



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2025 – 09:29 PM EDT

PDB ID : 2A5H
Title : 2.1 Angstrom X-ray crystal structure of lysine-2,3-aminomutase from Clostridium subterminale SB4, with Michaelis analog (L-alpha-lysine external aldimine form of pyridoxal-5'-phosphate).
Authors : Lepore, B.W.; Ruzicka, F.J.; Frey, P.A.; Ringe, D.
Deposited on : 2005-06-30
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

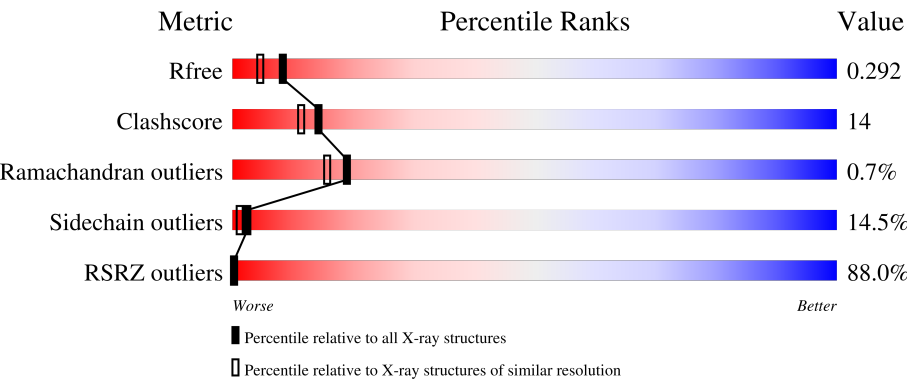
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	416	<div><div>86%</div><div><div>68%</div><div>22%</div><div>7%</div><div>..</div></div></div>
1	B	416	<div><div>90%</div><div><div>67%</div><div>24%</div><div>6%</div><div>..</div></div></div>
1	C	416	<div><div>82%</div><div><div>67%</div><div>23%</div><div>7%</div><div>..</div></div></div>
1	D	416	<div><div>80%</div><div><div>66%</div><div>24%</div><div>7%</div><div>..</div></div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14034 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called L-lysine 2,3-aminomutase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	Se	28	9	0
			3285	2067	591	607	11	9			
1	B	410	Total	C	N	O	S	Se	21	8	0
			3288	2071	589	608	11	9			
1	C	409	Total	C	N	O	S	Se	23	8	0
			3280	2065	588	607	11	9			
1	D	410	Total	C	N	O	S	Se	17	9	0
			3297	2074	595	608	11	9			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	GB 5410603
A	57	MSE	MET	modified residue	GB 5410603
A	124	MSE	MET	modified residue	GB 5410603
A	127	MSE	MET	modified residue	GB 5410603
A	145	MSE	MET	modified residue	GB 5410603
A	147	MSE	MET	modified residue	GB 5410603
A	218	MSE	MET	modified residue	GB 5410603
A	272	MSE	MET	modified residue	GB 5410603
A	341	MSE	MET	modified residue	GB 5410603
A	400	MSE	MET	modified residue	GB 5410603
B	1	MSE	MET	modified residue	GB 5410603
B	57	MSE	MET	modified residue	GB 5410603
B	124	MSE	MET	modified residue	GB 5410603
B	127	MSE	MET	modified residue	GB 5410603
B	145	MSE	MET	modified residue	GB 5410603
B	147	MSE	MET	modified residue	GB 5410603
B	218	MSE	MET	modified residue	GB 5410603
B	272	MSE	MET	modified residue	GB 5410603
B	341	MSE	MET	modified residue	GB 5410603
B	400	MSE	MET	modified residue	GB 5410603
C	1	MSE	MET	modified residue	GB 5410603

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Chain	Residue	Modelled	Actual	Comment	Reference
C	57	MSE	MET	modified residue	GB 5410603
C	124	MSE	MET	modified residue	GB 5410603
C	127	MSE	MET	modified residue	GB 5410603
C	145	MSE	MET	modified residue	GB 5410603
C	147	MSE	MET	modified residue	GB 5410603
C	218	MSE	MET	modified residue	GB 5410603
C	272	MSE	MET	modified residue	GB 5410603
C	341	MSE	MET	modified residue	GB 5410603
C	400	MSE	MET	modified residue	GB 5410603
D	1	MSE	MET	modified residue	GB 5410603
D	57	MSE	MET	modified residue	GB 5410603
D	124	MSE	MET	modified residue	GB 5410603
D	127	MSE	MET	modified residue	GB 5410603
D	145	MSE	MET	modified residue	GB 5410603
D	147	MSE	MET	modified residue	GB 5410603
D	218	MSE	MET	modified residue	GB 5410603
D	272	MSE	MET	modified residue	GB 5410603
D	341	MSE	MET	modified residue	GB 5410603
D	400	MSE	MET	modified residue	GB 5410603

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

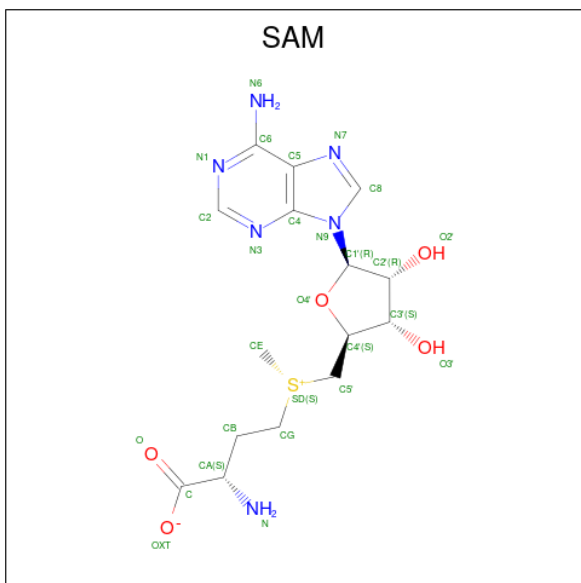
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



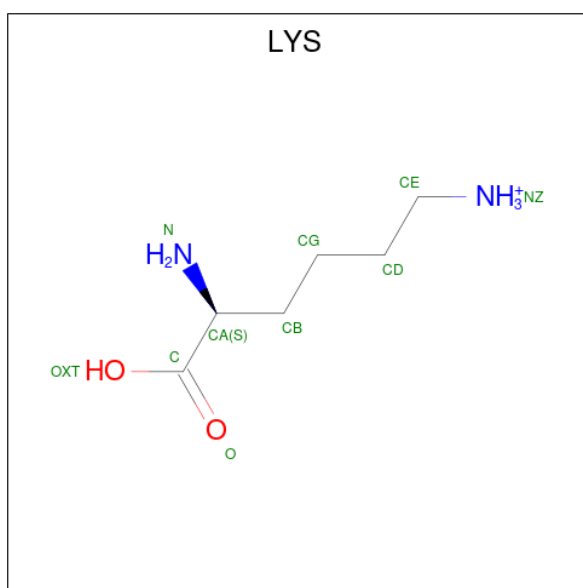
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



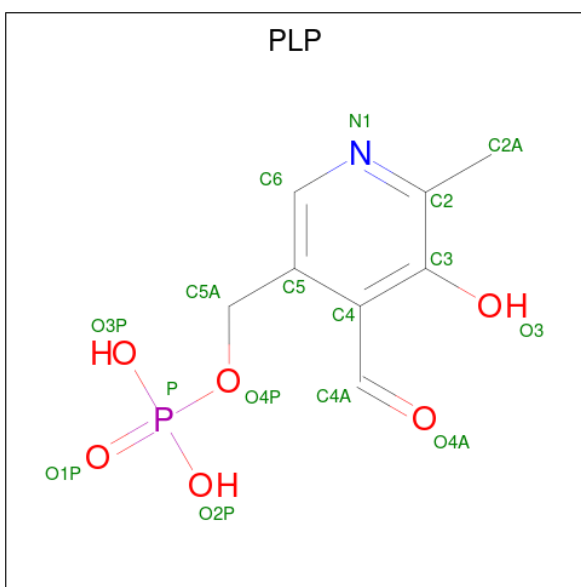
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	D	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 5 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).



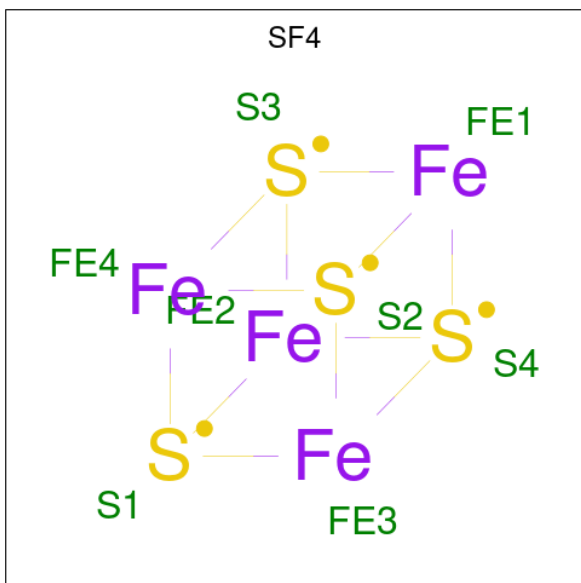
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	1
			13	9	2	2		
5	B	1	Total	C	N	O	0	1
			13	9	2	2		
5	C	1	Total	C	N	O	0	1
			13	9	2	2		
5	D	1	Total	C	N	O	0	1
			13	9	2	2		

- Molecule 6 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
6	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
6	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
6	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 8	Fe 4	S 4	0	0
7	B	1	Total 8	Fe 4	S 4	0	0
7	C	1	Total 8	Fe 4	S 4	0	0
7	D	1	Total 8	Fe 4	S 4	0	0

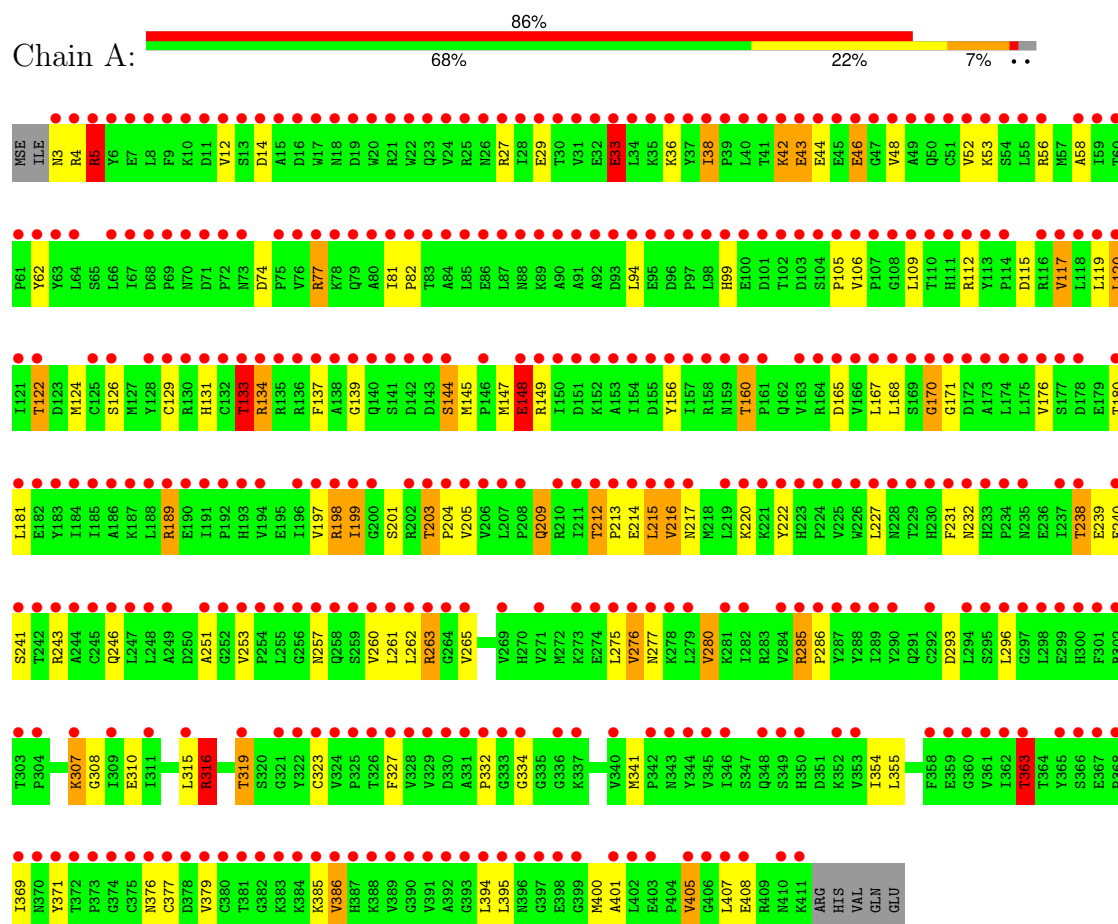
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	135	Total 135	O 135	0	0
8	B	116	Total 116	O 116	0	0
8	C	183	Total 183	O 183	0	0
8	D	174	Total 174	O 174	0	0

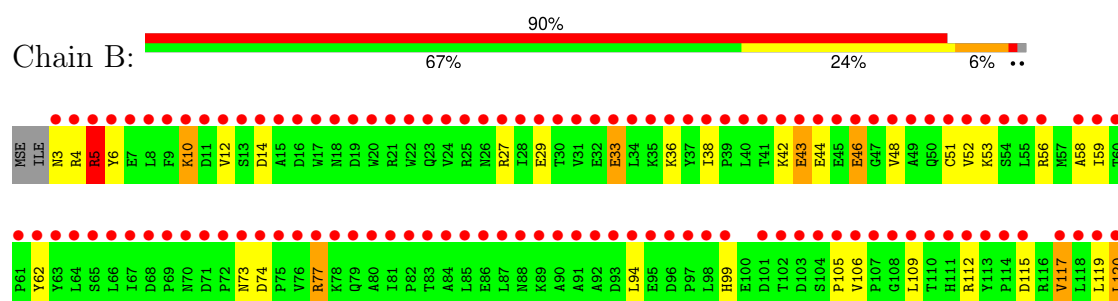
3 Residue-property plots

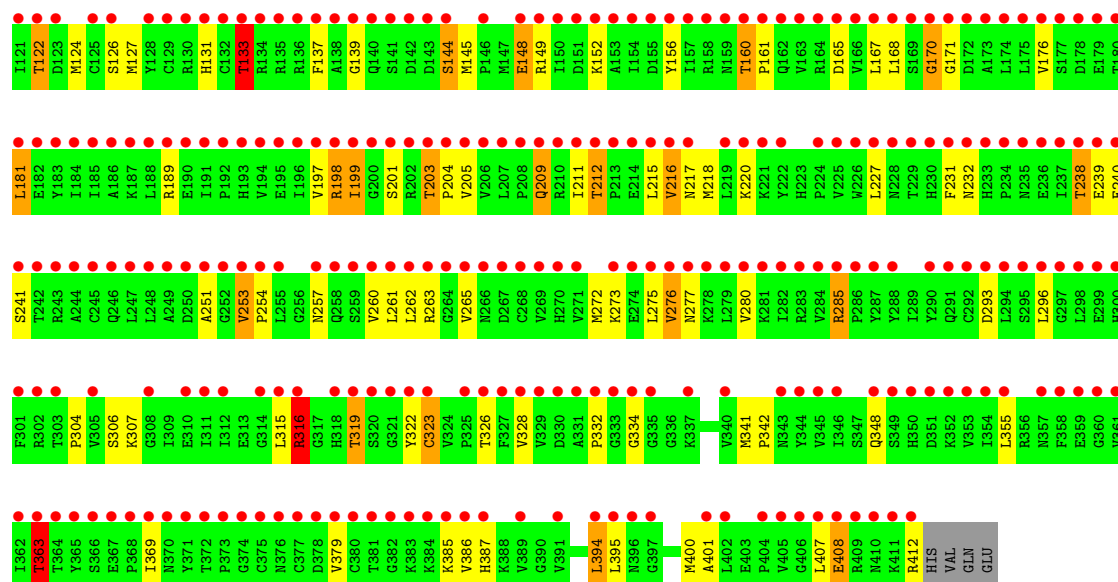
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: L-lysine 2,3-aminomutase

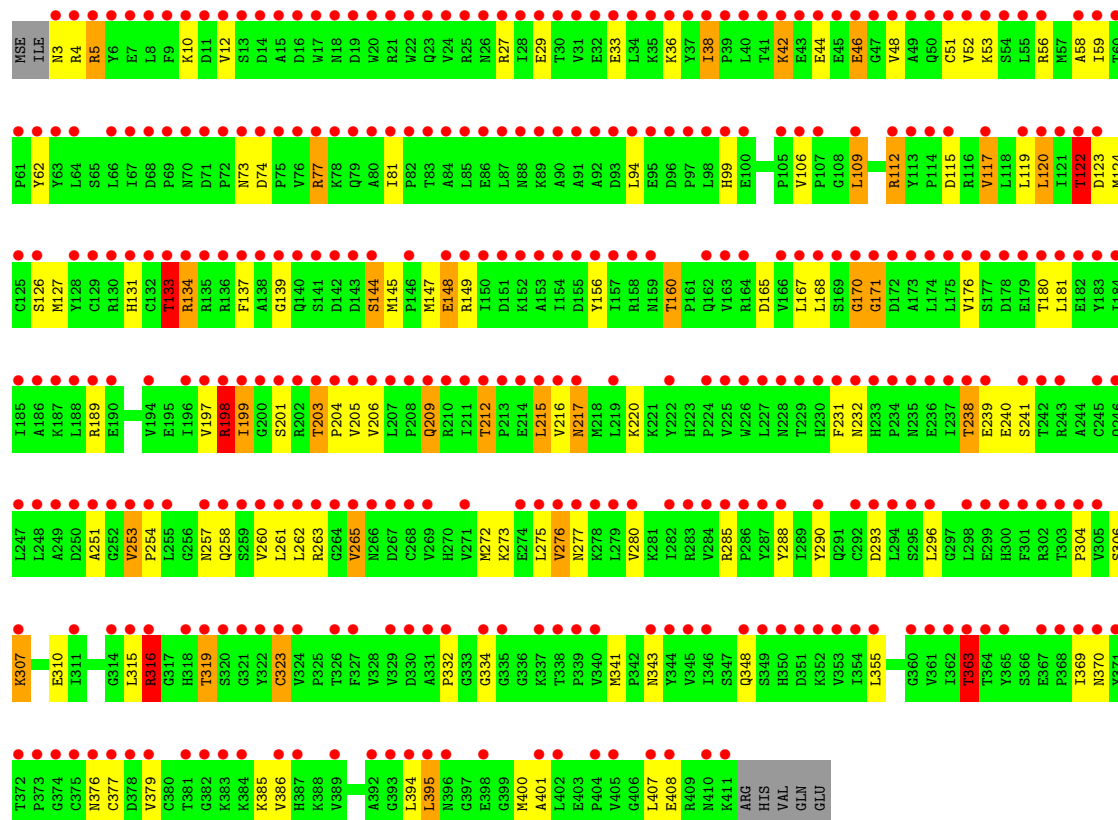
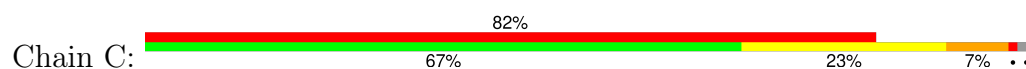


