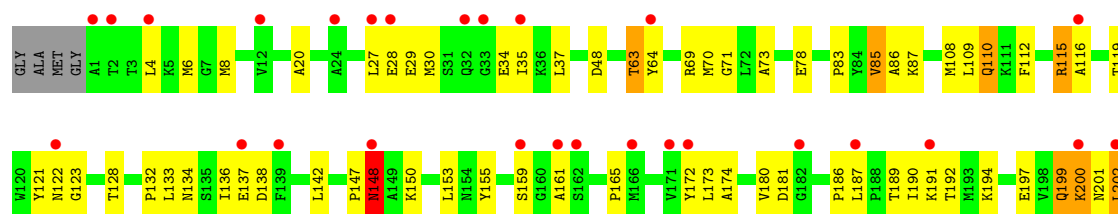
- Molecule 1: Sialic acid-binding periplasmic protein SiaP



- Molecule 1: Sialic acid-binding periplasmic protein SiaP

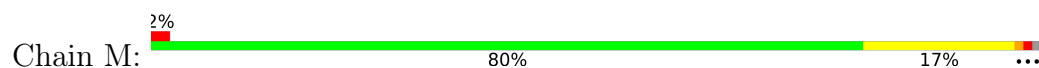


- Molecule 1: Sialic acid-binding periplasmic protein SiaP

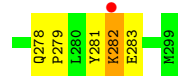
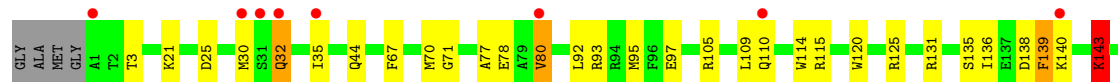
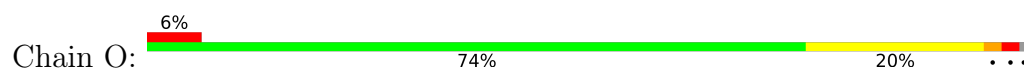




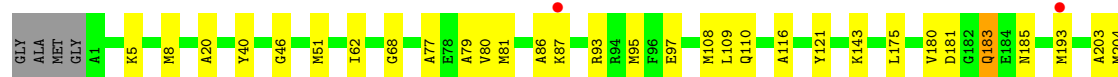
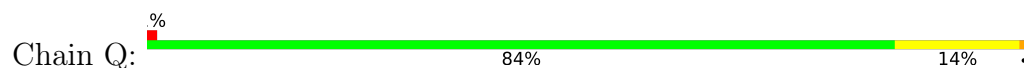
- Molecule 1: Sialic acid-binding periplasmic protein SiaP



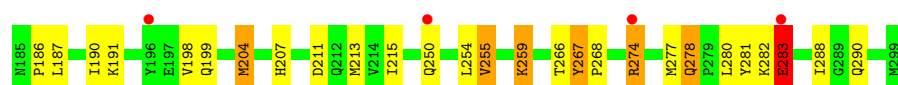
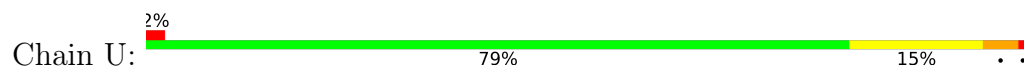
- Molecule 1: Sialic acid-binding periplasmic protein SiaP



- Molecule 1: Sialic acid-binding periplasmic protein SiaP

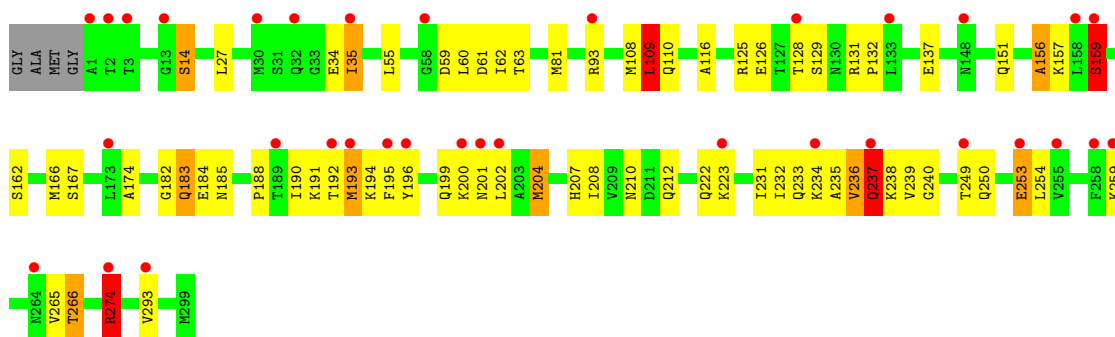


- Molecule 1: Sialic acid-binding periplasmic protein SiaP



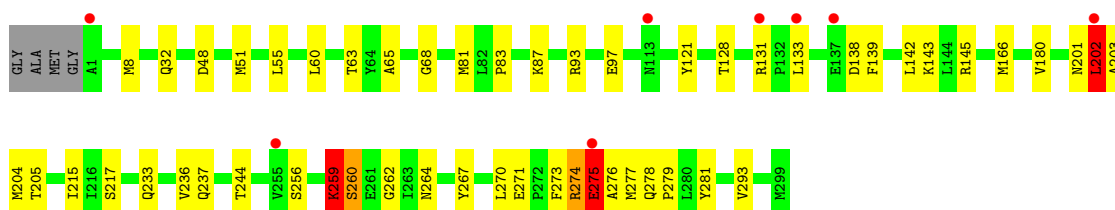
- Molecule 1: Sialic acid-binding periplasmic protein SiaP

Chain W: 



- Molecule 1: Sialic acid-binding periplasmic protein SiaP

Chain Y: 



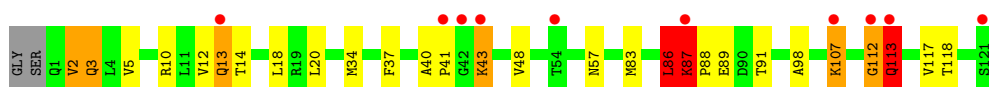
- Molecule 2: VHH_VcP#2

Chain B: 



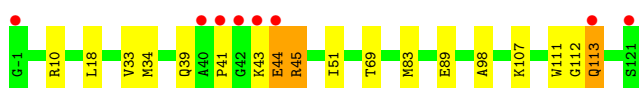
- Molecule 2: VHH_VcP#2

Chain D: 

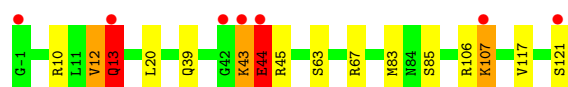
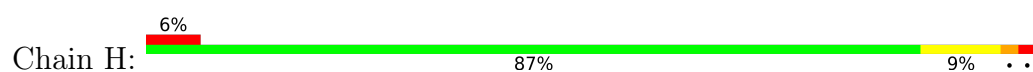


- Molecule 2: VHH_VcP#2

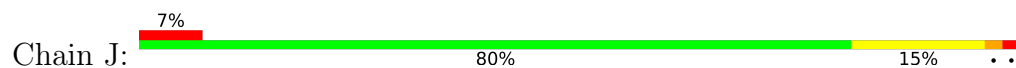
Chain F: 



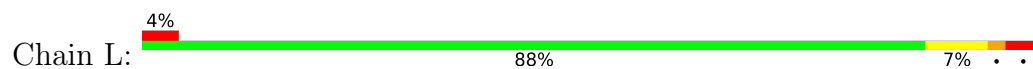
- Molecule 2: VHH_VcP#2



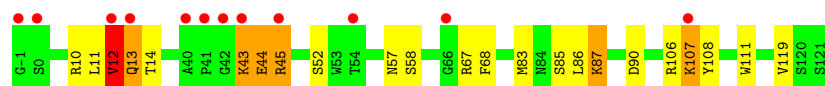
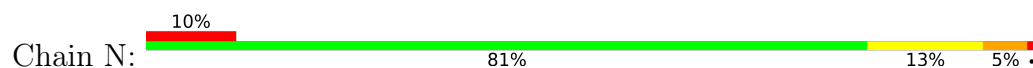
• Molecule 2: VHH_VcP#2



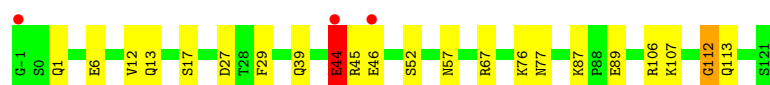
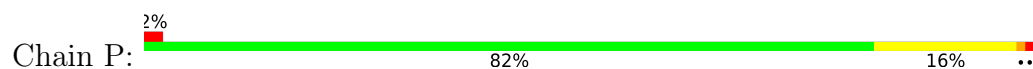
• Molecule 2: VHH_VcP#2



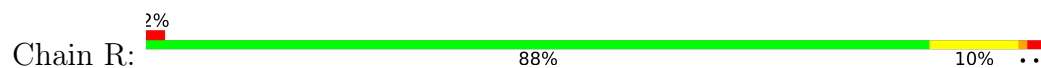
• Molecule 2: VHH_VcP#2



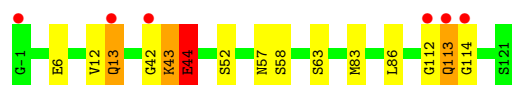
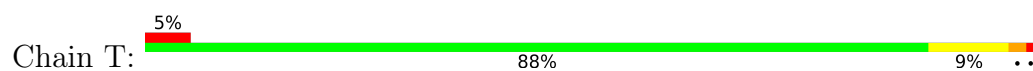
• Molecule 2: VHH_VcP#2



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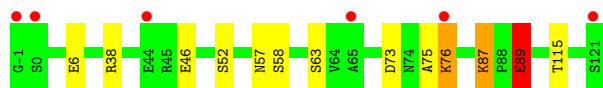


• Molecule 2: VHH_VcP#2



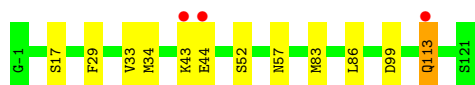
● Molecule 2: VHH_VcP#2

Chain V:  5% 89% 8% ..



● Molecule 2: VHH_VcP#2

Chain X:  2% 90% 9% .



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 0.232 , 0.264	Depositor DCC
R_{free} test set	2009 reflections (1.16%)	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	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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 $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.79	9/2404 (0.4%)	1.27	42/3248 (1.3%)
1	C	0.54	4/2404 (0.2%)	0.94	17/3248 (0.5%)
1	E	0.67	10/2413 (0.4%)	0.88	18/3260 (0.6%)
1	G	0.80	13/2404 (0.5%)	1.03	24/3248 (0.7%)
1	I	0.73	9/2404 (0.4%)	1.11	31/3248 (1.0%)
1	K	0.78	10/2404 (0.4%)	1.27	40/3248 (1.2%)
1	M	0.53	5/2404 (0.2%)	0.91	15/3248 (0.5%)
1	O	0.77	15/2404 (0.6%)	1.15	38/3248 (1.2%)
1	Q	0.35	2/2404 (0.1%)	0.67	9/3248 (0.3%)
1	U	0.67	8/2404 (0.3%)	0.80	17/3248 (0.5%)
1	W	0.50	3/2404 (0.1%)	1.00	29/3248 (0.9%)
1	Y	0.48	3/2404 (0.1%)	0.78	14/3248 (0.4%)
2	B	1.03	4/967 (0.4%)	1.06	8/1311 (0.6%)
2	D	0.65	3/961 (0.3%)	1.13	17/1303 (1.3%)
2	F	0.62	2/971 (0.2%)	1.27	20/1316 (1.5%)
2	H	0.61	2/971 (0.2%)	1.03	11/1316 (0.8%)
2	J	0.75	2/971 (0.2%)	0.94	11/1316 (0.8%)
2	L	0.57	3/971 (0.3%)	1.00	15/1316 (1.1%)
2	N	0.83	3/971 (0.3%)	1.01	14/1316 (1.1%)
2	P	0.61	2/971 (0.2%)	1.10	16/1316 (1.2%)
2	R	0.61	4/971 (0.4%)	0.93	7/1316 (0.5%)
2	T	0.26	0/971	0.67	5/1316 (0.4%)
2	V	0.50	2/971 (0.2%)	0.76	4/1316 (0.3%)
2	X	0.38	0/971	0.63	4/1316 (0.3%)
All	All	0.65	118/40495 (0.3%)	1.00	426/54762 (0.8%)

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 (118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	107	LYS	CE-NZ	24.35	2.22	1.49
2	J	87	LYS	N-CA	-15.14	1.33	1.45
1	U	173	LEU	CG-CD1	15.09	2.02	1.52
2	N	107	LYS	CD-CE	13.69	1.93	1.52
1	E	187	LEU	CG-CD1	13.61	1.97	1.52
1	U	173	LEU	CG-CD2	13.11	1.95	1.52
1	I	271	GLU	CD-OE2	13.02	1.50	1.25
2	N	107	LYS	CG-CD	12.77	1.90	1.52
1	K	234	LYS	CD-CE	12.26	1.89	1.52
1	O	200	LYS	CE-NZ	12.24	1.86	1.49
1	E	187	LEU	CG-CD2	11.80	1.91	1.52
2	N	107	LYS	CB-CG	11.44	1.86	1.52
1	I	271	GLU	CD-OE1	10.99	1.46	1.25
1	G	191	LYS	CE-NZ	10.91	1.82	1.49
1	Y	202	LEU	CG-CD2	10.79	1.88	1.52
1	G	140	LYS	CG-CD	10.69	1.84	1.52
1	O	282	LYS	CG-CD	10.16	1.82	1.52
1	G	234	LYS	CE-NZ	10.07	1.79	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	110	GLN	CD-NE2	-10.00	1.12	1.33
1	A	140	LYS	CE-NZ	9.61	1.78	1.49
2	B	43	LYS	CG-CD	9.52	1.81	1.52
1	K	212	GLN	CB-CG	9.28	1.80	1.52
1	M	140	LYS	CD-CE	9.25	1.80	1.52
1	G	259	LYS	CE-NZ	9.18	1.76	1.49
2	L	87	LYS	CE-NZ	9.15	1.76	1.49
2	B	43	LYS	CD-CE	9.02	1.79	1.52
1	A	234	LYS	CD-CE	-8.65	1.26	1.52
2	R	113	GLN	CG-CD	8.59	1.73	1.52
2	H	44	GLU	CD-OE1	8.36	1.41	1.25
2	R	44	GLU	CD-OE1	8.28	1.41	1.25
2	H	44	GLU	CD-OE2	8.26	1.41	1.25
1	Q	288	ILE	CG1-CD1	8.24	1.83	1.51
1	O	282	LYS	CE-NZ	8.12	1.73	1.49
1	K	234	LYS	CG-CD	8.11	1.76	1.52
1	K	293	VAL	CB-CG2	8.00	1.78	1.52
2	D	86	LEU	C-O	-7.96	1.14	1.23
1	A	234	LYS	CB-CG	7.85	1.76	1.52
1	M	180	VAL	CB-CG2	7.76	1.78	1.52
1	A	263	ILE	CG1-CD1	7.75	1.81	1.51
1	G	191	LYS	CD-CE	7.75	1.75	1.52
1	I	36	LYS	CE-NZ	7.71	1.72	1.49
1	U	278	GLN	CD-NE2	7.67	1.49	1.33
2	L	43	LYS	CB-CG	7.51	1.75	1.52
1	C	22	MET	CG-SD	7.46	1.99	1.80
1	I	131	ARG	CB-CG	7.42	1.74	1.52
2	F	44	GLU	CB-CG	7.33	1.74	1.52
1	M	237	GLN	CG-CD	7.31	1.70	1.52
1	O	32	GLN	CB-CG	7.13	1.73	1.52
1	K	223	LYS	CG-CD	7.12	1.73	1.52
1	E	187	LEU	CB-CG	7.11	1.67	1.53
1	G	234	LYS	CD-CE	6.96	1.73	1.52
1	O	143	LYS	CE-NZ	6.82	1.69	1.49
1	K	223	LYS	CB-CG	6.80	1.72	1.52
1	O	140	LYS	CB-CG	6.72	1.72	1.52
1	G	239	VAL	CB-CG1	6.69	1.74	1.52
2	V	76	LYS	CB-CG	6.68	1.72	1.52
1	O	110	GLN	CB-CG	6.66	1.72	1.52
1	G	27	LEU	CG-CD2	6.63	1.74	1.52
1	C	254	LEU	CG-CD1	6.62	1.74	1.52
1	G	34	GLU	CD-OE1	-6.56	1.12	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	U	143	LYS	CD-CE	6.55	1.72	1.52
1	Y	274	ARG	C-N	6.53	1.41	1.33
2	J	107	LYS	CD-CE	6.49	1.72	1.52
1	O	80	VAL	CB-CG2	-6.44	1.31	1.52
1	C	22	MET	CB-CG	6.43	1.71	1.52
1	I	131	ARG	CD-NE	6.42	1.55	1.46
1	G	140	LYS	CD-CE	6.40	1.71	1.52
1	M	29	GLU	CD-OE2	6.33	1.37	1.25
1	W	293	VAL	CB-CG2	6.31	1.73	1.52
2	D	113	GLN	CD-OE1	-6.25	1.11	1.23
1	E	238	LYS	CE-NZ	6.24	1.68	1.49
1	A	248	LYS	CE-NZ	6.24	1.68	1.49
1	A	234	LYS	CE-NZ	-6.23	1.30	1.49
1	C	295	LYS	CE-NZ	6.23	1.68	1.49
2	P	76	LYS	CD-CE	6.19	1.71	1.52
1	I	137	GLU	CB-CG	6.18	1.71	1.52
1	A	263	ILE	CB-CG2	6.17	1.73	1.52
2	R	44	GLU	CD-OE2	6.15	1.37	1.25
1	U	173	LEU	CA-CB	6.13	1.62	1.53
1	O	234	LYS	CD-CE	-6.12	1.34	1.52
1	I	172	TYR	C-N	6.09	1.41	1.33
1	W	293	VAL	CB-CG1	6.08	1.72	1.52
2	B	12	VAL	CB-CG2	6.04	1.72	1.52
1	O	263	ILE	CG1-CD1	6.03	1.75	1.51
1	G	34	GLU	CG-CD	-5.97	1.37	1.52
1	E	157	LYS	CE-NZ	5.95	1.67	1.49
1	Q	87	LYS	CB-CG	5.95	1.70	1.52
2	R	112	GLY	C-N	5.93	1.40	1.33
1	E	274	ARG	C-N	5.88	1.41	1.33
1	G	87	LYS	CB-CG	5.86	1.70	1.52
1	E	259	LYS	CE-NZ	5.84	1.66	1.49
1	U	259	LYS	CB-CG	5.82	1.70	1.52
1	A	164	THR	CB-CG2	5.80	1.71	1.52
2	V	89	GLU	CD-OE1	5.78	1.36	1.25
1	K	293	VAL	CB-CG1	5.75	1.71	1.52
2	P	113	GLN	CB-CG	5.73	1.69	1.52
1	I	143	LYS	CG-CD	5.72	1.69	1.52
1	O	80	VAL	CB-CG1	5.70	1.71	1.52
1	E	187	LEU	CA-CB	5.66	1.61	1.53
1	Y	202	LEU	CB-CG	5.58	1.64	1.53
1	O	200	LYS	CD-CE	5.54	1.69	1.52
1	O	80	VAL	CA-C	-5.52	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	275	GLU	CD-OE2	5.52	1.35	1.25
1	K	115	ARG	CG-CD	5.52	1.69	1.52
1	U	143	LYS	CA-C	-5.51	1.46	1.53
1	A	27	LEU	CG-CD2	5.49	1.70	1.52
1	K	283	GLU	CD-OE2	5.45	1.35	1.25
1	U	278	GLN	CB-CG	5.31	1.68	1.52
2	F	45	ARG	CA-CB	5.21	1.62	1.53
1	G	234	LYS	CG-CD	-5.21	1.36	1.52
2	D	12	VAL	CB-CG2	5.18	1.69	1.52
2	L	43	LYS	CE-NZ	5.18	1.64	1.49
1	E	255	VAL	CB-CG2	5.16	1.69	1.52
1	W	237	GLN	CB-CG	-5.11	1.37	1.52
1	M	29	GLU	CB-CG	5.11	1.67	1.52
1	O	140	LYS	CG-CD	5.08	1.67	1.52
1	E	157	LYS	CB-CG	5.05	1.67	1.52
1	K	234	LYS	CA-CB	5.01	1.61	1.53

