Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 11:54 AM 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:

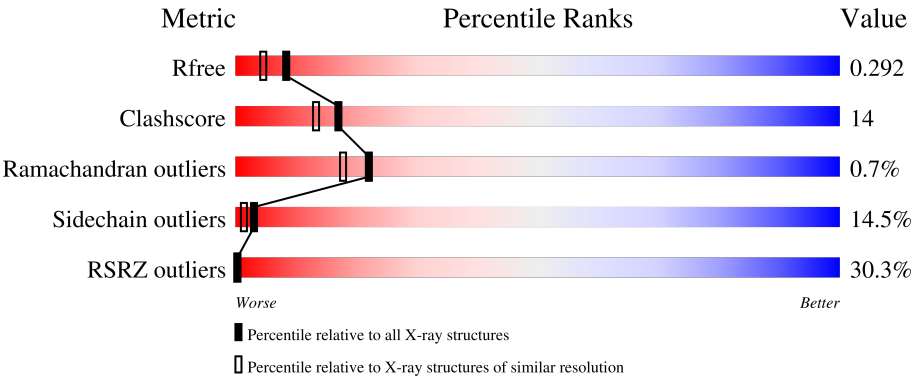
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 <=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	29% 68% 22% 7%
1	B	416	36% 67% 24% 6%
1	C	416	26% 67% 23% 7%
1	D	416	26% 66% 24% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	D	494	-	-	-	X

2 Entry composition (i)

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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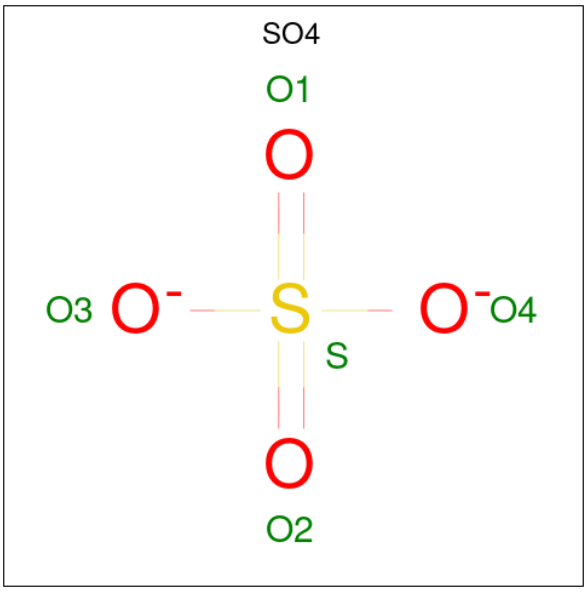
Chain	Residue	Modelled	Actual	Comment	Reference
C	57	MSE	MET	MODIFIED RESIDUE	GB 5410603
C	124	MSE	MET	MODIFIED RESIDUE	GB 5410603
C	127	MSE	MET	MODIFIED RESIDUE	GB 5410603
C	145	MSE	MET	MODIFIED RESIDUE	GB 5410603
C	147	MSE	MET	MODIFIED RESIDUE	GB 5410603
C	218	MSE	MET	MODIFIED RESIDUE	GB 5410603
C	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).

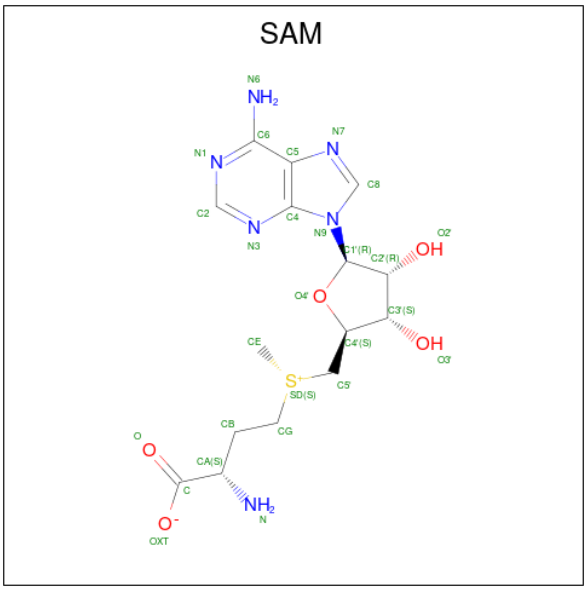
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



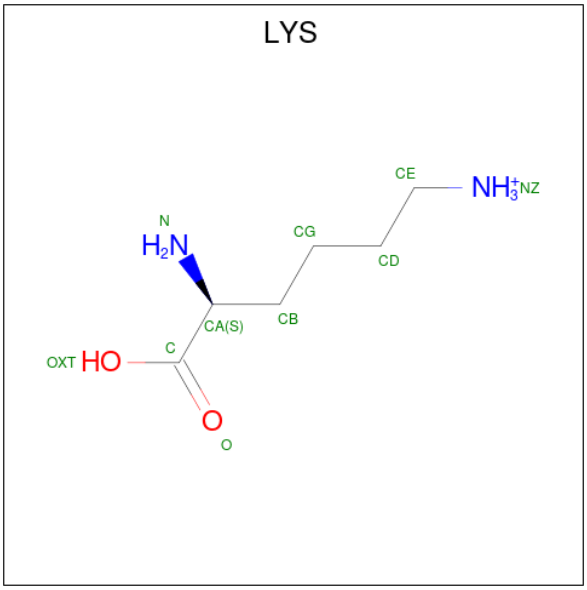
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

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



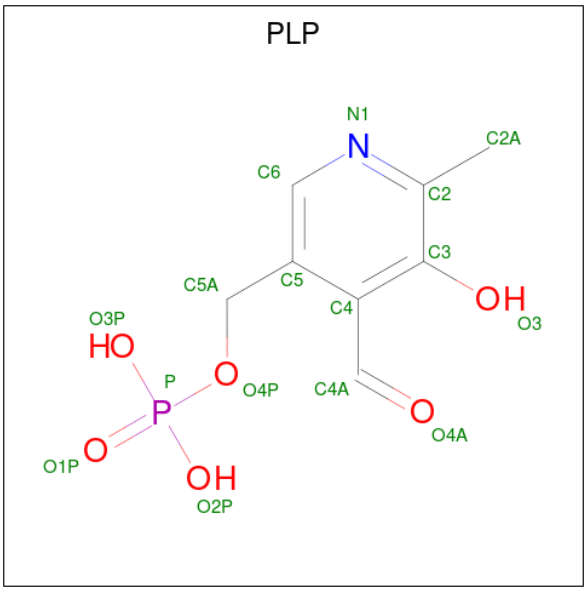
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	D	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

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



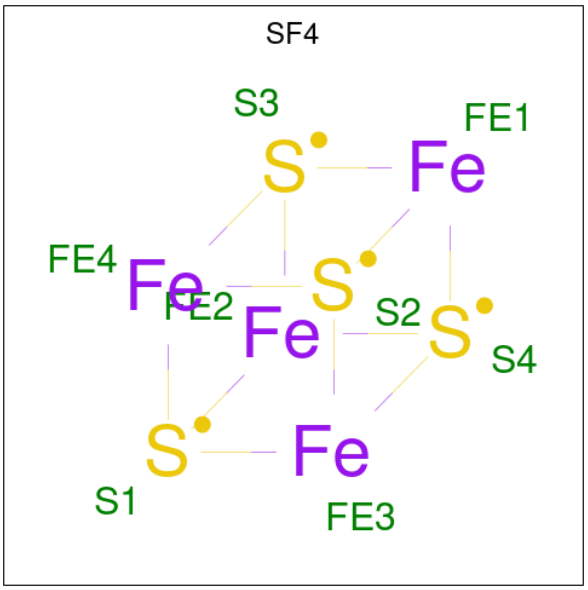
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	1
			13	9	2	2		
5	B	1	Total	C	N	O	0	1
			13	9	2	2		
5	C	1	Total	C	N	O	0	1
			13	9	2	2		
5	D	1	Total	C	N	O	0	1
			13	9	2	2		

- 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: Fe_4S_4).