• Molecule 1: L-lysine 2,3-aminomutase

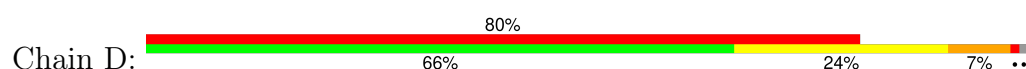


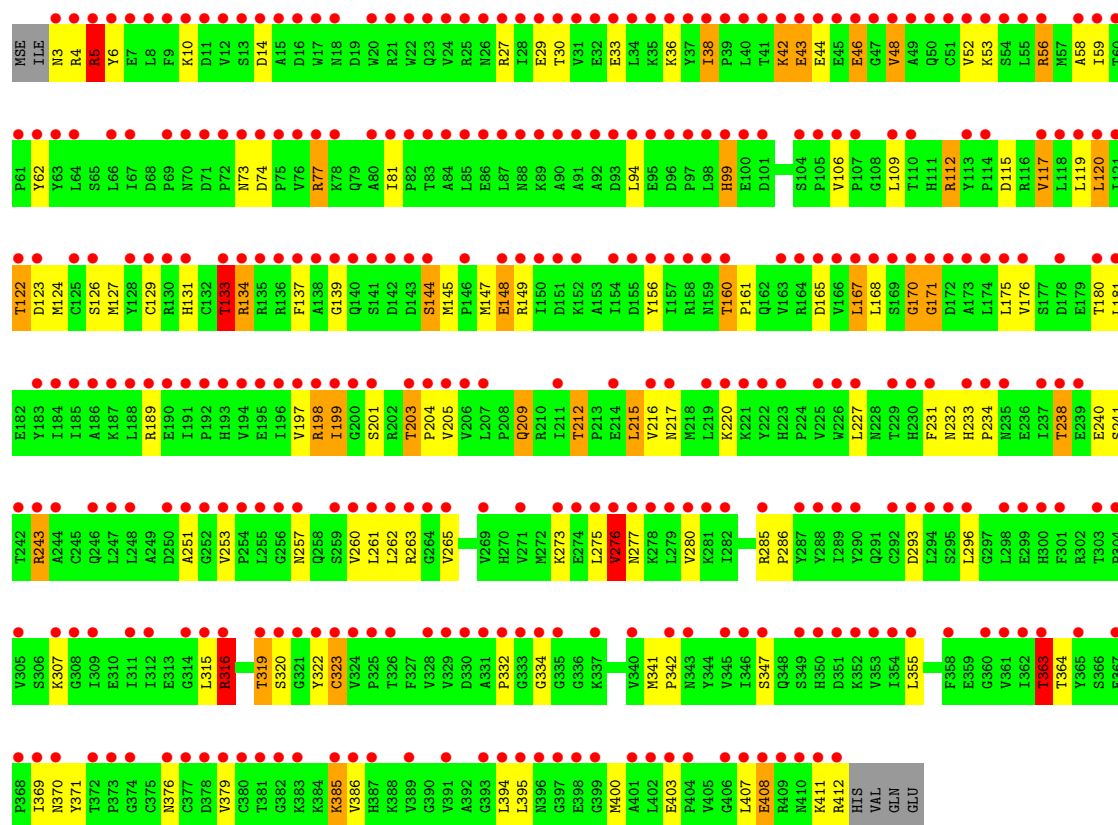


• Molecule 1: L-lysine 2,3-aminomutase



• Molecule 1: L-lysine 2,3-aminomutase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	118.89Å 92.93Å 177.74Å 90.00° 96.74° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 50.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	81.5 (50.00-2.10) 82.8 (50.00-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.19 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.184 , 0.225 0.266 , 0.292	Depositor DCC
R_{free} test set	10427 reflections (8.58%)	wwPDB-VP
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	1.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	14034	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SAM, ZN, SF4, PLP, SO4

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	1.47	7/3391 (0.2%)	1.17	35/4590 (0.8%)
1	B	1.50	8/3388 (0.2%)	1.14	25/4586 (0.5%)
1	C	1.05	6/3380 (0.2%)	1.18	34/4576 (0.7%)
1	D	1.19	7/3402 (0.2%)	1.15	35/4604 (0.8%)
All	All	1.32	28/13561 (0.2%)	1.16	129/18356 (0.7%)

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	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	408	GLU	CD-OE2	51.67	1.82	1.25
1	A	148	GLU	CG-CD	48.53	2.24	1.51
1	B	408	GLU	CD-OE1	-44.21	0.77	1.25
1	A	33	GLU	CG-CD	-38.65	0.94	1.51
1	A	46	GLU	CG-CD	-32.43	1.03	1.51
1	D	408	GLU	CD-OE1	29.24	1.57	1.25
1	B	46	GLU	CG-CD	-24.06	1.15	1.51
1	C	46	GLU	CG-CD	-22.62	1.18	1.51
1	D	408	GLU	CD-OE2	-19.86	1.03	1.25
1	D	148	GLU	CG-CD	18.61	1.79	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	42	LYS	CG-CD	18.45	2.15	1.52
1	C	148	GLU	CG-CD	15.83	1.75	1.51
1	C	239	GLU	CG-CD	15.14	1.74	1.51
1	A	43	GLU	CB-CG	-12.33	1.28	1.52
1	D	385	LYS	CG-CD	11.39	1.91	1.52
1	B	239	GLU	CG-CD	10.58	1.67	1.51
1	B	33	GLU	CG-CD	8.09	1.64	1.51
1	C	323	CYS	CB-SG	-7.64	1.69	1.82
1	A	408	GLU	CD-OE2	-7.50	1.17	1.25
1	B	385	LYS	CG-CD	7.19	1.76	1.52
1	A	239	GLU	CG-CD	6.62	1.61	1.51
1	D	46	GLU	CG-CD	6.62	1.61	1.51
1	A	42	LYS	CG-CD	-6.10	1.31	1.52
1	B	43	GLU	CB-CG	-5.97	1.40	1.52
1	C	385	LYS	CG-CD	-5.90	1.32	1.52
1	C	42	LYS	CG-CD	5.50	1.71	1.52
1	B	323	CYS	CB-SG	-5.43	1.73	1.81
1	D	323	CYS	CB-SG	-5.15	1.73	1.81

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	408	GLU	CG-CD-OE2	-25.33	67.64	118.30
1	A	33	GLU	CB-CG-CD	19.16	165.93	114.20
1	D	408	GLU	CG-CD-OE1	-16.68	84.94	118.30
1	B	408	GLU	CG-CD-OE1	15.71	149.73	118.30
1	B	263	ARG	NE-CZ-NH2	15.03	127.81	120.30
1	A	408	GLU	OE1-CD-OE2	13.73	139.77	123.30
1	A	148	GLU	CG-CD-OE2	-13.15	91.99	118.30
1	A	33	GLU	CG-CD-OE2	-12.69	92.93	118.30
1	C	4	ARG	NE-CZ-NH2	-12.49	114.06	120.30
1	C	5[A]	ARG	NE-CZ-NH2	-12.36	114.12	120.30
1	C	5[B]	ARG	NE-CZ-NH2	-12.36	114.12	120.30
1	D	4	ARG	NE-CZ-NH2	12.29	126.44	120.30
1	A	33	GLU	CG-CD-OE1	12.10	142.50	118.30
1	C	4	ARG	NE-CZ-NH1	11.82	126.21	120.30
1	D	4	ARG	NE-CZ-NH1	-11.69	114.45	120.30
1	C	5[A]	ARG	NE-CZ-NH1	11.11	125.86	120.30
1	C	5[B]	ARG	NE-CZ-NH1	11.11	125.86	120.30
1	D	42	LYS	CB-CG-CD	-10.93	83.19	111.60
1	A	4	ARG	NE-CZ-NH2	10.86	125.73	120.30
1	B	263	ARG	NE-CZ-NH1	-10.46	115.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	GLU	CB-CG-CD	10.45	142.41	114.20
1	A	4	ARG	NE-CZ-NH1	-10.44	115.08	120.30
1	C	134	ARG	NE-CZ-NH1	10.25	125.43	120.30
1	C	189	ARG	NE-CZ-NH1	10.25	125.42	120.30
1	C	189	ARG	NE-CZ-NH2	-10.07	115.27	120.30
1	A	198	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	C	134	ARG	NE-CZ-NH2	-9.93	115.33	120.30
1	A	408	GLU	CG-CD-OE1	-9.63	99.03	118.30
1	A	42	LYS	CG-CD-CE	-9.13	84.49	111.90
1	B	46	GLU	CB-CG-CD	9.02	138.56	114.20
1	D	316[A]	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	D	316[B]	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	C	198	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	B	4	ARG	NE-CZ-NH2	-8.79	115.91	120.30
1	A	263	ARG	NE-CZ-NH1	8.49	124.55	120.30
1	C	46	GLU	CB-CG-CD	8.46	137.03	114.20
1	D	316[A]	ARG	NE-CZ-NH2	-8.43	116.08	120.30
1	D	316[B]	ARG	NE-CZ-NH2	-8.43	116.08	120.30
1	B	198	ARG	NE-CZ-NH1	8.41	124.51	120.30
1	C	316[A]	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	C	316[B]	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	A	198	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	D	198	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	B	316[A]	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	B	316[B]	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	B	189	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	B	4	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	D	198	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	A	385	LYS	CG-CD-CE	-7.67	88.90	111.90
1	C	263	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	B	133	THR	CB-CA-C	-7.59	91.11	111.60
1	B	198	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	D	263	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	A	42	LYS	CB-CG-CD	7.49	131.08	111.60
1	B	408	GLU	OE1-CD-OE2	-7.45	114.36	123.30
1	A	133	THR	CB-CA-C	-7.36	91.74	111.60
1	C	133	THR	CB-CA-C	-7.29	91.90	111.60
1	A	189	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	D	112	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	D	133	THR	CB-CA-C	-7.07	92.51	111.60
1	D	46	GLU	CG-CD-OE1	-7.01	104.28	118.30
1	A	189	ARG	NE-CZ-NH2	-6.85	116.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	189	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	A	316[A]	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	316[B]	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	C	198	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	C	112	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	D	189	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	A	5[A]	ARG	NE-CZ-NH1	-6.48	117.06	120.30
1	A	5[B]	ARG	NE-CZ-NH1	-6.48	117.06	120.30
1	D	189	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	C	385	LYS	CG-CD-CE	-6.38	92.76	111.90
1	C	112	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	C	5[A]	ARG	CD-NE-CZ	6.23	132.32	123.60
1	C	5[B]	ARG	CD-NE-CZ	6.23	132.32	123.60
1	D	148	GLU	CG-CD-OE2	-6.22	105.87	118.30
1	A	148	GLU	CG-CD-OE1	6.12	130.55	118.30
1	B	5[A]	ARG	NE-CZ-NH1	-6.11	117.24	120.30
1	B	5[B]	ARG	NE-CZ-NH1	-6.11	117.24	120.30
1	B	5[A]	ARG	NE-CZ-NH2	6.10	123.35	120.30
1	B	5[B]	ARG	NE-CZ-NH2	6.10	123.35	120.30
1	C	263	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	C	316[A]	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	C	316[B]	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	D	363	THR	CB-CA-C	-5.96	95.50	111.60
1	D	148	GLU	CG-CD-OE1	5.95	130.19	118.30
1	B	316[A]	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	B	316[B]	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	C	148	GLU	CG-CD-OE2	-5.83	106.64	118.30
1	C	4	ARG	CD-NE-CZ	5.82	131.74	123.60
1	A	316[A]	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	316[B]	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	D	408	GLU	OE1-CD-OE2	-5.78	116.36	123.30
1	A	263	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	C	148	GLU	CG-CD-OE1	5.72	129.74	118.30
1	D	134	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	363	THR	CB-CA-C	-5.56	96.59	111.60
1	B	4	ARG	CD-NE-CZ	5.54	131.36	123.60
1	D	5[A]	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	D	5[B]	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	A	5[A]	ARG	NE-CZ-NH2	5.51	123.05	120.30
1	A	5[B]	ARG	NE-CZ-NH2	5.51	123.05	120.30
1	D	46	GLU	CG-CD-OE2	5.51	129.31	118.30
1	B	263	ARG	CD-NE-CZ	5.50	131.30	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	56	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	D	316[A]	ARG	CD-NE-CZ	5.47	131.26	123.60
1	D	316[B]	ARG	CD-NE-CZ	5.47	131.26	123.60
1	C	363	THR	CB-CA-C	-5.46	96.86	111.60
1	D	4	ARG	CD-NE-CZ	5.42	131.19	123.60
1	A	134	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	D	276	VAL	CG1-CB-CG2	5.42	119.57	110.90
1	A	285[A]	ARG	CB-CA-C	5.39	121.18	110.40
1	A	285[B]	ARG	CB-CA-C	5.39	121.18	110.40
1	A	4	ARG	CD-NE-CZ	5.37	131.12	123.60
1	D	385	LYS	CG-CD-CE	5.36	127.97	111.90
1	D	408	GLU	CG-CD-OE2	-5.35	107.59	118.30
1	C	109	LEU	CA-CB-CG	5.34	127.58	115.30
1	A	363	THR	CB-CA-C	-5.32	97.24	111.60
1	D	385	LYS	CB-CG-CD	-5.26	97.93	111.60
1	D	167	LEU	CB-CG-CD2	5.25	119.92	111.00
1	D	5[A]	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	D	5[B]	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	A	43	GLU	CA-CB-CG	5.22	124.88	113.40
1	C	316[A]	ARG	CG-CD-NE	5.14	122.60	111.80
1	C	316[B]	ARG	CG-CD-NE	5.14	122.60	111.80
1	C	385	LYS	CB-CG-CD	5.06	124.76	111.60
1	A	280	VAL	CG1-CB-CG2	5.04	118.96	110.90
1	B	394	LEU	CB-CG-CD1	5.02	119.53	111.00
1	C	122	THR	CB-CA-C	-5.01	98.08	111.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	GLU	Sidechain
1	A	170	GLY	Peptide
1	B	170	GLY	Peptide
1	B	408	GLU	Sidechain
1	C	170	GLY	Peptide
1	C	288	TYR	Peptide
1	D	170	GLY	Peptide
1	D	408	GLU	Sidechain