All (426) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	29	GLU	CG-CD-OE1	19.52	163.29	118.40
1	M	29	GLU	CG-CD-OE2	-17.93	77.16	118.40
2	B	107	LYS	CG-CD-CE	17.59	151.76	111.30
1	I	131	ARG	CG-CD-NE	-15.30	78.33	112.00
1	G	147	PRO	CA-C-N	14.66	149.54	121.54
1	G	147	PRO	C-N-CA	14.66	149.54	121.54
1	K	233	GLN	CA-C-N	14.52	152.57	121.64
1	K	233	GLN	C-N-CA	14.52	152.57	121.64
2	H	12	VAL	CA-C-N	14.17	141.62	122.77
2	H	12	VAL	C-N-CA	14.17	141.62	122.77
2	F	43	LYS	CA-C-N	-13.72	95.32	121.66
2	F	43	LYS	C-N-CA	-13.72	95.32	121.66
1	O	282	LYS	CB-CG-CD	-13.58	80.06	111.30
2	F	113	GLN	N-CA-CB	13.44	132.31	110.40
2	R	113	GLN	CA-CB-CG	13.05	140.20	114.10
1	W	223	LYS	CA-CB-CG	13.03	140.17	114.10
1	K	147	PRO	CA-C-N	13.00	146.37	121.54
1	K	147	PRO	C-N-CA	13.00	146.37	121.54
1	C	147	PRO	CA-C-N	12.84	146.06	121.54
1	C	147	PRO	C-N-CA	12.84	146.06	121.54
1	I	234	LYS	CA-CB-CG	-12.46	89.19	114.10
2	F	113	GLN	CB-CA-C	-12.42	84.03	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	LYS	CB-CG-CD	12.32	139.63	111.30
2	N	107	LYS	CD-CE-NZ	-12.29	72.57	111.90
1	M	140	LYS	CD-CE-NZ	-12.14	73.04	111.90
1	E	288	ILE	N-CA-C	-12.02	99.36	113.42
1	I	271	GLU	N-CA-CB	-11.86	92.04	110.43
2	D	13	GLN	CA-CB-CG	11.80	137.69	114.10
1	O	234	LYS	CB-CA-C	11.56	130.57	110.23
1	K	87	LYS	CG-CD-CE	-11.52	84.81	111.30
2	B	43	LYS	CD-CE-NZ	-11.50	75.10	111.90
1	O	147	PRO	CA-C-N	11.27	143.07	121.54
1	O	147	PRO	C-N-CA	11.27	143.07	121.54
1	W	223	LYS	N-CA-CB	11.13	129.10	110.41
1	E	287	ASN	CA-C-N	-10.90	108.88	121.85
1	E	287	ASN	C-N-CA	-10.90	108.88	121.85
1	U	173	LEU	CB-CG-CD2	10.79	143.08	110.70
1	Q	87	LYS	CA-CB-CG	10.69	135.48	114.10
2	P	76	LYS	CB-CG-CD	10.57	135.62	111.30
1	K	212	GLN	CB-CA-C	10.54	131.39	110.42
1	I	244	THR	CA-C-N	-10.51	106.78	120.44
1	I	244	THR	C-N-CA	-10.51	106.78	120.44
2	F	44	GLU	N-CA-CB	10.42	124.76	110.38
2	P	44	GLU	CB-CG-CD	10.41	130.30	112.60
2	L	45	ARG	CB-CG-CD	-10.40	87.37	111.30
1	I	173	LEU	CB-CG-CD1	10.38	141.83	110.70
2	P	76	LYS	CD-CE-NZ	10.37	145.07	111.90
1	M	237	GLN	CB-CG-CD	10.32	130.14	112.60
2	B	43	LYS	CG-CD-CE	10.31	135.00	111.30
1	A	234	LYS	CB-CA-C	10.30	130.45	110.46
1	K	28	GLU	CB-CG-CD	-10.16	95.32	112.60
1	C	278	GLN	N-CA-CB	-10.16	94.68	110.43
1	O	234	LYS	CG-CD-CE	10.15	134.65	111.30
1	Q	193	MET	CB-CG-SD	10.04	142.83	112.70
1	O	282	LYS	CB-CA-C	-9.99	95.19	110.88
2	R	113	GLN	N-CA-CB	9.97	125.55	110.79
1	C	148	ASN	CB-CA-C	9.95	130.22	110.42
1	Y	87	LYS	CB-CG-CD	9.94	134.16	111.30
2	R	112	GLY	CA-C-N	-9.88	106.55	122.95
2	R	112	GLY	C-N-CA	-9.88	106.55	122.95
2	V	76	LYS	CA-CB-CG	9.86	133.83	114.10
1	A	263	ILE	CG1-CB-CG2	9.84	140.21	110.70
1	C	148	ASN	N-CA-CB	-9.81	93.91	110.49
2	D	87	LYS	CB-CG-CD	-9.75	88.88	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	29	GLU	OE1-CD-OE2	-9.73	99.54	122.90
2	H	43	LYS	CA-C-N	9.67	135.33	121.50
2	H	43	LYS	C-N-CA	9.67	135.33	121.50
1	I	253	GLU	CA-CB-CG	9.65	133.40	114.10
1	K	212	GLN	CG-CD-NE2	-9.63	101.95	116.40
1	W	157	LYS	CB-CG-CD	9.62	133.42	111.30
1	Y	275	GLU	CA-CB-CG	9.62	133.33	114.10
1	C	140	LYS	CG-CD-CE	9.61	133.40	111.30
1	G	148	ASN	CB-CA-C	9.50	129.32	110.42
1	U	278	GLN	CA-CB-CG	-9.47	95.16	114.10
1	K	245	GLN	N-CA-CB	9.35	124.13	110.20
1	O	143	LYS	CD-CE-NZ	-9.31	82.10	111.90
1	A	131	ARG	CG-CD-NE	-9.26	91.62	112.00
1	O	282	LYS	N-CA-C	-9.26	101.16	111.07
1	O	140	LYS	CB-CG-CD	9.25	132.57	111.30
1	G	295	LYS	CB-CG-CD	9.19	132.43	111.30
1	O	148	ASN	CB-CA-C	9.18	128.69	110.42
1	O	282	LYS	CG-CD-CE	9.17	132.39	111.30
1	O	140	LYS	CG-CD-CE	-9.12	90.33	111.30
2	V	75	ALA	CA-C-N	9.06	138.85	121.54
2	V	75	ALA	C-N-CA	9.06	138.85	121.54
1	K	222	GLN	CA-C-N	9.05	136.99	121.14
1	K	222	GLN	C-N-CA	9.05	136.99	121.14
1	U	143	LYS	CA-CB-CG	-9.03	96.05	114.10
1	A	206	HIS	N-CA-CB	-9.01	98.61	112.30
1	M	29	GLU	CB-CG-CD	-8.99	97.32	112.60
2	L	42	GLY	CA-C-N	8.98	138.69	121.54
2	L	42	GLY	C-N-CA	8.98	138.69	121.54
1	A	247	VAL	CA-C-N	8.85	132.13	120.28
1	A	247	VAL	C-N-CA	8.85	132.13	120.28
1	E	187	LEU	CD1-CG-CD2	8.83	130.23	110.80
1	E	187	LEU	CB-CG-CD1	8.82	137.15	110.70
1	Y	275	GLU	N-CA-CB	8.78	123.16	109.82
1	O	282	LYS	CA-C-N	8.76	132.02	120.28
1	O	282	LYS	C-N-CA	8.76	132.02	120.28
2	L	45	ARG	CG-CD-NE	8.75	131.25	112.00
1	G	148	ASN	N-CA-CB	-8.71	95.76	110.49
1	O	143	LYS	CG-CD-CE	8.71	131.34	111.30
1	K	234	LYS	CB-CG-CD	8.69	131.28	111.30
2	F	113	GLN	CA-C-N	8.62	138.31	121.41
2	F	113	GLN	C-N-CA	8.62	138.31	121.41
1	Q	87	LYS	N-CA-CB	8.62	123.57	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	293	VAL	CG1-CB-CG2	8.61	129.73	110.80
2	L	87	LYS	CA-CB-CG	8.56	131.21	114.10
2	D	13	GLN	N-CA-CB	8.55	124.28	110.51
1	A	27	LEU	CB-CG-CD1	8.53	136.28	110.70
2	L	43	LYS	CB-CG-CD	8.52	130.89	111.30
1	K	223	LYS	N-CA-CB	-8.52	96.52	110.40
1	G	282	LYS	CD-CE-NZ	-8.51	84.66	111.90
2	F	44	GLU	CA-C-N	8.45	132.70	120.71
2	F	44	GLU	C-N-CA	8.45	132.70	120.71
1	A	34	GLU	N-CA-CB	-8.40	96.29	110.49
2	N	107	LYS	CG-CD-CE	-8.35	92.10	111.30
2	P	113	GLN	N-CA-C	-8.34	105.11	114.62
2	N	43	LYS	N-CA-C	8.31	122.35	110.14
1	K	148	ASN	CB-CA-C	8.27	126.87	110.42
1	A	248	LYS	CD-CE-NZ	8.23	138.22	111.90
2	N	44	GLU	N-CA-CB	8.20	122.08	110.36
1	Y	275	GLU	CB-CA-C	-8.17	97.93	110.92
1	C	274	ARG	N-CA-CB	-8.14	97.66	110.28
1	G	234	LYS	CB-CG-CD	8.10	129.94	111.30
2	D	13	GLN	CB-CA-C	-8.10	95.40	111.60
1	U	173	LEU	CB-CA-C	8.09	123.58	110.88
1	I	245	GLN	N-CA-CB	8.06	121.70	110.01
1	K	148	ASN	N-CA-CB	-8.04	96.91	110.49
1	K	87	LYS	CD-CE-NZ	7.94	137.31	111.90
1	K	234	LYS	CA-CB-CG	7.92	129.94	114.10
1	I	28	GLU	CG-CD-OE2	-7.89	100.24	118.40
1	C	245	GLN	CA-CB-CG	-7.88	98.34	114.10
1	I	253	GLU	CB-CA-C	-7.86	98.86	110.96
1	I	143	LYS	CB-CG-CD	7.83	129.31	111.30
1	K	245	GLN	CB-CG-CD	-7.81	99.32	112.60
2	H	44	GLU	CG-CD-OE2	-7.81	100.44	118.40
1	Q	110	GLN	N-CA-CB	7.79	121.81	110.20
1	U	142	LEU	CA-C-N	7.75	134.66	122.26
1	U	142	LEU	C-N-CA	7.75	134.66	122.26
1	W	237	GLN	CA-CB-CG	7.75	129.59	114.10
1	W	259	LYS	CA-CB-CG	7.72	129.55	114.10
1	W	236	VAL	CA-C-N	-7.72	109.95	120.44
1	W	236	VAL	C-N-CA	-7.72	109.95	120.44
1	W	259	LYS	CB-CG-CD	-7.70	93.60	111.30
1	A	205	THR	CA-C-N	-7.69	111.25	122.40
1	A	205	THR	C-N-CA	-7.69	111.25	122.40
1	E	234	LYS	CB-CG-CD	-7.67	93.65	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	76	LYS	N-CA-C	7.64	122.18	113.01
2	H	44	GLU	CB-CG-CD	7.60	125.52	112.60
1	W	234	LYS	CG-CD-CE	-7.57	93.90	111.30
1	K	234	LYS	N-CA-CB	-7.55	99.02	110.26
1	O	274	ARG	CB-CG-CD	7.55	128.66	111.30
2	R	44	GLU	CG-CD-OE2	-7.52	101.11	118.40
1	W	200	LYS	CB-CG-CD	7.50	128.55	111.30
1	A	34	GLU	CB-CA-C	7.49	125.33	110.42
2	B	12	VAL	CG1-CB-CG2	7.47	127.23	110.80
1	C	278	GLN	CA-CB-CG	7.47	129.04	114.10
1	A	131	ARG	CB-CG-CD	7.43	128.39	111.30
1	G	102	GLN	CB-CG-CD	7.41	125.20	112.60
2	D	112	GLY	CA-C-N	7.41	134.10	121.14
2	D	112	GLY	C-N-CA	7.41	134.10	121.14
1	O	110	GLN	N-CA-CB	-7.39	99.78	110.65
2	F	45	ARG	CB-CG-CD	7.38	128.27	111.30
1	E	275	GLU	CB-CG-CD	7.34	125.08	112.60
2	D	3	GLN	CA-CB-CG	7.31	128.73	114.10
2	F	89	GLU	N-CA-CB	7.31	122.74	110.32
1	E	187	LEU	CB-CG-CD2	-7.27	88.88	110.70
1	O	148	ASN	CA-C-N	7.27	134.55	121.89
1	O	148	ASN	C-N-CA	7.27	134.55	121.89
1	O	234	LYS	CB-CG-CD	7.27	128.02	111.30
1	O	30	MET	CA-CB-CG	7.18	128.47	114.10
2	T	113	GLN	CA-C-N	-7.16	98.80	120.92
2	T	113	GLN	C-N-CA	-7.16	98.80	120.92
1	Y	275	GLU	N-CA-C	-7.16	102.29	111.02
1	I	271	GLU	CB-CA-C	7.15	125.71	112.05
2	V	76	LYS	CG-CD-CE	7.13	127.71	111.30
1	O	148	ASN	N-CA-CB	-7.11	98.47	110.49
1	I	271	GLU	CG-CD-OE2	-7.09	102.10	118.40
1	Y	202	LEU	CD1-CG-CD2	7.07	126.35	110.80
1	W	237	GLN	N-CA-CB	7.07	120.32	110.07
2	P	107	LYS	N-CA-CB	-7.04	99.04	109.95
2	F	89	GLU	CA-CB-CG	7.03	128.17	114.10
1	K	283	GLU	CB-CG-CD	7.03	124.55	112.60
1	U	173	LEU	CA-CB-CG	-7.02	91.73	116.30
1	I	245	GLN	CA-CB-CG	-7.01	100.09	114.10
2	H	13	GLN	N-CA-CB	-6.99	99.03	110.42
1	M	253	GLU	N-CA-CB	6.97	121.31	110.44
1	O	110	GLN	CG-CD-NE2	-6.96	105.96	116.40
2	D	12	VAL	CA-C-N	-6.94	110.35	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	12	VAL	C-N-CA	-6.94	110.35	122.64
1	C	254	LEU	CD1-CG-CD2	6.93	126.04	110.80
1	U	274	ARG	CA-CB-CG	-6.92	100.26	114.10
1	U	143	LYS	N-CA-CB	-6.90	100.65	110.58
1	O	234	LYS	N-CA-C	-6.89	104.01	113.18
2	P	44	GLU	N-CA-CB	6.84	119.59	110.29
2	F	44	GLU	CA-CB-CG	6.83	127.77	114.10
1	A	233	GLN	CA-C-N	6.83	130.35	120.38
1	A	233	GLN	C-N-CA	6.83	130.35	120.38
1	K	223	LYS	CD-CE-NZ	-6.77	90.24	111.90
2	J	13	GLN	CA-CB-CG	6.75	127.61	114.10
2	P	76	LYS	CA-CB-CG	-6.74	100.63	114.10
1	G	259	LYS	CG-CD-CE	-6.71	95.86	111.30
1	I	173	LEU	N-CA-CB	6.70	120.01	109.82
1	Q	109	LEU	CA-C-N	-6.70	109.12	120.58
1	Q	109	LEU	C-N-CA	-6.70	109.12	120.58
2	D	87	LYS	N-CA-CB	6.70	122.29	110.37
1	I	143	LYS	CG-CD-CE	-6.68	95.94	111.30
2	F	45	ARG	CD-NE-CZ	-6.67	115.07	124.40
1	Q	87	LYS	CG-CD-CE	6.66	126.62	111.30
1	O	274	ARG	CG-CD-NE	6.66	126.65	112.00
1	E	110	GLN	CA-CB-CG	6.62	127.34	114.10
1	Y	87	LYS	CG-CD-CE	-6.61	96.10	111.30
2	H	44	GLU	OE1-CD-OE2	6.60	138.74	122.90
1	A	140	LYS	CD-CE-NZ	-6.58	90.86	111.90
2	R	113	GLN	CB-CA-C	-6.57	102.00	111.14
1	O	199	GLN	CA-C-N	6.57	133.38	122.54
1	O	199	GLN	C-N-CA	6.57	133.38	122.54
1	O	234	LYS	CA-C-N	6.55	128.96	120.44
1	O	234	LYS	C-N-CA	6.55	128.96	120.44
1	A	234	LYS	N-CA-CB	-6.55	99.79	110.14
2	L	43	LYS	CA-CB-CG	-6.54	101.01	114.10
2	N	43	LYS	CB-CA-C	-6.52	98.75	110.36
1	I	245	GLN	CB-CA-C	-6.50	100.67	110.88
2	F	112	GLY	CA-C-N	-6.50	109.77	121.14
2	F	112	GLY	C-N-CA	-6.50	109.77	121.14
1	U	173	LEU	N-CA-CB	-6.49	100.61	110.01
1	Y	259	LYS	CA-C-N	6.48	134.01	121.18
1	Y	259	LYS	C-N-CA	6.48	134.01	121.18
2	P	76	LYS	CB-CA-C	-6.47	96.97	110.17
1	O	80	VAL	CA-CB-CG2	6.46	121.39	110.40
1	W	234	LYS	CD-CE-NZ	6.46	132.58	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	200	LYS	CD-CE-NZ	6.46	132.57	111.90
1	K	200	LYS	CG-CD-CE	6.46	126.16	111.30
1	W	223	LYS	CB-CA-C	-6.45	97.12	109.95
1	G	295	LYS	CG-CD-CE	-6.45	96.47	111.30
1	W	233	GLN	CA-CB-CG	6.44	126.98	114.10
2	N	107	LYS	CA-CB-CG	-6.43	101.24	114.10
1	O	110	GLN	CG-CD-OE1	6.43	133.65	120.80
1	K	87	LYS	N-CA-CB	6.42	119.76	110.20
2	P	106	ARG	CA-C-N	6.41	130.67	121.50
2	P	106	ARG	C-N-CA	6.41	130.67	121.50
2	L	45	ARG	CB-CA-C	-6.40	99.40	109.70
2	J	12	VAL	CA-C-N	6.38	130.38	120.75
2	J	12	VAL	C-N-CA	6.38	130.38	120.75
2	T	113	GLN	CB-CG-CD	6.37	123.43	112.60
2	D	86	LEU	N-CA-C	-6.37	99.85	109.60
1	O	282	LYS	N-CA-CB	6.37	119.24	110.01
2	P	44	GLU	CG-CD-OE2	-6.37	103.76	118.40
1	Q	86	ALA	CA-C-N	-6.35	109.89	120.68
1	Q	86	ALA	C-N-CA	-6.35	109.89	120.68
2	X	113	GLN	CA-CB-CG	6.30	126.71	114.10
1	M	180	VAL	CG1-CB-CG2	6.30	124.66	110.80
2	N	44	GLU	CA-CB-CG	6.28	126.66	114.10
1	W	237	GLN	CG-CD-NE2	-6.26	107.00	116.40
1	A	248	LYS	CA-CB-CG	-6.26	101.57	114.10
1	W	191	LYS	CD-CE-NZ	6.23	131.85	111.90
2	F	113	GLN	CA-CB-CG	6.21	126.51	114.10
1	M	29	GLU	CA-CB-CG	6.19	126.48	114.10
1	M	237	GLN	N-CA-CB	6.19	120.95	110.49
1	I	28	GLU	CA-CB-CG	6.19	126.48	114.10
1	M	178	ASN	N-CA-CB	-6.17	103.09	112.28
2	J	113	GLN	CB-CA-C	-6.16	100.21	110.68
2	P	113	GLN	CB-CG-CD	6.16	123.06	112.60
2	B	112	GLY	CA-C-N	6.14	132.52	121.15
2	B	112	GLY	C-N-CA	6.14	132.52	121.15
1	A	131	ARG	CA-C-N	6.14	126.11	119.78
1	A	131	ARG	C-N-CA	6.14	126.11	119.78
1	I	200	LYS	CB-CG-CD	-6.14	97.17	111.30
1	U	172	TYR	CA-C-N	6.12	128.40	120.44
1	U	172	TYR	C-N-CA	6.12	128.40	120.44
1	A	23	LEU	CB-CG-CD1	6.11	129.04	110.70
1	Y	32	GLN	CA-CB-CG	6.11	126.31	114.10
2	J	89	GLU	CA-CB-CG	6.10	126.30	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	113	GLN	N-CA-CB	6.09	119.20	110.06
1	W	157	LYS	CG-CD-CE	-6.08	97.31	111.30
1	G	275	GLU	CB-CG-CD	6.08	122.93	112.60
1	G	287	ASN	CA-C-N	-6.07	109.86	120.29
1	G	287	ASN	C-N-CA	-6.07	109.86	120.29
2	P	113	GLN	CA-CB-CG	6.05	126.20	114.10
2	T	44	GLU	CA-CB-CG	6.03	126.16	114.10
1	O	234	LYS	CA-CB-CG	-6.02	102.06	114.10
1	U	259	LYS	CD-CE-NZ	-6.02	92.63	111.90
2	F	45	ARG	CG-CD-NE	-6.02	98.76	112.00
1	K	245	GLN	CB-CA-C	-6.02	99.69	110.70
2	L	45	ARG	CD-NE-CZ	-6.01	115.98	124.40
1	I	133	LEU	CB-CG-CD1	-6.01	92.67	110.70
1	O	234	LYS	CD-CE-NZ	6.00	131.10	111.90
1	K	87	LYS	CB-CA-C	-6.00	99.72	110.70
2	N	43	LYS	CA-C-N	-5.99	110.06	120.97
2	N	43	LYS	C-N-CA	-5.99	110.06	120.97
1	G	34	GLU	OE1-CD-OE2	-5.99	108.53	122.90
1	K	202	LEU	CB-CG-CD2	5.98	128.64	110.70
1	K	212	GLN	N-CA-CB	-5.98	100.39	110.49
1	I	143	LYS	CD-CE-NZ	-5.97	92.81	111.90
1	A	219	SER	N-CA-CB	5.96	120.28	110.39
1	E	259	LYS	CA-CB-CG	-5.94	102.22	114.10
2	D	2	VAL	CA-C-N	5.92	131.16	123.00
2	D	2	VAL	C-N-CA	5.92	131.16	123.00
1	K	244	THR	CA-C-N	-5.92	110.47	120.58
1	K	244	THR	C-N-CA	-5.92	110.47	120.58
1	K	200	LYS	CB-CG-CD	-5.91	97.70	111.30
1	U	283	GLU	CB-CG-CD	5.91	122.64	112.60
2	X	43	LYS	CA-C-N	-5.90	112.90	122.81
2	X	43	LYS	C-N-CA	-5.90	112.90	122.81
1	I	271	GLU	OE1-CD-OE2	5.89	137.04	122.90
2	H	107	LYS	CB-CA-C	-5.89	100.21	109.70
1	U	156	ALA	CA-C-N	-5.88	112.40	120.28
1	U	156	ALA	C-N-CA	-5.88	112.40	120.28
1	E	234	LYS	CG-CD-CE	5.88	124.82	111.30
2	R	112	GLY	N-CA-C	-5.88	103.61	112.60
2	J	107	LYS	CG-CD-CE	5.87	124.80	111.30
1	K	87	LYS	N-CA-C	5.85	118.89	111.69
1	U	259	LYS	CB-CG-CD	-5.85	97.84	111.30
1	G	148	ASN	CA-C-N	5.84	132.05	121.89
1	G	148	ASN	C-N-CA	5.84	132.05	121.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	274	ARG	CA-C-N	-5.84	112.68	120.79
1	Y	274	ARG	C-N-CA	-5.84	112.68	120.79
1	G	97	GLU	CG-CD-OE2	-5.81	105.03	118.40
1	A	35	ILE	CB-CA-C	5.79	118.52	110.99
1	E	259	LYS	CD-CE-NZ	5.79	130.44	111.90
2	L	87	LYS	CG-CD-CE	5.79	124.62	111.30
2	T	113	GLN	N-CA-C	5.79	123.13	110.80
1	Y	260	SER	N-CA-CB	5.78	120.50	110.39
1	K	110	GLN	CA-CB-CG	5.77	125.63	114.10
2	L	87	LYS	N-CA-CB	5.77	120.64	110.37
2	N	106	ARG	CA-C-N	-5.76	112.22	122.07
2	N	106	ARG	C-N-CA	-5.76	112.22	122.07
2	H	12	VAL	N-CA-C	5.75	116.46	108.23
1	A	232	ILE	CA-C-N	-5.74	113.08	120.65
1	A	232	ILE	C-N-CA	-5.74	113.08	120.65
1	I	275	GLU	N-CA-CB	5.73	119.17	110.28
1	W	156	ALA	CA-C-N	5.72	127.95	120.28
1	W	156	ALA	C-N-CA	5.72	127.95	120.28
1	G	87	LYS	CA-CB-CG	5.72	125.54	114.10
1	I	143	LYS	CA-CB-CG	-5.70	102.70	114.10
1	K	234	LYS	CD-CE-NZ	5.69	130.12	111.90
1	W	274	ARG	CG-CD-NE	-5.69	99.48	112.00
1	O	32	GLN	CB-CG-CD	5.69	122.27	112.60
1	K	223	LYS	CA-CB-CG	5.68	125.46	114.10
1	O	30	MET	CB-CG-SD	5.68	129.73	112.70
1	W	193	MET	CA-CB-CG	5.66	125.43	114.10
1	A	274	ARG	CA-C-N	5.66	128.33	120.29
1	A	274	ARG	C-N-CA	5.66	128.33	120.29
2	L	45	ARG	N-CA-CB	5.66	118.68	109.69
1	A	199	GLN	CA-C-N	-5.65	112.15	122.38
1	A	199	GLN	C-N-CA	-5.65	112.15	122.38
1	M	180	VAL	CA-CB-CG1	-5.65	100.80	110.40
1	K	234	LYS	CB-CA-C	5.61	120.72	110.11
2	D	113	GLN	OE1-CD-NE2	-5.59	117.01	122.60
2	D	107	LYS	CB-CG-CD	-5.57	98.49	111.30
2	N	45	ARG	CG-CD-NE	5.57	124.25	112.00
1	W	253	GLU	CA-CB-CG	5.56	125.22	114.10
1	Y	202	LEU	CA-CB-CG	5.55	135.71	116.30
1	I	15	VAL	CB-CA-C	-5.53	104.68	112.14
1	A	35	ILE	CA-C-N	5.51	131.74	122.87
1	A	35	ILE	C-N-CA	5.51	131.74	122.87
1	C	271	GLU	CB-CG-CD	5.50	121.95	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	LEU	CB-CG-CD2	-5.48	94.26	110.70
2	F	45	ARG	CB-CA-C	-5.48	100.63	109.72
2	P	46	GLU	CB-CG-CD	5.46	121.88	112.60
1	W	222	GLN	CA-C-N	-5.46	110.94	121.58
1	W	222	GLN	C-N-CA	-5.46	110.94	121.58
1	A	233	GLN	CA-CB-CG	5.45	125.00	114.10
1	E	275	GLU	N-CA-CB	5.45	118.66	109.78
2	N	43	LYS	N-CA-CB	5.45	118.81	110.70
2	J	89	GLU	N-CA-CB	5.44	119.91	110.39
1	A	33	GLY	CA-C-N	-5.43	111.16	121.54
1	A	33	GLY	C-N-CA	-5.43	111.16	121.54
1	A	131	ARG	CA-CB-CG	-5.42	103.25	114.10
1	E	237	GLN	CA-C-N	-5.42	113.07	120.44
1	E	237	GLN	C-N-CA	-5.42	113.07	120.44
1	A	159	SER	CA-C-O	-5.42	113.40	119.79
1	I	137	GLU	CB-CG-CD	5.41	121.80	112.60
2	H	12	VAL	CA-CB-CG2	5.40	119.58	110.40
1	O	110	GLN	OE1-CD-NE2	-5.40	117.20	122.60
2	D	43	LYS	CB-CA-C	5.39	118.61	109.50
1	K	200	LYS	CD-CE-NZ	-5.37	94.71	111.90
2	B	19	ARG	CG-CD-NE	-5.34	100.24	112.00
1	E	288	ILE	CA-C-O	5.33	123.59	118.90
1	K	115	ARG	CA-CB-CG	-5.30	103.50	114.10
1	W	191	LYS	CA-CB-CG	-5.29	103.52	114.10
1	I	252	ALA	CA-C-N	5.29	127.63	120.65
1	I	252	ALA	C-N-CA	5.29	127.63	120.65
1	A	140	LYS	CA-CB-CG	5.28	124.65	114.10
1	G	96	PHE	CA-C-N	5.27	130.94	121.66
1	G	96	PHE	C-N-CA	5.27	130.94	121.66
2	L	87	LYS	CB-CG-CD	-5.27	99.18	111.30
2	D	12	VAL	CG1-CB-CG2	5.26	122.38	110.80
1	A	275	GLU	N-CA-CB	-5.25	102.38	110.16
1	K	173	LEU	CA-CB-CG	5.25	134.68	116.30
1	C	96	PHE	CA-C-N	5.24	130.88	121.66
1	C	96	PHE	C-N-CA	5.24	130.88	121.66
1	A	32	GLN	N-CA-CB	5.23	119.44	111.70
1	M	253	GLU	CG-CD-OE2	-5.22	106.38	118.40
2	F	45	ARG	CA-CB-CG	5.21	124.51	114.10
1	A	222	GLN	CA-CB-CG	-5.19	103.72	114.10
2	X	44	GLU	CG-CD-OE1	5.17	130.29	118.40
2	J	88	PRO	CA-C-N	-5.14	111.00	121.18
2	J	88	PRO	C-N-CA	-5.14	111.00	121.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	143	LYS	CA-CB-CG	-5.12	103.85	114.10
1	G	27	LEU	CB-CG-CD2	-5.12	95.34	110.70
2	B	76	LYS	CG-CD-CE	-5.12	99.53	111.30
1	K	283	GLU	CA-CB-CG	-5.12	103.87	114.10
2	N	13	GLN	N-CA-C	5.11	116.84	109.07
1	I	93	ARG	CA-CB-CG	5.11	124.31	114.10
1	G	282	LYS	CB-CA-C	-5.11	102.80	110.92
1	I	253	GLU	CG-CD-OE2	-5.11	106.66	118.40
1	M	180	VAL	N-CA-C	5.10	116.06	108.46
1	W	234	LYS	N-CA-CB	-5.09	102.61	110.20
1	G	295	LYS	CA-CB-CG	5.08	124.25	114.10
1	C	277	MET	CA-C-N	5.07	126.43	120.09
1	C	277	MET	C-N-CA	5.07	126.43	120.09
2	P	107	LYS	CA-CB-CG	5.07	124.24	114.10
1	W	159	SER	CB-CA-C	5.07	119.30	110.68
1	C	253	GLU	CA-CB-CG	5.06	124.23	114.10
1	G	97	GLU	CB-CG-CD	5.06	121.20	112.60
1	W	109	LEU	CA-C-N	5.06	131.21	121.54
1	W	109	LEU	C-N-CA	5.06	131.21	121.54
1	C	140	LYS	CD-CE-NZ	-5.06	95.72	111.90
2	L	44	GLU	CA-C-N	-5.04	113.79	120.90
2	L	44	GLU	C-N-CA	-5.04	113.79	120.90
1	O	283	GLU	CA-CB-CG	5.03	124.17	114.10
1	E	276	ALA	N-CA-CB	-5.02	104.23	110.90
1	E	157	LYS	CB-CA-C	-5.01	102.79	110.81
2	J	113	GLN	CA-CB-CG	5.00	124.10	114.10