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

- Molecule 8 is water.

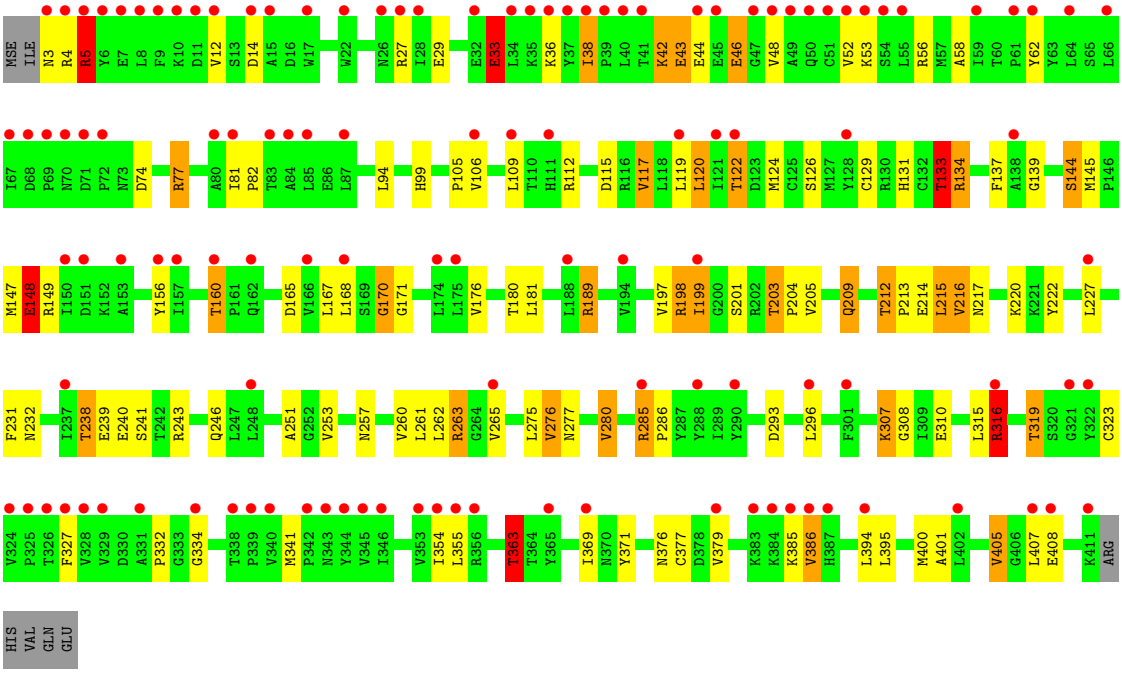
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	135	Total O 135 135	0	0
8	B	116	Total O 116 116	0	0
8	C	183	Total O 183 183	0	0
8	D	174	Total O 174 174	0	0

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.

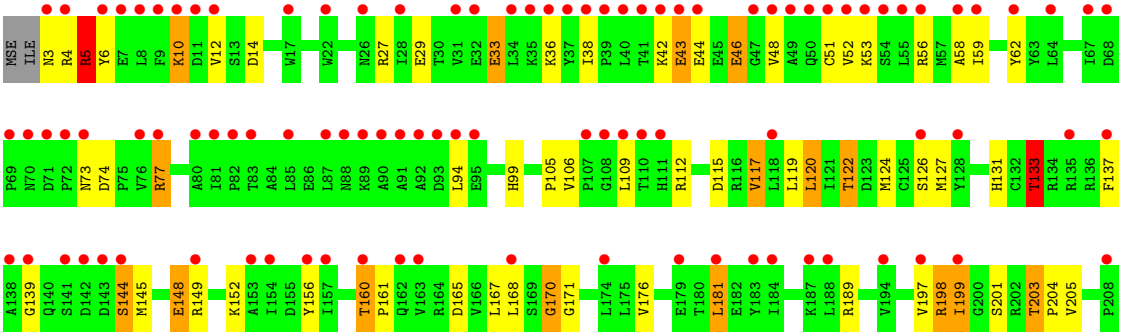
• Molecule 1: L-lysine 2,3-aminomutase

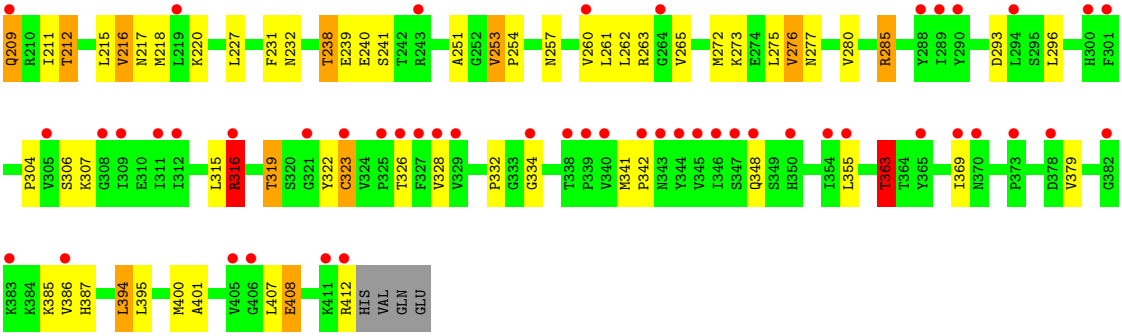
Chain A:



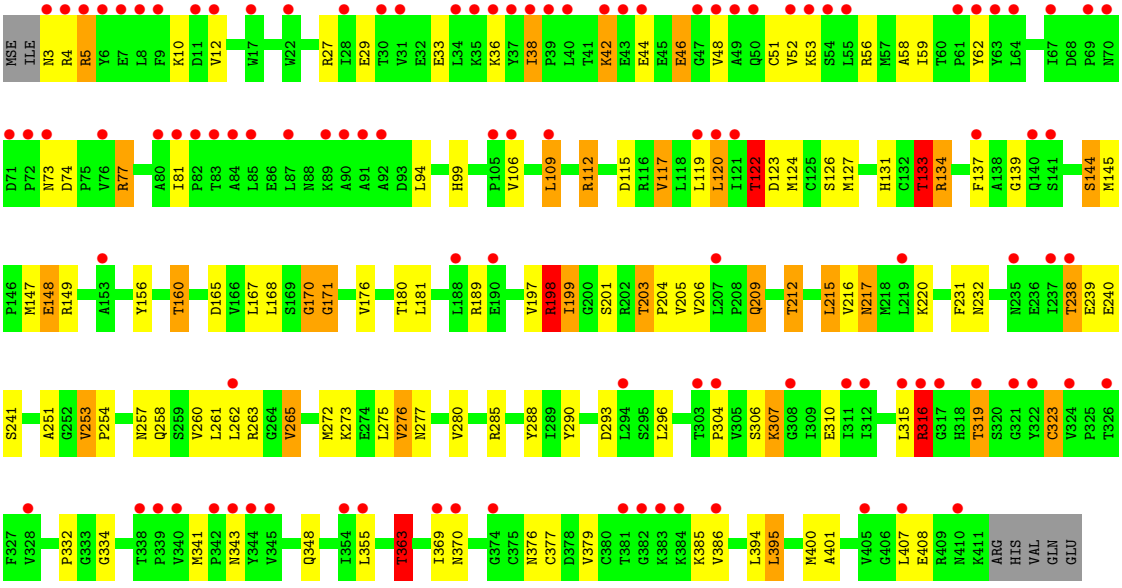
• Molecule 1: L-lysine 2,3-aminomutase

Chain B:

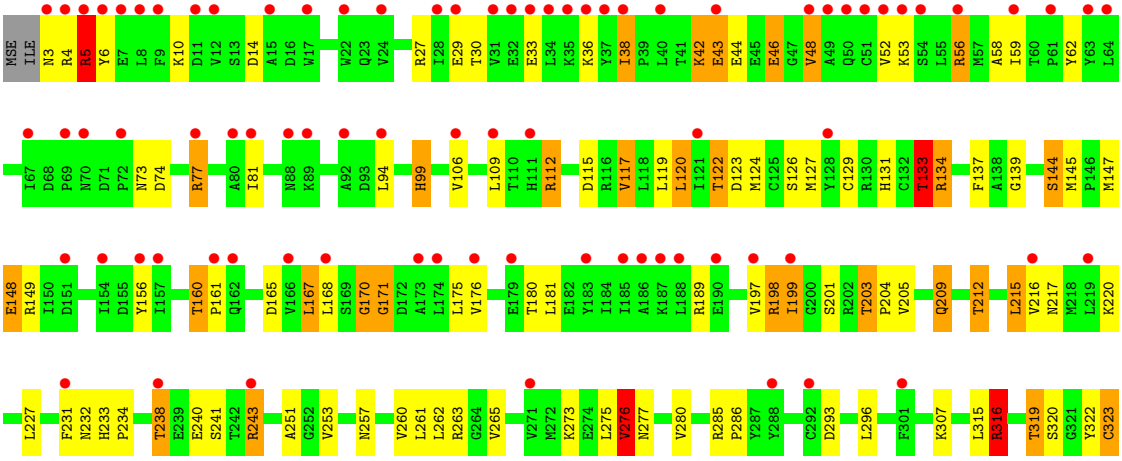


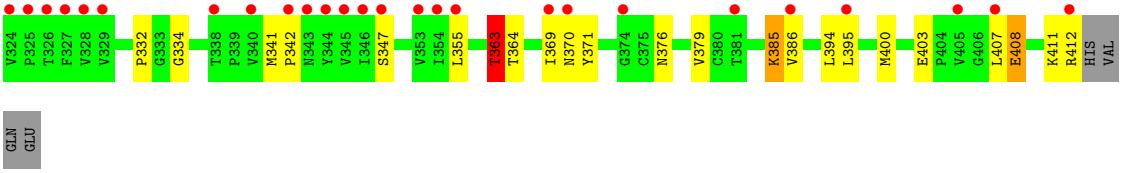


• Molecule 1: L-lysine 2,3-aminomutase



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




V324
P325
T326
F327
V328
V329
P332
G333
G334
T338
P339
V340
M341
P342
N343
Y344
V345
I346
S347
V353
I354
L355
T363
T364
I369
N370
Y371
G374
C375
N376
V379
C380
T381
K385
V386
L394
L395
M400
E403
P404
V405
G406
L407
E408
K411
R412
HIS
VAL
GLN
GLU

4 Data and refinement statistics (i)

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 46.61 – 3.00	Depositor EDS
% Data completeness (in resolution range)	81.5 (50.00-2.10) 96.8 (46.61-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [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	6418 reflections (8.40%)	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 , 41.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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%)	22	18
1	B	416/416 (100%)	398 (96%)	15 (4%)	3 (1%)	22	18
1	C	415/416 (100%)	397 (96%)	15 (4%)	3 (1%)	22	18
1	D	417/416 (100%)	397 (95%)	17 (4%)	3 (1%)	22	18
All	All	1664/1664 (100%)	1592 (96%)	60 (4%)	12 (1%)	22	18

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%)	3 1
1	D	375/362 (104%)	318 (85%)	57 (15%)	3 1
All	All	1496/1448 (103%)	1269 (85%)	227 (15%)	3 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 monosaccharides 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[B]	-	8,9,9	0.94	1 (12%)	7,10,10	1.12	1 (14%)
5	LYS	C	420[B]	-	8,9,9	1.02	0	7,10,10	0.90	0
7	SF4	C	418	4,1	0,12,12	-	-	-		
5	LYS	B	420[A]	-	8,9,9	0.74	0	7,10,10	1.02	1 (14%)
4	SAM	D	417	7	23,29,29	1.40	3 (13%)	20,42,42	1.82	5 (25%)
5	LYS	A	420[A]	-	8,9,9	0.85	1 (12%)	7,10,10	1.04	0
6	PLP	B	419	5	15,15,16	2.76	2 (13%)	21,22,23	0.93	0
3	SO4	A	592	-	4,4,4	0.30	0	6,6,6	0.22	0
4	SAM	B	417	7	23,29,29	1.64	3 (13%)	20,42,42	1.68	6 (30%)
6	PLP	D	419	5	15,15,16	2.88	2 (13%)	21,22,23	1.16	1 (4%)
3	SO4	D	494	-	4,4,4	0.31	0	6,6,6	0.34	0
7	SF4	B	418	4,1	0,12,12	-	-	-		
4	SAM	C	417	7	23,29,29	1.48	3 (13%)	20,42,42	1.83	5 (25%)
6	PLP	A	419	5	15,15,16	2.72	2 (13%)	21,22,23	1.18	2 (9%)
5	LYS	D	420[A]	-	8,9,9	0.94	1 (12%)	7,10,10	1.17	1 (14%)
4	SAM	A	417	7	23,29,29	1.57	3 (13%)	20,42,42	2.02	5 (25%)
5	LYS	C	420[A]	-	8,9,9	1.03	0	7,10,10	0.94	0
5	LYS	B	420[B]	-	8,9,9	0.75	0	7,10,10	0.99	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
3	SO4	C	593	-	4,4,4	0.24	0	6,6,6	0.47	0
7	SF4	A	418	4,1	0,12,12	-	-	-		
7	SF4	D	418	4,1	0,12,12	-	-	-		
3	SO4	B	495	-	4,4,4	0.25	0	6,6,6	0.31	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LYS	D	420[B]	-	-	1/9/9/9	-
5	LYS	C	420[B]	-	-	1/9/9/9	-
7	SF4	C	418	4,1	-	-	0/6/5/5
5	LYS	B	420[A]	-	-	1/9/9/9	-

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

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(^{o})	Ideal(^{o})
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

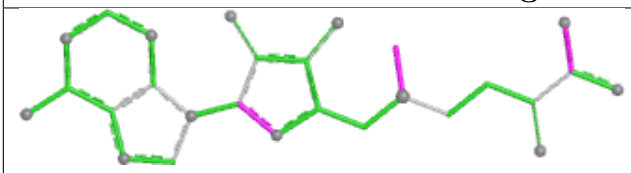
There are no ring outliers.

