



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 12:37 PM EDT

PDB ID : 2A5H / pdb_00002a5h
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:

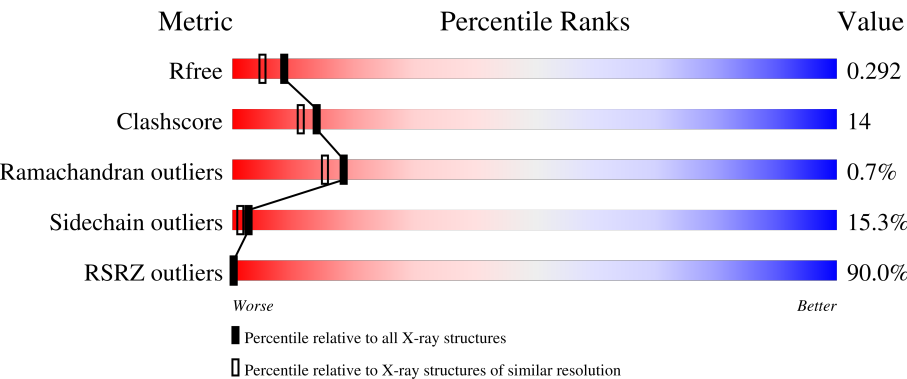
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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	88% 66%24%7%..
1	B	416	92% 66%25%6%..
1	C	416	84% 66%23%7%..
1	D	416	83% 65%25%7%..

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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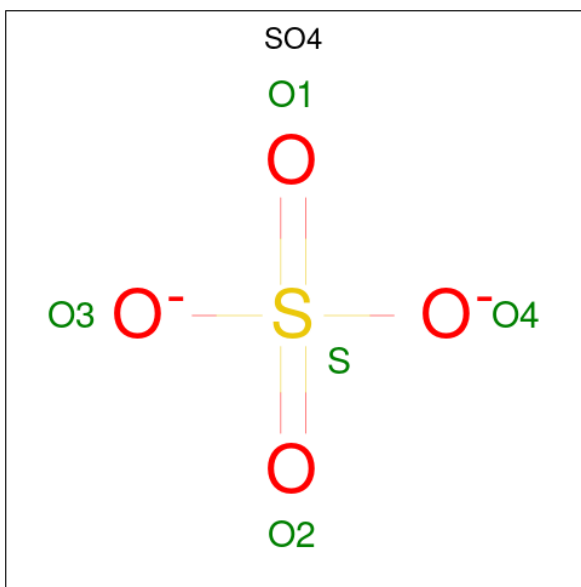
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Chain	Residue	Modelled	Actual	Comment	Reference
C	57	MSE	MET	modified residue	GB 5410603
C	124	MSE	MET	modified residue	GB 5410603
C	127	MSE	MET	modified residue	GB 5410603
C	145	MSE	MET	modified residue	GB 5410603
C	147	MSE	MET	modified residue	GB 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 (CCD ID: ZN) (formula: Zn).

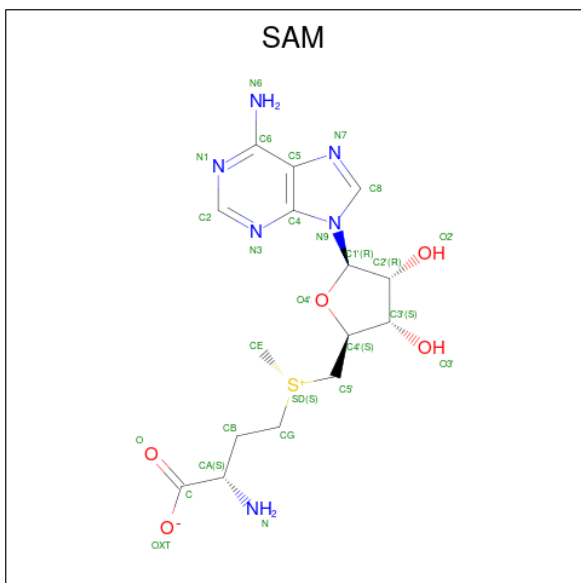
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



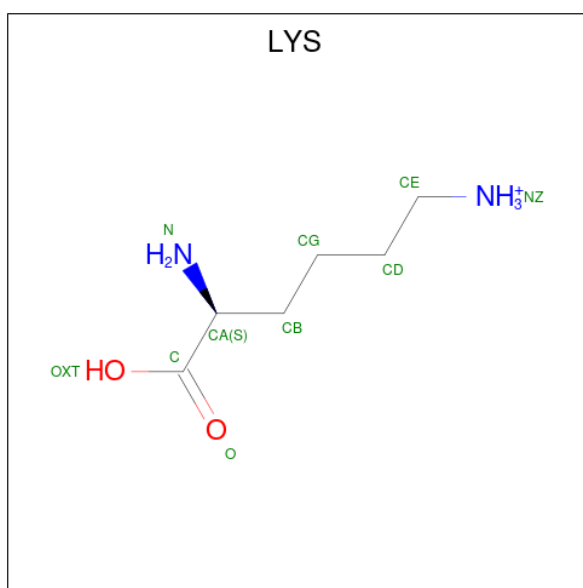
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