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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
1	Y	260	SER	Mainchain
1	Y	275	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2360	2341	2342	162	4
1	C	2360	2336	2342	53	0
1	E	2369	2348	2347	52	1
1	G	2360	2340	2342	65	0
1	I	2360	2342	2342	55	1
1	K	2360	2341	2342	74	0
1	M	2360	2341	2342	50	0
1	O	2360	2340	2342	81	3
1	Q	2360	2341	2342	27	0
1	U	2360	2341	2342	46	2
1	W	2360	2340	2342	52	1
1	Y	2360	2340	2342	40	1
2	B	945	891	893	19	0
2	D	939	887	888	25	2
2	F	949	896	896	13	0
2	H	949	896	896	13	0
2	J	949	896	896	11	3
2	L	949	898	896	19	1
2	N	949	896	896	35	2
2	P	949	897	896	9	0
2	R	949	896	896	13	0
2	T	949	896	896	11	3
2	V	949	896	896	10	0
2	X	949	896	896	6	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	39101	920	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 12.

All (920) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:275:GLU:OE2	1:I:278:GLN:NE2	2.06	0.87
2:H:12:VAL:CG2	2:H:13:GLN:H	1.86	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
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:A:255:VAL:HG12	1:A:259:LYS:HZ2	1.42	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
1:G:95:MET:HE3	1:G:296:LEU:HB3	1.61	0.81
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:E:22:MET:HE2	1:E:239:VAL:HG22	1.66	0.78
1:G:213:MET:HE2	1:G:215:ILE:HD11	1.64	0.78
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
1:M:95:MET:HE2	1:M:296:LEU:HB3	1.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:235:ALA:C	1:A:239:VAL:HG23	2.12	0.74
1:A:23:LEU:HD12	1:A:235:ALA:HB1	1.69	0.74
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
2:T:6:GLU:CD	2:T:114:GLY:H	1.95	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
2:T:83:MET:HE2	2:T:86:LEU:HD21	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:133:LEU:HD22	1:Y:139:PHE:CD1	2.28	0.69
1:A:70:MET:HE2	1:A:70:MET:HA	1.75	0.69
2:T:44:GLU:CD	2:T:44:GLU:H	2.00	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
1:K:83:PRO:HB2	1:K:277:MET:HE3	1.74	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:A:35:ILE:HD11	1:A:228:ASP:CG	2.20	0.67
1:E:274:ARG:O	1:E:275:GLU:C	2.38	0.67
1:E:187:LEU:HG	1:E:187:LEU:HD12	1.68	0.67
1:U:187:LEU:HD11	1:U:204:MET:HE1	1.75	0.67
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
2:R:6:GLU:CD	2:R:114:GLY:H	2.02	0.67
1:O:233:GLN:C	1:O:236:VAL:HG22	2.20	0.66
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
1:W:61:ASP:C	1:W:62:ILE:HD13	2.20	0.66
2:B:91:THR:HG23	2:B:118:THR:HA	1.77	0.66
1:G:95:MET:CE	1:G:296:LEU:HB3	2.25	0.66
2:H:12:VAL:HG22	2:H:13:GLN:H	1.59	0.65
2:J:12:VAL:HG22	2:J:13:GLN:H	1.62	0.65
1:E:166:MET:HE1	1:E:174:ALA:CB	2.26	0.65
1:K:109:LEU:HD23	1:K:110:GLN:HB2	1.78	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:W:183:GLN:HG2	1:W:184:GLU:N	2.09	0.64
1:C:295:LYS:NZ	1:C:295:LYS:CD	2.59	0.64
1:W:193:MET:C	1:W:194:LYS:HG2	2.22	0.64
1:E:275:GLU:HB2	1:E:276:ALA:HB2	1.80	0.64
1:G:23:LEU:C	1:G:27:LEU:HD12	2.23	0.64
1:K:155:TYR:HA	1:K:277:MET:HE1	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:237:GLN:O	1:W:238:LYS:C	2.39	0.64
2:X:29:PHE:CE1	2:X:34:MET:HE3	2.33	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:8:MET:HE1	1:A:20:ALA:CB	2.27	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:K:29:GLU:HG2	1:K:30:MET:HE2	1.81	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:W:188:PRO:O	1:W:192:THR:OG1	2.11	0.62
1:C:213:MET:HE3	1:C:215:ILE:HD11	1.81	0.62
1:O:143:LYS:NZ	1:O:143:LYS:HD3	2.10	0.62
1:Y:128:THR:HG22	1:Y:202:LEU:HD23	1.81	0.62
1:A:255:VAL:HG12	1:A:259:LYS:NZ	2.14	0.62
2:H:39:GLN:NE2	2:H:43:LYS:O	2.27	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
2:D:83:MET:HB3	2:D:86:LEU:HD21	1.82	0.61
1:O:262:GLY:O	1:O:263:ILE:C	2.42	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: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
2:L:44:GLU:O	2:L:45:ARG:C	2.41	0.61
1:M:30:MET:HE3	1:M:30:MET:HA	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:259:LYS:HZ1	1:G:265:VAL:HB	1.64	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
2:J:6:GLU:CD	2:J:114:GLY:H	2.10	0.59
1:A:23:LEU:HD23	1:A:37:LEU:CD2	2.33	0.59
1:O:143:LYS:CD	1:O:143:LYS:HZ3	2.08	0.59
1:I:16:GLU:HG2	1:I:212:GLN:HE22	1.66	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: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:E:213:MET:HE3	1:E:215:ILE:HD11	1.84	0.59
2:H:83:MET:HE1	2:H:117:VAL:HG21	1.84	0.59
1:I:55:LEU:HD23	1:I:215:ILE:CG2	2.33	0.59
2:B:83:MET:HE2	2:B:86:LEU:HD11	1.85	0.58
1:U:81:MET:HE2	1:U:151:GLN:HB2	1.85	0.58
2:D:83:MET:HE1	2:D:117:VAL:HG21	1.84	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:234:LYS:CG	1:K:234:LYS:CE	2.81	0.58
2:N:12:VAL:C	2:N:13:GLN:HG2	2.28	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
2:D:20:LEU:HG	2:D:83:MET:HE2	1.85	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:W:34:GLU:C	1:W:35:ILE:HD13	2.28	0.58
1:A:102:GLN:HA	1:A:105:ARG:HG3	1.86	0.57
1:A:128:THR:C	1:A:199:GLN:OE1	2.47	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:Q:68:GLY:C	1:Q:81:MET:HE2	2.30	0.57
1:Y:201:ASN:HD22	1:Y:264:ASN:HB3	1.69	0.57
1:A:8:MET:HE1	1:A:20:ALA:HB3	1.86	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:A:271:GLU:HA	1:A:274:ARG:HB2	1.87	0.57
1:K:83:PRO:CB	1:K:277:MET:HE3	2.35	0.57
1:O:271:GLU:HA	1:O:274:ARG:HG3	1.87	0.57
2:F:34:MET:HE1	2:F:98:ALA:HB2	1.87	0.56
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
1:E:272:PRO:HA	1:E:275:GLU:CD	2.31	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
1:W:250:GLN:HA	1:W:253:GLU:HG3	1.87	0.56
1:M:145:ARG:HG3	1:M:166:MET:HE3	1.87	0.56
1:Y:8:MET:CA	1:Y:51:MET:HE1	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Y:274:ARG:O	1:Y:275:GLU:C	2.45	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:W:166:MET:HE1	1:W:174:ALA:HB3	1.88	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
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:296:LEU:HA	1:A:299:MET:HE3	1.88	0.55
1:A:133:LEU:HD23	1:A:139:PHE:CZ	2.41	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
2:N:13:GLN:O	2:N:14:THR:C	2.50	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
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:U:143:LYS:HB2	1:U:181:ASP:CG	2.32	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
1:Y:133:LEU:HD21	1:Y:142:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:17:SER:HB2	2:V:58:SER:HB2	1.89	0.54
1:Y:8:MET:C	1:Y:51:MET:HE1	2.33	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
2:H:20:LEU:HG	2:H:83:MET:HE2	1.90	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:V:73:ASP:CB	2:V:76:LYS:HG3	2.33	0.53
1:Y:145:ARG:HG3	1:Y:166:MET:HE3	1.89	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:K:212:GLN:CB	1:K:212:GLN:CD	2.76	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:A:273:PHE:O	1:A:277:MET:HE2	2.08	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
2:X:29:PHE:CD1	2:X:34:MET:HE3	2.44	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:A:96:PHE:HE2	1:A:213:MET:HE3	1.75	0.52
1:A:205:THR:O	1:A:206:HIS:C	2.49	0.52
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:Y:133:LEU:HD23	1:Y:138:ASP:C	2.34	0.52
1:A:175:LEU:CD2	1:A:180:VAL:HG23	2.39	0.52
1:A:244:THR:C	1:A:248:LYS:HD2	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:12:VAL:HG22	2:H:13:GLN:N	2.22	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
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:C:46:GLY:O	1:C:51:MET:HE2	2.10	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:I:263:ILE:N	1:I:263:ILE:HD13	2.25	0.52
1:W:81:MET:HE3	1:W:151:GLN:HB2	1.92	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
2:J:42:GLY:C	2:J:43:LYS:HG2	2.35	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
2:D:34:MET:HE1	2:D:98:ALA:HB2	1.92	0.51
1:O:70:MET:HE2	1:O:70:MET:HA	1.91	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:K:243:HIS:O	1:K:244:THR:C	2.54	0.51
1:O:232:ILE:C	1:O:234:LYS:N	2.68	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: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:239:VAL:CG1	1:G:239:VAL:HB	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:244:THR:O	1:I:245:GLN:C	2.50	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: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
2:N:12:VAL:C	2:N:13:GLN:CG	2.85	0.50
1:K:63:THR:HG23	1:K:64:TYR:N	2.25	0.50
1:O:232:ILE:C	1:O:234:LYS:H	2.20	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:M:213:MET:HE2	1:M:215:ILE:HD11	1.93	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
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
2:R:39:GLN:CD	2:R:45:ARG:HG3	2.36	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
1:G:125:ARG:HE	1:G:184:GLU:CD	2.20	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:U:158:LEU:HB2	1:U:277:MET:HE1	1.94	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:M:166:MET:HE1	1:M:180:VAL:HG21	1.92	0.49
1:U:213:MET:HE3	1:U:215:ILE:HD11	1.94	0.49
1:A:30:MET:CE	1:A:238:LYS:HZ3	2.25	0.49
1:A:234:LYS:CB	1:A:234:LYS:CD	2.80	0.49
2:H:20:LEU:CD1	2:H:83:MET:HE2	2.42	0.49
1:Q:8:MET:HE1	1:Q:20:ALA:CB	2.43	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
1:A:166:MET:HE3	1:A:180:VAL:HG11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:T:6:GLU:CD	2:T:114:GLY:N	2.68	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:33:GLY:C	1:A:34:GLU:HG3	2.38	0.48
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
1:O:125:ARG:HE	1:O:184:GLU:CD	2.21	0.48
2:H:67:ARG:NH1	2:H:85:SER:O	2.46	0.48
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:O:143:LYS:HD3	1:O:143:LYS:HZ3	1.71	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:Y:233:GLN:O	1:Y:236:VAL:HG22	2.12	0.48
1:C:83:PRO:HG2	1:C:277:MET:HE2	1.95	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:U:250:GLN:C	1:U:254:LEU:HD23	2.38	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:245:GLN:O	1:I:246:THR:C	2.57	0.48
1:O:279:PRO:HA	1:O:282:LYS:HD3	1.94	0.48
1:W:108:MET:HE1	1:W:116:ALA:HB2	1.95	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:70:MET:SD	1:A:108:MET:HE3	2.54	0.48
1:E:3:THR:HG23	1:E:3:THR:O	2.12	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:W:235:ALA:O	1:W:236:VAL:C	2.56	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
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:M:236:VAL:C	1:M:237:GLN:O	2.58	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
2:N:83:MET:HE2	2:N:86:LEU:HD21	1.95	0.47
1:C:83:PRO:CG	1:C:277:MET:HE2	2.44	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:E:272:PRO:C	1:E:275:GLU:H	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:259:LYS:C	1:A:261:GLU:H	2.22	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:O:143:LYS:HD2	1:O:143:LYS:HZ2	1.77	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
1:A:273:PHE:O	1:A:274:ARG:C	2.59	0.46
1:G:284:PHE:O	1:G:288:ILE:HG12	2.15	0.46
1:K:8:MET:HE1	1:K:20:ALA:HB3	1.97	0.46
1:C:48:ASP:OD1	1:C:48:ASP:N	2.49	0.46
1:G:213:MET:CE	1:G:215:ILE:HD11	2.40	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
1:U:29:GLU:OE1	1:U:30:MET:HE2	2.16	0.46
1:A:70:MET:HE2	1:A:70:MET:CA	2.43	0.46
1:O:35:ILE:HD11	1:O:228:ASP:CG	2.40	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
2:F:18:LEU:HB3	2:F:83:MET:HE3	1.97	0.46
1:G:143:LYS:O	1:G:180:VAL:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:71:GLY:HA3	1:K:78:GLU:CG	2.46	0.46
1:M:199:GLN:C	1:M:200:LYS:HE2	2.41	0.46
2:N:107:LYS:HG2	2:N:111:TRP:CZ2	2.51	0.46
1:Q:8:MET:HE1	1:Q:20:ALA:HB3	1.98	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:E:68:GLY:C	1:E:81:MET:HE2	2.41	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: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
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
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:259:LYS:HZ2	1:G:265:VAL:HB	1.81	0.45
1:G:292:ILE:O	1:G:295:LYS:HB3	2.16	0.45
1:M:108:MET:HE1	1:M:213:MET:HE3	1.99	0.45
1:M:180:VAL:CG1	1:M:181:ASP:N	2.78	0.45
1:Y:8:MET:HA	1:Y:51:MET:HE1	1.98	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:243:HIS:C	1:K:245:GLN:N	2.72	0.45
1:O:80:VAL:HG13	1:O:95:MET:HE3	1.98	0.45
1:C:270:LEU:O	1:C:271:GLU:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:120:TRP:O	1:O:212:GLN:N	2.49	0.45
1:O:281:TYR:O	1:O:282:LYS:C	2.60	0.45
1:A:256:SER:O	1:A:259:LYS:HB2	2.16	0.45
1:K:257:PHE:C	1:K:257:PHE:CD2	2.93	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:A:30:MET:HE2	1:A:238:LYS:NZ	2.31	0.45
1:A:232:ILE:O	1:A:233:GLN:C	2.55	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: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:W:166:MET:HE1	1:W:174:ALA:CB	2.46	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:G:23:LEU:O	1:G:27:LEU:HD12	2.16	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:Q:93:ARG:HH11	1:Q:97:GLU:CD	2.25	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:O:21:LYS:HD3	1:O:21:LYS:C	2.42	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
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
2:L:48:VAL:CG2	2:L:49:ALA:N	2.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:108:MET:HE1	1:K:116:ALA:HB2	2.00	0.44
1:A:234:LYS:O	1:A:238:LYS:CB	2.66	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
2:T:113:GLN:O	2:T:114:GLY:C	2.55	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: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
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
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:E:272:PRO:C	1:E:275:GLU:HG2	2.42	0.43
1:G:51:MET:HE3	1:G:63:THR:OG1	2.18	0.43
1:M:200:LYS:HE2	1:M:200:LYS:N	2.33	0.43
1:C:55:LEU:CD1	1:C:63:THR:HG22	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:U:175:LEU:HD23	1:U:199:GLN:HG2	2.00	0.43
1:U:282:LYS:O	1:U:283:GLU:C	2.58	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: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
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:238:LYS:C	2.61	0.43
1:M:237:GLN:O	1:M:240:GLY:N	2.37	0.43
1:Q:46:GLY:O	1:Q:51:MET:HE2	2.18	0.43
1:Q:121:TYR:HB3	1:Q:244:THR:HG23	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:8:MET:HG2	1:M:41:PRO:HA	2.01	0.43
2:N:11:LEU:HG	2:N:13:GLN:HE21	1.83	0.43
1:Q:95:MET:HE2	1:Q:296:LEU:HB3	2.01	0.43
1:Q:108:MET:HE1	1:Q:116:ALA:HB2	2.01	0.43
1:A:88:ASP:C	1:A:88:ASP:OD1	2.60	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:23:LEU:O	1:G:24:ALA:C	2.62	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:W:237:GLN:C	1:W:239:VAL:N	2.73	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
1:A:30:MET:CE	1:A:238:LYS:NZ	2.82	0.42
2:D:37:PHE:HA	2:D:48:VAL:HG23	2.01	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
1:E:22:MET:HA	1:E:25:ASP:HB2	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:108:MET:HE1	1:G:213:MET:HE1	2.02	0.42
1:K:293:VAL:CG1	2:R:41:PRO:CB	2.97	0.42
1:M:68:GLY:C	1:M:81:MET:HE2	2.45	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:I:232:ILE:O	1:I:233:GLN:C	2.62	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:C	1:A:277:MET:HE2	2.45	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
1:U:156:ALA:O	1:U:157:LYS:C	2.59	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:136:ILE:O	1:O:139:PHE:HB2	2.19	0.41
1:G:96:PHE:CE1	1:G:105:ARG:HD2	2.56	0.41
1:U:280:LEU:O	1:U:283:GLU:HB3	2.20	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:ASP:OD1	1:E:48:ASP:N	2.52	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:O:70:MET:HE2	1:O:70:MET:CA	2.50	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
1:A:81:MET:O	1:A:82:LEU:C	2.63	0.41
1:I:131:ARG:CG	1:I:131:ARG:C	2.93	0.41
2:L:44:GLU:H	2:L:44:GLU:HG2	1.43	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:A:186:PRO:C	1:A:190:ILE:HD12	2.46	0.41
1:K:122:ASN:CG	1:K:212:GLN:HG2	2.46	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
1:I:145:ARG:C	1:I:145:ARG:HD3	2.46	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
1:A:6:MET:HE2	1:A:64:TYR:CE2	2.55	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
2:D:112:GLY:C	2:D:113:GLN:HE21	2.28	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:22:MET:O	1:A:23:LEU:C	2.63	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: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
2:H:20:LEU:CG	2:H:83:MET:HE2	2.50	0.41
1:I:26:THR:O	1:I:30:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:44:GLN:HG3	1:I:45:LEU:HD13	2.03	0.41
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:33:GLY:C	1:A:34:GLU:CG	2.93	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: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:K:132:PRO:HA	1:K:201:ASN:OD1	2.21	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:A:243:HIS:O	1:A:244:THR:C	2.64	0.40
1:G:48:ASP:OD1	1:G:48:ASP:N	2.54	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:C:275:GLU:HA	1:C:278:GLN:HE21	1.85	0.40
2:F:45:ARG:HD2	2:F:107:LYS:HZ1	1.87	0.40
1:I:55:LEU:HD21	1:I:215:ILE:HG22	1.98	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
2:R:40:ALA:HB1	2:R:41:PRO:HD2	2.03	0.40
1:W:55:LEU:HD23	1:W:60:LEU:C	2.47	0.40
1:Y:274:ARG:O	1:Y:275:GLU:O	2.39	0.40
1:C:144:LEU:HD12	1:C:182:GLY:C	2.46	0.40
1:G:108:MET:HE1	1:G:213:MET:CE	2.51	0.40
1:M:237:GLN:C	1:M:239:VAL:N	2.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	18	45
1	C	297/303 (98%)	290 (98%)	6 (2%)	1 (0%)	36	64
1	E	299/303 (99%)	289 (97%)	9 (3%)	1 (0%)	36	64
1	G	297/303 (98%)	286 (96%)	9 (3%)	2 (1%)	18	45
1	I	297/303 (98%)	290 (98%)	5 (2%)	2 (1%)	18	45
1	K	297/303 (98%)	286 (96%)	8 (3%)	3 (1%)	12	36
1	M	297/303 (98%)	288 (97%)	4 (1%)	5 (2%)	7	23
1	O	297/303 (98%)	285 (96%)	8 (3%)	4 (1%)	9	29
1	Q	297/303 (98%)	292 (98%)	4 (1%)	1 (0%)	36	64
1	U	297/303 (98%)	289 (97%)	5 (2%)	3 (1%)	12	36
1	W	297/303 (98%)	290 (98%)	5 (2%)	2 (1%)	18	45
1	Y	297/303 (98%)	292 (98%)	3 (1%)	2 (1%)	18	45
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	41
2	L	121/123 (98%)	117 (97%)	3 (2%)	1 (1%)	16	41
2	N	121/123 (98%)	121 (100%)	0	0	100	100
2	P	121/123 (98%)	115 (95%)	5 (4%)	1 (1%)	16	41
2	R	121/123 (98%)	119 (98%)	1 (1%)	1 (1%)	16	41
2	T	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
2	V	121/123 (98%)	119 (98%)	1 (1%)	1 (1%)	16	41
2	X	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
All	All	5015/5112 (98%)	4888 (98%)	94 (2%)	33 (1%)	18	45