2 monomers are involved in 2 short contacts:

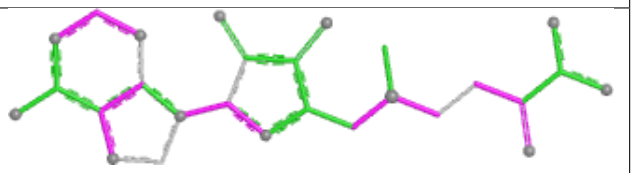
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	418	SF4	1	0
7	D	418	SF4	1	0

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

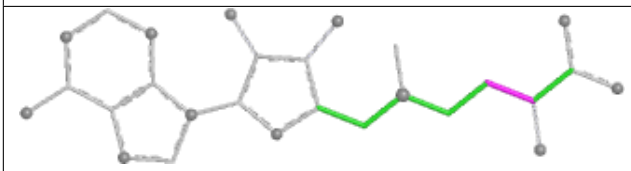
Ligand SAM D 417



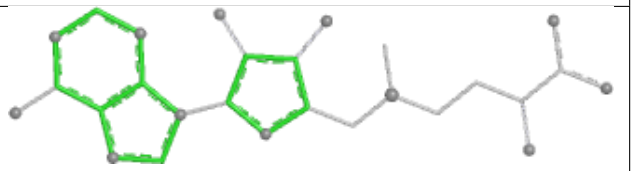
Bond lengths



Bond angles

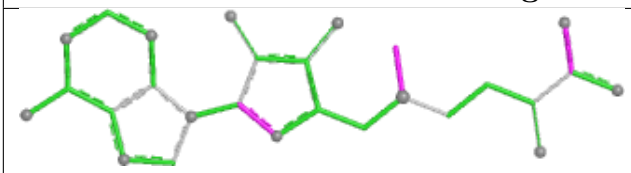


Torsions

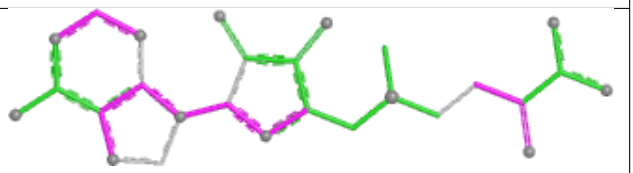


Rings

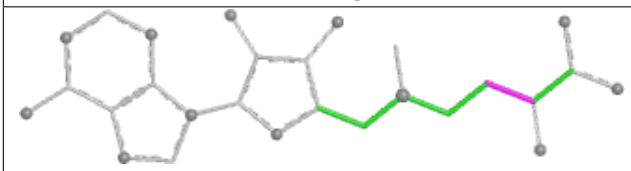
Ligand SAM B 417



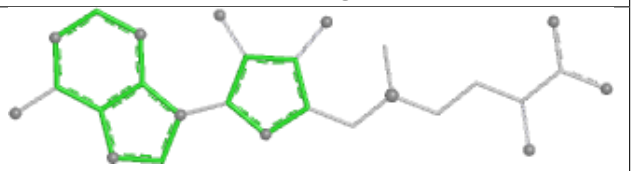
Bond lengths



Bond angles

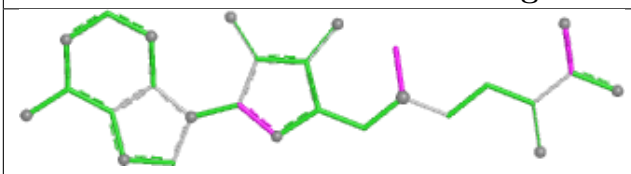


Torsions

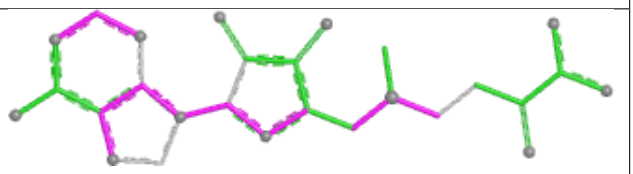


Rings

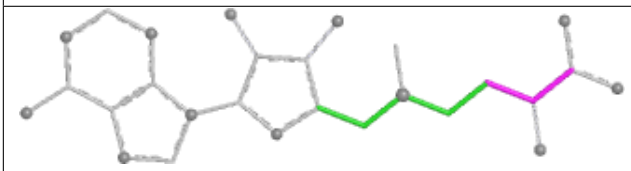
Ligand SAM C 417



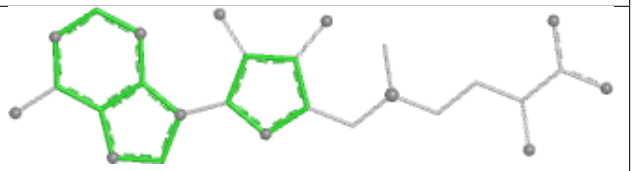
Bond lengths



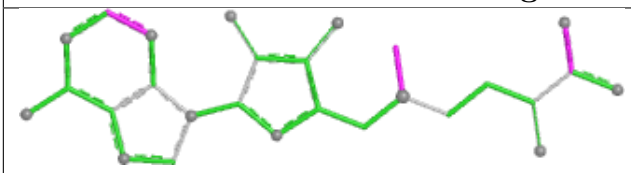
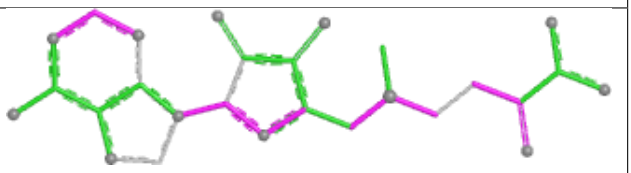
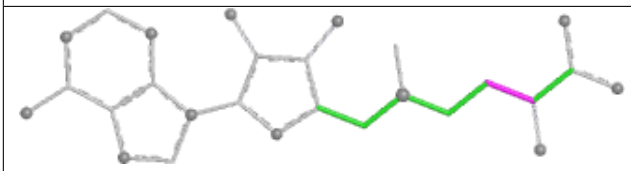
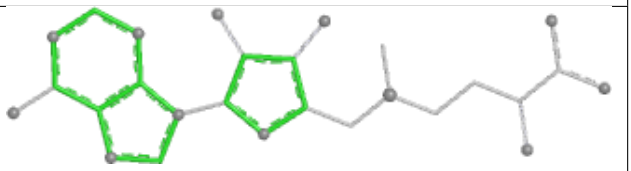
Bond angles



Torsions



Rings

Ligand SAM A 417	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	400/416 (96%)	1.57	121 (30%)	0	0	18, 39, 61, 72	9 (2%)
1	B	401/416 (96%)	1.81	149 (37%)	0	0	20, 43, 79, 98	7 (1%)
1	C	400/416 (96%)	1.52	107 (26%)	0	0	16, 32, 59, 73	7 (1%)
1	D	401/416 (96%)	1.48	108 (26%)	0	0	15, 32, 55, 69	6 (1%)
All	All	1602/1664 (96%)	1.60	485 (30%)	0	0	15, 36, 65, 98	29 (1%)

All (485) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	48	VAL	10.9
1	B	38	ILE	7.5
1	D	6	TYR	7.3
1	B	22	TRP	6.9
1	B	54	SER	6.9
1	B	85	LEU	6.8
1	C	64	LEU	6.7
1	B	81	ILE	6.5
1	B	40	LEU	6.4
1	C	40	LEU	6.3
1	A	6	TYR	6.2
1	C	8	LEU	6.2
1	A	49	ALA	6.2
1	C	369	ILE	6.1
1	B	48	VAL	6.0
1	B	126	SER	5.9
1	C	38	ILE	5.8
1	B	53	LYS	5.8
1	D	9	PHE	5.7
1	D	52	VAL	5.7
1	D	40	LEU	5.7