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	3285	0	3300	99	0
1	B	3288	0	3306	91	0
1	C	3280	0	3295	112	0
1	D	3297	0	3313	121	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	27	0	21	0	0
4	B	27	0	21	0	0
4	C	27	0	21	0	0
4	D	27	0	21	0	0
5	A	13	0	22	0	0
5	B	13	0	22	0	0
5	C	13	0	22	0	0
5	D	13	0	22	0	0
6	A	15	0	6	0	0
6	B	15	0	6	0	0
6	C	15	0	6	0	0
6	D	15	0	6	0	0
7	A	8	0	0	0	0
7	B	8	0	0	0	0
7	C	8	0	0	1	0
7	D	8	0	0	1	0
8	A	135	0	0	7	0
8	B	116	0	0	3	0
8	C	183	0	0	10	1
8	D	174	0	0	8	0
All	All	14034	0	13410	376	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (376) 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:C:285[B]:ARG:CD	1:D:285[B]:ARG:HD2	1.54	1.37
1:C:285[B]:ARG:CD	1:D:285[B]:ARG:CD	2.09	1.31
1:C:285[B]:ARG:HD2	1:D:285[B]:ARG:CD	1.65	1.23
1:C:285[B]:ARG:HD2	1:D:285[B]:ARG:NE	1.62	1.14
1:D:243[A]:ARG:HD2	8:D:578:HOH:O	1.48	1.11
1:A:214:GLU:OE1	8:A:713:HOH:O	1.68	1.10
1:C:285[B]:ARG:HD3	1:D:285[B]:ARG:HD2	1.33	1.06
1:B:231:PHE:H	1:B:257:ASN:HD21	1.08	0.97
1:D:212:THR:HG22	1:D:215:LEU:H	1.30	0.95
1:A:231:PHE:H	1:A:257:ASN:HD21	1.16	0.94
1:C:231:PHE:H	1:C:257:ASN:HD21	1.15	0.93
1:C:285[B]:ARG:NE	1:D:285[B]:ARG:HD2	1.83	0.93
1:A:212:THR:HG22	1:A:215:LEU:H	1.32	0.92
1:C:285[B]:ARG:HD3	1:D:285[B]:ARG:CD	1.93	0.92
1:D:137:PHE:CZ	1:D:145:MSE:HE2	2.04	0.91
1:B:112:ARG:HD3	8:B:501:HOH:O	1.69	0.91
1:A:216:VAL:HG13	1:A:251:ALA:HB2	1.53	0.90
1:B:216:VAL:HG13	1:B:251:ALA:HB2	1.54	0.90
1:D:112:ARG:HD2	1:D:334:GLY:O	1.70	0.90
1:A:112:ARG:HD2	1:A:334:GLY:O	1.71	0.90
1:C:112:ARG:HD2	1:C:334:GLY:O	1.71	0.90
1:C:212:THR:HG22	1:C:215:LEU:H	1.36	0.89
1:D:44:GLU:O	1:D:48:VAL:HG13	1.73	0.89
1:D:243[A]:ARG:HH11	1:D:243[A]:ARG:HG3	1.38	0.88
1:D:276:VAL:HG13	1:D:323:CYS:HB3	1.52	0.88
1:A:400:MSE:HE1	1:D:94:LEU:HD11	1.56	0.87
1:B:400:MSE:HE1	1:C:94:LEU:HD11	1.57	0.86
1:D:231:PHE:H	1:D:257:ASN:HD21	1.19	0.86
1:D:216:VAL:HG13	1:D:251:ALA:HB2	1.56	0.86
1:C:44:GLU:O	1:C:48:VAL:HG13	1.76	0.85
1:D:212:THR:HG21	8:D:626:HOH:O	1.77	0.85
1:C:145:MSE:HE3	1:C:149:ARG:NH2	1.92	0.85
1:B:94:LEU:HD11	1:C:400:MSE:HE1	1.58	0.84
1:B:44:GLU:O	1:B:48:VAL:HG13	1.78	0.84
1:A:44:GLU:O	1:A:48:VAL:HG13	1.79	0.83
1:A:363:THR:HG21	1:B:332:PRO:O	1.79	0.82
1:A:145:MSE:HE3	1:A:149:ARG:NH2	1.92	0.82
1:C:137:PHE:CE2	1:C:145:MSE:HE2	2.13	0.82
1:B:112:ARG:HD2	1:B:334:GLY:O	1.79	0.82
1:A:332:PRO:O	1:B:363:THR:HG21	1.80	0.81
1:C:27[B]:ARG:NH2	1:C:29:GLU:OE2	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:PHE:CZ	1:B:145:MSE:HE2	2.15	0.81
1:A:276:VAL:HG13	1:A:323:CYS:HB3	1.61	0.81
1:B:203:THR:HG22	1:B:204:PRO:HD3	1.63	0.80
1:C:168:LEU:HB2	1:C:199[B]:ILE:HG22	1.63	0.80
1:C:62:TYR:OH	1:C:238:THR:HG21	1.82	0.80
1:A:122:THR:HG23	1:A:144:SER:HA	1.65	0.79
1:D:137:PHE:CE2	1:D:145:MSE:HE2	2.18	0.79
1:C:137:PHE:CZ	1:C:145:MSE:HE2	2.16	0.78
1:D:112:ARG:HD3	8:D:500:HOH:O	1.83	0.78
1:D:122:THR:HG23	1:D:144:SER:HA	1.66	0.78
1:C:216:VAL:HG13	1:C:251:ALA:HB2	1.64	0.77
1:B:168:LEU:HB2	1:B:199[B]:ILE:HG22	1.66	0.77
1:B:145:MSE:HE3	1:B:149:ARG:NH2	1.99	0.77
1:B:122:THR:HG23	1:B:144:SER:HA	1.67	0.77
1:C:276:VAL:HG13	1:C:323:CYS:HB3	1.67	0.76
1:D:168:LEU:HB2	1:D:199[B]:ILE:HG22	1.67	0.76
1:D:145:MSE:HE3	1:D:149:ARG:NH2	2.00	0.76
1:B:33:GLU:O	1:B:36:LYS:HG2	1.86	0.76
1:A:27[B]:ARG:NH2	1:A:29:GLU:OE2	2.19	0.75
1:D:33:GLU:O	1:D:36:LYS:HG2	1.86	0.75
1:A:137:PHE:CZ	1:A:145:MSE:HE2	2.22	0.75
1:B:276:VAL:HG13	1:B:323:CYS:HB3	1.68	0.75
1:B:137:PHE:CE2	1:B:145:MSE:HE2	2.23	0.74
1:D:137:PHE:CE2	1:D:145:MSE:CE	2.71	0.74
1:B:27[B]:ARG:NH2	1:B:29:GLU:OE2	2.18	0.74
1:D:165:ASP:OD2	1:D:198:ARG:HD3	1.87	0.74
1:B:201:SER:OG	1:B:203:THR:HB	1.88	0.74
1:A:316[A]:ARG:HG2	1:A:316[A]:ARG:HH11	1.51	0.73
1:A:168:LEU:HB2	1:A:199[B]:ILE:HG22	1.71	0.73
1:A:33:GLU:O	1:A:36:LYS:HG2	1.89	0.73
1:A:216:VAL:HG13	1:A:251:ALA:CB	2.19	0.73
1:C:285[B]:ARG:CD	1:D:285[B]:ARG:HD3	2.17	0.73
1:B:165:ASP:OD2	1:B:198:ARG:HD3	1.89	0.72
1:A:137:PHE:CE2	1:A:145:MSE:HE2	2.24	0.72
1:C:122:THR:HG23	1:C:144:SER:HA	1.69	0.72
1:D:62:TYR:OH	1:D:238:THR:HG21	1.89	0.72
1:C:137:PHE:CE2	1:C:145:MSE:CE	2.73	0.72
1:C:137:PHE:HE2	1:C:145:MSE:CE	2.02	0.71
1:B:5[A]:ARG:NH1	1:B:14:ASP:OD1	2.22	0.71
1:D:27[B]:ARG:NH2	1:D:29:GLU:OE2	2.23	0.71
1:D:243[A]:ARG:HD3	8:D:654:HOH:O	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316[A]:ARG:HH11	1:C:316[A]:ARG:HG2	1.56	0.71
1:A:165:ASP:OD2	1:A:198:ARG:HD3	1.91	0.70
1:C:115:ASP:OD1	1:D:319:THR:HG22	1.91	0.70
1:C:363:THR:HG21	1:D:332:PRO:O	1.91	0.70
1:A:201:SER:OG	1:A:203:THR:HB	1.90	0.70
1:B:316[A]:ARG:HG2	1:B:316[A]:ARG:HH11	1.57	0.70
1:D:156:TYR:O	1:D:160:THR:HG23	1.91	0.69
1:B:137:PHE:CE2	1:B:145:MSE:CE	2.75	0.69
1:A:94:LEU:HD11	1:D:400:MSE:HE1	1.73	0.69
1:B:400:MSE:CE	8:C:744:HOH:O	2.40	0.69
1:C:343:ASN:HB3	8:C:615:HOH:O	1.92	0.69
1:C:112:ARG:HD3	8:C:599:HOH:O	1.92	0.67
1:B:216:VAL:HG13	1:B:251:ALA:CB	2.24	0.67
1:C:201:SER:OG	1:C:203:THR:HB	1.93	0.67
1:C:33:GLU:O	1:C:36:LYS:HG2	1.95	0.67
1:D:201:SER:OG	1:D:203:THR:HB	1.94	0.67
1:C:156:TYR:O	1:C:160:THR:HG23	1.95	0.66
1:D:137:PHE:HE2	1:D:145:MSE:CE	2.09	0.66
1:A:122:THR:HG21	8:A:633:HOH:O	1.95	0.66
1:C:122:THR:CG2	8:C:732:HOH:O	2.43	0.66
1:C:217:ASN:ND2	8:C:661:HOH:O	2.28	0.65
1:B:137:PHE:HE2	1:B:145:MSE:CE	2.10	0.65
1:A:133:THR:CG2	1:A:293:ASP:OD2	2.45	0.64
1:D:216:VAL:HG13	1:D:251:ALA:CB	2.27	0.64
1:B:62:TYR:OH	1:B:238:THR:HG21	1.96	0.64
1:B:156:TYR:O	1:B:160:THR:CG2	2.45	0.64
1:C:156:TYR:O	1:C:160:THR:CG2	2.45	0.64
1:B:231:PHE:H	1:B:257:ASN:ND2	1.90	0.63
1:A:115:ASP:OD1	1:B:319:THR:HG22	1.99	0.63
1:C:203:THR:HG22	1:C:204:PRO:HD3	1.80	0.63
1:D:137:PHE:HE2	1:D:145:MSE:HE1	1.63	0.63
1:C:285[B]:ARG:HD2	1:D:285[B]:ARG:HD3	1.73	0.63
1:C:319:THR:HG22	1:D:115:ASP:OD1	1.98	0.63
1:A:341:MSE:HG2	1:B:341:MSE:HE2	1.80	0.63
1:A:56:ARG:HD2	1:A:139:GLY:O	1.99	0.62
1:B:133:THR:HG23	1:B:293:ASP:OD2	1.99	0.62
1:D:316[A]:ARG:HG2	1:D:316[A]:ARG:HH11	1.64	0.62
1:D:156:TYR:O	1:D:160:THR:CG2	2.47	0.62
1:A:137:PHE:CE2	1:A:145:MSE:CE	2.82	0.62
1:C:231:PHE:H	1:C:257:ASN:ND2	1.91	0.62
1:D:27[A]:ARG:NH1	1:D:124:MSE:HE2	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:TYR:OH	1:A:238:THR:HG21	1.99	0.61
1:D:137:PHE:HZ	1:D:145:MSE:HE2	1.60	0.61
1:B:137:PHE:HE2	1:B:145:MSE:HE1	1.65	0.61
1:C:332:PRO:O	1:D:363:THR:HG21	2.00	0.61
1:C:341:MSE:HG2	1:D:341:MSE:HE2	1.82	0.61
1:B:131:HIS:CD2	1:B:260[A]:VAL:HG11	2.35	0.61
1:A:212:THR:HG21	8:A:683:HOH:O	2.01	0.61
1:A:319:THR:HG22	1:B:115:ASP:OD1	2.00	0.60
1:A:137:PHE:HE2	1:A:145:MSE:CE	2.13	0.60
1:D:43:GLU:HG2	1:D:44:GLU:N	2.14	0.60
1:C:137:PHE:HE2	1:C:145:MSE:HE1	1.65	0.60
1:D:131:HIS:CD2	1:D:260[A]:VAL:HG11	2.37	0.60
1:C:56:ARG:HD2	1:C:139:GLY:O	2.02	0.60
1:C:307:LYS:HE3	1:C:310:GLU:OE1	2.01	0.60
1:A:209:GLN:H	1:A:209:GLN:NE2	2.00	0.59
1:A:112:ARG:HD3	8:A:598:HOH:O	2.02	0.59
1:A:307:LYS:HE3	1:A:310:GLU:OE1	2.01	0.59
1:A:133:THR:HG23	1:A:293:ASP:OD2	2.03	0.59
1:C:232:ASN:HD21	1:C:260[B]:VAL:H	1.49	0.59
1:C:165:ASP:OD2	1:C:198:ARG:HD3	2.02	0.58
1:D:199[B]:ILE:HG13	1:D:227:LEU:HD12	1.86	0.58
1:A:5[A]:ARG:NH1	1:A:14:ASP:OD1	2.36	0.58
1:A:156:TYR:O	1:A:160:THR:CG2	2.52	0.58
1:A:263:ARG:HD3	8:A:629:HOH:O	2.03	0.58
1:B:133:THR:CG2	1:B:293:ASP:OD2	2.51	0.58
1:C:216:VAL:HG13	1:C:251:ALA:CB	2.34	0.58
1:D:363:THR:HG22	1:D:364:THR:H	1.69	0.58
1:C:209:GLN:H	1:C:209:GLN:NE2	2.03	0.57
1:D:56:ARG:HD2	1:D:139:GLY:O	2.04	0.57
1:C:232:ASN:HD21	1:C:260[A]:VAL:H	1.50	0.57
1:B:238:THR:HG22	1:B:241:SER:H	1.69	0.57
1:A:27[A]:ARG:NH1	1:A:124:MSE:HE2	2.19	0.57
1:B:156:TYR:O	1:B:160:THR:HG23	2.05	0.57
1:A:131:HIS:CD2	1:A:260[A]:VAL:HG11	2.40	0.57
1:A:109:LEU:HD21	1:A:117:VAL:CG1	2.35	0.56
1:B:56:ARG:HD2	1:B:139:GLY:O	2.04	0.56
1:C:231:PHE:N	1:C:257:ASN:HD21	1.93	0.56
1:A:341:MSE:HE2	1:B:341:MSE:HG2	1.86	0.56
1:C:232:ASN:ND2	1:C:260[A]:VAL:H	2.02	0.56
1:C:232:ASN:ND2	1:C:260[B]:VAL:H	2.03	0.56
1:D:238:THR:HG23	1:D:240:GLU:OE1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:GLU:OE2	1:B:152:LYS:HE3	2.06	0.56
1:D:243[A]:ARG:HG3	1:D:243[A]:ARG:NH1	2.10	0.56
1:D:238:THR:HG22	1:D:241:SER:H	1.71	0.56
1:C:277:ASN:OD1	1:C:319:THR:HG21	2.06	0.55
1:C:238:THR:HG22	1:C:241:SER:H	1.72	0.55
1:C:38:ILE:HD11	1:C:81:ILE:HD11	1.88	0.55
1:D:133:THR:CG2	1:D:293:ASP:OD2	2.55	0.55
1:D:232:ASN:HD21	1:D:260[B]:VAL:H	1.54	0.55
1:C:77:ARG:HD3	8:C:727:HOH:O	2.07	0.55
1:D:109:LEU:HD21	1:D:117:VAL:CG1	2.36	0.55
1:C:122:THR:HG21	8:C:732:HOH:O	2.04	0.55
1:A:133:THR:HG21	1:A:293:ASP:OD2	2.06	0.54
1:A:216:VAL:CG1	1:A:251:ALA:HB2	2.30	0.54
8:B:610:HOH:O	1:D:370:ASN:HA	2.07	0.54
1:A:231:PHE:H	1:A:257:ASN:ND2	1.97	0.54
1:C:341:MSE:HE2	1:D:341:MSE:HG2	1.88	0.54
1:C:238:THR:HG23	1:C:240:GLU:OE1	2.07	0.54
1:B:156:TYR:O	1:B:160:THR:HG22	2.07	0.54
1:C:131:HIS:CD2	1:C:260[A]:VAL:HG11	2.43	0.53
1:D:99:HIS:HD2	8:D:649:HOH:O	1.91	0.53
1:D:109:LEU:HD21	1:D:117:VAL:HG11	1.90	0.53
1:C:133:THR:HG23	1:C:293:ASP:HB2	1.89	0.53
1:C:285[B]:ARG:HD3	1:D:285[B]:ARG:HD3	1.82	0.53
1:A:156:TYR:O	1:A:160:THR:HG23	2.07	0.53
1:B:5[A]:ARG:NH2	1:B:12:VAL:O	2.42	0.53
1:C:376:ASN:CG	1:D:73:ASN:HD22	2.11	0.53
1:D:232:ASN:HD21	1:D:260[A]:VAL:H	1.55	0.53
1:D:273:LYS:NZ	1:D:277:ASN:HD21	2.06	0.53
1:B:387:HIS:NE2	1:C:408:GLU:OE1	2.41	0.53
1:B:74:ASP:HB3	1:B:77:ARG:HG2	1.92	0.52
1:B:74:ASP:HB3	1:B:77:ARG:CG	2.39	0.52
1:A:277:ASN:OD1	1:A:319:THR:HG21	2.09	0.52
1:B:306:SER:HB2	1:C:348:GLN:HG3	1.90	0.52
1:A:231:PHE:N	1:A:257:ASN:HD21	1.98	0.52
1:B:209:GLN:H	1:B:209:GLN:NE2	2.07	0.52
1:C:285[B]:ARG:CD	1:D:285[B]:ARG:NE	2.45	0.52
1:B:260[B]:VAL:HG22	1:B:262:LEU:HG	1.92	0.52
1:B:27[A]:ARG:NH1	1:B:124:MSE:HE2	2.25	0.52
1:B:231:PHE:N	1:B:257:ASN:HD21	1.92	0.52
1:B:120:LEU:HD12	1:B:170:GLY:HA2	1.90	0.52
1:C:133:THR:CG2	1:C:293:ASP:OD2	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:PHE:HE2	1:A:145:MSE:HE1	1.75	0.52
1:B:216:VAL:CG1	1:B:251:ALA:HB2	2.34	0.52
1:C:74:ASP:HB3	1:C:77:ARG:CG	2.39	0.52
1:D:341:MSE:HB2	1:D:342:PRO:CD	2.40	0.52
1:B:277:ASN:OD1	1:B:319:THR:HG21	2.09	0.51
1:C:122:THR:HG23	8:C:732:HOH:O	2.08	0.51
1:D:5[A]:ARG:NH2	8:D:623:HOH:O	2.40	0.51
1:D:5[A]:ARG:NH1	1:D:14:ASP:OD1	2.41	0.51
1:A:260[B]:VAL:HG22	1:A:262:LEU:HG	1.92	0.51
1:A:308:GLY:HA3	1:A:327:PHE:CE2	2.45	0.51
1:A:401:ALA:HB2	1:C:363:THR:HG23	1.93	0.51
1:A:376:ASN:CG	1:B:73:ASN:HD22	2.14	0.51
1:D:145:MSE:HE3	1:D:149:ARG:HH22	1.71	0.51
1:D:411:LYS:O	1:D:412:ARG:HG3	2.11	0.51
1:A:122:THR:CG2	8:A:633:HOH:O	2.55	0.51
1:D:133:THR:HG23	1:D:293:ASP:OD2	2.10	0.51
1:A:232:ASN:ND2	1:A:260[A]:VAL:H	2.09	0.51
1:A:199[B]:ILE:HG13	1:A:227:LEU:HD12	1.93	0.50
1:C:285[B]:ARG:CZ	1:D:285[B]:ARG:HD2	2.40	0.50
1:C:319:THR:CG2	1:D:115:ASP:OD1	2.60	0.50
1:B:137:PHE:HZ	1:B:145:MSE:HE2	1.71	0.50
1:A:109:LEU:CD2	1:A:117:VAL:HG13	2.41	0.50
1:D:232:ASN:ND2	1:D:260[A]:VAL:H	2.09	0.50
1:A:238:THR:HG23	1:A:240:GLU:OE1	2.12	0.50
1:C:171:GLY:HA2	7:C:418:SF4:S4	2.52	0.50
1:D:232:ASN:ND2	1:D:260[B]:VAL:H	2.09	0.50
1:A:213:PRO:HD2	8:A:713:HOH:O	2.12	0.49
1:B:109:LEU:HD21	1:B:117:VAL:HG11	1.93	0.49
1:C:258:GLN:HB3	1:C:290:TYR:HE1	1.76	0.49
1:D:209:GLN:H	1:D:209:GLN:NE2	2.10	0.49
1:A:232:ASN:ND2	1:A:260[B]:VAL:H	2.10	0.49
1:B:232:ASN:ND2	1:B:260[A]:VAL:H	2.11	0.49
1:C:272:MSE:O	1:C:276:VAL:HB	2.13	0.49
1:D:341:MSE:HB2	1:D:342:PRO:HD2	1.94	0.49
1:A:203:THR:HG22	1:A:204:PRO:HD3	1.96	0.48
1:B:59:ILE:HA	1:B:127:MSE:HG2	1.95	0.48
1:D:129:CYS:HB3	1:D:131:HIS:CE1	2.48	0.48
1:D:260[A]:VAL:HG13	1:D:262:LEU:HG	1.94	0.48
1:C:73:ASN:HD22	1:D:376:ASN:CG	2.17	0.48
1:B:109:LEU:HD21	1:B:117:VAL:CG1	2.43	0.48
1:A:276:VAL:HG22	1:A:286:PRO:CG	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:ASN:OD1	1:D:319:THR:HG21	2.14	0.48
1:D:233:HIS:CG	1:D:234:PRO:HD2	2.48	0.47
1:D:273:LYS:HZ2	1:D:277:ASN:HD21	1.61	0.47
1:A:109:LEU:HD21	1:A:117:VAL:HG11	1.94	0.47
1:A:260[A]:VAL:HG13	1:A:262:LEU:HG	1.94	0.47
1:C:137:PHE:HZ	1:C:145:MSE:HE2	1.78	0.47
1:A:276:VAL:HG22	1:A:286:PRO:HG2	1.96	0.47
1:C:74:ASP:HB3	1:C:77:ARG:HG2	1.97	0.47
1:B:238:THR:HG23	1:B:240:GLU:OE1	2.15	0.47
1:C:133:THR:HG21	1:C:293:ASP:OD2	2.14	0.47
1:B:203:THR:HG22	1:B:204:PRO:CD	2.40	0.47
1:B:232:ASN:HD21	1:B:260[B]:VAL:H	1.63	0.47
1:D:6:TYR:O	1:D:10:LYS:HB3	2.15	0.47
1:A:147:MSE:HE1	1:A:180:THR:HG23	1.97	0.47
1:B:232:ASN:ND2	1:B:260[B]:VAL:H	2.12	0.47
1:C:262:LEU:HB2	1:C:265:VAL:HG13	1.98	0.46
1:A:74:ASP:HB3	1:A:77:ARG:CG	2.45	0.46
1:A:319:THR:CG2	1:B:115:ASP:OD1	2.63	0.46
1:A:371:TYR:CG	1:B:304:PRO:HD3	2.50	0.46
1:B:326:THR:HG22	1:B:328:VAL:HG13	1.96	0.46
1:D:243[A]:ARG:CD	8:D:578:HOH:O	2.31	0.46
1:A:74:ASP:HB3	1:A:77:ARG:HG2	1.97	0.46
1:B:6:TYR:O	1:B:10:LYS:HG3	2.15	0.46
1:A:308:GLY:HA3	1:A:327:PHE:CZ	2.50	0.46
1:D:203:THR:HG22	1:D:204:PRO:HD3	1.98	0.46
1:C:285[B]:ARG:HD2	1:D:285[B]:ARG:CZ	2.40	0.46
1:D:109:LEU:CD2	1:D:117:VAL:HG13	2.45	0.46
1:C:260[B]:VAL:HG22	1:C:262:LEU:HG	1.96	0.46
1:D:276:VAL:HG22	1:D:286:PRO:HG2	1.98	0.46
1:A:115:ASP:OD1	1:B:319:THR:CG2	2.63	0.46
1:A:386:VAL:HG21	8:B:581:HOH:O	2.16	0.46
1:B:272:MSE:O	1:B:276:VAL:HB	2.17	0.45
1:B:341:MSE:HB2	1:B:342:PRO:CD	2.45	0.45
1:C:38:ILE:CD1	1:C:81:ILE:HD11	2.46	0.45
1:B:232:ASN:HD21	1:B:260[A]:VAL:H	1.63	0.45
1:C:370:ASN:HA	8:C:775:HOH:O	2.17	0.45
1:A:232:ASN:HD21	1:A:260[B]:VAL:H	1.64	0.45
1:D:124:MSE:SE	1:D:175:LEU:HD12	2.66	0.45
1:A:133:THR:HG23	1:A:293:ASP:HB2	1.99	0.45
1:B:160:THR:HA	1:B:161:PRO:HD3	1.73	0.45
1:D:74:ASP:HB3	1:D:77:ARG:CG	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:SER:HB3	1:D:322:TYR:CE1	2.52	0.45
1:A:38:ILE:HD11	1:A:81:ILE:HD11	1.97	0.45
1:A:145:MSE:HE3	1:A:149:ARG:HH22	1.79	0.45
1:D:122:THR:HG21	8:D:621:HOH:O	2.17	0.45
1:D:212:THR:CG2	1:D:215:LEU:H	2.15	0.45
1:B:348:GLN:HG3	1:C:306:SER:HB2	1.99	0.45
1:C:109:LEU:HD21	1:C:117:VAL:CG1	2.48	0.45
1:D:120:LEU:HD12	1:D:170:GLY:HA2	1.98	0.45
1:C:59:ILE:HA	1:C:127:MSE:HG2	1.98	0.44
1:D:30:THR:OG1	1:D:33:GLU:HB2	2.17	0.44
1:A:156:TYR:O	1:A:160:THR:HG22	2.17	0.44
1:A:232:ASN:HD21	1:A:260[A]:VAL:H	1.65	0.44
1:B:253:VAL:HA	1:B:254:PRO:HD3	1.91	0.44
1:A:48:VAL:HG12	1:A:82:PRO:HD2	1.99	0.44
1:A:129:CYS:HB3	1:A:131:HIS:CE1	2.53	0.44
1:C:27[A]:ARG:NH1	1:C:124:MSE:HE2	2.33	0.44
1:D:133:THR:HG23	1:D:293:ASP:HB2	1.98	0.44
1:A:363:THR:HG23	1:C:401:ALA:HB2	2.00	0.44
1:B:273:LYS:NZ	1:B:277:ASN:HD21	2.15	0.44
1:C:5[A]:ARG:NH2	1:C:12:VAL:O	2.50	0.43
1:D:59:ILE:HA	1:D:127:MSE:HG2	2.00	0.43
1:D:123:ASP:C	1:D:123:ASP:OD1	2.56	0.43
1:C:206:VAL:HG21	8:C:635:HOH:O	2.18	0.43
1:B:401:ALA:HB2	1:D:363:THR:HG23	2.00	0.43
1:B:199[B]:ILE:HG13	1:B:227:LEU:HD12	2.00	0.43
1:C:123:ASP:OD1	1:C:123:ASP:C	2.57	0.43
1:D:133:THR:HG21	1:D:293:ASP:OD2	2.19	0.43
1:B:122:THR:HG22	1:B:124:MSE:H	1.83	0.43
1:B:285:ARG:HD3	1:B:322:TYR:O	2.18	0.43
1:C:109:LEU:CD2	1:C:117:VAL:HG13	2.49	0.43
1:D:160:THR:HA	1:D:161:PRO:HD3	1.65	0.43
1:A:120:LEU:HD12	1:A:170:GLY:HA2	2.00	0.43
1:C:262:LEU:CB	1:C:265:VAL:HG13	2.48	0.43
1:C:115:ASP:OD1	1:D:319:THR:CG2	2.65	0.43
1:C:120:LEU:HD12	1:C:170:GLY:HA2	2.01	0.42
1:C:133:THR:HG23	1:C:293:ASP:CB	2.49	0.42
1:C:133:THR:HG23	1:C:293:ASP:OD2	2.19	0.42
1:A:238:THR:HG22	1:A:241:SER:H	1.82	0.42
1:C:209:GLN:H	1:C:209:GLN:HE21	1.67	0.42
1:D:137:PHE:CE2	1:D:145:MSE:HE1	2.41	0.42
1:D:231:PHE:H	1:D:257:ASN:ND2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LEU:HD21	1:A:117:VAL:HG13	1.99	0.42
1:D:171:GLY:HA2	7:D:418:SF4:S4	2.60	0.42
1:D:276:VAL:HG22	1:D:286:PRO:CG	2.49	0.42
1:D:38:ILE:HD11	1:D:81:ILE:HD11	2.01	0.42
1:D:199[A]:ILE:HD11	1:D:201:SER:HB2	2.01	0.42
1:A:5[A]:ARG:NH2	1:A:12:VAL:O	2.53	0.42
1:A:189:ARG:HD2	1:A:222:TYR:O	2.20	0.42
1:B:145:MSE:HE3	1:B:149:ARG:HH22	1.82	0.42
1:C:109:LEU:HD21	1:C:117:VAL:HG11	2.02	0.42
1:C:253:VAL:HA	1:C:254:PRO:HD3	1.91	0.41
1:D:122:THR:HG22	1:D:124:MSE:H	1.84	0.41
1:D:216:VAL:CG1	1:D:251:ALA:HB2	2.40	0.41
1:A:105:PRO:HG2	1:A:109:LEU:HD12	2.01	0.41
1:C:273:LYS:HZ2	1:C:319:THR:HG23	1.84	0.41
1:A:238:THR:HG22	1:A:240:GLU:N	2.35	0.41
1:C:147:MSE:HE1	1:C:180:THR:HG23	2.02	0.41
1:B:137:PHE:CE2	1:B:145:MSE:HE1	2.46	0.41
1:B:181:LEU:HD13	1:B:218:MSE:HE1	2.02	0.41
1:C:307:LYS:O	1:C:307:LYS:HD3	2.20	0.41
1:A:354:ILE:HD11	1:C:395:LEU:HD13	2.02	0.41
1:C:156:TYR:O	1:C:160:THR:HG22	2.18	0.41
1:D:238:THR:CG2	1:D:240:GLU:OE1	2.68	0.41
1:A:238:THR:CG2	1:A:240:GLU:OE1	2.69	0.41
1:B:203:THR:CG2	1:B:211:ILE:HD11	2.51	0.41
1:B:260[A]:VAL:HG13	1:B:262:LEU:HG	2.02	0.41
1:C:304:PRO:HD3	1:D:371:TYR:CG	2.56	0.41
1:A:260[A]:VAL:HG13	1:A:262:LEU:CG	2.51	0.41
1:A:405:VAL:HG13	1:D:403:GLU:O	2.20	0.41
1:B:27[B]:ARG:HH21	1:B:58:ALA:HB1	1.86	0.40
1:D:147:MSE:HE1	1:D:180:THR:HG23	2.03	0.40
1:A:243[B]:ARG:NH1	1:A:246:GLN:OE1	2.47	0.40
1:B:260[A]:VAL:HG13	1:B:262:LEU:CD1	2.51	0.40
1:D:38:ILE:CD1	1:D:81:ILE:HD11	2.51	0.40
1:A:363:THR:HG22	1:C:400:MSE:HG2	2.03	0.40
1:B:109:LEU:CD2	1:B:117:VAL:HG13	2.52	0.40