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 ⓘ

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%)	238 (92%)	20 (8%)	11	34
1	C	258/259 (100%)	249 (96%)	9 (4%)	32	65
1	E	258/259 (100%)	254 (98%)	4 (2%)	55	82
1	G	258/259 (100%)	254 (98%)	4 (2%)	55	82
1	I	258/259 (100%)	254 (98%)	4 (2%)	55	82
1	K	258/259 (100%)	250 (97%)	8 (3%)	35	69
1	M	258/259 (100%)	257 (100%)	1 (0%)	84	94
1	O	258/259 (100%)	252 (98%)	6 (2%)	44	76
1	Q	258/259 (100%)	254 (98%)	4 (2%)	55	82
1	U	258/259 (100%)	254 (98%)	4 (2%)	55	82
1	W	258/259 (100%)	249 (96%)	9 (4%)	32	65
1	Y	258/259 (100%)	254 (98%)	4 (2%)	55	82
2	B	98/98 (100%)	93 (95%)	5 (5%)	21	52
2	D	97/98 (99%)	94 (97%)	3 (3%)	35	69
2	F	98/98 (100%)	95 (97%)	3 (3%)	35	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	98/98 (100%)	94 (96%)	4 (4%)	27	60
2	J	98/98 (100%)	93 (95%)	5 (5%)	21	52
2	L	98/98 (100%)	94 (96%)	4 (4%)	27	60
2	N	98/98 (100%)	95 (97%)	3 (3%)	35	69
2	P	98/98 (100%)	97 (99%)	1 (1%)	68	88
2	R	98/98 (100%)	96 (98%)	2 (2%)	48	79
2	T	98/98 (100%)	94 (96%)	4 (4%)	27	60
2	V	98/98 (100%)	96 (98%)	2 (2%)	48	79
2	X	98/98 (100%)	97 (99%)	1 (1%)	68	88
All	All	4271/4284 (100%)	4157 (97%)	114 (3%)	39	72

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLU
1	A	32	GLN
1	A	102	GLN
1	A	131	ARG
1	A	136	ILE
1	A	140	LYS
1	A	144	LEU
1	A	153	LEU
1	A	157	LYS
1	A	202	LEU
1	A	206	HIS
1	A	217	SER
1	A	233	GLN
1	A	246	THR
1	A	249	THR
1	A	255	VAL
1	A	264	ASN
1	A	271	GLU
1	A	274	ARG
1	A	275	GLU
2	B	13	GLN
2	B	44	GLU
2	B	52	SER
2	B	113	GLN
2	B	116	GLN

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Mol	Chain	Res	Type
1	C	2	THR
1	C	15	VAL
1	C	32	GLN
1	C	63	THR
1	C	110	GLN
1	C	216	ILE
1	C	230	ASP
1	C	260	SER
1	C	265	VAL
2	D	2	VAL
2	D	5	VAL
2	D	107	LYS
1	E	159	SER
1	E	173	LEU
1	E	255	VAL
1	E	288	ILE
2	F	44	GLU
2	F	69	THR
2	F	113	GLN
1	G	148	ASN
1	G	184	GLU
1	G	212	GLN
1	G	234	LYS
2	H	13	GLN
2	H	44	GLU
2	H	63	SER
2	H	121	SER
1	I	28	GLU
1	I	137	GLU
1	I	217	SER
1	I	263	ILE
2	J	20	LEU
2	J	44	GLU
2	J	93	ILE
2	J	107	LYS
2	J	113	GLN
1	K	63	THR
1	K	85	VAL
1	K	137	GLU
1	K	148	ASN
1	K	159	SER
1	K	199	GLN

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Mol	Chain	Res	Type
1	K	227	THR
1	K	266	THR
2	L	44	GLU
2	L	48	VAL
2	L	87	LYS
2	L	107	LYS
1	M	217	SER
2	N	12	VAL
2	N	44	GLU
2	N	87	LYS
1	O	32	GLN
1	O	143	LYS
1	O	148	ASN
1	O	184	GLU
1	O	217	SER
1	O	237	GLN
2	P	67	ARG
1	Q	183	GLN
1	Q	212	GLN
1	Q	236	VAL
1	Q	260	SER
2	R	44	GLU
2	R	113	GLN
2	T	13	GLN
2	T	43	LYS
2	T	44	GLU
2	T	63	SER
1	U	102	GLN
1	U	153	LEU
1	U	184	GLU
1	U	255	VAL
2	V	63	SER
2	V	87	LYS
1	W	14	SER
1	W	35	ILE
1	W	109	LEU
1	W	129	SER
1	W	162	SER
1	W	167	SER
1	W	183	GLN
1	W	266	THR
1	W	274	ARG

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Mol	Chain	Res	Type
2	X	113	GLN
1	Y	202	LEU
1	Y	217	SER
1	Y	256	SER
1	Y	259	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	233	GLN
2	B	13	GLN
1	C	54	GLN
1	C	110	GLN
1	C	176	GLN
1	C	183	GLN
1	C	278	GLN
2	D	113	GLN
1	E	44	GLN
1	E	154	ASN
1	E	287	ASN
1	G	9	GLN
1	G	110	GLN
1	G	148	ASN
1	G	222	GLN
1	G	264	ASN
2	H	100	HIS
2	H	113	GLN
1	I	134	ASN
1	I	212	GLN
1	I	222	GLN
2	J	1	GLN
2	J	31	ASN
2	J	39	GLN
2	J	100	HIS
1	K	9	GLN
1	K	110	GLN
1	K	212	GLN
1	K	233	GLN
2	L	105	HIS
1	M	54	GLN
1	M	110	GLN

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Mol	Chain	Res	Type
1	M	178	ASN
1	M	222	GLN
1	M	264	ASN
2	N	13	GLN
2	N	100	HIS
1	O	54	GLN
1	O	110	GLN
1	O	185	ASN
1	O	250	GLN
1	O	278	GLN
2	P	100	HIS
1	Q	9	GLN
1	Q	32	GLN
1	Q	233	GLN
1	Q	237	GLN
1	Q	250	GLN
2	R	100	HIS
2	R	113	GLN
2	R	116	GLN
1	U	54	GLN
1	U	148	ASN
1	U	212	GLN
1	U	222	GLN
1	U	233	GLN
1	W	44	GLN
1	W	102	GLN
1	W	183	GLN
1	W	185	ASN
1	W	233	GLN
1	W	237	GLN
1	W	250	GLN
1	W	287	ASN
2	X	102	HIS
2	X	116	GLN
1	Y	32	GLN
1	Y	54	GLN
1	Y	201	ASN
1	Y	206	HIS
1	Y	222	GLN
1	Y	278	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	$\# Z > 2$
4	GOL	U	302	-	5,5,5	0.87	0	5,5,5	1.06	0
4	GOL	U	303	-	5,5,5	0.91	0	5,5,5	1.16	1 (20%)
3	SLB	A	301	-	20,20,21	1.43	2 (10%)	21,28,31	1.39	3 (14%)
3	SLB	K	301	-	20,20,21	1.34	2 (10%)	21,28,31	1.22	3 (14%)
3	SLB	E	301	-	20,20,21	1.38	2 (10%)	21,28,31	1.09	1 (4%)
4	GOL	U	304	-	5,5,5	0.85	0	5,5,5	1.14	1 (20%)
3	SLB	C	301	-	20,20,21	1.34	2 (10%)	21,28,31	1.29	3 (14%)
3	SLB	U	301	-	20,20,21	1.41	2 (10%)	21,28,31	1.24	2 (9%)
4	GOL	E	302	-	5,5,5	0.95	0	5,5,5	1.07	0
3	SLB	W	301	-	20,20,21	1.39	2 (10%)	21,28,31	1.18	3 (14%)
4	GOL	G	302	-	5,5,5	1.22	1 (20%)	5,5,5	1.52	1 (20%)
3	SLB	O	301	-	20,20,21	1.34	2 (10%)	21,28,31	1.23	4 (19%)
3	SLB	Q	301	-	20,20,21	1.34	2 (10%)	21,28,31	1.12	2 (9%)
3	SLB	M	301	-	20,20,21	1.35	2 (10%)	21,28,31	1.15	2 (9%)
3	SLB	I	301	-	20,20,21	1.31	2 (10%)	21,28,31	1.20	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SLB	Y	301	-	20,20,21	1.34	2 (10%)	21,28,31	1.15	2 (9%)
4	GOL	Q	302	-	5,5,5	1.34	1 (20%)	5,5,5	1.44	1 (20%)
3	SLB	G	301	-	20,20,21	1.34	2 (10%)	21,28,31	1.24	2 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	U	302	-	-	0/4/4/4	-
4	GOL	U	303	-	-	0/4/4/4	-
3	SLB	A	301	-	-	5/18/34/38	0/1/1/1
3	SLB	K	301	-	-	1/18/34/38	0/1/1/1
3	SLB	E	301	-	-	1/18/34/38	0/1/1/1
4	GOL	U	304	-	-	0/4/4/4	-
3	SLB	C	301	-	-	1/18/34/38	0/1/1/1
3	SLB	U	301	-	-	5/18/34/38	0/1/1/1
4	GOL	E	302	-	-	2/4/4/4	-
3	SLB	W	301	-	-	3/18/34/38	0/1/1/1
4	GOL	G	302	-	-	0/4/4/4	-
3	SLB	O	301	-	-	1/18/34/38	0/1/1/1
3	SLB	Q	301	-	-	1/18/34/38	0/1/1/1
3	SLB	M	301	-	-	1/18/34/38	0/1/1/1
3	SLB	I	301	-	-	1/18/34/38	0/1/1/1
3	SLB	Y	301	-	-	1/18/34/38	0/1/1/1
4	GOL	Q	302	-	-	2/4/4/4	-
3	SLB	G	301	-	-	1/18/34/38	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	301	SLB	C10-N5	3.70	1.46	1.34
3	A	301	SLB	C10-N5	3.63	1.46	1.34
3	E	301	SLB	C10-N5	3.53	1.45	1.34
3	W	301	SLB	C10-N5	3.52	1.45	1.34
3	M	301	SLB	C10-N5	3.52	1.45	1.34
3	Q	301	SLB	C10-N5	3.52	1.45	1.34
3	I	301	SLB	C10-N5	3.51	1.45	1.34
3	O	301	SLB	C10-N5	3.50	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	301	SLB	C10-N5	3.48	1.45	1.34
3	C	301	SLB	C10-N5	3.45	1.45	1.34
3	Y	301	SLB	C10-N5	3.45	1.45	1.34
3	G	301	SLB	C10-N5	3.39	1.45	1.34
3	A	301	SLB	O6-C6	-2.80	1.39	1.44
3	U	301	SLB	O6-C6	-2.75	1.39	1.44
3	W	301	SLB	O6-C6	-2.64	1.39	1.44
3	E	301	SLB	O6-C6	-2.62	1.39	1.44
4	Q	302	GOL	O2-C2	-2.49	1.36	1.43
3	M	301	SLB	O6-C6	-2.28	1.40	1.44
3	Q	301	SLB	O6-C6	-2.21	1.40	1.44
3	G	301	SLB	O6-C6	-2.20	1.40	1.44
4	G	302	GOL	O2-C2	-2.19	1.37	1.43
3	Y	301	SLB	O6-C6	-2.13	1.40	1.44
3	O	301	SLB	O6-C6	-2.12	1.40	1.44
3	C	301	SLB	O6-C6	-2.07	1.40	1.44
3	I	301	SLB	O6-C6	-2.03	1.40	1.44
3	K	301	SLB	O6-C6	-2.00	1.40	1.44

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	SLB	C9-C8-C7	-3.67	104.69	112.17
4	G	302	GOL	C3-C2-C1	-3.04	100.63	111.80
3	I	301	SLB	O1B-C1-C2	2.87	120.18	112.71
3	M	301	SLB	O1B-C1-C2	2.85	120.12	112.71
3	C	301	SLB	O1B-C1-C2	2.84	120.10	112.71
3	U	301	SLB	C9-C8-C7	-2.84	106.39	112.17
3	O	301	SLB	O1B-C1-C2	2.83	120.08	112.71
3	K	301	SLB	O1B-C1-C2	2.78	119.95	112.71
3	U	301	SLB	O1B-C1-C2	2.75	119.85	112.71
3	A	301	SLB	O1B-C1-C2	2.74	119.85	112.71
3	E	301	SLB	O1B-C1-C2	2.73	119.80	112.71
3	G	301	SLB	O1B-C1-C2	2.71	119.77	112.71
4	Q	302	GOL	C3-C2-C1	-2.71	101.85	111.80
3	Q	301	SLB	O1B-C1-C2	2.71	119.76	112.71
3	W	301	SLB	C9-C8-C7	-2.71	106.65	112.17
3	Y	301	SLB	O1B-C1-C2	2.71	119.75	112.71
3	W	301	SLB	O1B-C1-C2	2.64	119.58	112.71
3	C	301	SLB	C8-C7-C6	-2.61	108.14	113.05
3	I	301	SLB	C8-C7-C6	-2.41	108.53	113.05
3	A	301	SLB	C11-C10-N5	2.33	119.98	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	301	SLB	C11-C10-N5	2.31	119.95	116.12
3	G	301	SLB	C8-C7-C6	-2.26	108.81	113.05
3	K	301	SLB	C11-C10-N5	2.20	119.77	116.12
3	O	301	SLB	C11-C10-N5	2.16	119.69	116.12
3	O	301	SLB	C8-C7-C6	-2.15	109.02	113.05
3	M	301	SLB	C11-C10-N5	2.14	119.66	116.12
3	W	301	SLB	C11-C10-N5	2.12	119.63	116.12
3	Y	301	SLB	C11-C10-N5	2.12	119.63	116.12
3	I	301	SLB	C11-C10-N5	2.08	119.57	116.12
3	K	301	SLB	O1B-C1-O1A	-2.07	119.39	124.08
3	Q	301	SLB	C11-C10-N5	2.06	119.54	116.12
4	U	304	GOL	C3-C2-C1	-2.05	104.28	111.80
3	O	301	SLB	O1B-C1-O1A	-2.04	119.45	124.08
3	I	301	SLB	O1B-C1-O1A	-2.01	119.51	124.08
4	U	303	GOL	C3-C2-C1	-2.01	104.42	111.80

There are no chirality outliers.

All (26) 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	U	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
4	E	302	GOL	O2-C2-C3-O3
3	U	301	SLB	O7-C7-C8-C9
4	Q	302	GOL	O2-C2-C3-O3
3	U	301	SLB	C6-C7-C8-C9
3	W	301	SLB	O8-C8-C9-O9

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Mol	Chain	Res	Type	Atoms
3	U	301	SLB	O7-C7-C8-O8
4	E	302	GOL	C1-C2-C3-O3
4	Q	302	GOL	C1-C2-C3-O3
3	W	301	SLB	C7-C8-C9-O9

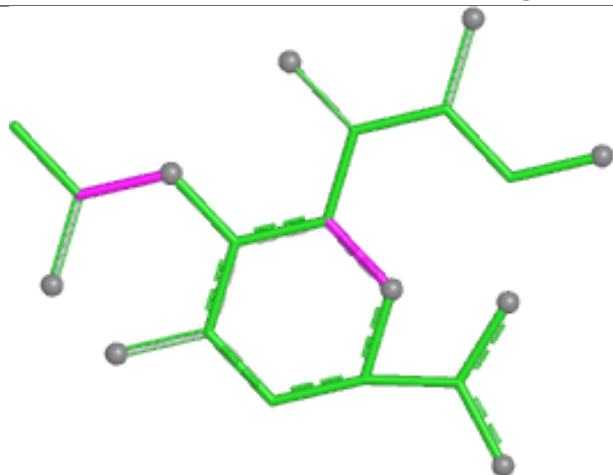
There are no ring outliers.