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Mol	Chain	Res	Type	RSRZ
1	C	84	ALA	5.7
1	A	17	TRP	5.6
1	B	90	ALA	5.6
1	C	70	ASN	5.5
1	C	31	VAL	5.4
1	B	37	TYR	5.4
1	C	9	PHE	5.3
1	A	51	CYS	5.3
1	B	31	VAL	5.2
1	B	59	ILE	5.1
1	C	85	LEU	5.1
1	A	52	VAL	5.1
1	D	8	LEU	5.1
1	D	38	ILE	5.0
1	D	4	ARG	5.0
1	C	43	GLU	5.0
1	A	9	PHE	4.9
1	A	15	ALA	4.9
1	D	386	VAL	4.9
1	C	4	ARG	4.9
1	C	80	ALA	4.8
1	C	6	TYR	4.8
1	B	139	GLY	4.8
1	B	138	ALA	4.8
1	B	4	ARG	4.7
1	B	143	ASP	4.7
1	B	87	LEU	4.6
1	A	85	LEU	4.6
1	C	383	LYS	4.6
1	C	69	PRO	4.6
1	C	67	ILE	4.6
1	A	22	TRP	4.5
1	D	34	LEU	4.5
1	D	369	ILE	4.5
1	B	9	PHE	4.5
1	C	54	SER	4.5
1	A	37	TYR	4.4
1	B	80	ALA	4.4
1	C	3	ASN	4.4
1	A	40	LEU	4.4
1	B	71	ASP	4.4
1	C	386	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	92	ALA	4.3
1	A	81	ILE	4.3
1	B	108	GLY	4.3
1	D	157	ILE	4.3
1	B	8	LEU	4.3
1	C	50	GLN	4.3
1	D	106	VAL	4.3
1	B	70	ASN	4.3
1	C	90	ALA	4.2
1	A	38	ILE	4.2
1	C	37	TYR	4.2
1	D	67	ILE	4.2
1	D	156	TYR	4.2
1	D	37	TYR	4.2
1	A	369	ILE	4.2
1	C	106	VAL	4.1
1	B	52	VAL	4.1
1	C	49	ALA	4.1
1	D	11	ASP	4.1
1	D	69	PRO	4.1
1	B	88	ASN	4.0
1	C	7	GLU	4.0
1	A	14	ASP	4.0
1	D	49	ALA	4.0
1	D	190	GLU	3.9
1	C	87	LEU	3.9
1	C	105	PRO	3.9
1	B	153	ALA	3.9
1	A	345	VAL	3.9
1	D	342	PRO	3.9
1	A	11	ASP	3.9
1	C	47	GLY	3.9
1	A	10	LYS	3.9
1	C	89	LYS	3.9
1	A	80	ALA	3.8
1	A	54	SER	3.8
1	B	107	PRO	3.8
1	B	326	THR	3.8
1	D	340	VAL	3.8
1	A	45	GLU	3.8
1	C	73	ASN	3.8
1	C	343	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	95	GLU	3.7
1	C	81	ILE	3.7
1	B	312	ILE	3.7
1	D	168	LEU	3.7
1	B	94	LEU	3.7
1	B	6	TYR	3.6
1	B	35	LYS	3.6
1	B	39	PRO	3.6
1	B	28	ILE	3.6
1	B	51	CYS	3.6
1	B	339	PRO	3.6
1	D	154	ILE	3.5
1	A	27[A]	ARG	3.5
1	B	26	ASN	3.5
1	C	11	ASP	3.5
1	C	62	TYR	3.5
1	A	168	LEU	3.5
1	B	156	TYR	3.5
1	B	93	ASP	3.5
1	C	235	ASN	3.5
1	A	36	LYS	3.5
1	C	34	LEU	3.5
1	B	11	ASP	3.4
1	A	12	VAL	3.4
1	B	41	THR	3.4
1	A	53	LYS	3.4
1	B	184	ILE	3.4
1	B	55	LEU	3.4
1	D	72	PRO	3.4
1	A	72	PRO	3.4
1	A	194	VAL	3.4
1	C	381	THR	3.4
1	A	4	ARG	3.4
1	B	34	LEU	3.4
1	B	36	LYS	3.3
1	C	53	LYS	3.3
1	C	344	TYR	3.3
1	A	387	HIS	3.3
1	B	32	GLU	3.3
1	D	36	LYS	3.3
1	B	328	VAL	3.3
1	D	183	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	84	ALA	3.3
1	B	149	ARG	3.3
1	B	72	PRO	3.3
1	D	370	ASN	3.3
1	A	379	VAL	3.3
1	D	48	VAL	3.3
1	D	173	ALA	3.3
1	D	412	ARG	3.2
1	A	3	ASN	3.2
1	B	343	ASN	3.2
1	B	355	LEU	3.2
1	C	61	PRO	3.2
1	D	162	GLN	3.2
1	B	329	VAL	3.2
1	D	28	ILE	3.2
1	B	12	VAL	3.2
1	D	326	THR	3.2
1	C	39	PRO	3.2
1	B	89	LYS	3.2
1	C	17	TRP	3.2
1	A	70	ASN	3.2
1	B	43	GLU	3.2
1	D	188	LEU	3.2
1	B	386	VAL	3.2
1	B	405	VAL	3.2
1	B	142	ASP	3.1
1	D	77	ARG	3.1
1	A	344	TYR	3.1
1	D	185	ILE	3.1
1	C	153	ALA	3.1
1	A	301	PHE	3.1
1	B	83	THR	3.1
1	D	43	GLU	3.1
1	D	186	ALA	3.1
1	A	28	ILE	3.1
1	A	386	VAL	3.1
1	D	344	TYR	3.1
1	C	52	VAL	3.1
1	D	405	VAL	3.1
1	A	408	GLU	3.1
1	B	342	PRO	3.1
1	D	22	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	64	LEU	3.1
1	A	59	ILE	3.1
1	A	346[A]	ILE	3.1
1	D	343	ASN	3.0
1	B	50	GLN	3.0
1	C	48	VAL	3.0
1	C	345	VAL	3.0
1	C	384	LYS	3.0
1	B	412	ARG	3.0
1	A	343	ASN	3.0
1	A	340	VAL	3.0
1	C	55	LEU	3.0
1	A	342	PRO	3.0
1	A	150	ILE	3.0
1	D	12	VAL	3.0
1	B	10	LYS	3.0
1	D	35	LYS	3.0
1	B	49	ALA	3.0
1	D	179	GLU	3.0
1	A	329	VAL	3.0
1	B	309	ILE	3.0
1	C	72	PRO	3.0
1	D	53	LYS	2.9
1	A	109	LEU	2.9
1	C	109	LEU	2.9
1	D	94	LEU	2.9
1	A	41	THR	2.9
1	B	340	VAL	2.9
1	D	345	VAL	2.9
1	A	157	ILE	2.9
1	A	237	ILE	2.9
1	D	50	GLN	2.9
1	B	338	THR	2.9
1	A	44	GLU	2.9
1	B	288	TYR	2.9
1	B	344	TYR	2.9
1	D	3	ASN	2.9
1	A	354	ILE	2.8
1	B	327	PHE	2.8
1	D	111	HIS	2.8
1	D	301	PHE	2.8
1	A	121	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	121	ILE	2.8
1	C	237	ILE	2.8
1	D	70	ASN	2.8
1	A	383	LYS	2.8
1	A	39	PRO	2.8
1	C	35	LYS	2.8
1	B	91	ALA	2.8
1	B	157	ILE	2.8
1	A	326	THR	2.8
1	A	5[A]	ARG	2.8
1	A	153	ALA	2.8
1	B	7	GLU	2.8
1	B	82	PRO	2.8
1	B	305	VAL	2.8
1	C	92	ALA	2.8
1	C	340	VAL	2.8
1	A	69	PRO	2.8
1	B	345	VAL	2.7
1	C	30	THR	2.7
1	B	77	ARG	2.7
1	B	64	LEU	2.7
1	A	67	ILE	2.7
1	A	199[A]	ILE	2.7
1	B	67	ILE	2.7
1	C	407	LEU	2.7
1	B	118	LEU	2.7
1	D	329	VAL	2.7
1	B	162	GLN	2.7
1	A	66	LEU	2.7
1	C	71	ASP	2.7
1	C	321	GLY	2.7
1	B	58	ALA	2.7
1	C	91	ALA	2.7
1	B	209	GLN	2.7
1	B	135	ARG	2.7
1	B	181	LEU	2.7
1	A	111	HIS	2.6
1	A	83	THR	2.6
1	B	168	LEU	2.6
1	A	339	PRO	2.6
1	B	316[A]	ARG	2.6
1	D	51	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	199[A]	ILE	2.6
1	C	311	ILE	2.6
1	B	44	GLU	2.6
1	D	5[A]	ARG	2.6
1	B	42	LYS	2.6
1	B	301	PHE	2.6
1	D	338	THR	2.6
1	D	381	THR	2.6
1	A	68	ASP	2.6