All (1) 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)
8:C:764:HOH:O	8:C:764:HOH:O[2_454]	1.88	0.32

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	416/416 (100%)	400 (96%)	13 (3%)	3 (1%)	19	16
1	B	416/416 (100%)	398 (96%)	15 (4%)	3 (1%)	19	16
1	C	415/416 (100%)	397 (96%)	15 (4%)	3 (1%)	19	16
1	D	417/416 (100%)	397 (95%)	17 (4%)	3 (1%)	19	16
All	All	1664/1664 (100%)	1592 (96%)	60 (4%)	12 (1%)	19	16

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	GLY
1	B	52	VAL
1	B	171	GLY
1	C	171	GLY
1	D	52	VAL
1	D	171	GLY
1	A	53	LYS
1	D	53	LYS
1	C	52	VAL
1	C	53	LYS
1	A	52	VAL
1	B	53	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	374/362 (103%)	316 (84%)	58 (16%)	2	1
1	B	374/362 (103%)	315 (84%)	59 (16%)	2	1
1	C	373/362 (103%)	320 (86%)	53 (14%)	2	1
1	D	375/362 (104%)	318 (85%)	57 (15%)	2	1
All	All	1496/1448 (103%)	1269 (85%)	227 (15%)	2	1

All (227) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	5[A]	ARG
1	A	5[B]	ARG
1	A	33	GLU
1	A	38	ILE
1	A	42	LYS
1	A	43	GLU
1	A	46	GLU
1	A	77	ARG
1	A	99	HIS
1	A	106	VAL
1	A	117	VAL
1	A	119	LEU
1	A	120	LEU
1	A	122	THR
1	A	133	THR
1	A	144	SER
1	A	148	GLU
1	A	160	THR
1	A	167	LEU
1	A	176	VAL
1	A	181	LEU
1	A	197	VAL
1	A	199[A]	ILE
1	A	199[B]	ILE
1	A	203	THR
1	A	205	VAL
1	A	209	GLN
1	A	212	THR
1	A	215	LEU
1	A	216	VAL
1	A	217	ASN
1	A	220	LYS

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Mol	Chain	Res	Type
1	A	238	THR
1	A	253	VAL
1	A	261	LEU
1	A	265	VAL
1	A	275	LEU
1	A	276	VAL
1	A	280	VAL
1	A	285[A]	ARG
1	A	285[B]	ARG
1	A	296	LEU
1	A	307	LYS
1	A	315	LEU
1	A	316[A]	ARG
1	A	316[B]	ARG
1	A	319	THR
1	A	355	LEU
1	A	363	THR
1	A	369	ILE
1	A	377	CYS
1	A	379	VAL
1	A	386	VAL
1	A	394	LEU
1	A	395	LEU
1	A	405	VAL
1	A	407	LEU
1	B	3	ASN
1	B	5[A]	ARG
1	B	5[B]	ARG
1	B	10	LYS
1	B	38	ILE
1	B	42	LYS
1	B	43	GLU
1	B	46	GLU
1	B	51	CYS
1	B	77	ARG
1	B	99	HIS
1	B	105	PRO
1	B	106	VAL
1	B	117	VAL
1	B	119	LEU
1	B	120	LEU
1	B	122	THR

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Mol	Chain	Res	Type
1	B	133	THR
1	B	144	SER
1	B	148	GLU
1	B	160	THR
1	B	167	LEU
1	B	176	VAL
1	B	181	LEU
1	B	197	VAL
1	B	199[A]	ILE
1	B	199[B]	ILE
1	B	203	THR
1	B	205	VAL
1	B	209	GLN
1	B	212	THR
1	B	215[A]	LEU
1	B	215[B]	LEU
1	B	216	VAL
1	B	217	ASN
1	B	220	LYS
1	B	238	THR
1	B	253	VAL
1	B	261	LEU
1	B	265	VAL
1	B	275	LEU
1	B	276	VAL
1	B	280	VAL
1	B	285	ARG
1	B	296	LEU
1	B	307	LYS
1	B	315	LEU
1	B	316[A]	ARG
1	B	316[B]	ARG
1	B	319	THR
1	B	355	LEU
1	B	363	THR
1	B	369	ILE
1	B	379	VAL
1	B	386	VAL
1	B	394	LEU
1	B	395	LEU
1	B	407	LEU
1	B	412	ARG

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Mol	Chain	Res	Type
1	C	3	ASN
1	C	10	LYS
1	C	38	ILE
1	C	42	LYS
1	C	46	GLU
1	C	51	CYS
1	C	77	ARG
1	C	99	HIS
1	C	106	VAL
1	C	117	VAL
1	C	119	LEU
1	C	120	LEU
1	C	122	THR
1	C	133	THR
1	C	144	SER
1	C	148	GLU
1	C	160	THR
1	C	167	LEU
1	C	176	VAL
1	C	181	LEU
1	C	197	VAL
1	C	198	ARG
1	C	199[A]	ILE
1	C	199[B]	ILE
1	C	203	THR
1	C	205	VAL
1	C	209	GLN
1	C	212	THR
1	C	215	LEU
1	C	217	ASN
1	C	220	LYS
1	C	238	THR
1	C	253	VAL
1	C	261	LEU
1	C	265	VAL
1	C	275	LEU
1	C	276	VAL
1	C	280	VAL
1	C	296	LEU
1	C	307	LYS
1	C	315	LEU
1	C	316[A]	ARG

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Mol	Chain	Res	Type
1	C	316[B]	ARG
1	C	319	THR
1	C	355	LEU
1	C	363	THR
1	C	369	ILE
1	C	377	CYS
1	C	379	VAL
1	C	386	VAL
1	C	394	LEU
1	C	395	LEU
1	C	407	LEU
1	D	3	ASN
1	D	5[A]	ARG
1	D	5[B]	ARG
1	D	38	ILE
1	D	42	LYS
1	D	43	GLU
1	D	46	GLU
1	D	48	VAL
1	D	77	ARG
1	D	99	HIS
1	D	106	VAL
1	D	117	VAL
1	D	119	LEU
1	D	120	LEU
1	D	122	THR
1	D	133	THR
1	D	144	SER
1	D	148	GLU
1	D	160	THR
1	D	167	LEU
1	D	176	VAL
1	D	181	LEU
1	D	197	VAL
1	D	199[A]	ILE
1	D	199[B]	ILE
1	D	203	THR
1	D	205	VAL
1	D	209	GLN
1	D	212	THR
1	D	215	LEU
1	D	217	ASN

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Mol	Chain	Res	Type
1	D	220	LYS
1	D	238	THR
1	D	243[A]	ARG
1	D	243[B]	ARG
1	D	253	VAL
1	D	261	LEU
1	D	265	VAL
1	D	275	LEU
1	D	276	VAL
1	D	280	VAL
1	D	296	LEU
1	D	307	LYS
1	D	315	LEU
1	D	316[A]	ARG
1	D	316[B]	ARG
1	D	319	THR
1	D	347	SER
1	D	355	LEU
1	D	363	THR
1	D	369	ILE
1	D	379	VAL
1	D	385	LYS
1	D	386	VAL
1	D	394	LEU
1	D	395	LEU
1	D	407	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	88	ASN
1	A	159	ASN
1	A	162	GLN
1	A	209	GLN
1	A	232	ASN
1	A	257	ASN
1	A	343	ASN
1	B	3	ASN
1	B	88	ASN
1	B	159	ASN
1	B	209	GLN