4 monomers are involved in 5 short contacts:

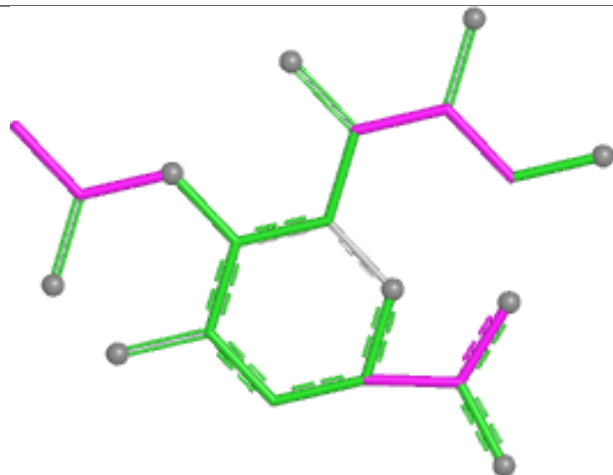
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	SLB	2	0
3	W	301	SLB	1	0
3	Q	301	SLB	1	0
4	Q	302	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

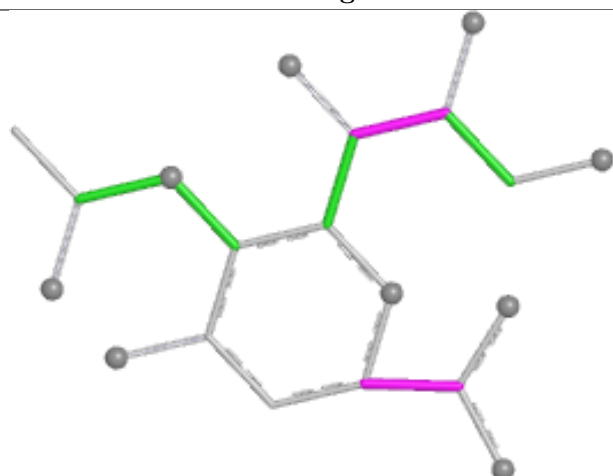
Ligand SLB A 301



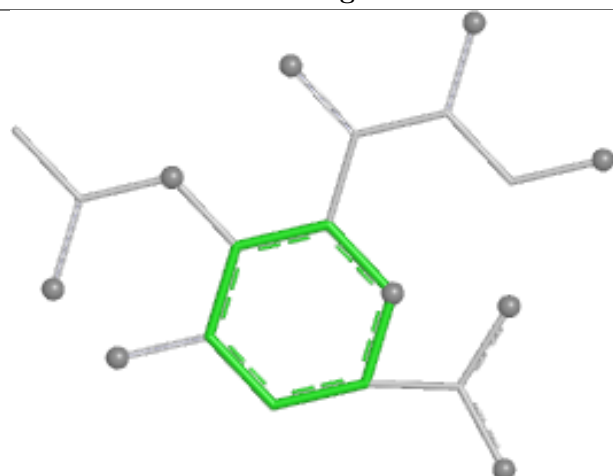
Bond lengths



Bond angles

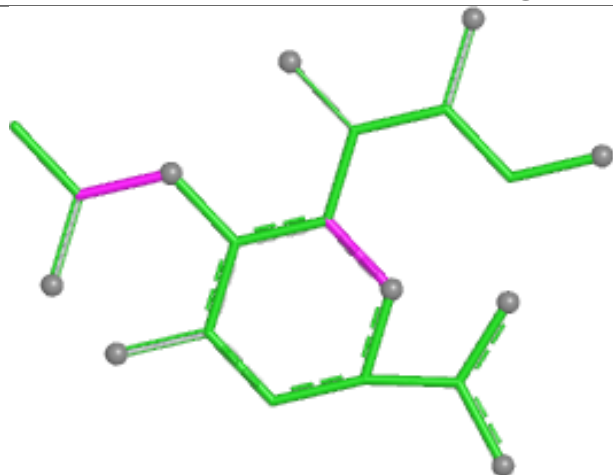


Torsions

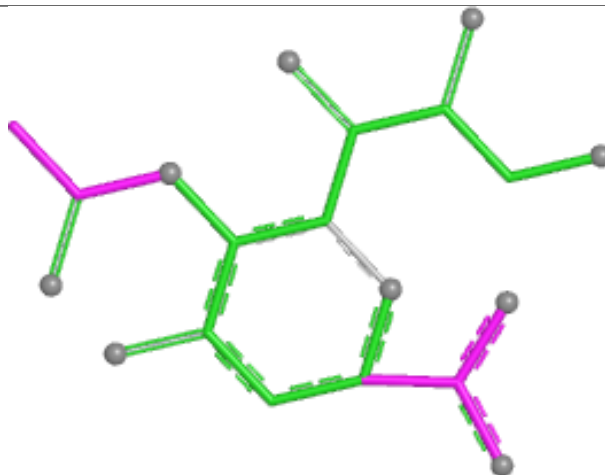


Rings

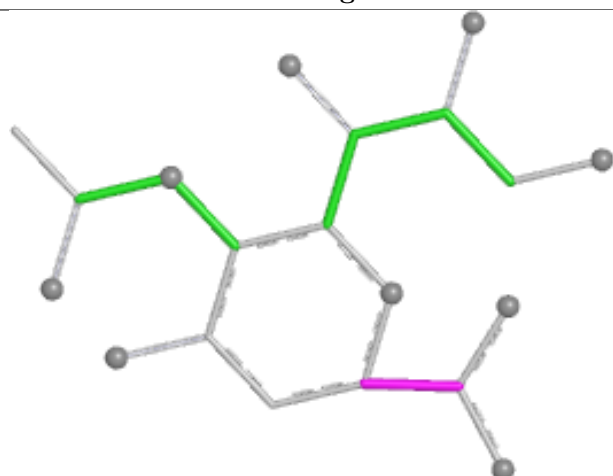
Ligand SLB K 301



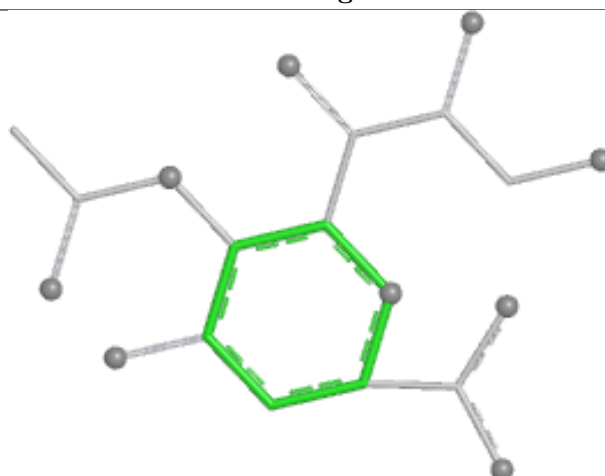
Bond lengths



Bond angles

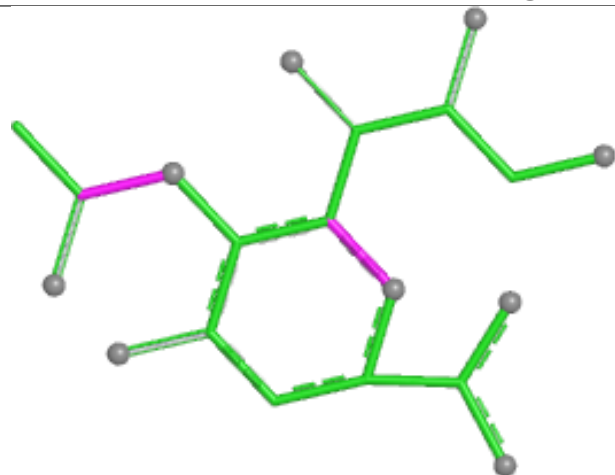


Torsions

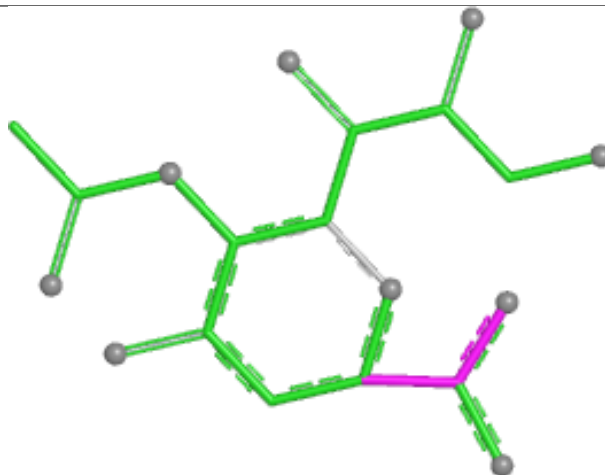


Rings

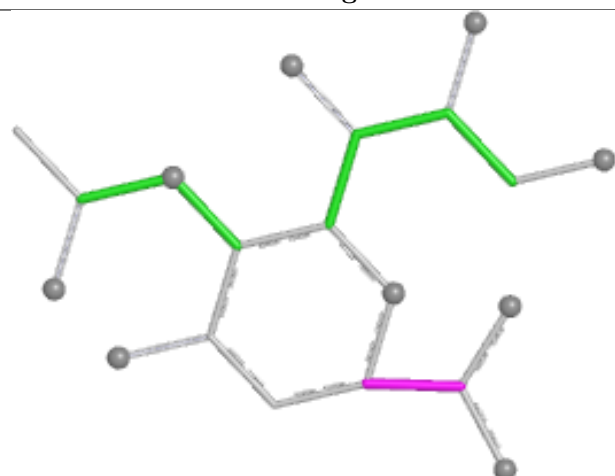
Ligand SLB E 301



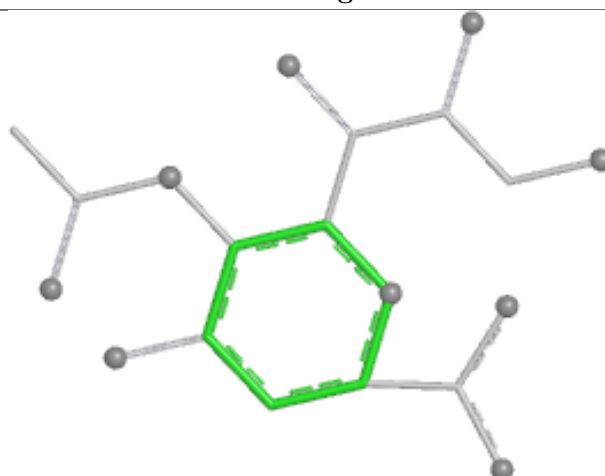
Bond lengths



Bond angles

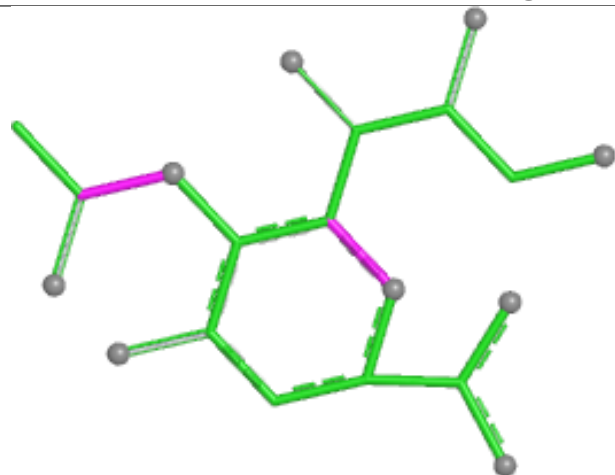


Torsions

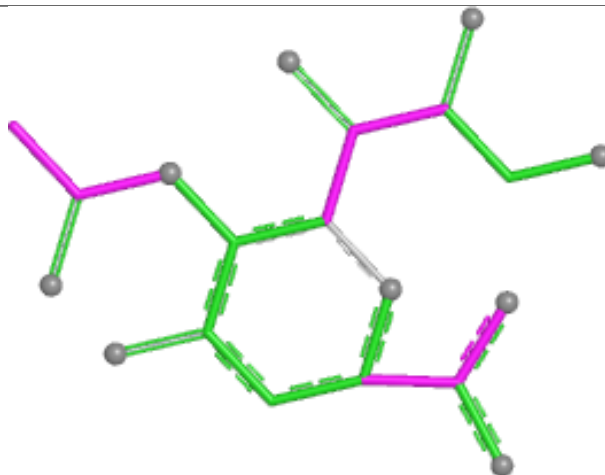


Rings

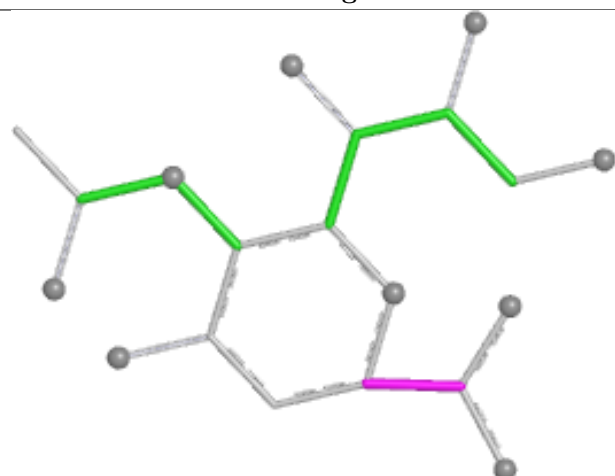
Ligand SLB C 301



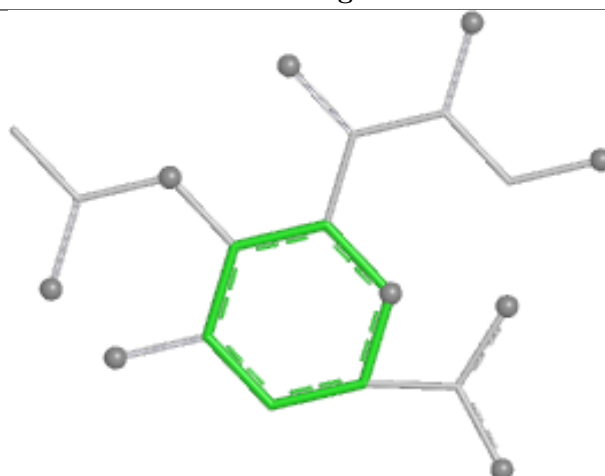
Bond lengths



Bond angles

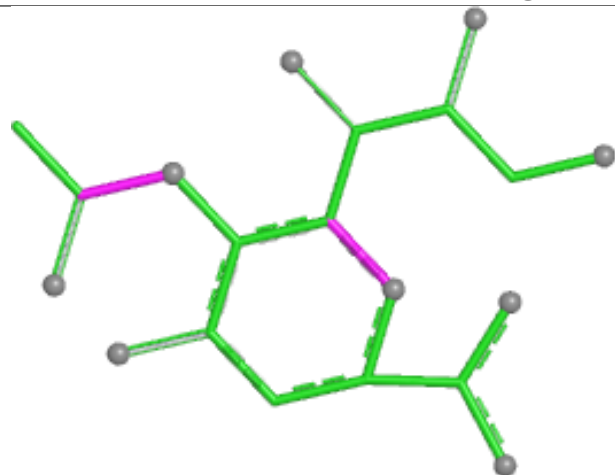


Torsions

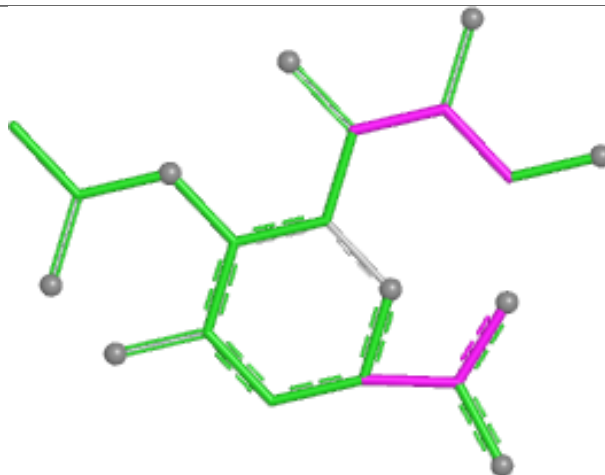


Rings

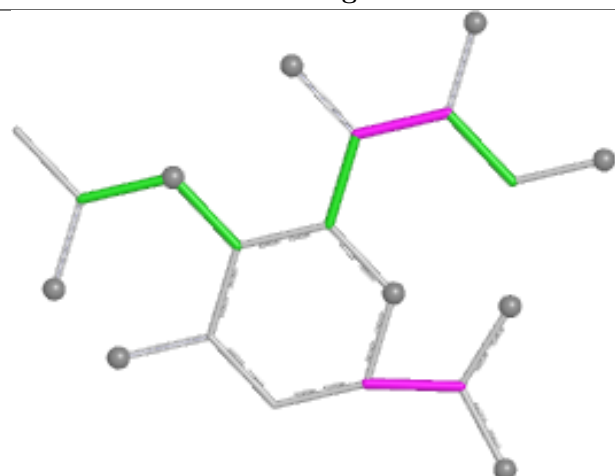
Ligand SLB U 301



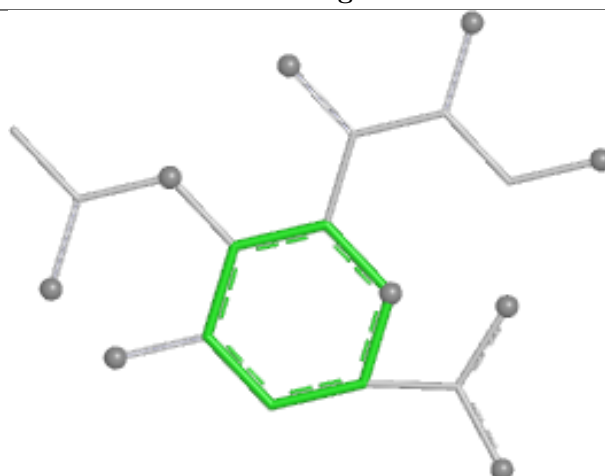
Bond lengths



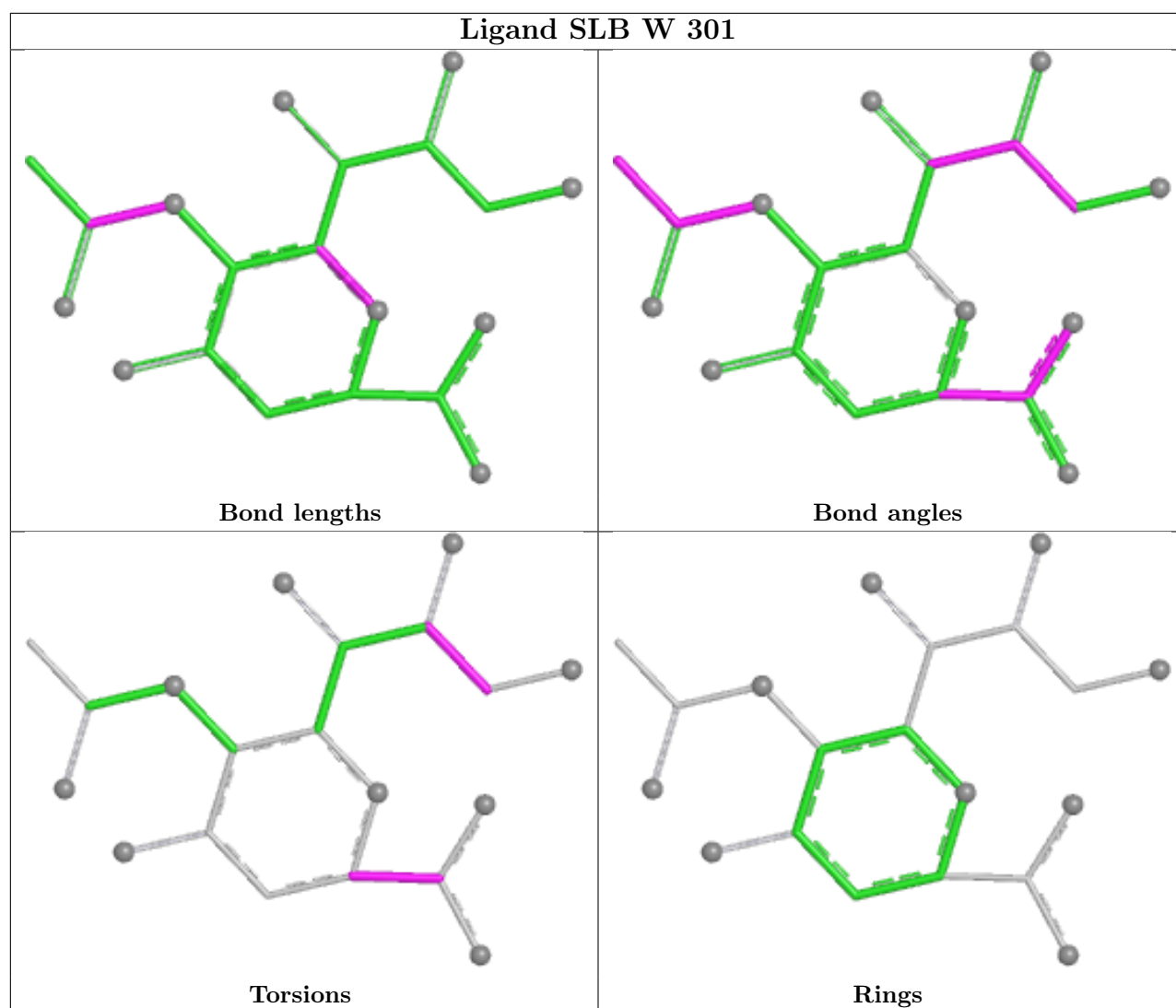
Bond angles



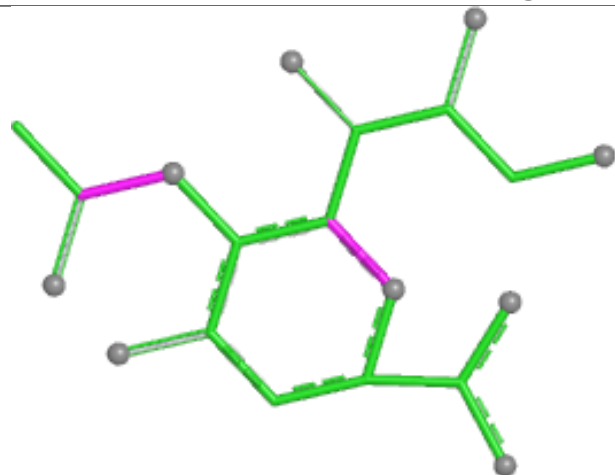
Torsions



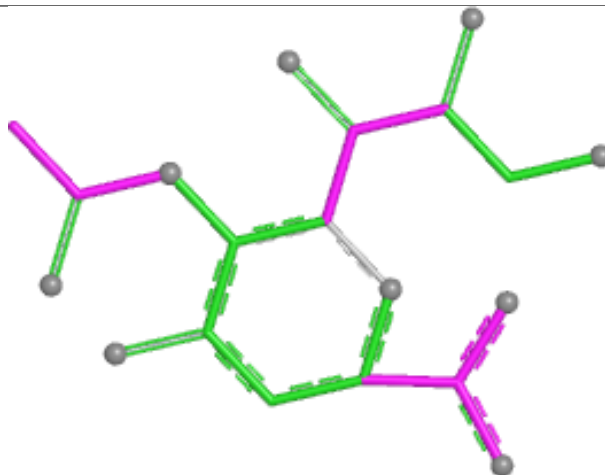
Rings



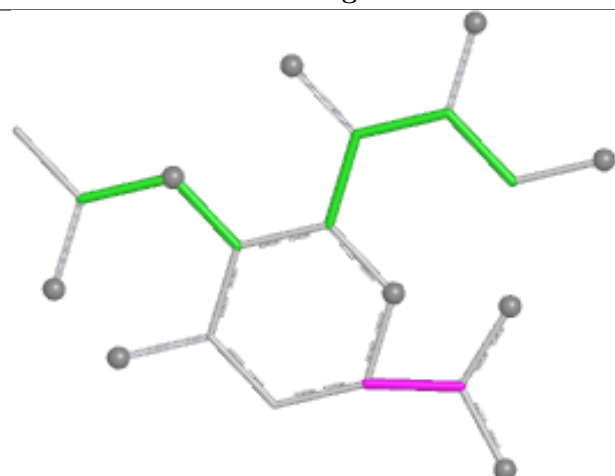
Ligand SLB O 301



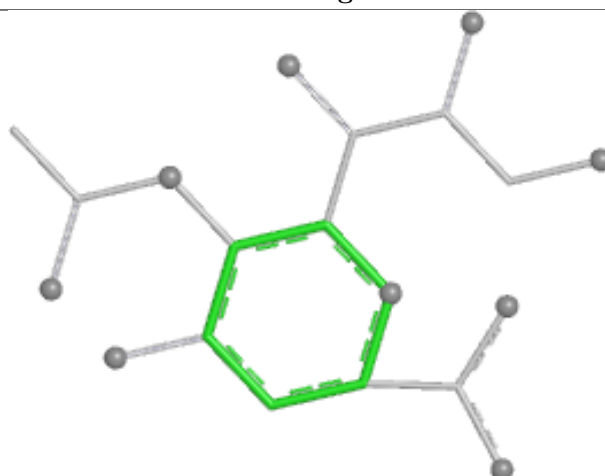
Bond lengths



Bond angles

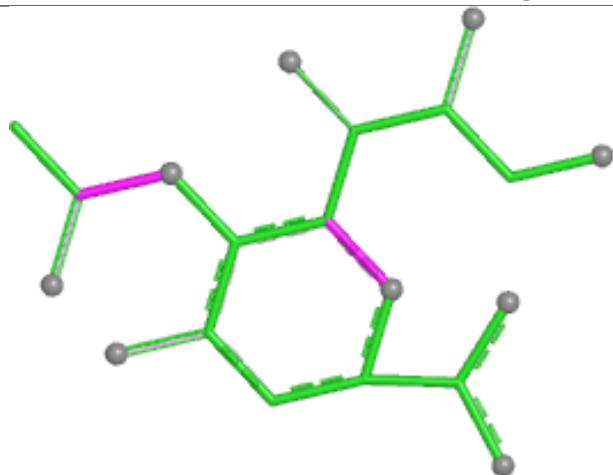


Torsions

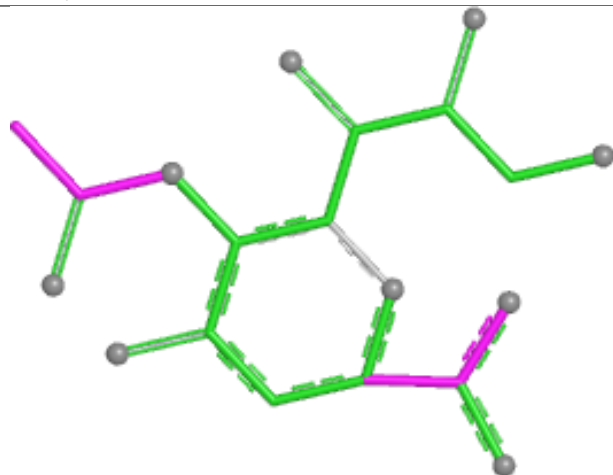


Rings

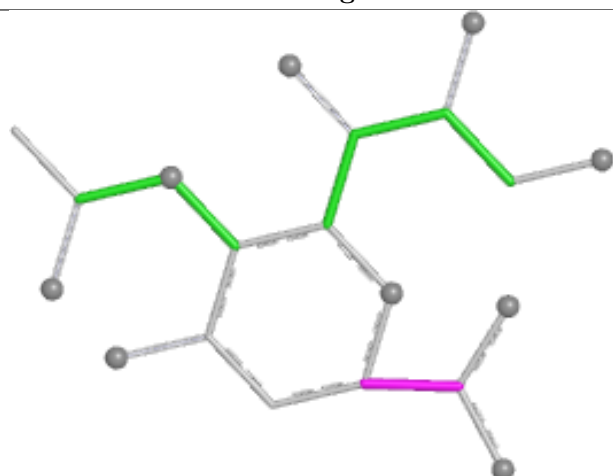
Ligand SLB Q 301



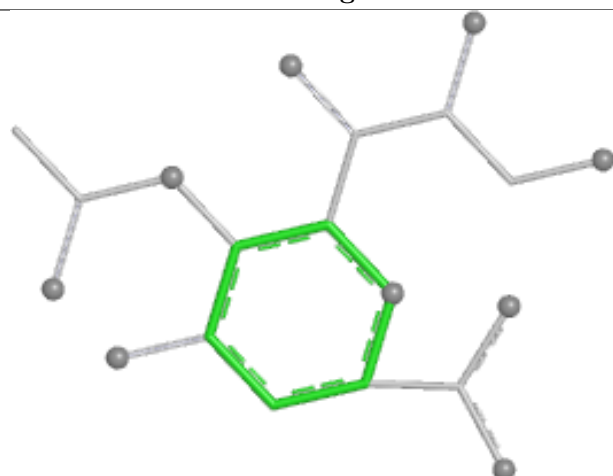
Bond lengths



Bond angles

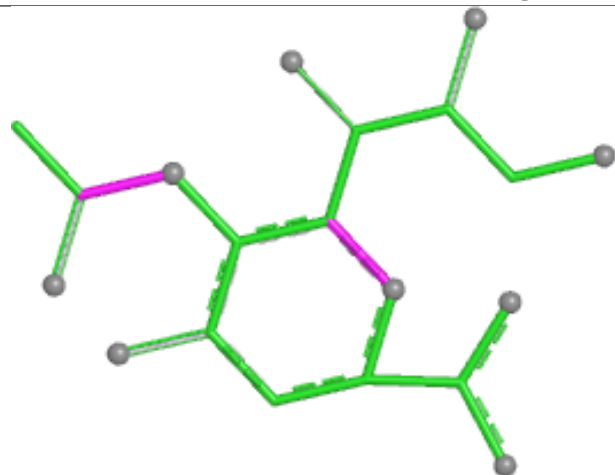


Torsions

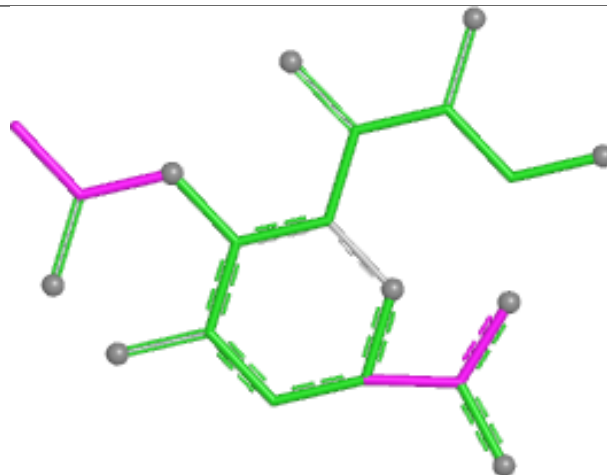


Rings

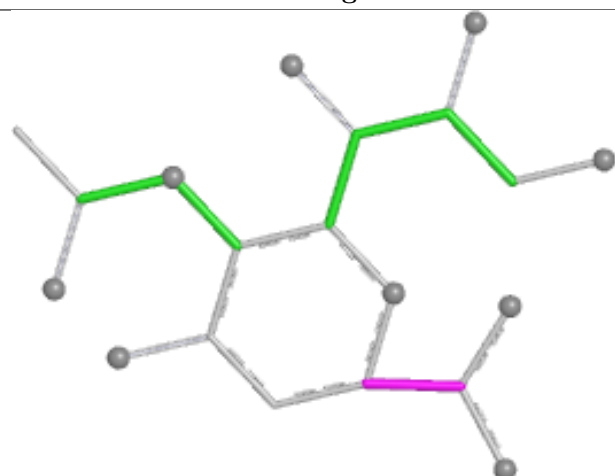
Ligand SLB M 301