1	C	374	GLY	2.6
1	C	382	GLY	2.6
1	A	35	LYS	2.6
1	B	373	PRO	2.6
1	B	197	VAL	2.6
1	C	405	VAL	2.6
1	C	316[A]	ARG	2.6
1	D	199[A]	ILE	2.6
1	B	308	GLY	2.6
1	B	334	GLY	2.6
1	A	325	PRO	2.6
1	C	410	ASN	2.6
1	B	382	GLY	2.6
1	A	26	ASN	2.6
1	D	32	GLU	2.6
1	C	119	LEU	2.6
1	A	411	LYS	2.5
1	C	63	TYR	2.5
1	B	321	GLY	2.5
1	B	370	ASN	2.5
1	B	187	LYS	2.5
1	A	353	VAL	2.5
1	D	31	VAL	2.5
1	B	128	TYR	2.5
1	B	154	ILE	2.5
1	D	328	VAL	2.5
1	B	160	THR	2.5
1	A	50	GLN	2.5
1	C	294	LEU	2.5
1	D	174	LEU	2.5
1	A	324	VAL	2.5
1	B	289	ILE	2.5
1	C	137	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	174	LEU	2.5
1	B	383	LYS	2.5
1	B	411	LYS	2.5
1	C	342	PRO	2.4
1	B	56	ARG	2.4
1	D	24	VAL	2.4
1	B	323	CYS	2.4
1	D	15	ALA	2.4
1	D	231	PHE	2.4
1	A	87	LEU	2.4
1	B	73	ASN	2.4
1	C	207	LEU	2.4
1	B	163	VAL	2.4
1	B	183	TYR	2.4
1	C	338	THR	2.4
1	D	238	THR	2.4
1	A	119	LEU	2.4
1	A	227	LEU	2.4
1	A	355	LEU	2.4
1	A	106	VAL	2.4
1	A	7	GLU	2.4
1	C	322	TYR	2.4
1	C	339	PRO	2.4
1	A	175	LEU	2.4
1	B	188	LEU	2.4
1	C	308	GLY	2.4
1	C	315	LEU	2.4
1	A	356[A]	ARG	2.4
1	C	12	VAL	2.4
1	B	17	TRP	2.4
1	D	288	TYR	2.4
1	C	140	GLN	2.4
1	D	327	PHE	2.4
1	D	151	ASP	2.4
1	D	325	PRO	2.4
1	C	36	LYS	2.4
1	D	89	LYS	2.4
1	D	17	TRP	2.4
1	A	32	GLU	2.3
1	C	370	ASN	2.3
1	D	33	GLU	2.3
1	A	128	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	42	LYS	2.3
1	B	174	LEU	2.3
1	D	56	ARG	2.3
1	B	47	GLY	2.3
1	C	317	GLY	2.3
1	D	54	SER	2.3
1	B	179	GLU	2.3
1	C	83	THR	2.3
1	B	346[A]	ILE	2.3
1	D	346[A]	ILE	2.3
1	A	384	LYS	2.3
1	A	285[A]	ARG	2.3
1	C	82	PRO	2.3
1	C	354	ILE	2.3
1	A	8	LEU	2.3
1	A	156	TYR	2.3
1	A	394	LEU	2.3
1	B	290	TYR	2.3
1	C	5[A]	ARG	2.3
1	D	407	LEU	2.3
1	A	122	THR	2.3
1	B	260[A]	VAL	2.3
1	C	324	VAL	2.3
1	B	325	PRO	2.3
1	A	385	LYS	2.2
1	C	219	LEU	2.2
1	D	63	TYR	2.2
1	D	216	VAL	2.2
1	C	44	GLU	2.2
1	B	294	LEU	2.2
1	A	327	PHE	2.2
1	D	7	GLU	2.2
1	B	144	SER	2.2
1	B	208	PRO	2.2
1	A	331	ALA	2.2
1	B	350	HIS	2.2
1	A	402	LEU	2.2
1	B	219	LEU	2.2
1	D	219	LEU	2.2
1	A	288	TYR	2.2
1	D	161	PRO	2.2
1	D	324	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	22	TRP	2.2
1	B	369	ILE	2.2
1	C	312	ILE	2.2
1	D	88	ASN	2.2
1	D	92	ALA	2.2
1	A	55	LEU	2.2
1	A	64	LEU	2.2
1	A	296	LEU	2.2
1	D	292	CYS	2.2
1	D	374	GLY	2.2
1	C	76	VAL	2.2
1	B	110	THR	2.2
1	A	321	GLY	2.2
1	D	109	LEU	2.2
1	A	162	GLN	2.2
1	A	188	LEU	2.1
1	B	76	VAL	2.1
1	B	365	TYR	2.1
1	D	128	TYR	2.1
1	A	138	ALA	2.1
1	C	238	THR	2.1
1	D	243[A]	ARG	2.1
1	A	61	PRO	2.1
1	D	61	PRO	2.1
1	A	34	LEU	2.1
1	A	407	LEU	2.1
1	A	328	VAL	2.1
1	A	365	TYR	2.1
1	B	62	TYR	2.1
1	C	319	THR	2.1
1	B	354	ILE	2.1
1	C	28	ILE	2.1
1	D	355	LEU	2.1
1	A	334	GLY	2.1
1	D	29	GLU	2.1
1	A	322	TYR	2.1
1	B	68	ASP	2.1
1	D	354	ILE	2.1
1	A	47	GLY	2.1
1	B	406	GLY	2.1
1	D	395	LEU	2.1
1	D	347	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	194	VAL	2.1
1	D	271	VAL	2.1
1	D	353	VAL	2.1
1	A	160	THR	2.1
1	A	338	THR	2.1
1	A	290	TYR	2.1
1	B	300	HIS	2.1
1	D	59	ILE	2.1
1	D	81	ILE	2.1
1	C	355	LEU	2.1
1	C	304	PRO	2.1
1	B	243	ARG	2.1
1	D	166	VAL	2.1
1	D	80	ALA	2.1
1	B	137	PHE	2.1
1	D	187	LYS	2.1
1	B	141	SER	2.0
1	A	248	LEU	2.0
1	C	262	LEU	2.0
1	A	166	VAL	2.0
1	C	328	VAL	2.0
1	D	176	VAL	2.0
1	B	264	GLY	2.0
1	C	190	GLU	2.0
1	A	151	ASP	2.0
1	B	378	ASP	2.0
1	B	311	ILE	2.0
1	D	121	ILE	2.0
1	B	111	HIS	2.0
1	C	326	THR	2.0
1	D	197	VAL	2.0
1	A	316[A]	ARG	2.0
1	B	3	ASN	2.0
1	B	347	SER	2.0
1	B	348	GLN	2.0
1	A	62	TYR	2.0
1	C	141	SER	2.0
1	B	69	PRO	2.0
1	B	109	LEU	2.0
1	C	120	LEU	2.0
1	C	188	LEU	2.0
1	C	303	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	71	ASP	2.0
1	A	265	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	D	494	5/5	0.77	0.52	88,88,88,89	0
2	ZN	D	421	1/1	0.82	0.10	31,31,31,31	0
2	ZN	C	421	1/1	0.83	0.09	36,36,36,36	0
4	SAM	B	417	27/27	0.84	0.25	32,34,39,43	1
5	LYS	B	420[A]	10/10	0.86	0.23	32,34,39,39	3
5	LYS	B	420[B]	10/10	0.86	0.23	32,34,39,39	3
3	SO4	C	593	5/5	0.90	0.51	79,80,81,81	0
4	SAM	C	417	27/27	0.90	0.21	21,23,25,31	1
5	LYS	D	420[A]	10/10	0.90	0.23	24,25,28,29	3
5	LYS	D	420[B]	10/10	0.90	0.23	24,25,28,29	3
3	SO4	A	592	5/5	0.91	0.33	98,98,99,99	0
5	LYS	C	420[A]	10/10	0.91	0.19	22,24,27,27	3
5	LYS	C	420[B]	10/10	0.91	0.19	22,24,27,27	3
3	SO4	B	495	5/5	0.91	0.37	101,101,101,101	0
4	SAM	A	417	27/27	0.91	0.19	25,27,31,36	1
4	SAM	D	417	27/27	0.92	0.19	21,23,26,33	1
5	LYS	A	420[A]	10/10	0.94	0.19	27,29,32,33	3
5	LYS	A	420[B]	10/10	0.94	0.19	27,29,32,33	3
7	SF4	B	418	8/8	0.94	0.10	35,38,40,40	0
6	PLP	B	419	15/16	0.95	0.20	27,34,36,37	0
6	PLP	C	419	15/16	0.95	0.17	18,24,25,26	0