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Mol	Chain	Res	Type
1	B	232	ASN
1	B	257	ASN
1	B	343	ASN
1	B	370	ASN
1	C	3	ASN
1	C	88	ASN
1	C	159	ASN
1	C	209	GLN
1	C	232	ASN
1	C	257	ASN
1	C	343	ASN
1	C	370	ASN
1	D	3	ASN
1	D	88	ASN
1	D	159	ASN
1	D	162	GLN
1	D	209	GLN
1	D	232	ASN
1	D	257	ASN
1	D	343	ASN
1	D	370	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 4 are monoatomic - leaving 24 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	LYS	D	420[A]	-	8,9,9	0.94	1 (12%)	7,10,10	1.17	1 (14%)
6	PLP	C	419	5	15,15,16	2.80	3 (20%)	21,22,23	0.97	0
5	LYS	A	420[B]	-	8,9,9	0.85	1 (12%)	7,10,10	1.05	0
5	LYS	C	420[B]	-	8,9,9	1.02	0	7,10,10	0.90	0
6	PLP	A	419	5	15,15,16	2.72	2 (13%)	21,22,23	1.18	2 (9%)
4	SAM	B	417	7	23,29,29	1.64	3 (13%)	20,42,42	1.68	6 (30%)
5	LYS	B	420[A]	-	8,9,9	0.74	0	7,10,10	1.02	1 (14%)
7	SF4	B	418	4,1	0,12,12	-	-	-	-	-
7	SF4	D	418	4,1	0,12,12	-	-	-	-	-
5	LYS	A	420[A]	-	8,9,9	0.85	1 (12%)	7,10,10	1.04	0
3	SO4	B	495	-	4,4,4	0.25	0	6,6,6	0.31	0
5	LYS	C	420[A]	-	8,9,9	1.03	0	7,10,10	0.94	0
4	SAM	D	417	7	23,29,29	1.40	3 (13%)	20,42,42	1.82	5 (25%)
7	SF4	A	418	4,1	0,12,12	-	-	-	-	-
6	PLP	B	419	5	15,15,16	2.76	2 (13%)	21,22,23	0.93	0
4	SAM	C	417	7	23,29,29	1.48	3 (13%)	20,42,42	1.83	5 (25%)
7	SF4	C	418	4,1	0,12,12	-	-	-	-	-
3	SO4	A	592	-	4,4,4	0.30	0	6,6,6	0.22	0
5	LYS	D	420[B]	-	8,9,9	0.94	1 (12%)	7,10,10	1.12	1 (14%)
3	SO4	D	494	-	4,4,4	0.31	0	6,6,6	0.34	0
6	PLP	D	419	5	15,15,16	2.88	2 (13%)	21,22,23	1.16	1 (4%)
3	SO4	C	593	-	4,4,4	0.24	0	6,6,6	0.47	0
4	SAM	A	417	7	23,29,29	1.57	3 (13%)	20,42,42	2.02	5 (25%)
5	LYS	B	420[B]	-	8,9,9	0.75	0	7,10,10	0.99	1 (14%)

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
5	LYS	D	420[A]	-	-	1/9/9/9	-
6	PLP	C	419	5	-	0/6/6/8	0/1/1/1
5	LYS	A	420[B]	-	-	1/9/9/9	-
5	LYS	C	420[B]	-	-	1/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PLP	A	419	5	-	1/6/6/8	0/1/1/1
4	SAM	B	417	7	-	2/13/33/33	0/3/3/3
5	LYS	B	420[A]	-	-	1/9/9/9	-
7	SF4	B	418	4,1	-	-	0/6/5/5
7	SF4	D	418	4,1	-	-	0/6/5/5
5	LYS	A	420[A]	-	-	1/9/9/9	-
5	LYS	C	420[A]	-	-	1/9/9/9	-
4	SAM	D	417	7	-	2/13/33/33	0/3/3/3
7	SF4	A	418	4,1	-	-	0/6/5/5
6	PLP	B	419	5	-	0/6/6/8	0/1/1/1
4	SAM	C	417	7	-	3/13/33/33	0/3/3/3
7	SF4	C	418	4,1	-	-	0/6/5/5
5	LYS	D	420[B]	-	-	1/9/9/9	-
6	PLP	D	419	5	-	0/6/6/8	0/1/1/1
4	SAM	A	417	7	-	2/13/33/33	0/3/3/3
5	LYS	B	420[B]	-	-	1/9/9/9	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	419	PLP	C4A-C4	-9.92	1.31	1.51
6	C	419	PLP	C4A-C4	-9.65	1.32	1.51
6	B	419	PLP	C4A-C4	-9.47	1.32	1.51
6	A	419	PLP	C4A-C4	-9.10	1.33	1.51
4	B	417	SAM	OXT-C	5.04	1.46	1.30
4	A	417	SAM	OXT-C	4.78	1.45	1.30
4	C	417	SAM	OXT-C	4.41	1.44	1.30
4	D	417	SAM	OXT-C	3.95	1.43	1.30
4	A	417	SAM	C2-N3	3.60	1.37	1.32
4	D	417	SAM	CE-SD	3.17	1.98	1.78
6	D	419	PLP	P-O2P	-3.08	1.43	1.54
4	B	417	SAM	O4'-C1'	2.92	1.44	1.40
4	A	417	SAM	CE-SD	2.91	1.97	1.78
4	B	417	SAM	CE-SD	2.79	1.96	1.78
4	C	417	SAM	CE-SD	2.65	1.95	1.78
4	C	417	SAM	O4'-C1'	2.63	1.44	1.40
6	C	419	PLP	P-O2P	-2.46	1.45	1.54
6	A	419	PLP	P-O2P	-2.44	1.45	1.54
6	C	419	PLP	O4P-C5A	2.22	1.53	1.44
5	D	420[A]	LYS	O-C	2.20	1.28	1.22
5	D	420[B]	LYS	O-C	2.20	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	419	PLP	C6-C5	2.14	1.42	1.37
4	D	417	SAM	O4'-C1'	2.12	1.43	1.40
5	A	420[A]	LYS	O-C	2.09	1.28	1.22
5	A	420[B]	LYS	O-C	2.09	1.28	1.22

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	417	SAM	C4'-O4'-C1'	-4.99	105.36	109.92
4	D	417	SAM	O4'-C1'-N9	4.69	114.96	108.75
4	A	417	SAM	O4'-C1'-N9	4.49	114.70	108.75
4	A	417	SAM	CG-SD-C5'	-4.00	93.65	103.43
4	C	417	SAM	CG-SD-C5'	-3.92	93.85	103.43
4	A	417	SAM	CB-CA-N	3.69	119.73	110.12
4	B	417	SAM	N3-C2-N1	-3.33	124.15	128.67
4	D	417	SAM	CB-CA-N	3.28	118.66	110.12
4	A	417	SAM	C4'-O4'-C1'	-3.17	107.02	109.92
4	B	417	SAM	C4'-O4'-C1'	-3.16	107.03	109.92
4	D	417	SAM	N3-C2-N1	-3.16	124.39	128.67
4	B	417	SAM	CB-CA-N	3.13	118.28	110.12
4	A	417	SAM	N3-C2-N1	-2.86	124.79	128.67
6	D	419	PLP	C4A-C4-C5	2.81	123.83	120.94
6	A	419	PLP	O4P-P-O1P	-2.74	99.02	106.44
6	A	419	PLP	O2P-P-O4P	2.64	113.56	106.67
4	D	417	SAM	CG-SD-C5'	-2.63	97.01	103.43
4	C	417	SAM	N3-C2-N1	-2.58	125.17	128.67
4	B	417	SAM	O4'-C1'-N9	2.58	112.16	108.75
4	C	417	SAM	C1'-N9-C4	-2.42	122.38	126.64
4	B	417	SAM	C1'-N9-C4	-2.36	122.50	126.64
4	D	417	SAM	C4-C5-N7	-2.33	106.87	109.34
4	B	417	SAM	C4-C5-N7	-2.25	106.96	109.34
5	D	420[A]	LYS	OXT-C-O	-2.24	118.99	124.08
5	D	420[B]	LYS	OXT-C-O	-2.24	118.99	124.08
4	C	417	SAM	C4-C5-N7	-2.17	107.04	109.34
5	B	420[A]	LYS	CB-CA-N	2.13	115.66	110.12
5	B	420[B]	LYS	CB-CA-N	2.13	115.66	110.12

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	417	SAM	N-CA-CB-CG

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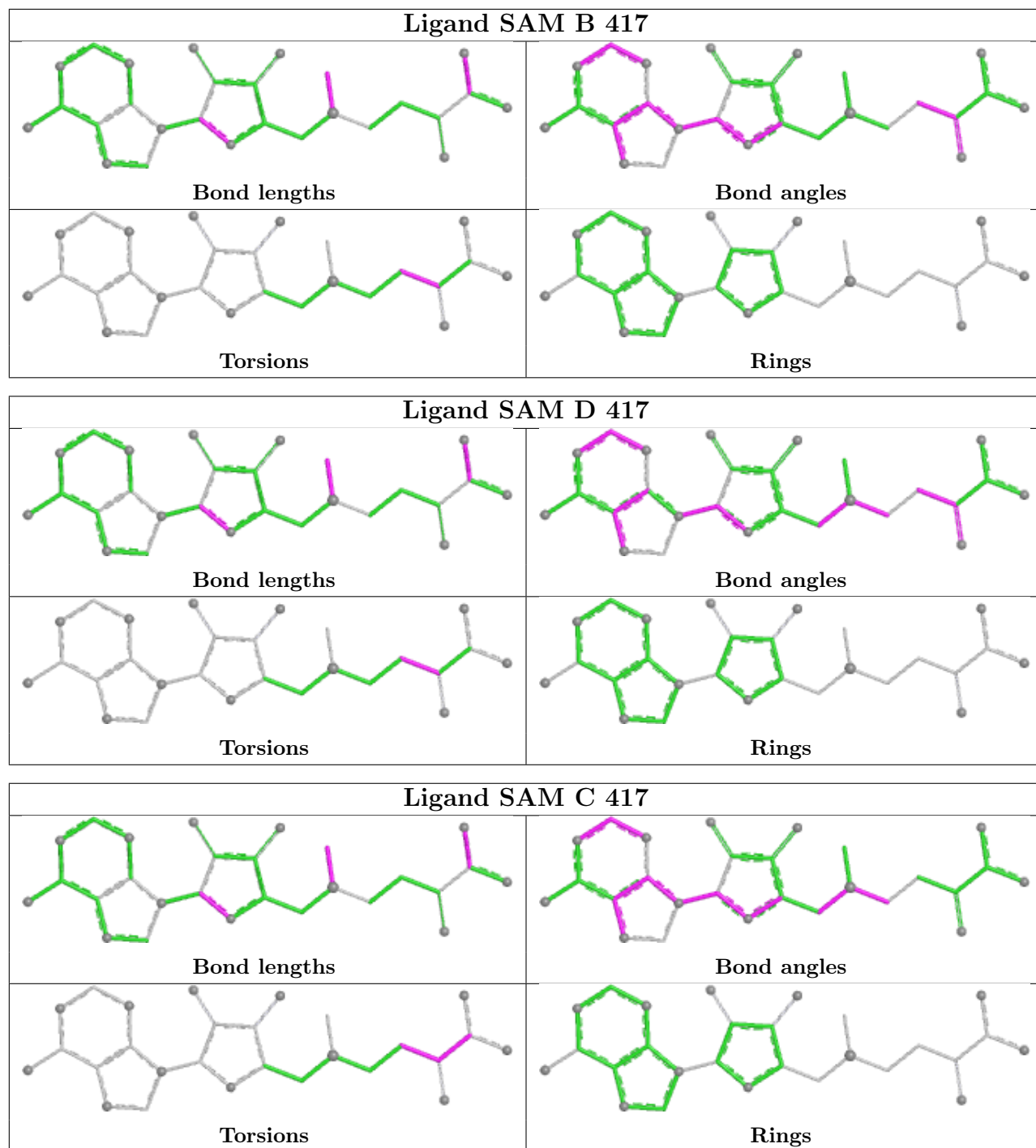
Mol	Chain	Res	Type	Atoms
4	D	417	SAM	N-CA-CB-CG
4	A	417	SAM	C-CA-CB-CG
4	B	417	SAM	C-CA-CB-CG
4	C	417	SAM	C-CA-CB-CG
4	D	417	SAM	C-CA-CB-CG
4	A	417	SAM	N-CA-CB-CG
4	B	417	SAM	N-CA-CB-CG
6	A	419	PLP	C5A-O4P-P-O1P
5	A	420[A]	LYS	OXT-C-CA-N
5	A	420[B]	LYS	OXT-C-CA-N
4	C	417	SAM	O-C-CA-N
5	B	420[A]	LYS	OXT-C-CA-N
5	B	420[B]	LYS	OXT-C-CA-N
5	D	420[A]	LYS	OXT-C-CA-N
5	D	420[B]	LYS	OXT-C-CA-N
5	C	420[A]	LYS	OXT-C-CA-N
5	C	420[B]	LYS	OXT-C-CA-N

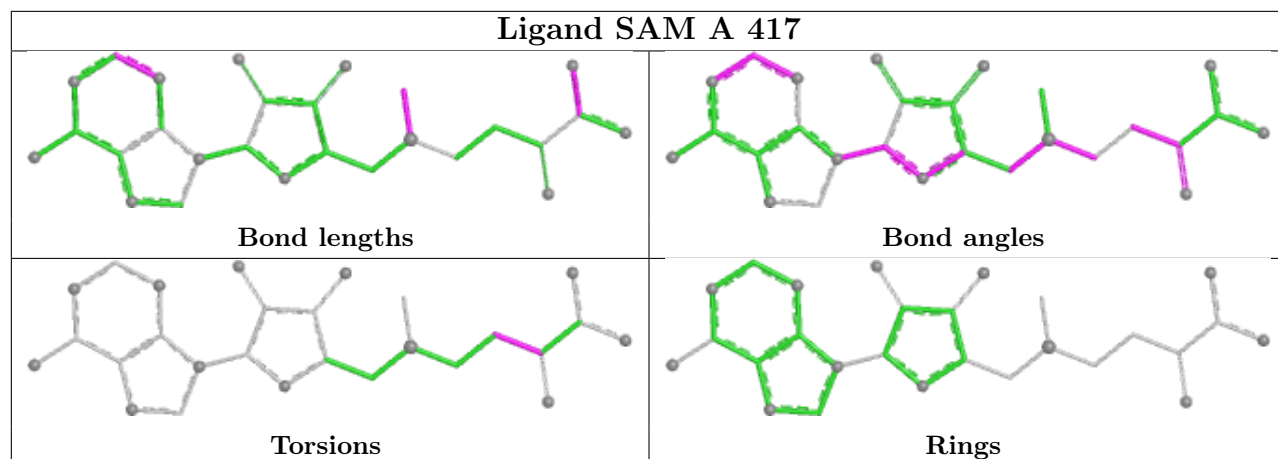
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	418	SF4	1	0
7	C	418	SF4	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.





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	400/416 (96%)	3.65	357 (89%) 0 0	12, 38, 60, 72	18 (4%)
1	B	401/416 (96%)	4.14	376 (93%) 0 0	13, 42, 78, 98	15 (3%)
1	C	400/416 (96%)	3.48	343 (85%) 0 0	11, 32, 58, 73	15 (3%)
1	D	401/416 (96%)	3.27	334 (83%) 0 0	9, 32, 54, 69	15 (3%)
All	All	1602/1664 (96%)	3.63	1410 (88%) 0 0	9, 36, 64, 98	63 (3%)

All (1410) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	47	GLY	13.3
1	D	52	VAL	12.2
1	A	48	VAL	12.0
1	B	31	VAL	11.5
1	A	46	GLU	10.0
1	A	90	ALA	9.7
1	B	81	ILE	9.6
1	B	138	ALA	9.6
1	C	38	ILE	9.3
1	A	52	VAL	9.2
1	B	48	VAL	8.9
1	C	48	VAL	8.8
1	B	66	LEU	8.7
1	B	88	ASN	8.7
1	B	176	VAL	8.6
1	B	4	ARG	8.6
1	C	30	THR	8.5
1	C	369	ILE	8.4
1	A	34	LEU	8.3
1	B	30	THR	8.3
1	B	38	ILE	8.0

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Mol	Chain	Res	Type	RSRZ
1	A	206	VAL	8.0
1	D	34	LEU	8.0
1	B	6	TYR	8.0
1	B	64	LEU	7.9
1	C	52	VAL	7.9
1	B	92	ALA	7.9
1	D	48	VAL	7.9
1	B	14	ASP	7.9
1	B	175	LEU	7.8
1	C	153	ALA	7.8
1	A	53	LYS	7.8
1	C	31	VAL	7.7
1	B	55	LEU	7.7
1	D	92	ALA	7.6
1	B	35	LYS	7.6
1	B	8	LEU	7.6
1	B	32	GLU	7.6
1	D	43	GLU	7.6
1	B	12	VAL	7.5
1	B	93	ASP	7.4
1	C	51	CYS	7.4
1	A	10	LYS	7.3
1	A	120	LEU	7.3
1	C	12	VAL	7.3
1	D	128	TYR	7.3
1	A	406	GLY	7.2
1	A	368	PRO	7.2
1	C	175	LEU	7.2
1	A	38	ILE	7.1
1	D	40	LEU	7.1
1	B	95	GLU	7.1
1	C	53	LYS	7.1
1	C	73	ASN	7.1
1	B	98	LEU	7.0
1	D	33	GLU	7.0
1	D	120	LEU	7.0
1	B	369	ILE	7.0
1	B	22	TRP	7.0
1	B	229	THR	6.9
1	C	11	ASP	6.9
1	A	51	CYS	6.9
1	A	89	LYS	6.9