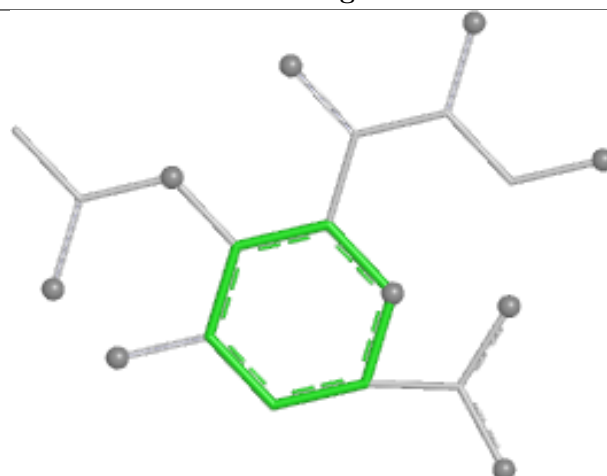
Bond lengths



Bond angles

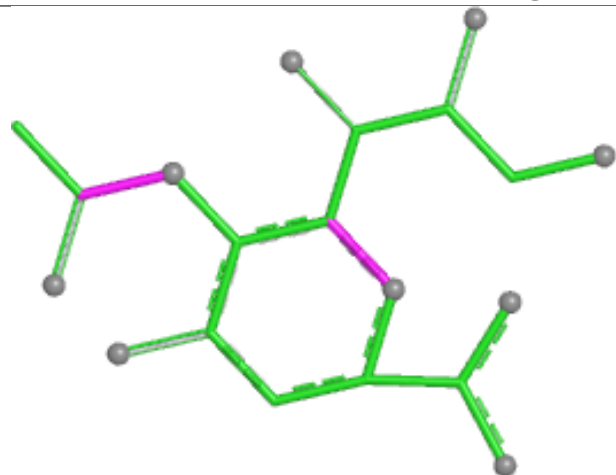


Torsions

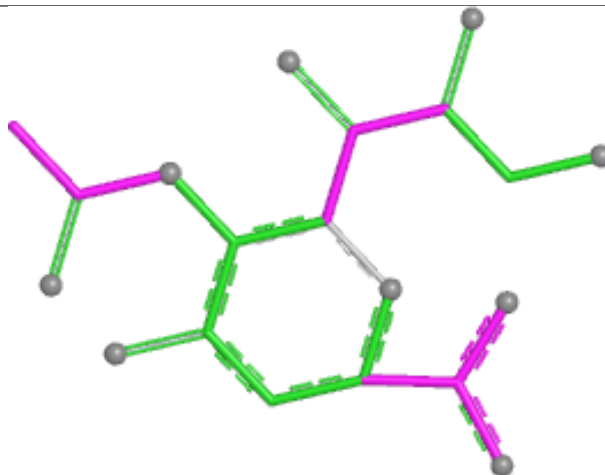


Rings

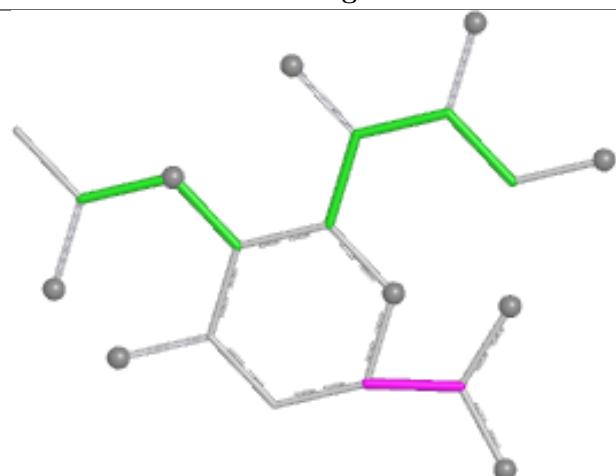
Ligand SLB I 301



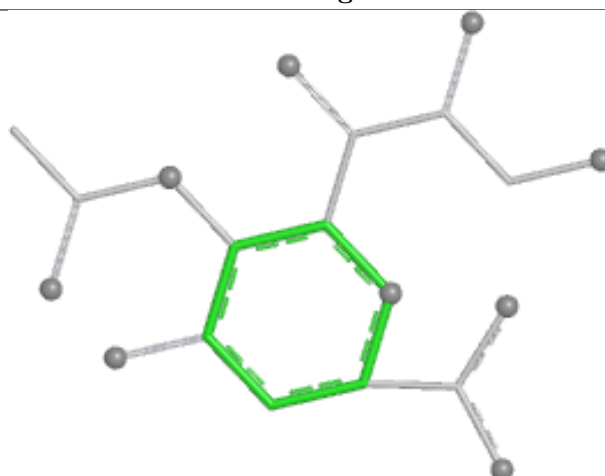
Bond lengths



Bond angles

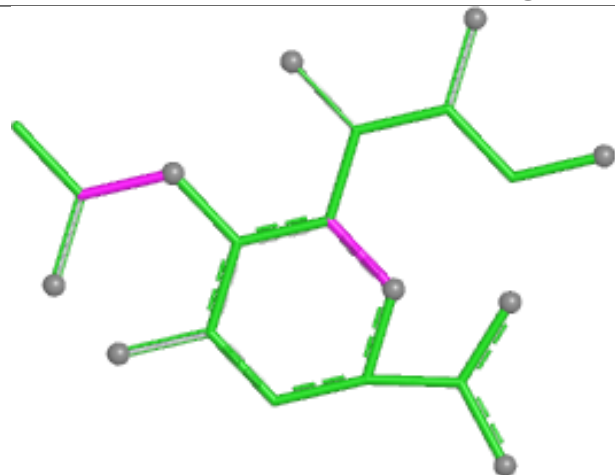


Torsions

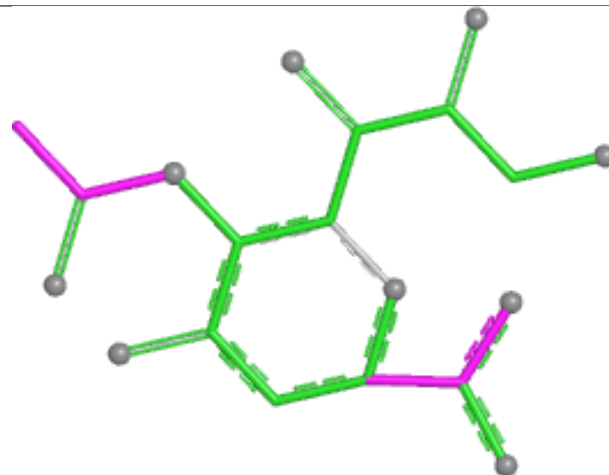


Rings

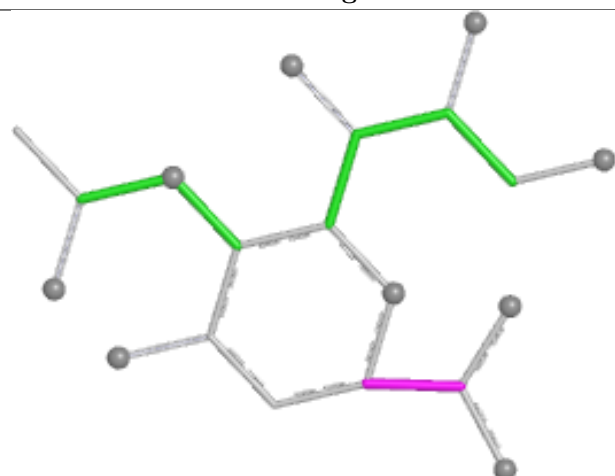
Ligand SLB Y 301



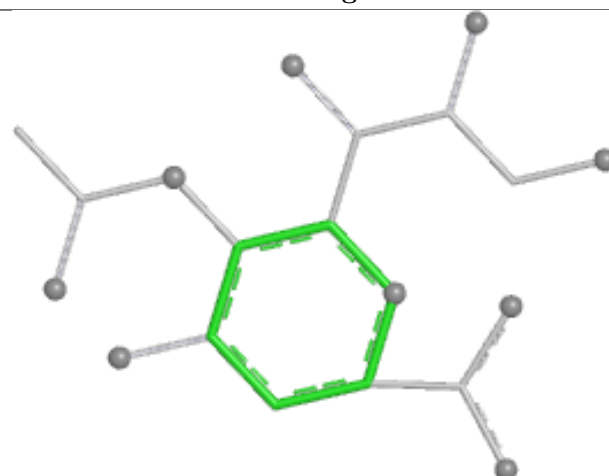
Bond lengths



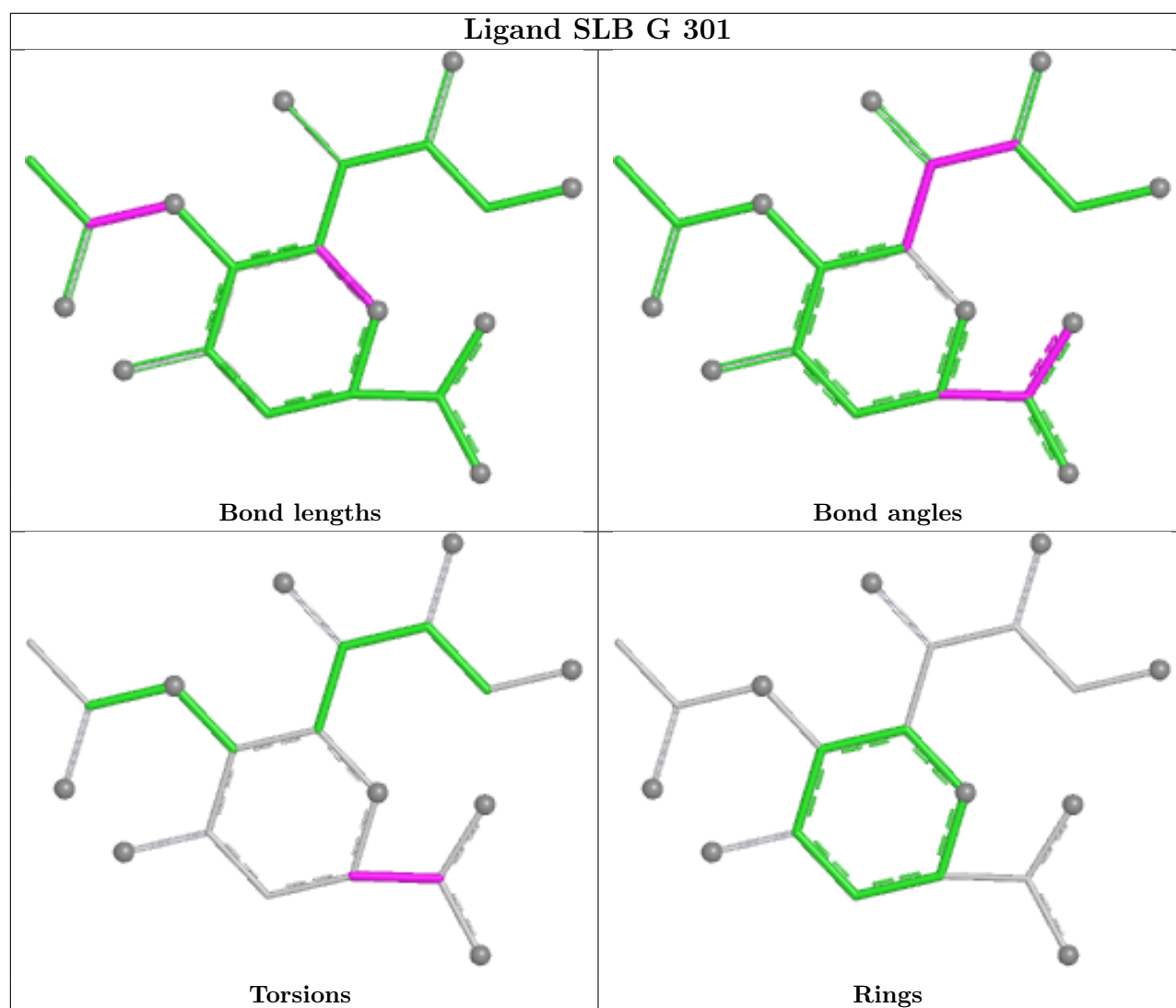
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	299/303 (98%)	1.96	143 (47%) 0 0	37, 82, 117, 133	0
1	C	299/303 (98%)	0.83	24 (8%) 18 13	33, 60, 81, 93	0
1	E	301/303 (99%)	0.19	8 (2%) 56 46	24, 42, 62, 98	0
1	G	299/303 (98%)	0.59	17 (5%) 29 22	27, 56, 81, 93	0
1	I	299/303 (98%)	0.63	14 (4%) 36 28	32, 55, 82, 100	0
1	K	299/303 (98%)	0.99	37 (12%) 8 6	30, 63, 85, 96	0
1	M	299/303 (98%)	0.12	6 (2%) 65 55	26, 42, 58, 77	0
1	O	299/303 (98%)	0.57	18 (6%) 27 20	29, 54, 79, 92	0
1	Q	299/303 (98%)	0.07	2 (0%) 84 78	26, 42, 63, 78	0
1	U	299/303 (98%)	0.25	7 (2%) 61 51	23, 44, 68, 81	0
1	W	299/303 (98%)	0.79	34 (11%) 10 7	32, 61, 88, 103	0
1	Y	299/303 (98%)	0.27	8 (2%) 56 46	23, 45, 70, 91	0
2	B	122/123 (99%)	0.55	10 (8%) 17 12	30, 45, 72, 94	0
2	D	121/123 (98%)	0.52	10 (8%) 17 12	34, 48, 76, 97	0
2	F	123/123 (100%)	0.28	8 (6%) 25 18	25, 40, 74, 92	0
2	H	123/123 (100%)	0.17	7 (5%) 29 22	25, 35, 70, 86	0
2	J	123/123 (100%)	0.48	9 (7%) 21 15	27, 42, 76, 93	0
2	L	123/123 (100%)	0.21	5 (4%) 41 32	28, 38, 67, 83	0
2	N	123/123 (100%)	0.43	12 (9%) 13 9	26, 39, 70, 92	0
2	P	123/123 (100%)	0.13	3 (2%) 59 49	25, 34, 55, 78	0
2	R	123/123 (100%)	-0.05	2 (1%) 70 61	22, 32, 59, 90	0
2	T	123/123 (100%)	0.04	6 (4%) 35 27	23, 34, 59, 92	0
2	V	123/123 (100%)	0.05	6 (4%) 35 27	23, 32, 56, 70	0
2	X	123/123 (100%)	0.06	3 (2%) 59 49	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%)	0.50	399 (7%) 18 13	22, 48, 84, 133	0