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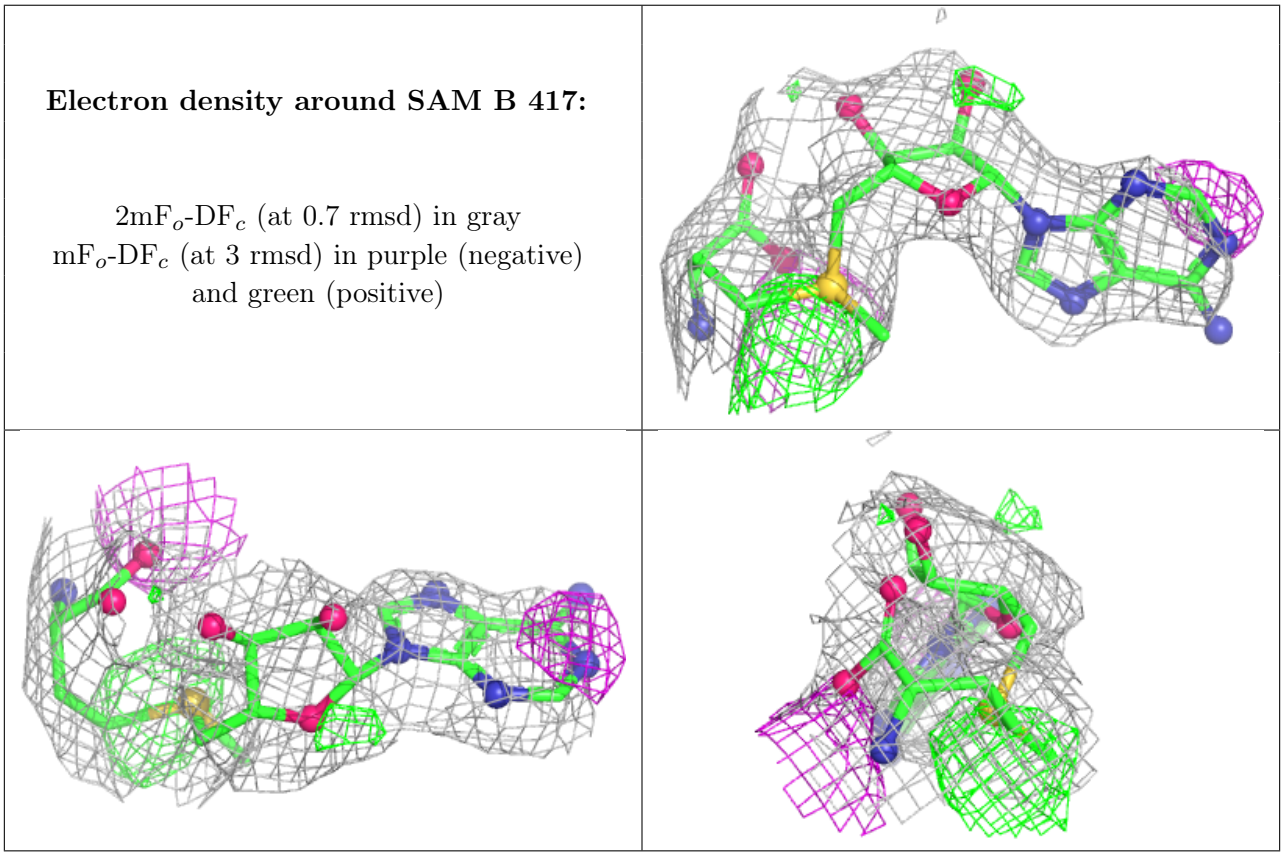
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	PLP	D	419	15/16	0.95	0.20	20,27,29,30	0
6	PLP	A	419	15/16	0.95	0.18	24,31,32,33	0
7	SF4	D	418	8/8	0.96	0.08	21,22,25,26	0
2	ZN	B	421	1/1	0.97	0.06	45,45,45,45	0
7	SF4	C	418	8/8	0.97	0.07	22,24,25,26	0
7	SF4	A	418	8/8	0.97	0.07	24,27,29,29	0
2	ZN	A	421	1/1	0.99	0.07	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.