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Mol	Chain	Res	Type	RSRZ
1	B	37	TYR	6.9
1	A	174	LEU	6.9
1	D	55	LEU	6.9
1	D	254	PRO	6.8
1	B	119	LEU	6.8
1	B	181	LEU	6.8
1	C	62	TYR	6.8
1	D	46	GLU	6.7
1	C	7	GLU	6.7
1	B	59	ILE	6.7
1	D	35	LYS	6.7
1	B	139	GLY	6.7
1	B	239	GLU	6.7
1	B	40	LEU	6.7
1	A	92	ALA	6.6
1	B	50	GLN	6.6
1	B	10	LYS	6.6
1	A	117	VAL	6.6
1	C	58	ALA	6.6
1	B	47	GLY	6.5
1	A	31	VAL	6.5
1	C	128	TYR	6.5
1	A	395	LEU	6.5
1	D	29	GLU	6.4
1	C	81	ILE	6.4
1	C	90	ALA	6.4
1	C	59	ILE	6.4
1	A	128	TYR	6.4
1	C	95	GLU	6.4
1	B	211	ILE	6.4
1	A	85	LEU	6.3
1	A	71	ASP	6.3
1	A	28	ILE	6.3
1	B	264	GLY	6.3
1	B	87	LEU	6.3
1	D	265	VAL	6.3
1	A	369	ILE	6.3
1	A	47	GLY	6.3
1	A	40	LEU	6.3
1	D	69	PRO	6.3
1	B	126	SER	6.2
1	D	31	VAL	6.2

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Mol	Chain	Res	Type	RSRZ
1	C	241	SER	6.2
1	D	49	ALA	6.2
1	B	128	TYR	6.2
1	B	44	GLU	6.2
1	A	55	LEU	6.2
1	B	34	LEU	6.2
1	C	37	TYR	6.2
1	A	87	LEU	6.1
1	B	143	ASP	6.1
1	B	39	PRO	6.1
1	B	140	GLN	6.1
1	A	37	TYR	6.1
1	A	9	PHE	6.1
1	A	66	LEU	6.1
1	A	91	ALA	6.1
1	C	253	VAL	6.1
1	D	334	GLY	6.1
1	B	9	PHE	6.1
1	C	54	SER	6.1
1	A	258	GLN	6.1
1	B	75	PRO	6.0
1	D	38	ILE	6.0
1	B	89	LYS	6.0
1	B	254	PRO	6.0
1	D	54	SER	6.0
1	D	84	ALA	6.0
1	B	246	GLN	6.0
1	C	10	LYS	5.9
1	B	24	VAL	5.9
1	B	63	TYR	5.9
1	B	154	ILE	5.9
1	B	260[A]	VAL	5.9
1	B	203	THR	5.9
1	B	94	LEU	5.9
1	A	84	ALA	5.9
1	B	76	VAL	5.9
1	B	83	THR	5.9
1	A	362	ILE	5.8
1	B	28	ILE	5.8
1	B	53	LYS	5.8
1	D	47	GLY	5.8
1	D	53	LYS	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	13	SER	5.8
1	B	134	ARG	5.8
1	A	188	LEU	5.8
1	B	135	ARG	5.8
1	C	56	ARG	5.8
1	B	52	VAL	5.8
1	B	227	LEU	5.8
1	B	296	LEU	5.8
1	C	40	LEU	5.8
1	D	196	ILE	5.8
1	B	58	ALA	5.8
1	D	51	CYS	5.7
1	B	46	GLU	5.7
1	B	160	THR	5.7
1	B	85	LEU	5.7
1	B	69	PRO	5.7
1	D	39	PRO	5.7
1	D	381	THR	5.7
1	C	6	TYR	5.6
1	C	8	LEU	5.6
1	C	55	LEU	5.6
1	B	54	SER	5.6
1	C	9	PHE	5.6
1	A	346[A]	ILE	5.6
1	D	96	ASP	5.6
1	D	190	GLU	5.6
1	B	184	ILE	5.5
1	C	32	GLU	5.5
1	D	56	ARG	5.5
1	A	69	PRO	5.5
1	B	121	ILE	5.5
1	B	33	GLU	5.5
1	C	170	GLY	5.5
1	A	166	VAL	5.5
1	B	3	ASN	5.5
1	A	119	LEU	5.5
1	C	22	TRP	5.5
1	A	49	ALA	5.5
1	A	199[A]	ILE	5.5
1	B	334	GLY	5.5
1	B	370	ASN	5.5
1	C	176	VAL	5.5