All (399) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	V	0	SER	8.2
2	H	42	GLY	5.9
2	L	43	LYS	5.9
1	E	187	LEU	5.8
2	B	0	SER	5.4
1	A	118	ASP	5.4
1	A	273	PHE	5.3
2	J	13	GLN	5.1
1	A	206	HIS	5.1
1	A	265	VAL	5.1
1	A	34	GLU	5.1
1	A	136	ILE	5.1
1	A	133	LEU	4.9
1	A	158	LEU	4.8
1	A	202	LEU	4.8
1	A	266	THR	4.7
1	A	254	LEU	4.7
2	B	101	PHE	4.6
1	W	2	THR	4.5
1	A	134	ASN	4.5
1	A	84	TYR	4.5
1	A	32	GLN	4.4
1	G	1	ALA	4.4
1	A	258	PHE	4.3
2	L	42	GLY	4.2
1	A	281	TYR	4.2
1	A	211	ASP	4.2
1	A	159	SER	4.1
2	R	-1	GLY	4.1
2	F	113	GLN	4.1
1	A	27	LEU	4.1
1	A	260	SER	4.0
1	A	285	ASP	4.0
1	A	205	THR	4.0
1	A	132	PRO	4.0
1	K	28	GLU	4.0
1	A	246	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	O	263	ILE	3.9
1	W	195	PHE	3.9
1	A	1	ALA	3.9
1	Y	133	LEU	3.9
2	N	12	VAL	3.9
1	E	-1	MET	3.9
1	A	116	ALA	3.9
2	H	107	LYS	3.8
1	A	270	LEU	3.8
2	V	-1	GLY	3.8
1	A	35	ILE	3.8
1	C	81	MET	3.8
2	J	107	LYS	3.8
2	L	45	ARG	3.8
1	A	238	LYS	3.8
1	W	1	ALA	3.8
2	N	40	ALA	3.7
1	A	201	ASN	3.7
1	A	282	LYS	3.7
1	A	138	ASP	3.7
1	A	87	LYS	3.7
1	U	159	SER	3.7
1	W	237	GLN	3.7
1	C	274	ARG	3.7
1	A	26	THR	3.7
1	A	255	VAL	3.6
1	A	263	ILE	3.6
1	W	159	SER	3.6
2	H	-1	GLY	3.6
1	W	3	THR	3.6
1	A	22	MET	3.6
1	A	139	PHE	3.6
1	O	262	GLY	3.6
1	E	275	GLU	3.6
1	A	155	TYR	3.5
1	A	272	PRO	3.5
1	I	28	GLU	3.5
1	K	182	GLY	3.5
1	A	120	TRP	3.5
2	F	41	PRO	3.5
1	K	148	ASN	3.5
1	A	161	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	127	THR	3.5
1	A	86	ALA	3.5
1	G	148	ASN	3.5
1	K	203	ALA	3.5
1	Y	113	ASN	3.5
1	W	128	THR	3.4
1	A	92	LEU	3.4
1	A	251	GLU	3.4
1	A	248	LYS	3.4
1	O	182	GLY	3.4
2	P	-1	GLY	3.4
2	J	41	PRO	3.4
1	K	35	ILE	3.4
1	K	245	GLN	3.4
1	C	254	LEU	3.3
1	A	277	MET	3.3
1	A	203	ALA	3.3
1	O	1	ALA	3.3
2	T	13	GLN	3.3
2	D	121	SER	3.3
1	A	204	MET	3.3
1	W	193	MET	3.3
2	R	113	GLN	3.3
2	B	121	SER	3.3
1	A	181	ASP	3.2
1	A	264	ASN	3.2
1	A	297	ALA	3.2
1	C	291	PRO	3.2
1	A	130	ASN	3.2
2	N	43	LYS	3.2
1	A	15	VAL	3.2
1	M	215	ILE	3.2
1	A	252	ALA	3.1
2	B	13	GLN	3.1
1	C	77	ALA	3.1
1	A	245	GLN	3.1
2	X	113	GLN	3.1
1	A	141	GLY	3.1
2	N	42	GLY	3.1
1	A	231	ILE	3.1
2	L	44	GLU	3.1
1	A	119	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	85	VAL	3.1
1	A	129	SER	3.1
1	C	32	GLN	3.1
1	I	245	GLN	3.1
2	F	-1	GLY	3.1
1	W	234	LYS	3.1
1	Q	193	MET	3.0
1	A	199	GLN	3.0
2	D	13	GLN	3.0
1	A	247	VAL	3.0
1	A	257	PHE	3.0
1	A	290	GLN	3.0
1	K	212	GLN	3.0
2	D	41	PRO	3.0
2	N	41	PRO	3.0
1	A	90	ASP	3.0
1	M	29	GLU	3.0
1	A	79	ALA	3.0
1	A	189	THR	3.0
1	A	31	SER	2.9
1	A	275	GLU	2.9
2	V	65	ALA	2.9
1	M	238	LYS	2.9
1	W	200	LYS	2.9
2	D	42	GLY	2.9
1	A	102	GLN	2.9
1	A	278	GLN	2.9
1	E	197	GLU	2.9
1	C	148	ASN	2.9
2	N	0	SER	2.9
1	C	276	ALA	2.9
1	Q	87	LYS	2.9
2	N	54	THR	2.9
1	C	290	GLN	2.9
1	A	236	VAL	2.9
1	A	82	LEU	2.9
1	E	0	GLY	2.9
1	A	222	GLN	2.9
1	A	81	MET	2.8
1	E	97	GLU	2.8
1	M	180	VAL	2.8
1	A	200	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	Y	275	GLU	2.8
1	U	274	ARG	2.8
2	J	42	GLY	2.8
1	K	1	ALA	2.8
1	K	161	ALA	2.8
1	A	207	HIS	2.8
2	B	25	SER	2.8
1	A	157	LYS	2.8
2	J	-1	GLY	2.8
1	O	32	GLN	2.8
1	A	126	GLU	2.8
1	C	296	LEU	2.8
1	A	21	LYS	2.8
1	A	83	PRO	2.8
2	N	13	GLN	2.7
1	I	174	ALA	2.7
1	A	249	THR	2.7
2	D	113	GLN	2.7
1	W	255	VAL	2.7
1	A	142	LEU	2.7
1	A	235	ALA	2.7
1	W	264	ASN	2.7
1	C	135	SER	2.7
1	O	31	SER	2.7
1	K	233	GLN	2.7
2	F	40	ALA	2.7
1	A	162	SER	2.7
1	A	293	VAL	2.7
2	V	44	GLU	2.7
1	A	186	PRO	2.7
1	I	289	GLY	2.7
1	O	180	VAL	2.7
2	L	107	LYS	2.6
1	A	262	GLY	2.6
2	F	121	SER	2.6
1	A	221	TRP	2.6
1	A	140	LYS	2.6
1	A	143	LYS	2.6
1	G	87	LYS	2.6
1	G	134	ASN	2.6
2	H	43	LYS	2.6
1	K	159	SER	2.6

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Mol	Chain	Res	Type	RSRZ
2	N	45	ARG	2.6
1	A	220	THR	2.6
1	A	208	ILE	2.6
1	G	34	GLU	2.6
1	O	35	ILE	2.6
1	O	30	MET	2.6
1	O	110	GLN	2.6
2	P	44	GLU	2.6
1	C	295	LYS	2.6
1	A	33	GLY	2.6
1	W	196	TYR	2.6
2	T	112	GLY	2.6
1	I	30	MET	2.6
1	M	197	GLU	2.6
1	A	67	PHE	2.6
1	M	237	GLN	2.5
1	A	223	LYS	2.5
2	H	121	SER	2.5
1	G	275	GLU	2.5
2	B	44	GLU	2.5
2	H	13	GLN	2.5
2	V	76	LYS	2.5
1	A	153	LEU	2.5
1	C	255	VAL	2.5
1	U	283	GLU	2.5
2	J	89	GLU	2.5
1	A	276	ALA	2.5
1	G	259	LYS	2.5
1	W	148	ASN	2.5
1	K	202	LEU	2.5
1	G	135	SER	2.5
1	W	258	PHE	2.5
1	A	274	ARG	2.5
1	K	4	LEU	2.4
1	A	209	VAL	2.4
2	V	121	SER	2.4
1	W	253	GLU	2.4
1	C	1	ALA	2.4
1	G	102	GLN	2.4
1	K	122	ASN	2.4
1	C	269	ASP	2.4
1	I	211	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	W	58	GLY	2.4
1	I	271	GLU	2.4
2	N	107	LYS	2.4
2	J	113	GLN	2.4
2	T	113	GLN	2.4
1	K	2	THR	2.4
1	C	134	ASN	2.4
1	A	163	PRO	2.4
1	A	123	GLY	2.4
1	K	12	VAL	2.4
1	O	282	LYS	2.4
1	K	27	LEU	2.4
1	Y	202	LEU	2.4
1	I	178	ASN	2.4
1	I	234	LYS	2.4
1	W	259	LYS	2.4
1	W	274	ARG	2.4
2	X	43	LYS	2.4
1	A	135	SER	2.4
1	A	64	TYR	2.4
1	W	192	THR	2.4
1	K	191	LYS	2.3
2	F	43	LYS	2.3
2	B	65	ALA	2.3
2	J	120	SER	2.3
1	A	267	TYR	2.3
1	W	189	THR	2.3
1	O	140	LYS	2.3
2	J	43	LYS	2.3
1	W	13	GLY	2.3
2	N	-1	GLY	2.3
2	T	114	GLY	2.3
1	A	242	ALA	2.3
1	K	116	ALA	2.3
1	A	30	MET	2.3
1	A	233	GLN	2.3
1	A	294	SER	2.3
1	W	173	LEU	2.3
1	K	244	THR	2.3
1	G	272	PRO	2.3
1	G	265	VAL	2.3
1	W	201	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	257	PHE	2.3
2	H	44	GLU	2.3
1	A	175	LEU	2.3
1	A	228	ASP	2.3
1	A	3	THR	2.3
2	T	42	GLY	2.3
1	E	166	MET	2.2
1	A	28	GLU	2.2
1	K	137	GLU	2.2
2	F	44	GLU	2.2
1	O	202	LEU	2.2
1	A	234	LYS	2.2
1	I	215	ILE	2.2
1	A	268	PRO	2.2
1	A	172	TYR	2.2
1	A	224	LEU	2.2
1	A	271	GLU	2.2
1	K	32	GLN	2.2
1	A	241	ASP	2.2
1	I	131	ARG	2.2
1	A	164	THR	2.2
1	A	188	PRO	2.2
1	O	80	VAL	2.2
1	A	11	SER	2.2
1	U	196	TYR	2.2
2	T	-1	GLY	2.2
1	A	89	PHE	2.2
1	K	187	LEU	2.2
1	A	91	HIS	2.2
1	W	293	VAL	2.2
1	A	95	MET	2.2
1	C	22	MET	2.2
1	K	33	GLY	2.2
2	D	112	GLY	2.2
2	N	66	GLY	2.2
1	W	202	LEU	2.2
1	K	253	GLU	2.2
2	X	44	GLU	2.2
1	I	176	GLN	2.2
1	A	279	PRO	2.2
1	K	64	TYR	2.2
1	A	117	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	U	173	LEU	2.2
1	C	253	GLU	2.2
1	Y	1	ALA	2.2
1	Y	137	GLU	2.2
1	W	93	ARG	2.1
1	W	32	GLN	2.1
1	Y	255	VAL	2.1
1	W	30	MET	2.1
1	A	195	PHE	2.1
1	C	196	TYR	2.1
1	A	253	GLU	2.1
1	A	232	ILE	2.1
1	G	288	ILE	2.1
1	A	122	ASN	2.1
1	U	178	ASN	2.1
1	K	293	VAL	2.1
2	B	41	PRO	2.1
1	G	295	LYS	2.1
2	D	54	THR	2.1
1	C	153	LEU	2.1
1	G	139	PHE	2.1
1	I	133	LEU	2.1
1	W	133	LEU	2.1
1	O	203	ALA	2.1
1	O	274	ARG	2.1
1	C	278	GLN	2.1
1	K	207	HIS	2.1
1	K	171	VAL	2.1
2	D	107	LYS	2.1
2	B	42	GLY	2.1
1	Y	131	ARG	2.1
1	C	35	ILE	2.1
1	K	24	ALA	2.1
1	W	35	ILE	2.1
1	U	250	GLN	2.1
1	K	166	MET	2.1
1	C	265	VAL	2.1
1	O	200	LYS	2.1
1	A	227	THR	2.1
1	A	216	ILE	2.1
1	E	267	TYR	2.1
1	A	250	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	107	LYS	2.0
1	A	214	VAL	2.0
1	C	80	VAL	2.0
1	I	173	LEU	2.0
1	K	254	LEU	2.0
1	A	100	PHE	2.0
1	A	131	ARG	2.0
1	A	160	GLY	2.0
1	A	244	THR	2.0
1	W	249	THR	2.0
1	K	172	TYR	2.0
1	K	200	LYS	2.0
1	W	223	LYS	2.0
2	D	43	LYS	2.0
1	G	209	VAL	2.0
1	K	162	SER	2.0
1	G	133	LEU	2.0
1	W	158	LEU	2.0
1	K	139	PHE	2.0
2	F	42	GLY	2.0
1	O	266	THR	2.0
2	D	87	LYS	2.0
2	P	46	GLU	2.0
1	A	299	MET	2.0
1	A	196	TYR	2.0
1	G	267	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

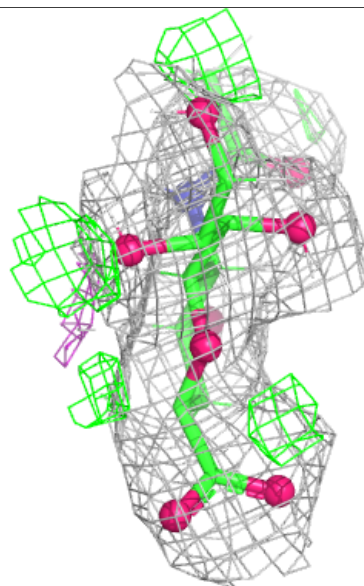
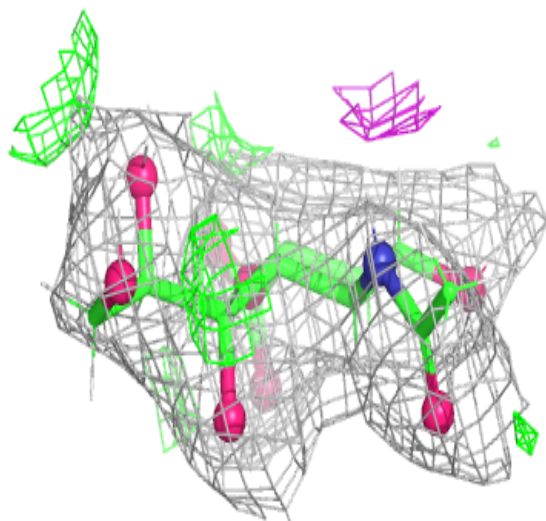
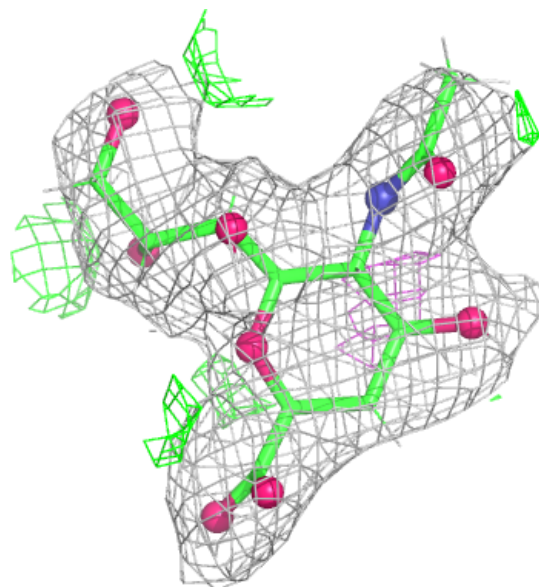
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	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
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.

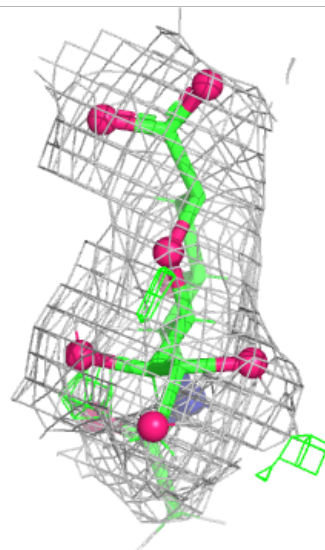
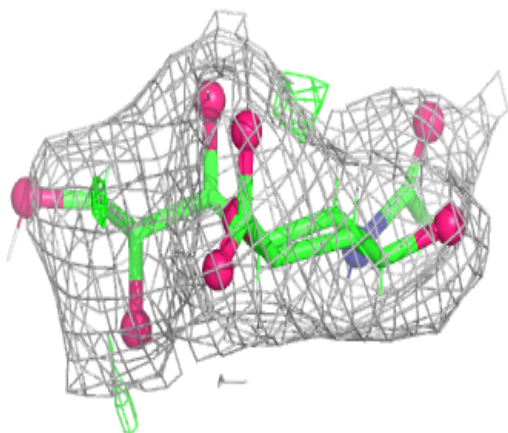
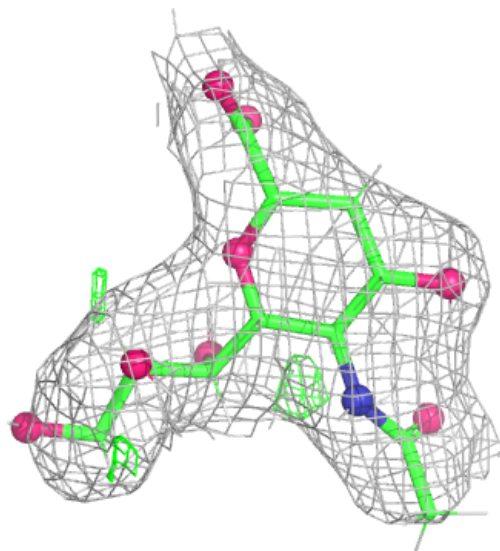
Electron density around SLB K 301:

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



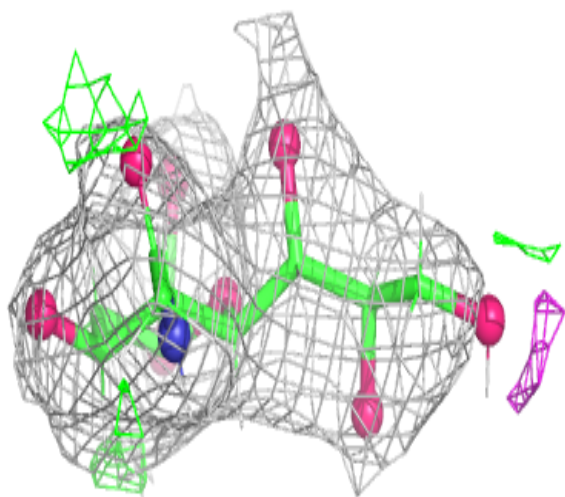
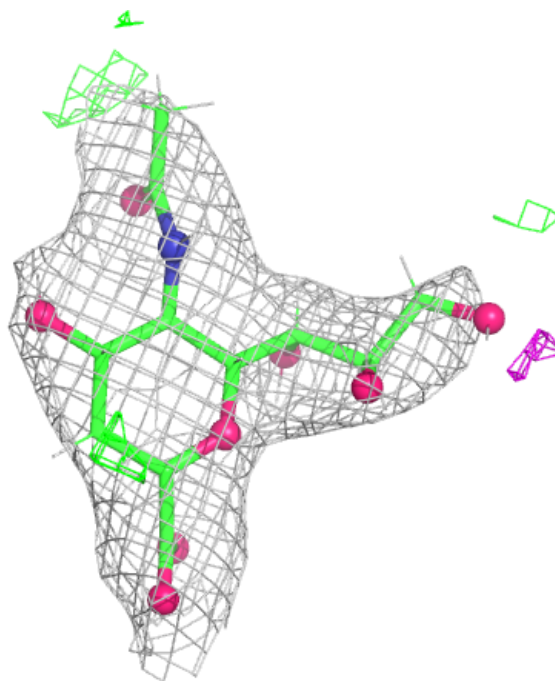
Electron density around SLB W 301:

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



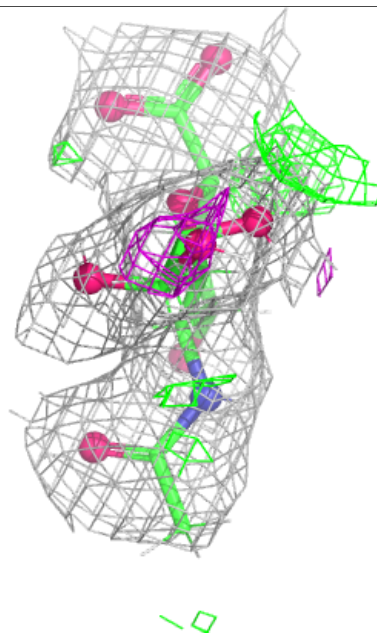
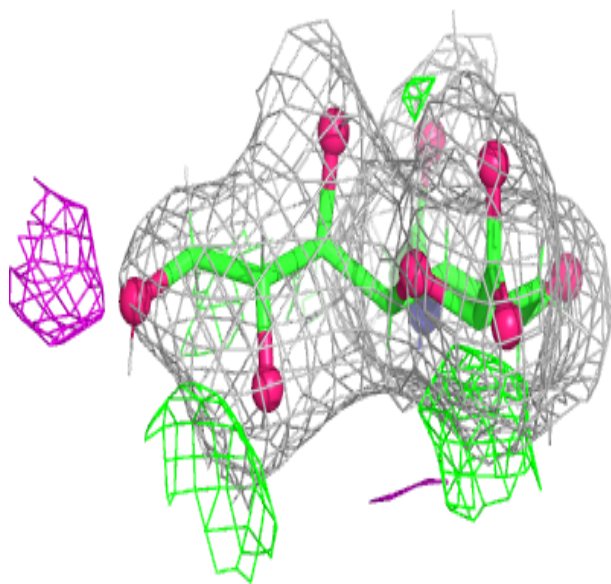
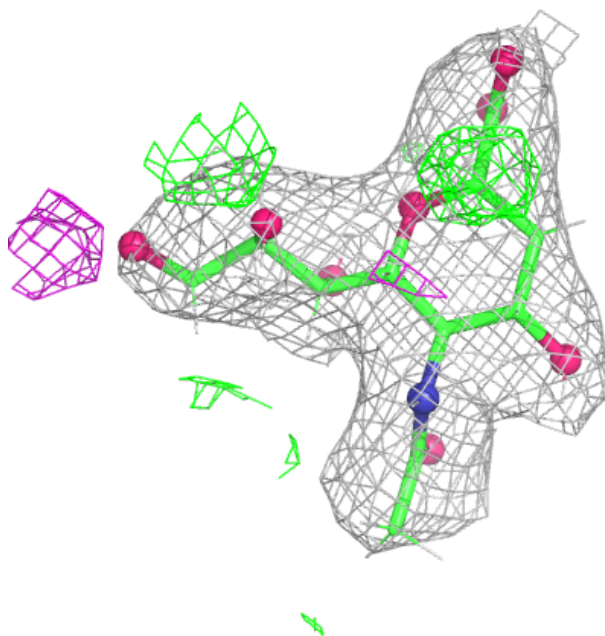
Electron density around SLB A 301:

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



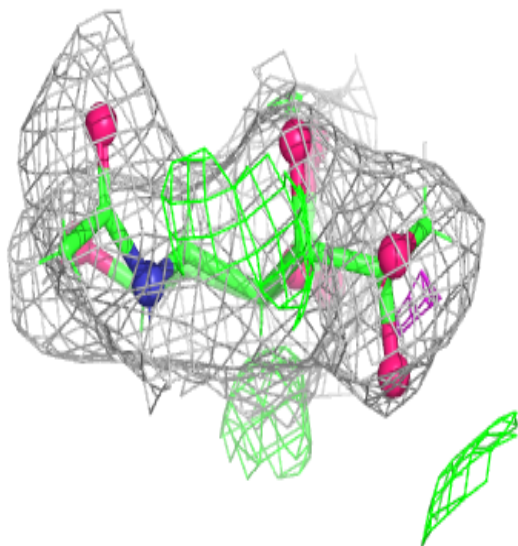
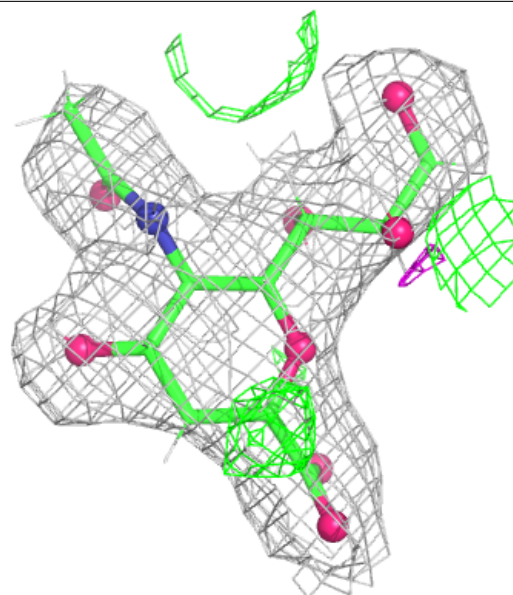
Electron density around SLB U 301:

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



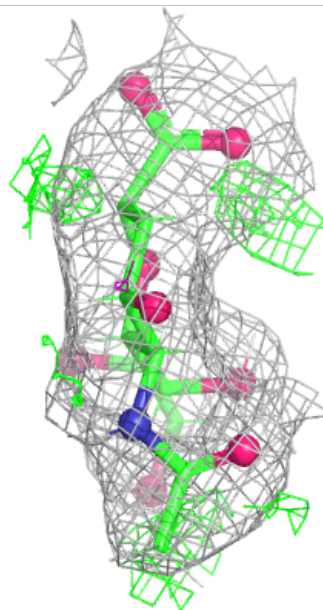
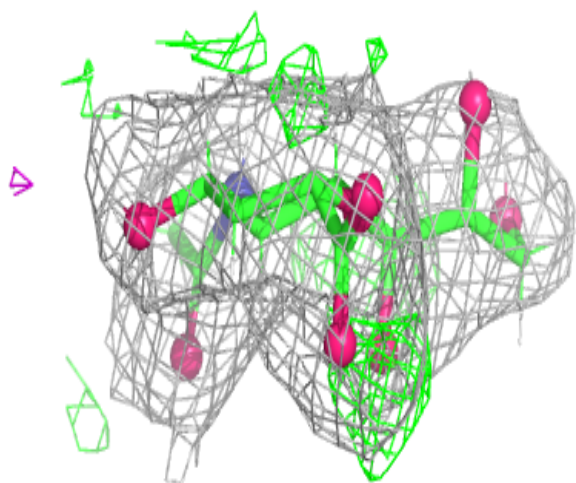
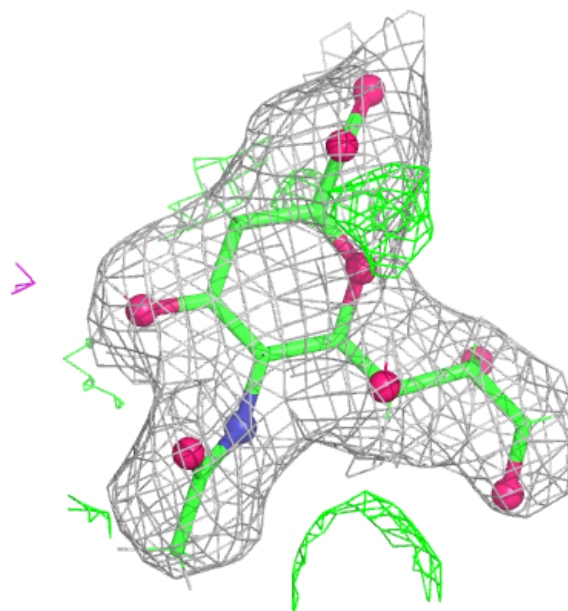
Electron density around SLB E 301:

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



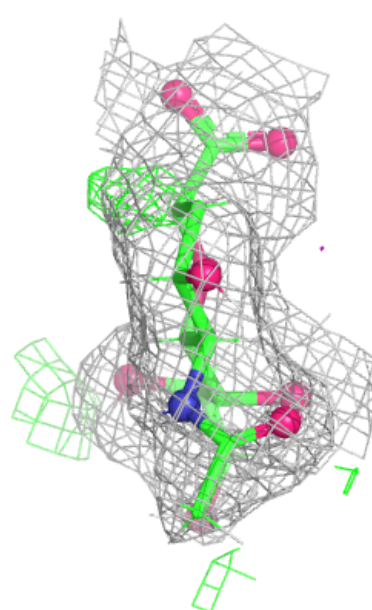
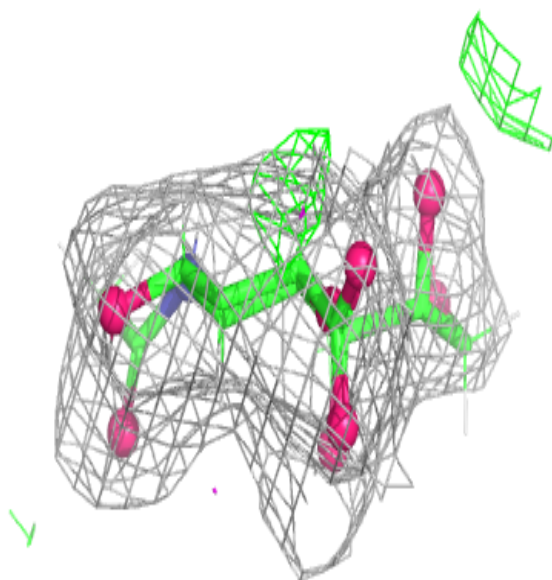
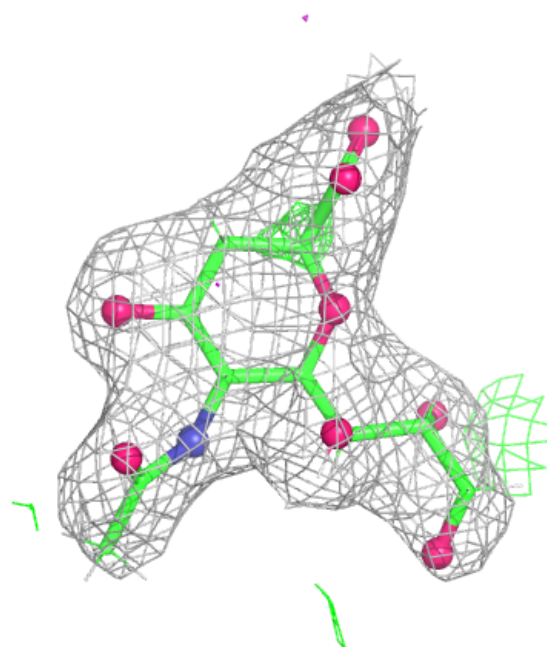
Electron density around SLB M 301:

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



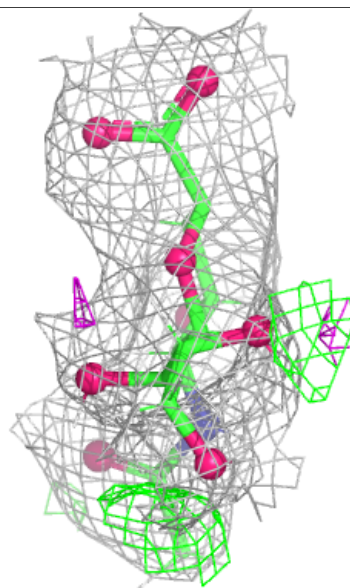
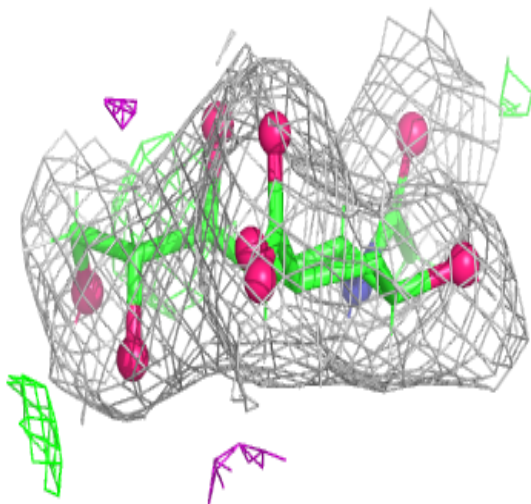
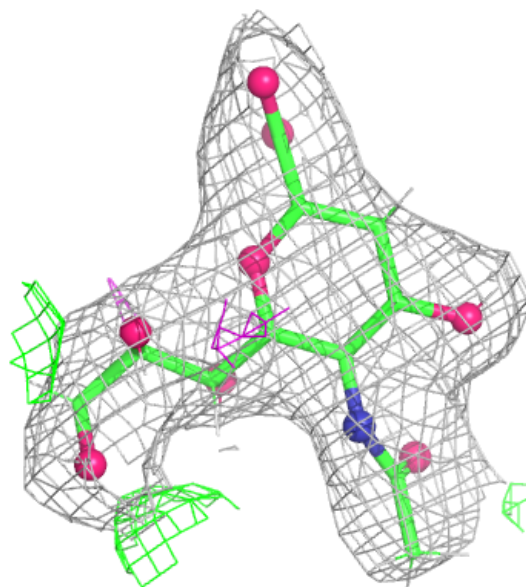
Electron density around SLB I 301:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



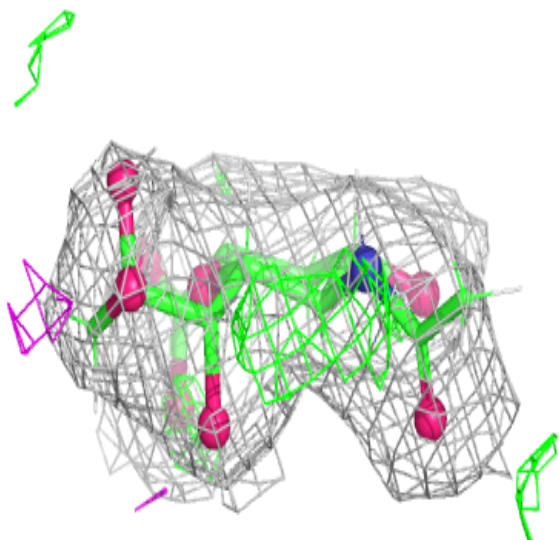
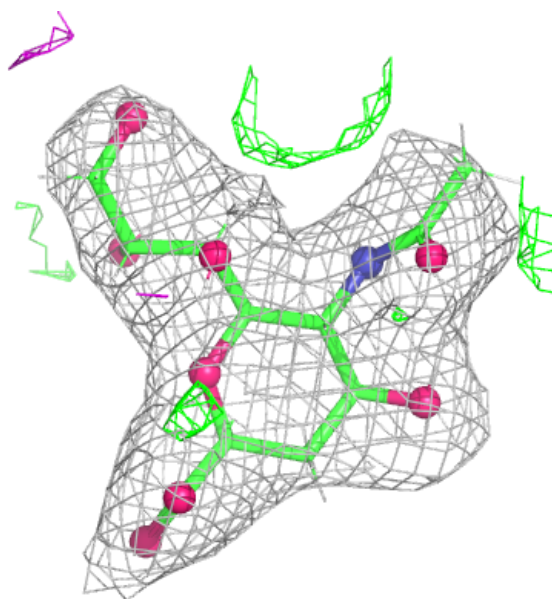
Electron density around SLB C 301:

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



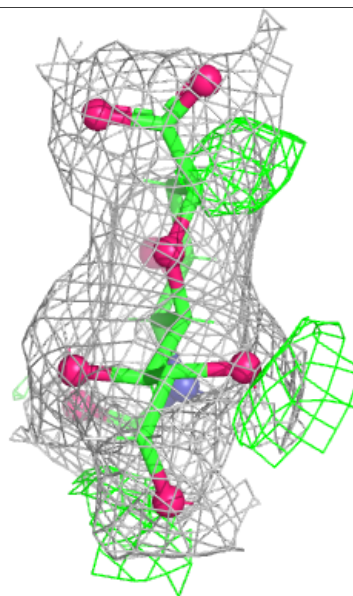
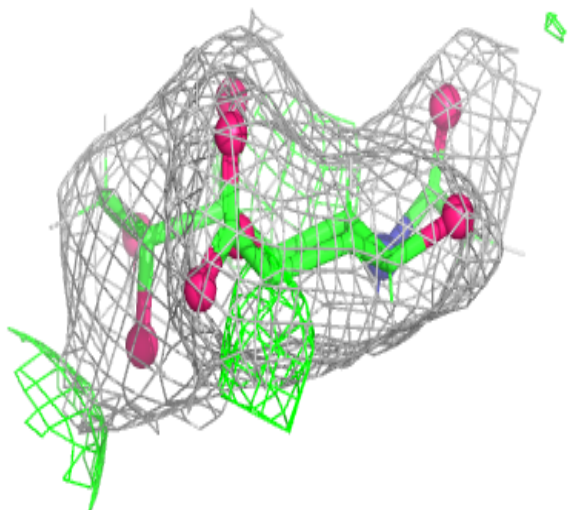
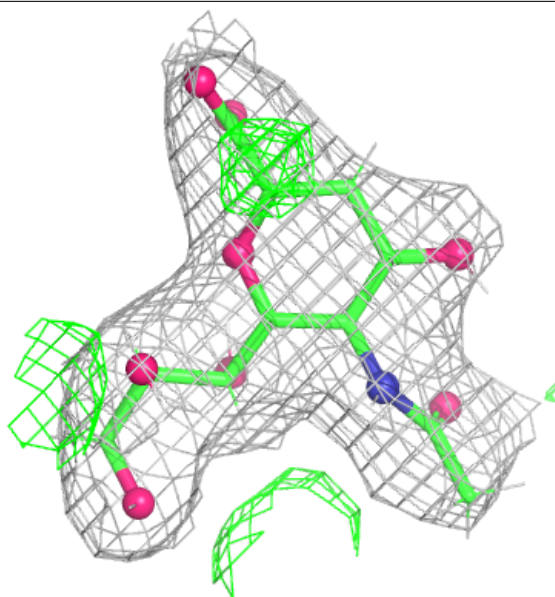
Electron density around SLB G 301:

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



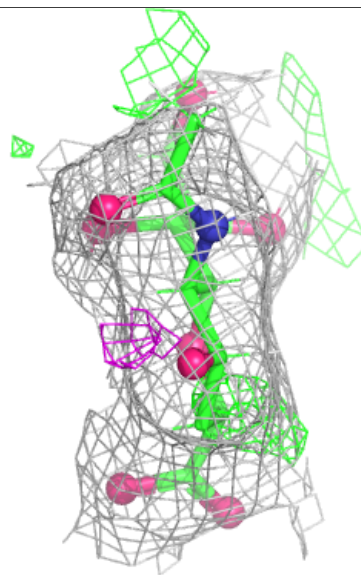
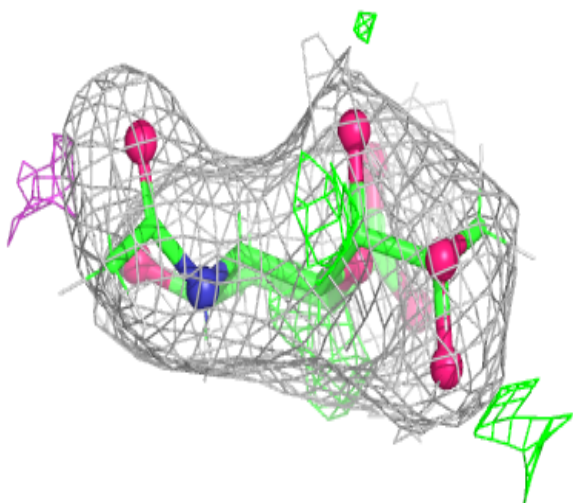
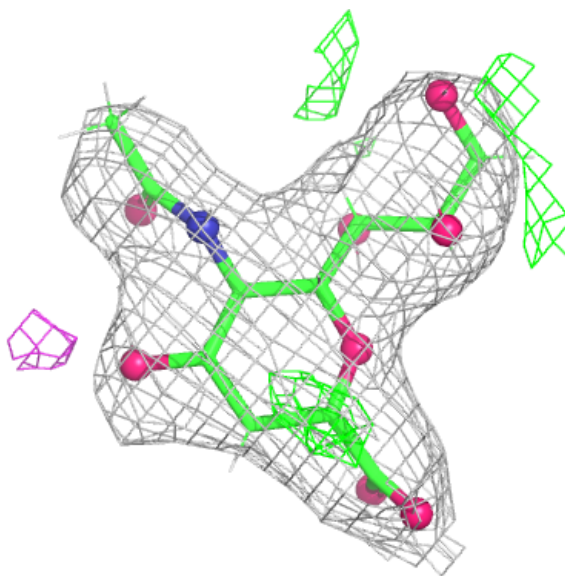
Electron density around SLB Q 301:

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



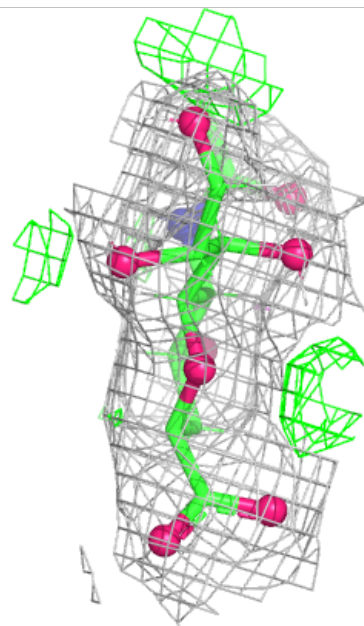
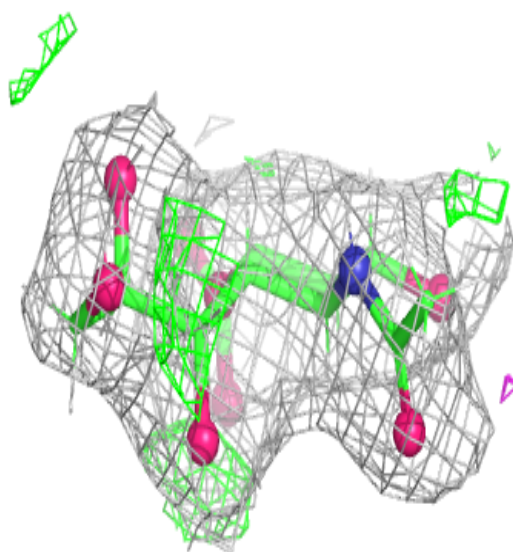
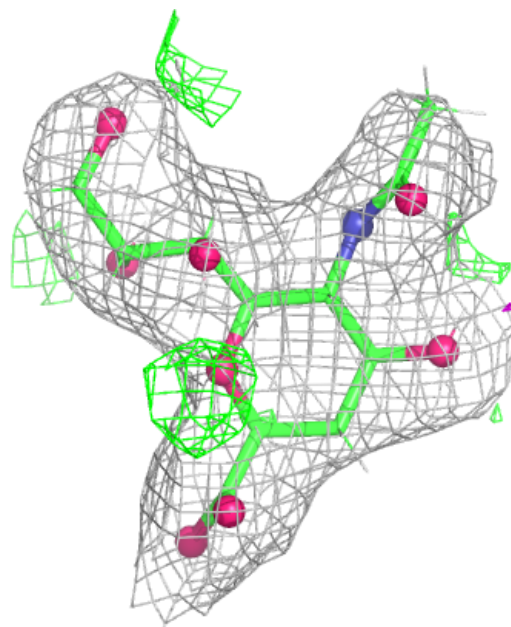
Electron density around SLB O 301:

$2mF_o-DF_c$ (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.