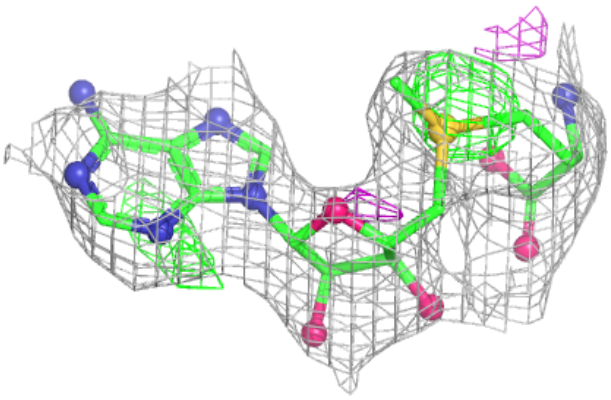
Electron density around SAM B 417:

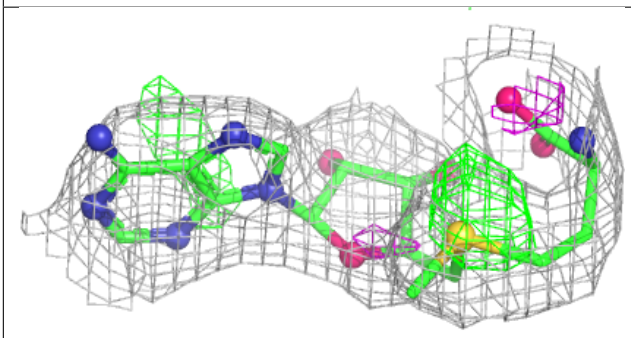
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

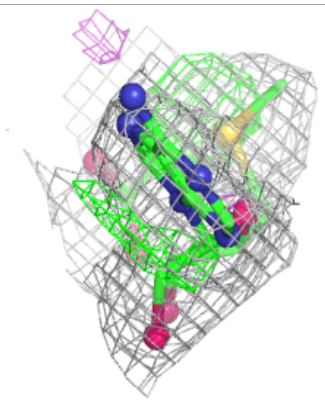


Electron density around SAM C 417:

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

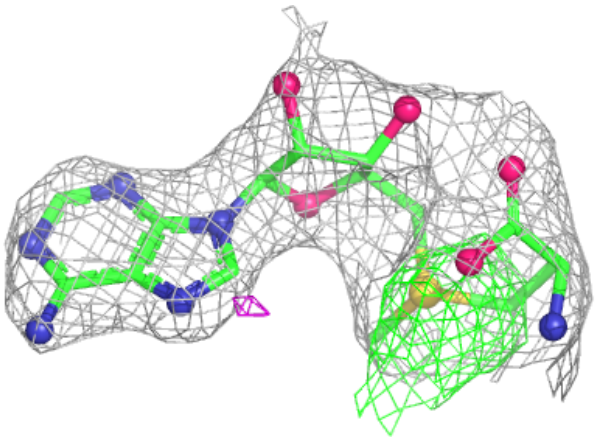


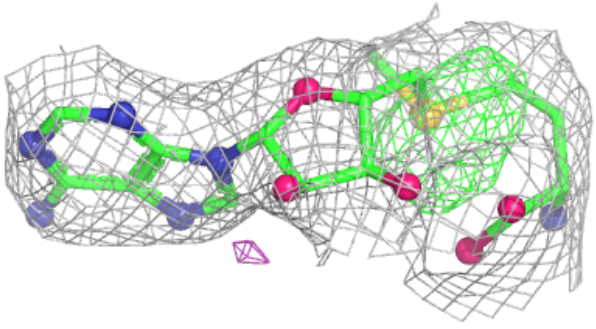


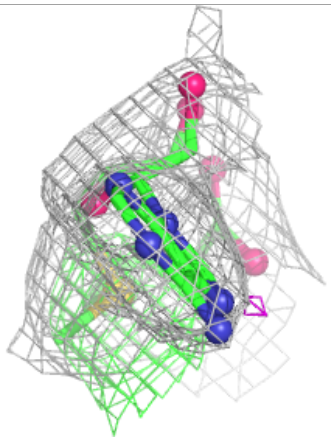


Electron density around SAM A 417:

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

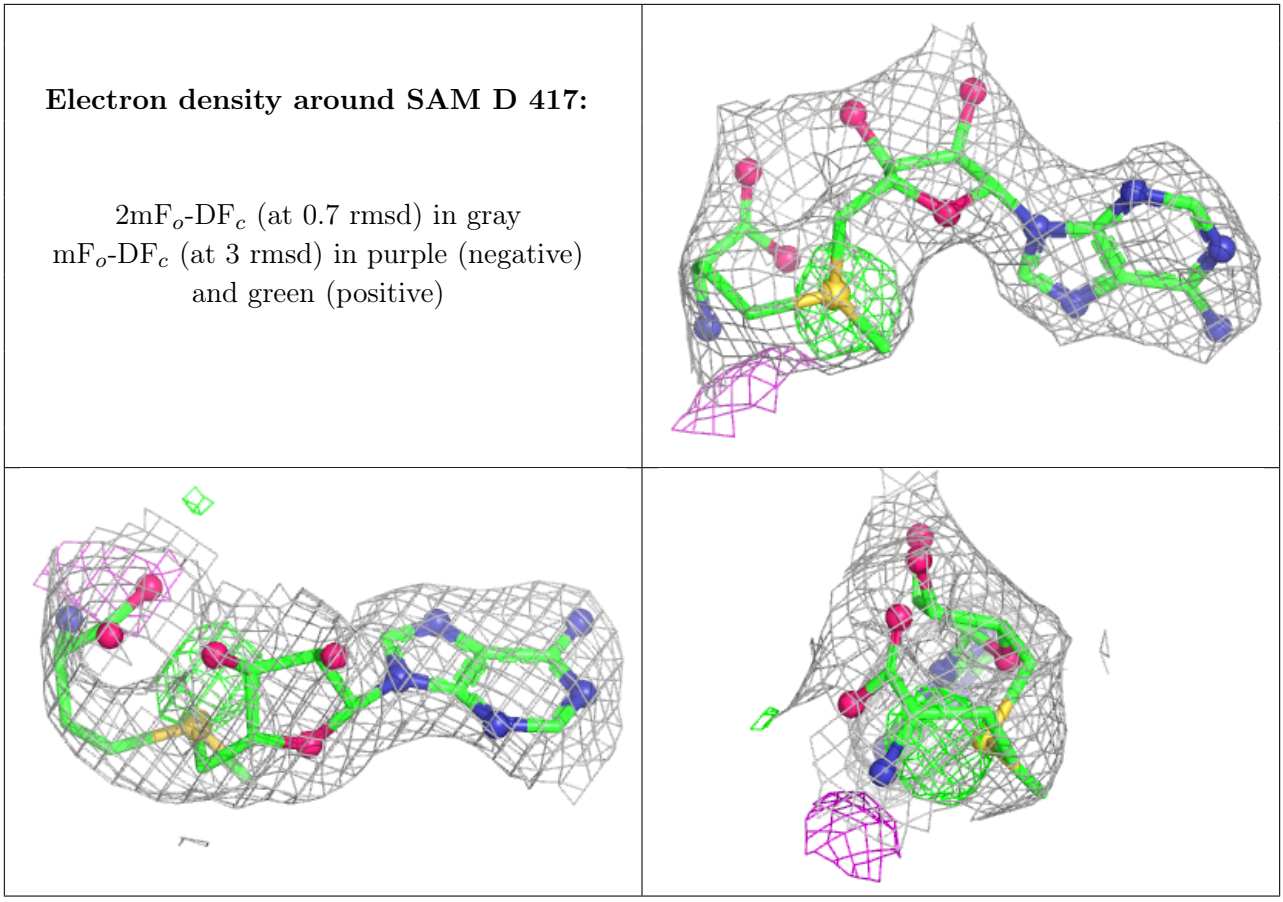






Electron density around SAM D 417:

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



6.5 Other polymers (i)

There are no such residues in this entry.