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Mol	Chain	Res	Type	RSRZ
1	C	408	GLU	5.5
1	B	11	ASP	5.5
1	D	412	ARG	5.5
1	B	137	PHE	5.5
1	C	137	PHE	5.5
1	D	369	ILE	5.5
1	C	370	ASN	5.4
1	C	152	LYS	5.4
1	A	263	ARG	5.4
1	B	27[A]	ARG	5.4
1	B	247	LEU	5.4
1	B	262	LEU	5.4
1	A	146	PRO	5.4
1	B	146	PRO	5.4
1	B	26	ASN	5.4
1	A	386	VAL	5.4
1	B	389	VAL	5.4
1	C	64	LEU	5.4
1	A	95	GLU	5.4
1	A	214	GLU	5.4
1	A	296	LEU	5.4
1	C	389	VAL	5.4
1	D	83	THR	5.4
1	B	73	ASN	5.4
1	A	62	TYR	5.3
1	D	382	GLY	5.3
1	D	122	THR	5.3
1	B	231	PHE	5.3
1	B	82	PRO	5.3
1	A	205	VAL	5.3
1	B	276	VAL	5.3
1	C	171	GLY	5.3
1	D	89	LYS	5.3
1	D	185	ILE	5.3
1	C	119	LEU	5.3
1	C	35	LYS	5.3
1	A	191	ILE	5.3
1	A	186	ALA	5.3
1	A	6	TYR	5.3
1	A	311	ILE	5.2
1	B	157	ILE	5.2
1	C	121	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	237	ILE	5.2
1	B	7	GLU	5.2
1	D	36	LYS	5.2
1	A	12	VAL	5.2
1	B	84	ALA	5.2
1	A	122	THR	5.2
1	B	156	TYR	5.2
1	B	412	ARG	5.2
1	C	43	GLU	5.2
1	A	167	LEU	5.2
1	C	34	LEU	5.2
1	D	106	VAL	5.2
1	D	50	GLN	5.2
1	C	299	GLU	5.2
1	C	279	LEU	5.2
1	D	64	LEU	5.2
1	A	138	ALA	5.2
1	B	80	ALA	5.2
1	A	7	GLU	5.2
1	B	192	PRO	5.2
1	B	150	ILE	5.2
1	A	298	LEU	5.1
1	D	181	LEU	5.1
1	A	319	THR	5.1
1	B	186	ALA	5.1
1	B	86	GLU	5.1
1	A	157	ILE	5.1
1	B	207	LEU	5.1
1	A	126	SER	5.1
1	A	350	HIS	5.1
1	D	154	ILE	5.1
1	D	199[A]	ILE	5.1
1	B	149	ARG	5.1
1	A	64	LEU	5.1
1	B	19	ASP	5.1
1	C	15	ALA	5.1
1	C	84	ALA	5.1
1	C	138	ALA	5.1
1	B	56	ARG	5.0
1	C	346[A]	ILE	5.0
1	B	230	HIS	5.0
1	B	153	ALA	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	50	GLN	5.0
1	B	65	SER	5.0
1	B	294	LEU	5.0
1	B	61	PRO	5.0
1	D	117	VAL	5.0
1	C	36	LYS	5.0
1	A	181	LEU	5.0
1	C	216	VAL	5.0
1	B	183	TYR	4.9
1	D	87	LEU	4.9
1	D	45	GLU	4.9
1	C	72	PRO	4.9
1	B	199[A]	ILE	4.9
1	B	17	TRP	4.9
1	B	298	LEU	4.9
1	C	235	ASN	4.9
1	B	252	GLY	4.9
1	D	9	PHE	4.9
1	A	98	LEU	4.9
1	D	226	TRP	4.9
1	A	156	TYR	4.9
1	B	49	ALA	4.9
1	B	103	ASP	4.9
1	A	43	GLU	4.9
1	A	121	ILE	4.9
1	A	207	LEU	4.9
1	C	181	LEU	4.9
1	C	75	PRO	4.8
1	D	126	SER	4.8
1	C	383	LYS	4.8
1	D	150	ILE	4.8
1	C	248	LEU	4.8
1	C	375	CYS	4.8
1	D	171	GLY	4.8
1	C	33	GLU	4.8
1	A	54	SER	4.8
1	B	141	SER	4.8
1	A	73	ASN	4.8
1	A	245	CYS	4.8
1	C	373	PRO	4.8
1	B	91	ALA	4.8
1	C	24	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	260[A]	VAL	4.8
1	B	180	THR	4.8
1	B	315	LEU	4.8
1	C	296	LEU	4.8
1	D	399	GLY	4.8
1	B	90	ALA	4.8
1	B	25	ARG	4.7
1	D	41	THR	4.7
1	D	90	ALA	4.7
1	D	91	ALA	4.7
1	C	89	LYS	4.7
1	A	76	VAL	4.7
1	B	271	VAL	4.7
1	A	79	GLN	4.7
1	B	174	LEU	4.7
1	C	315	LEU	4.7
1	C	374	GLY	4.7
1	A	208	PRO	4.7
1	B	281	LYS	4.7
1	A	22	TRP	4.7
1	B	282	ILE	4.7
1	A	254	PRO	4.7
1	D	27[A]	ARG	4.7
1	B	329	VAL	4.7
1	D	197	VAL	4.7
1	C	46	GLU	4.7
1	C	20	TRP	4.7
1	B	360	GLY	4.7
1	B	397	GLY	4.7
1	A	352	LYS	4.7
1	A	8	LEU	4.7
1	A	109	LEU	4.7
1	B	224	PRO	4.6
1	B	368	PRO	4.6
1	B	301	PHE	4.6
1	C	4	ARG	4.6
1	C	260[A]	VAL	4.6
1	A	399	GLY	4.6
1	B	109	LEU	4.6
1	B	373	PRO	4.6
1	D	58	ALA	4.6
1	B	349	SER	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	376	ASN	4.6
1	A	260[A]	VAL	4.6
1	D	78	LYS	4.6
1	B	122	THR	4.6
1	A	150	ILE	4.6
1	B	72	PRO	4.6
1	B	332	PRO	4.6
1	C	154	ILE	4.6
1	D	311	ILE	4.6
1	A	29	GLU	4.6
1	B	232	ASN	4.6
1	D	88	ASN	4.6
1	D	11	ASP	4.6
1	D	130	ARG	4.6
1	D	229	THR	4.6
1	A	82	PRO	4.6
1	D	148	GLU	4.6
1	D	362	ILE	4.6
1	B	70	ASN	4.6
1	A	27[A]	ARG	4.5
1	D	142	ASP	4.5
1	D	143	ASP	4.5
1	D	280	VAL	4.5
1	A	300	HIS	4.5
1	D	379	VAL	4.5
1	A	212	THR	4.5
1	D	86	GLU	4.5
1	C	66	LEU	4.5
1	D	294	LEU	4.5
1	B	278	LYS	4.5
1	C	252	GLY	4.5
1	B	36	LYS	4.5
1	A	67	ILE	4.5
1	C	144	SER	4.5
1	B	378	ASP	4.5
1	A	44	GLU	4.5
1	A	24	VAL	4.5
1	A	60	THR	4.5
1	A	110	THR	4.5
1	C	379	VAL	4.5
1	A	159	ASN	4.4
1	D	32	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	301	PHE	4.4
1	A	83	THR	4.4
1	B	41	THR	4.4
1	B	97	PRO	4.4
1	C	27[A]	ARG	4.4
1	A	94	LEU	4.4
1	A	402	LEU	4.4
1	B	144	SER	4.4
1	B	200	GLY	4.4
1	C	139	GLY	4.4
1	C	87	LEU	4.4
1	A	68	ASP	4.4
1	C	151	ASP	4.4
1	A	137	PHE	4.4
1	A	56	ARG	4.4
1	B	5[A]	ARG	4.4
1	B	77	ARG	4.4
1	C	21	ARG	4.4
1	C	212	THR	4.4
1	A	197	VAL	4.4
1	C	204	PRO	4.4
1	B	43	GLU	4.4
1	B	275	LEU	4.4
1	C	402	LEU	4.4
1	A	63	TYR	4.3
1	A	171	GLY	4.3
1	B	187	LYS	4.3
1	C	130	ARG	4.3
1	A	30	THR	4.3
1	A	343	ASN	4.3
1	B	51	CYS	4.3
1	B	133	THR	4.3
1	C	133	THR	4.3
1	D	376	ASN	4.3
1	A	389	VAL	4.3
1	B	305	VAL	4.3
1	D	22	TRP	4.3
1	B	168	LEU	4.3
1	C	131	HIS	4.3
1	A	237	ILE	4.3
1	A	411	LYS	4.3
1	C	150	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	121	ILE	4.3
1	A	135	ARG	4.3
1	A	243[A]	ARG	4.3
1	C	301	PHE	4.3
1	B	381	THR	4.3
1	A	107	PRO	4.3
1	B	166	VAL	4.3
1	B	206	VAL	4.3
1	B	265	VAL	4.3
1	C	50	GLN	4.3
1	B	20	TRP	4.3
1	B	255	LEU	4.3
1	C	17	TRP	4.3
1	B	42	LYS	4.3
1	B	158	ARG	4.3
1	A	334	GLY	4.3
1	B	244	ALA	4.3
1	C	360	GLY	4.3
1	A	371	TYR	4.3
1	B	287	TYR	4.3
1	D	129	CYS	4.3
1	A	35	LYS	4.3
1	B	21	ARG	4.3
1	C	94	LEU	4.3
1	D	296	LEU	4.3
1	B	171	GLY	4.3
1	C	92	ALA	4.3
1	C	264	GLY	4.3
1	A	196	ILE	4.3
1	B	274	GLU	4.3
1	C	106	VAL	4.2
1	B	297	GLY	4.2
1	B	376	ASN	4.2
1	A	160	THR	4.2
1	D	10	LYS	4.2
1	D	24	VAL	4.2
1	D	402	LEU	4.2
1	A	382	GLY	4.2
1	B	195	GLU	4.2
1	B	299	GLU	4.2
1	C	3	ASN	4.2
1	A	226	TRP	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	309	ILE	4.2
1	C	157	ILE	4.2
1	C	41	THR	4.2
1	A	136	ARG	4.2
1	B	104	SER	4.2
1	A	39	PRO	4.2
1	A	224	PRO	4.2
1	A	33	GLU	4.2
1	B	45	GLU	4.2
1	C	109	LEU	4.2
1	D	94	LEU	4.2
1	B	191	ILE	4.2
1	D	157	ILE	4.2
1	A	17	TRP	4.2
1	B	243	ARG	4.2
1	B	384	LYS	4.2
1	A	133	THR	4.2
1	C	13	SER	4.2
1	B	62	TYR	4.2
1	C	113	TYR	4.2
1	B	190	GLU	4.2
1	C	125	CYS	4.2
1	B	170	GLY	4.2
1	C	382	GLY	4.2
1	D	217	ASN	4.2
1	D	251	ALA	4.1
1	D	28	ILE	4.1
1	D	377	CYS	4.1
1	B	194	VAL	4.1
1	C	205	VAL	4.1
1	A	153	ALA	4.1
1	C	211	ILE	4.1
1	C	126	SER	4.1
1	D	155	ASP	4.1
1	D	319	THR	4.1
1	A	45	GLU	4.1
1	A	86	GLU	4.1
1	A	20	TRP	4.1
1	A	297	GLY	4.1
1	D	156	TYR	4.1
1	A	194	VAL	4.1
1	A	248	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	276	VAL	4.1
1	B	331	ALA	4.1
1	D	244	ALA	4.1
1	C	311	ILE	4.1
1	C	69	PRO	4.1
1	C	410	ASN	4.1
1	A	230	HIS	4.1
1	D	389	VAL	4.1
1	C	80	ALA	4.1
1	D	141	SER	4.1
1	C	258	GLN	4.1
1	A	200	GLY	4.0
1	D	206	VAL	4.0
1	D	386	VAL	4.0
1	A	80	ALA	4.0
1	A	349	SER	4.0
1	D	363	THR	4.0
1	B	411	LYS	4.0
1	C	88	ASN	4.0
1	A	111	HIS	4.0
1	B	280	VAL	4.0
1	B	142	ASP	4.0
1	D	110	THR	4.0
1	D	221	LYS	4.0
1	D	411	LYS	4.0
1	A	70	ASN	4.0
1	A	376	ASN	4.0
1	B	108	GLY	4.0
1	B	367	GLU	4.0
1	C	206	VAL	4.0
1	C	63	TYR	4.0
1	B	286	PRO	4.0
1	D	107	PRO	4.0
1	C	29	GLU	4.0
1	C	86	GLU	4.0
1	D	100	GLU	4.0
1	B	219	LEU	4.0
1	D	222	TYR	3.9
1	C	362	ILE	3.9
1	D	191	ILE	3.9
1	A	149	ARG	3.9
1	B	120	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	279	LEU	3.9
1	D	85	LEU	3.9
1	D	207	LEU	3.9
1	A	36	LYS	3.9
1	A	244	ALA	3.9
1	C	78	LYS	3.9
1	C	329	VAL	3.9
1	A	375	CYS	3.9
1	A	322	TYR	3.9
1	D	365	TYR	3.9
1	A	3	ASN	3.9
1	B	217	ASN	3.9
1	A	190	GLU	3.9
1	C	134	ARG	3.9
1	D	25	ARG	3.9
1	A	172	ASP	3.9
1	A	378	ASP	3.9
1	C	115	ASP	3.9
1	B	383	LYS	3.9
1	C	231	PHE	3.9
1	A	104	SER	3.9
1	B	253	VAL	3.9
1	A	26	ASN	3.9
1	A	240	GLU	3.9
1	D	17	TRP	3.9
1	B	285	ARG	3.9
1	C	316[A]	ARG	3.9
1	B	151	ASP	3.9
1	B	78	LYS	3.9
1	A	262	LEU	3.9
1	A	163	VAL	3.9
1	C	91	ALA	3.9
1	D	7	GLU	3.9
1	D	173	ALA	3.9
1	B	212	THR	3.9
1	B	380	CYS	3.9
1	D	3	ASN	3.9
1	C	209	GLN	3.8
1	D	82	PRO	3.8
1	A	383	LYS	3.8
1	C	141	SER	3.8
1	C	247	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	119	LEU	3.8
1	A	358	PHE	3.8
1	B	266	ASN	3.8
1	B	372	THR	3.8
1	C	322	TYR	3.8
1	D	37	TYR	3.8
1	D	62	TYR	3.8
1	A	154	ILE	3.8
1	C	19	ASP	3.8
1	C	398	GLU	3.8
1	A	407	LEU	3.8
1	C	229	THR	3.8
1	A	139	GLY	3.8
1	C	129	CYS	3.8
1	C	224	PRO	3.8
1	D	152	LYS	3.8
1	D	6	TYR	3.8
1	C	71	ASP	3.8
1	B	354	ILE	3.8
1	C	45	GLU	3.8
1	B	131	HIS	3.8
1	B	248	LEU	3.8
1	D	8	LEU	3.8
1	A	285[A]	ARG	3.8
1	B	235	ASN	3.8
1	C	266	ASN	3.8
1	B	348	GLN	3.8
1	D	30	THR	3.8
1	D	372	THR	3.8
1	A	269	VAL	3.8
1	A	353	VAL	3.8
1	A	379	VAL	3.8
1	B	374	GLY	3.8
1	C	197	VAL	3.8
1	A	385	LYS	3.8
1	D	42	LYS	3.8
1	C	39	PRO	3.8
1	C	146	PRO	3.8
1	B	16	ASP	3.8
1	B	123	ASP	3.8
1	B	351	ASP	3.8
1	C	354	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	230	HIS	3.8
1	C	202	ARG	3.7
1	B	394	LEU	3.7
1	C	98	LEU	3.7
1	C	207	LEU	3.7
1	C	255	LEU	3.7
1	D	174	LEU	3.7
1	C	337	LYS	3.7
1	C	76	VAL	3.7
1	A	97	PRO	3.7
1	B	375	CYS	3.7
1	C	378	ASP	3.7
1	B	167	LEU	3.7
1	C	215	LEU	3.7
1	B	106	VAL	3.7
1	B	225	VAL	3.7
1	A	96	ASP	3.7
1	A	367	GLU	3.7
1	A	373	PRO	3.7
1	B	107	PRO	3.7
1	D	99	HIS	3.7
1	D	59	ILE	3.7
1	C	201	SER	3.7
1	D	170	GLY	3.7
1	A	398	GLU	3.7
1	C	214	GLU	3.7
1	A	213	PRO	3.7
1	A	253	VAL	3.7
1	B	353	VAL	3.7
1	B	379	VAL	3.7
1	B	302	ARG	3.7
1	C	140	GLN	3.7
1	B	228	ASN	3.7
1	B	277	ASN	3.7
1	A	247	LEU	3.7
1	A	275	LEU	3.7
1	C	407	LEU	3.7
1	C	314	GLY	3.7
1	D	403	GLU	3.7
1	A	327	PHE	3.7
1	C	136	ARG	3.7
1	D	136	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	276	VAL	3.6
1	C	61	PRO	3.6
1	C	82	PRO	3.6
1	C	345	VAL	3.6
1	B	162	GLN	3.6
1	A	78	LYS	3.6
1	D	312	ILE	3.6
1	A	227	LEU	3.6
1	A	255	LEU	3.6
1	A	390	GLY	3.6
1	D	175	LEU	3.6
1	A	189	ARG	3.6
1	B	112	ARG	3.6
1	C	68	ASP	3.6
1	C	172	ASP	3.6
1	D	158	ARG	3.6
1	A	131	HIS	3.6
1	C	387	HIS	3.6
1	D	61	PRO	3.6
1	D	75	PRO	3.6
1	B	340	VAL	3.6
1	A	287	TYR	3.6
1	B	222	TYR	3.6
1	B	382	GLY	3.6
1	B	60	THR	3.6
1	C	83	THR	3.6
1	A	348	GLN	3.6
1	B	173	ALA	3.6
1	D	401	ALA	3.6
1	A	225	VAL	3.6
1	B	328	VAL	3.6
1	A	295	SER	3.6
1	B	366	SER	3.6
1	B	196	ILE	3.6
1	D	282	ILE	3.6
1	C	335	GLY	3.6
1	B	118	LEU	3.6
1	C	85	LEU	3.6
1	C	14	ASP	3.6
1	B	110	THR	3.6
1	C	60	THR	3.6
1	A	286	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	404	PRO	3.6
1	B	205	VAL	3.6
1	C	217	ASN	3.6
1	B	29	GLU	3.6
1	A	132	CYS	3.6
1	C	292	CYS	3.6
1	C	67	ILE	3.5
1	C	199[A]	ILE	3.5
1	B	74	ASP	3.5
1	C	120	LEU	3.5
1	C	142	ASP	3.5
1	C	278	LYS	3.5
1	A	32	GLU	3.5
1	D	176	VAL	3.5
1	D	349	SER	3.5
1	A	19	ASP	3.5
1	C	282	ILE	3.5
1	A	118	LEU	3.5
1	C	262	LEU	3.5
1	B	15	ALA	3.5
1	D	138	ALA	3.5
1	D	73	ASN	3.5
1	D	137	PHE	3.5
1	B	284	VAL	3.5
1	B	345	VAL	3.5
1	C	340	VAL	3.5
1	B	226	TRP	3.5
1	C	377	CYS	3.5
1	A	155	ASP	3.5
1	D	178	ASP	3.5
1	A	81	ILE	3.5
1	D	160	THR	3.5
1	A	72	PRO	3.5
1	B	251	ALA	3.5
1	A	169	SER	3.5
1	D	320	SER	3.5
1	B	233	HIS	3.5
1	A	11	ASP	3.5
1	D	172	ASP	3.5
1	A	184	ILE	3.5
1	B	67	ILE	3.5
1	A	299	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	408	GLU	3.5
1	B	214	GLU	3.5
1	B	215[A]	LEU	3.5
1	C	44	GLU	3.5
1	D	98	LEU	3.5
1	D	407	LEU	3.5
1	C	77	ARG	3.5
1	A	88	ASN	3.5
1	C	228	ASN	3.5
1	A	105	PRO	3.4
1	A	176	VAL	3.4
1	A	387	HIS	3.4
1	D	12	VAL	3.4
1	D	151	ASP	3.4
1	B	132	CYS	3.4
1	B	148	GLU	3.4
1	B	164	ARG	3.4
1	B	237	ILE	3.4
1	B	188	LEU	3.4
1	D	298	LEU	3.4
1	A	13	SER	3.4
1	D	169	SER	3.4
1	A	183	TYR	3.4
1	A	222	TYR	3.4
1	B	387	HIS	3.4
1	A	220	LYS	3.4
1	B	172	ASP	3.4
1	C	117	VAL	3.4
1	C	163	VAL	3.4
1	B	310	GLU	3.4
1	B	408	GLU	3.4
1	A	164	ARG	3.4
1	C	122	THR	3.4
1	C	174	LEU	3.4
1	D	67	ILE	3.4
1	D	255	LEU	3.4
1	A	246	GLN	3.4
1	C	105	PRO	3.4
1	A	187	LYS	3.4
1	B	330	ASP	3.4
1	D	330	ASP	3.4
1	A	170	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	360	GLY	3.4
1	D	194	VAL	3.4
1	C	189	ARG	3.4
1	C	277	ASN	3.4
1	A	211	ILE	3.4
1	A	114	PRO	3.4
1	B	213	PRO	3.4
1	D	373	PRO	3.4
1	D	295	SER	3.4
1	A	388	LYS	3.4
1	A	142	ASP	3.4
1	D	44	GLU	3.4
1	A	329	VAL	3.3
1	B	245	CYS	3.3
1	D	247	LEU	3.3
1	D	350	HIS	3.3
1	A	330	ASP	3.3
1	A	333	GLY	3.3
1	D	333	GLY	3.3
1	A	216	VAL	3.3
1	A	271	VAL	3.3
1	B	327	PHE	3.3
1	B	391	VAL	3.3
1	D	205	VAL	3.3
1	D	246	GLN	3.3
1	A	102	THR	3.3
1	A	279	LEU	3.3
1	A	294	LEU	3.3
1	A	152	LYS	3.3
1	A	75	PRO	3.3
1	B	114	PRO	3.3
1	D	274	GLU	3.3
1	A	77	ARG	3.3
1	C	25	ARG	3.3
1	B	68	ASP	3.3
1	A	393	GLY	3.3
1	A	284	VAL	3.3
1	B	371	TYR	3.3
1	B	386	VAL	3.3
1	C	353	VAL	3.3
1	D	322	TYR	3.3
1	C	242	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	4	ARG	3.3
1	A	100	GLU	3.3
1	D	95	GLU	3.3
1	D	16	ASP	3.3
1	B	216	VAL	3.3
1	C	386	VAL	3.3
1	C	5[A]	ARG	3.3
1	B	169	SER	3.3
1	C	298	LEU	3.3
1	D	66	LEU	3.3
1	D	259	SER	3.3
1	A	61	PRO	3.2
1	B	257	ASN	3.2
1	C	42	LYS	3.2
1	B	198	ARG	3.2
1	A	41	THR	3.2
1	D	60	THR	3.2
1	C	355	LEU	3.2
1	D	97	PRO	3.2
1	C	268	CYS	3.2
1	C	23	GLN	3.2
1	C	49	ALA	3.2
1	C	173	ALA	3.2
1	D	200	GLY	3.2
1	D	374	GLY	3.2
1	B	189	ARG	3.2
1	C	148	GLU	3.2
1	D	149	ARG	3.2
1	D	353	VAL	3.2
1	B	113	TYR	3.2
1	B	241	SER	3.2
1	D	144	SER	3.2
1	A	14	ASP	3.2
1	A	168	LEU	3.2
1	A	215	LEU	3.2
1	B	268	CYS	3.2
1	A	173	ALA	3.2
1	A	374	GLY	3.2
1	A	410	ASN	3.2
1	A	134	ARG	3.2
1	D	164	ARG	3.2
1	C	233	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	358	PHE	3.2
1	C	238	THR	3.2
1	B	96	ASP	3.2
1	B	325	PRO	3.2
1	C	261	LEU	3.2
1	D	368	PRO	3.2
1	D	395	LEU	3.2
1	A	282	ILE	3.2
1	A	130	ARG	3.2
1	B	136	ARG	3.2
1	B	210	ARG	3.2
1	D	220	LYS	3.2
1	C	182	GLU	3.2
1	D	214	GLU	3.2
1	B	326	THR	3.1
1	B	361	VAL	3.1
1	C	381	THR	3.1
1	D	163	VAL	3.1
1	D	329	VAL	3.1
1	A	103	ASP	3.1
1	A	178	ASP	3.1
1	A	175	LEU	3.1
1	A	290	TYR	3.1
1	D	114	PRO	3.1
1	A	221	LYS	3.1
1	B	362	ILE	3.1
1	B	125	CYS	3.1
1	B	182	GLU	3.1
1	C	112	ARG	3.1
1	C	196	ILE	3.1
1	D	195	GLU	3.1
1	B	350	HIS	3.1
1	A	229	THR	3.1
1	B	363	THR	3.1
1	B	220	LYS	3.1
1	B	263	ARG	3.1
1	B	316[A]	ARG	3.1
1	A	182	GLU	3.1
1	A	252	GLY	3.1
1	A	264	GLY	3.1
1	D	183	TYR	3.1
1	A	257	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	28	ILE	3.1
1	A	129	CYS	3.1
1	A	381	THR	3.1
1	A	5[A]	ARG	3.1
1	B	152	LYS	3.1
1	B	352	LYS	3.1
1	C	283	ARG	3.1
1	B	234	PRO	3.1
1	D	168	LEU	3.1
1	D	188	LEU	3.1
1	C	18	ASN	3.1
1	C	26	ASN	3.1
1	D	277	ASN	3.1
1	B	23	GLN	3.1
1	D	140	GLN	3.1
1	D	250	ASP	3.1
1	A	202	ARG	3.1
1	C	263	ARG	3.1
1	D	281	LYS	3.1
1	D	303	THR	3.1
1	C	107	PRO	3.0
1	C	339	PRO	3.0
1	A	256	GLY	3.0
1	C	70	ASN	3.0
1	C	275	LEU	3.0
1	C	321	GLY	3.0
1	B	18	ASN	3.0
1	D	257	ASN	3.0
1	C	183	TYR	3.0
1	B	209	GLN	3.0
1	B	130	ARG	3.0
1	B	236	GLU	3.0
1	A	363	THR	3.0
1	B	261	LEU	3.0
1	A	58	ALA	3.0
1	B	79	GLN	3.0
1	A	59	ILE	3.0
1	B	365	TYR	3.0
1	D	211	ILE	3.0
1	B	377	CYS	3.0
1	D	134	ARG	3.0
1	A	143	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	352	LYS	3.0
1	D	193	HIS	3.0
1	B	269	VAL	3.0
1	C	200	GLY	3.0
1	C	208	PRO	3.0
1	A	231	PHE	3.0
1	D	167	LEU	3.0
1	D	287	TYR	3.0
1	D	380	CYS	3.0
1	B	295	SER	3.0
1	D	13	SER	3.0
1	C	203	THR	3.0
1	C	114	PRO	3.0
1	D	72	PRO	3.0
1	B	405	VAL	3.0
1	C	219	LEU	3.0
1	C	411	LYS	3.0
1	A	101	ASP	2.9
1	B	346[A]	ILE	2.9
1	C	351	ASP	2.9
1	C	371	TYR	2.9
1	A	99	HIS	2.9
1	B	238	THR	2.9
1	B	410	ASN	2.9
1	C	396	ASN	2.9
1	D	26	ASN	2.9
1	D	204	PRO	2.9
1	D	404	PRO	2.9
1	B	197	VAL	2.9
1	A	219	LEU	2.9
1	B	283	ARG	2.9
1	D	109	LEU	2.9
1	D	118	LEU	2.9
1	C	384	LYS	2.9
1	C	293	ASP	2.9
1	D	293	ASP	2.9
1	D	351	ASP	2.9
1	B	185	ILE	2.9
1	A	113	TYR	2.9
1	A	288	TYR	2.9
1	A	372	THR	2.9
1	C	393	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	393	GLY	2.9
1	D	4	ARG	2.9
1	D	77	ARG	2.9
1	A	265	VAL	2.9
1	B	179	GLU	2.9
1	A	23	GLN	2.9
1	C	79	GLN	2.9
1	B	344	TYR	2.9
1	C	100	GLU	2.9
1	C	332	PRO	2.9
1	B	337	LYS	2.9
1	A	324	VAL	2.9
1	D	76	VAL	2.9
1	D	328	VAL	2.9
1	A	301	PHE	2.9
1	D	14	ASP	2.9
1	D	346[A]	ILE	2.9
1	A	217	ASN	2.9
1	D	21	ARG	2.9
1	D	285[A]	ARG	2.9
1	A	180	THR	2.9
1	A	377	CYS	2.9
1	C	290	TYR	2.9
1	C	363	THR	2.9
1	B	314	GLY	2.9
1	B	335	GLY	2.9
1	D	367	GLU	2.9
1	A	384	LYS	2.9
1	D	352	LYS	2.9
1	D	304	PRO	2.8
1	C	394	LEU	2.8
1	D	391	VAL	2.8
1	B	71	ASP	2.8
1	A	251	ALA	2.8
1	C	185	ILE	2.8
1	D	370	ASN	2.8
1	A	273	LYS	2.8
1	A	278	LYS	2.8
1	C	334	GLY	2.8
1	D	273	LYS	2.8
1	D	321	GLY	2.8
1	C	156	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	204	PRO	2.8
1	C	250	ASP	2.8
1	D	101	ASP	2.8
1	D	233	HIS	2.8
1	B	249	ALA	2.8
1	B	401	ALA	2.8
1	D	15	ALA	2.8
1	C	149	ARG	2.8
1	B	159	ASN	2.8
1	B	240	GLU	2.8
1	C	184	ILE	2.8
1	D	309	ILE	2.8
1	A	203	THR	2.8
1	A	193	HIS	2.8
1	C	123	ASP	2.8
1	D	219	LEU	2.8
1	D	216	VAL	2.8
1	A	144	SER	2.8
1	C	186	ALA	2.8
1	D	186	ALA	2.8
1	D	187	LYS	2.8
1	A	108	GLY	2.8
1	D	238	THR	2.8
1	A	161	PRO	2.8
1	A	140	GLN	2.8
1	C	162	GLN	2.8
1	D	230	HIS	2.8
1	A	401	ALA	2.7
1	C	295	SER	2.8
1	D	231	PHE	2.7
1	B	312	ILE	2.7
1	C	97	PRO	2.7
1	A	210	ARG	2.7
1	A	302	ARG	2.7
1	B	409	ARG	2.7
1	C	158	ARG	2.7
1	C	294	LEU	2.7
1	A	228	ASN	2.7
1	A	281	LYS	2.7
1	A	370	ASN	2.7
1	C	284	VAL	2.7
1	C	343	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	104	SER	2.7
1	B	319	THR	2.7
1	C	364	THR	2.7
1	C	372	THR	2.7
1	D	81	ILE	2.7
1	C	246	GLN	2.7
1	D	23	GLN	2.7
1	A	151	ASP	2.7
1	A	234	PRO	2.7
1	C	254	PRO	2.7
1	C	304	PRO	2.7
1	D	325	PRO	2.7
1	C	367	GLU	2.7
1	C	188	LEU	2.7
1	D	315	LEU	2.7
1	A	391	VAL	2.7
1	D	340	VAL	2.7
1	C	251	ALA	2.7
1	D	139	GLY	2.7
1	B	291	GLN	2.7
1	D	133	THR	2.7
1	D	223	HIS	2.7
1	C	143	ASP	2.7
1	C	267	ASP	2.7
1	D	234	PRO	2.7
1	C	190	GLU	2.7
1	B	177	SER	2.7
1	B	355	LEU	2.7
1	D	355	LEU	2.7
1	B	308	GLY	2.7
1	B	202	ARG	2.7
1	A	125	CYS	2.6
1	A	396	ASN	2.6
1	B	323	CYS	2.6
1	A	261	LEU	2.6
1	A	394	LEU	2.6
1	B	201	SER	2.6
1	B	290	TYR	2.6
1	C	135	ARG	2.6
1	C	405	VAL	2.6
1	D	135	ARG	2.6
1	D	271	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	409	ARG	2.6
1	A	192	PRO	2.6
1	D	105	PRO	2.6
1	D	237	ILE	2.6
1	C	159	ASN	2.6
1	B	320	SER	2.6
1	A	198	ARG	2.6
1	C	302	ARG	2.6
1	B	288	TYR	2.6
1	A	106	VAL	2.6
1	A	321	GLY	2.6
1	C	288	TYR	2.6
1	D	113	TYR	2.6
1	D	256	GLY	2.6
1	D	276	VAL	2.6
1	C	179	GLU	2.6
1	B	273	LYS	2.6
1	C	155	ASP	2.6
1	D	93	ASP	2.6
1	C	368	PRO	2.6
1	D	192	PRO	2.6
1	D	20	TRP	2.6
1	C	245	CYS	2.6
1	D	125	CYS	2.6
1	A	359	GLU	2.6
1	B	117	VAL	2.6
1	B	163	VAL	2.6
1	D	290	TYR	2.6
1	C	319	THR	2.6
1	D	180	THR	2.6
1	B	404	PRO	2.6
1	D	70	ASN	2.6
1	C	227	LEU	2.6
1	A	397	GLY	2.5
1	B	321	GLY	2.5
1	A	392	ALA	2.5
1	B	385	LYS	2.5
1	C	280	VAL	2.5
1	C	330	ASP	2.5
1	A	238	THR	2.5
1	D	242	THR	2.5
1	D	189	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	410	ASN	2.5
1	A	185	ILE	2.5
1	A	223	HIS	2.5
1	D	299	GLU	2.5
1	D	300	HIS	2.5
1	B	115	ASP	2.5
1	C	265	VAL	2.5
1	C	327	PHE	2.5
1	D	159	ASN	2.5
1	B	311	ILE	2.5
1	C	236	GLU	2.5
1	D	337	LYS	2.5
1	B	395	LEU	2.5
1	B	407	LEU	2.5
1	A	112	ARG	2.5
1	A	405	VAL	2.5
1	D	225	VAL	2.5
1	D	263	ARG	2.5
1	C	180	THR	2.5
1	A	235	ASN	2.5
1	B	322	TYR	2.5
1	D	235	ASN	2.5
1	B	208	PRO	2.5
1	B	300	HIS	2.5
1	C	300	HIS	2.5
1	D	383	LYS	2.5
1	D	248	LEU	2.5
1	C	93	ASP	2.5
1	C	132	CYS	2.5
1	A	21	ARG	2.5
1	A	337	LYS	2.4
1	C	210	ARG	2.4
1	D	74	ASP	2.4
1	A	18	ASN	2.4
1	A	328	VAL	2.4
1	A	345	VAL	2.4
1	C	194	VAL	2.4
1	C	213	PRO	2.4
1	A	42	LYS	2.4
1	C	259	SER	2.4
1	C	365	TYR	2.4
1	D	288	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	285[A]	ARG	2.4
1	B	267	ASP	2.4
1	B	293	ASP	2.4
1	C	167	LEU	2.4
1	D	262	LEU	2.4
1	B	129	CYS	2.4
1	A	303	THR	2.4
1	B	303	THR	2.4
1	D	326	THR	2.4
1	A	233	HIS	2.4
1	A	340	VAL	2.4
1	D	131	HIS	2.4
1	C	349	SER	2.4
1	C	164	ARG	2.4
1	D	358	PHE	2.4
1	C	16	ASP	2.4
1	C	168	LEU	2.4
1	D	239	GLU	2.4
1	B	357	ASN	2.4
1	D	343	ASN	2.4
1	B	221	LYS	2.4
1	B	242	THR	2.4
1	C	269	VAL	2.4
1	D	166	VAL	2.4
1	D	324	VAL	2.4
1	D	361	VAL	2.4
1	A	241	SER	2.4
1	B	259	SER	2.4
1	D	347	SER	2.4
1	A	25	ARG	2.4
1	D	198	ARG	2.4
1	A	365	TYR	2.4
1	D	264	GLY	2.4
1	D	289	ILE	2.4
1	D	275	LEU	2.3
1	D	279	LEU	2.3
1	B	343	ASN	2.3
1	C	318	HIS	2.3
1	D	385	LYS	2.3
1	A	15	ALA	2.3
1	C	331	ALA	2.3
1	A	361	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	269	VAL	2.3
1	B	258	GLN	2.3
1	B	178	ASP	2.3
1	D	397	GLY	2.3
1	D	63	TYR	2.3
1	D	18	ASN	2.3
1	A	249	ALA	2.3
1	A	331	ALA	2.3
1	C	338	THR	2.3
1	D	80	ALA	2.3
1	A	323	CYS	2.3
1	D	123	ASP	2.3
1	C	257	ASN	2.3
1	B	111	HIS	2.3
1	A	158	ARG	2.3
1	C	249	ALA	2.3
1	D	331	ALA	2.3
1	A	336	GLY	2.3
1	B	333	GLY	2.3
1	D	360	GLY	2.3
1	C	187	LYS	2.3
1	C	232	ASN	2.3
1	C	243	ARG	2.3
1	C	401	ALA	2.3
1	A	259	SER	2.3
1	C	169	SER	2.3
1	B	292	CYS	2.2
1	C	239	GLU	2.2
1	C	323	CYS	2.2
1	C	350	HIS	2.2
1	C	226	TRP	2.2
1	D	184	ILE	2.2
1	A	315	LEU	2.2
1	A	344	TYR	2.2
1	C	344	TYR	2.2
1	D	227	LEU	2.2
1	A	274	GLU	2.2
1	D	201	SER	2.2
1	D	406	GLY	2.2
1	C	166	VAL	2.2
1	B	270	HIS	2.2
1	D	387	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	222	TYR	2.2
1	A	16	ASP	2.2
1	B	105	PRO	2.2
1	D	146	PRO	2.2
1	D	165	ASP	2.2
1	C	307	LYS	2.2
1	D	252	GLY	2.2
1	D	323	CYS	2.2
1	D	335	GLY	2.2
1	C	99	HIS	2.2
1	C	271	VAL	2.2
1	C	361	VAL	2.2
1	A	148	GLU	2.2
1	B	359	GLU	2.2
1	B	102	THR	2.2
1	C	303	THR	2.2
1	D	203	THR	2.2
1	A	177	SER	2.2
1	A	165	ASP	2.2
1	C	96	ASP	2.2
1	D	378	ASP	2.2
1	C	198	ARG	2.2
1	D	5[A]	ARG	2.2
1	D	243[A]	ARG	2.2
1	D	308	GLY	2.2
1	D	316[A]	ARG	2.2
1	B	193	HIS	2.2
1	B	318	HIS	2.2
1	C	324	VAL	2.2
1	D	261	LEU	2.1
1	A	307	LYS	2.1
1	C	326	THR	2.1
1	C	320	SER	2.1
1	D	307	LYS	2.1
1	B	165	ASP	2.1
1	C	74	ASP	2.1
1	C	392	ALA	2.1
1	B	161	PRO	2.1
1	D	253	VAL	2.1
1	D	398	GLU	2.1
1	A	289	ILE	2.1
1	B	402	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	278	LYS	2.1
1	D	354	ILE	2.1
1	A	242	THR	2.1
1	A	304	PRO	2.1
1	A	403	GLU	2.1
1	D	408	GLU	2.1
1	A	380	CYS	2.1
1	D	305	VAL	2.1
1	C	178	ASP	2.1
1	C	395	LEU	2.1
1	A	141	SER	2.1
1	D	71	ASP	2.1
1	A	204	PRO	2.1
1	A	325	PRO	2.1
1	A	332	PRO	2.1
1	D	314	GLY	2.1
1	A	277	ASN	2.1
1	C	274	GLU	2.1
1	D	345	VAL	2.1
1	A	116	ARG	2.1
1	B	101	ASP	2.1
1	B	250	ASP	2.1
1	D	394	LEU	2.1
1	A	326	THR	2.1
1	B	406	GLY	2.0
1	A	232	ASN	2.0
1	A	342	PRO	2.0
1	C	234	PRO	2.0
1	C	286	PRO	2.0
1	D	342	PRO	2.0
1	A	292	CYS	2.0
1	C	225	VAL	2.0
1	B	155	ASP	2.0
1	A	366	SER	2.0
1	C	177	SER	2.0
1	B	364	THR	2.0
1	C	348	GLN	2.0
1	B	396	ASN	2.0
1	D	396	ASN	2.0
1	D	332	PRO	2.0
1	C	287	TYR	2.0
1	C	305	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	292	CYS	2.0
1	A	93	ASP	2.0
1	B	99	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	C	593	5/5	0.37	0.31	79,80,81,81	0
3	SO4	A	592	5/5	0.48	0.28	98,98,99,99	0
5	LYS	C	420[A]	10/10	0.51	0.28	22,24,27,27	3
5	LYS	C	420[B]	10/10	0.51	0.28	22,24,27,27	3
3	SO4	D	494	5/5	0.55	0.25	88,88,88,89	0
5	LYS	B	420[B]	10/10	0.64	0.30	32,34,39,39	3
4	SAM	B	417	27/27	0.64	0.27	32,34,39,43	1
5	LYS	B	420[A]	10/10	0.64	0.30	32,34,39,39	3
3	SO4	B	495	5/5	0.66	0.27	101,101,101,101	0
4	SAM	D	417	27/27	0.76	0.23	21,23,26,33	1
4	SAM	A	417	27/27	0.77	0.20	25,27,31,36	1
5	LYS	A	420[A]	10/10	0.79	0.20	27,29,32,33	3
5	LYS	A	420[B]	10/10	0.79	0.20	27,29,32,33	3
4	SAM	C	417	27/27	0.79	0.21	21,23,25,31	1
6	PLP	A	419	15/16	0.84	0.20	24,31,32,33	0
5	LYS	D	420[B]	10/10	0.86	0.15	24,25,28,29	3
5	LYS	D	420[A]	10/10	0.86	0.15	24,25,28,29	3
6	PLP	B	419	15/16	0.88	0.17	27,34,36,37	0
7	SF4	B	418	8/8	0.88	0.12	35,38,40,40	0
6	PLP	D	419	15/16	0.90	0.14	20,27,29,30	0

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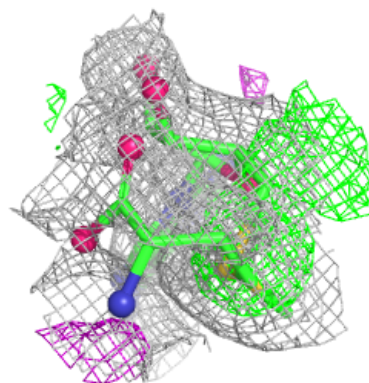
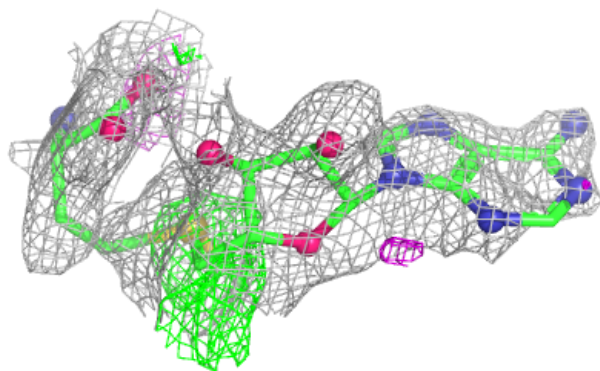
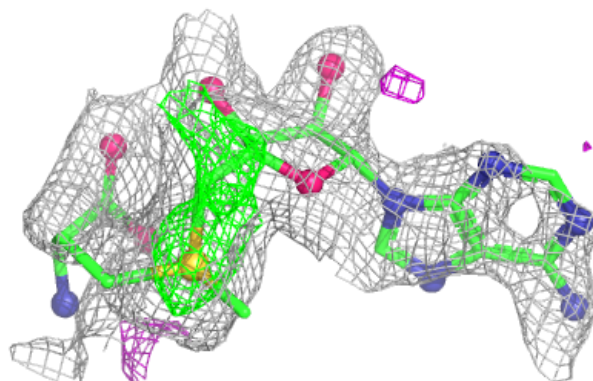
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	PLP	C	419	15/16	0.90	0.16	18,24,25,26	0
7	SF4	D	418	8/8	0.90	0.08	21,22,25,26	0
2	ZN	D	421	1/1	0.91	0.08	31,31,31,31	0
7	SF4	C	418	8/8	0.92	0.08	22,24,25,26	0
7	SF4	A	418	8/8	0.93	0.08	24,27,29,29	0
2	ZN	B	421	1/1	0.94	0.07	45,45,45,45	0
2	ZN	C	421	1/1	0.97	0.04	36,36,36,36	0
2	ZN	A	421	1/1	0.98	0.05	36,36,36,36	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.

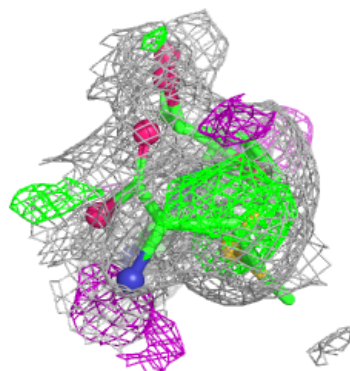
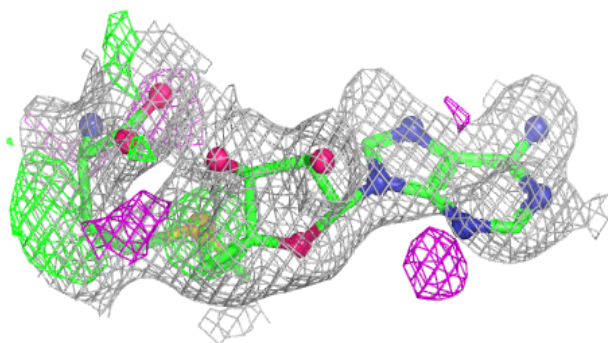
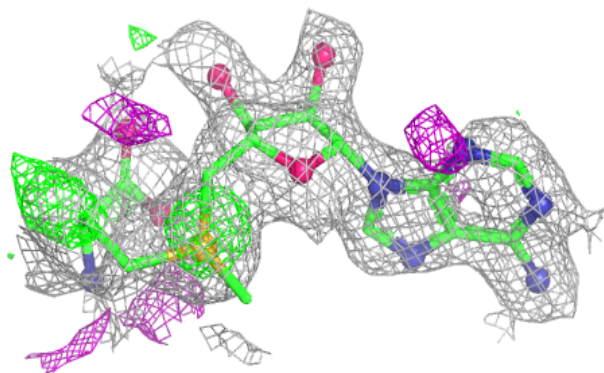
Electron density around SAM B 417:

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

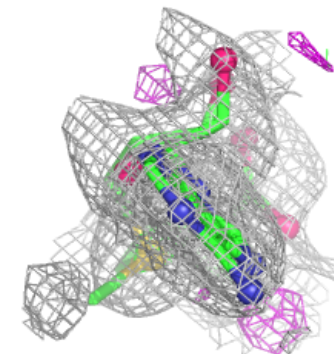
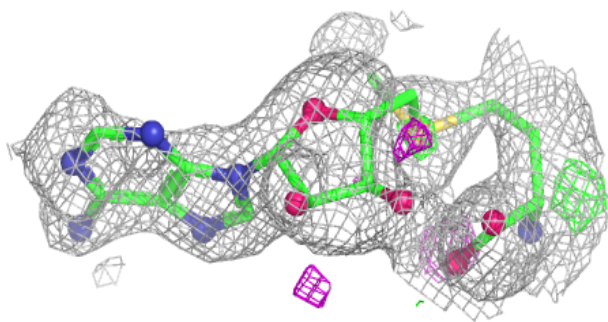
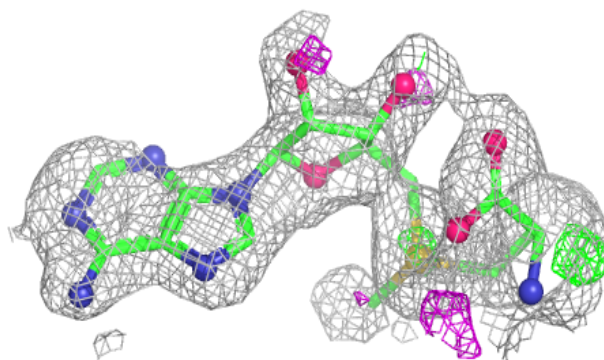


Electron density around SAM D 417:

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

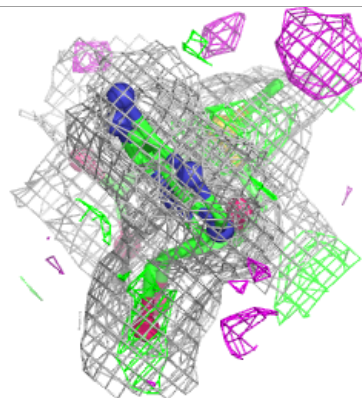
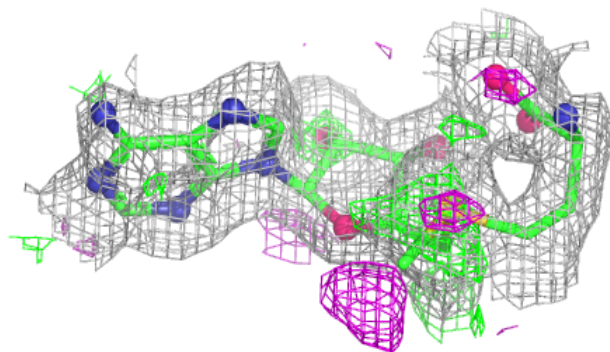
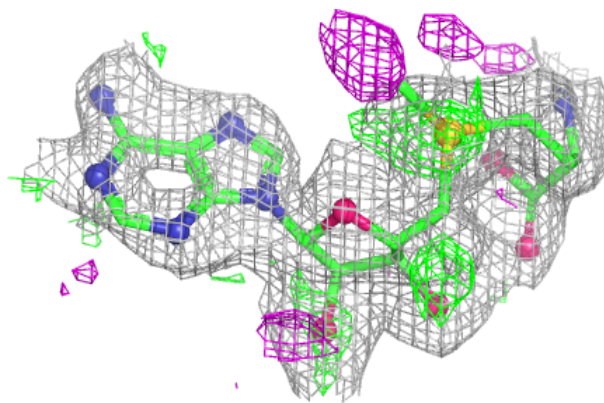
**Electron density around SAM A 417:**

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



Electron density around SAM C 417:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.