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



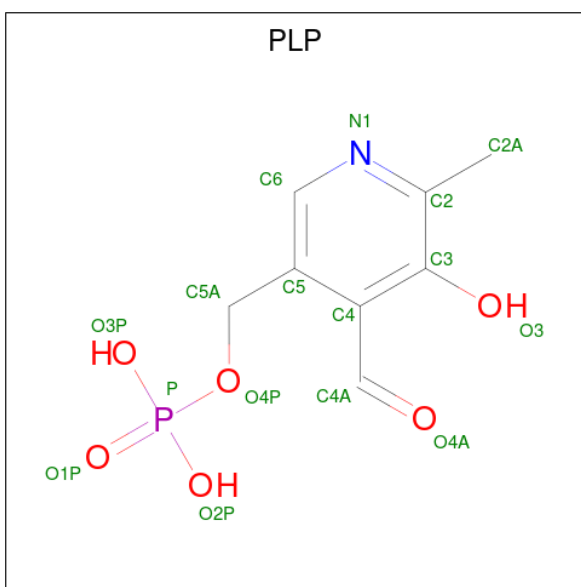
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	D	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 5 is LYSINE (CCD ID: LYS) (formula: $C_6H_{15}N_2O_2$).



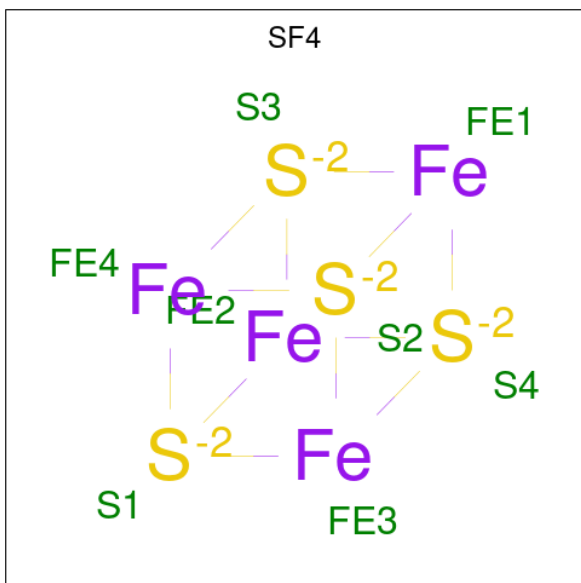
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	1
			13	9	2	2		
5	B	1	Total	C	N	O	0	1
			13	9	2	2		
5	C	1	Total	C	N	O	0	1
			13	9	2	2		
5	D	1	Total	C	N	O	0	1
			13	9	2	2		

- Molecule 6 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: 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		

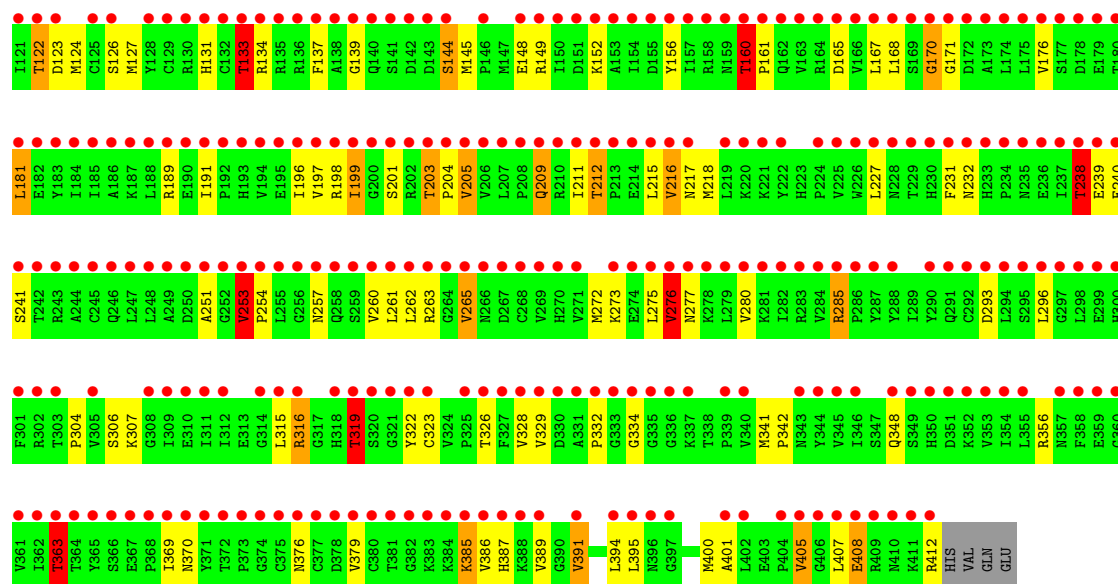
- Molecule 7 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



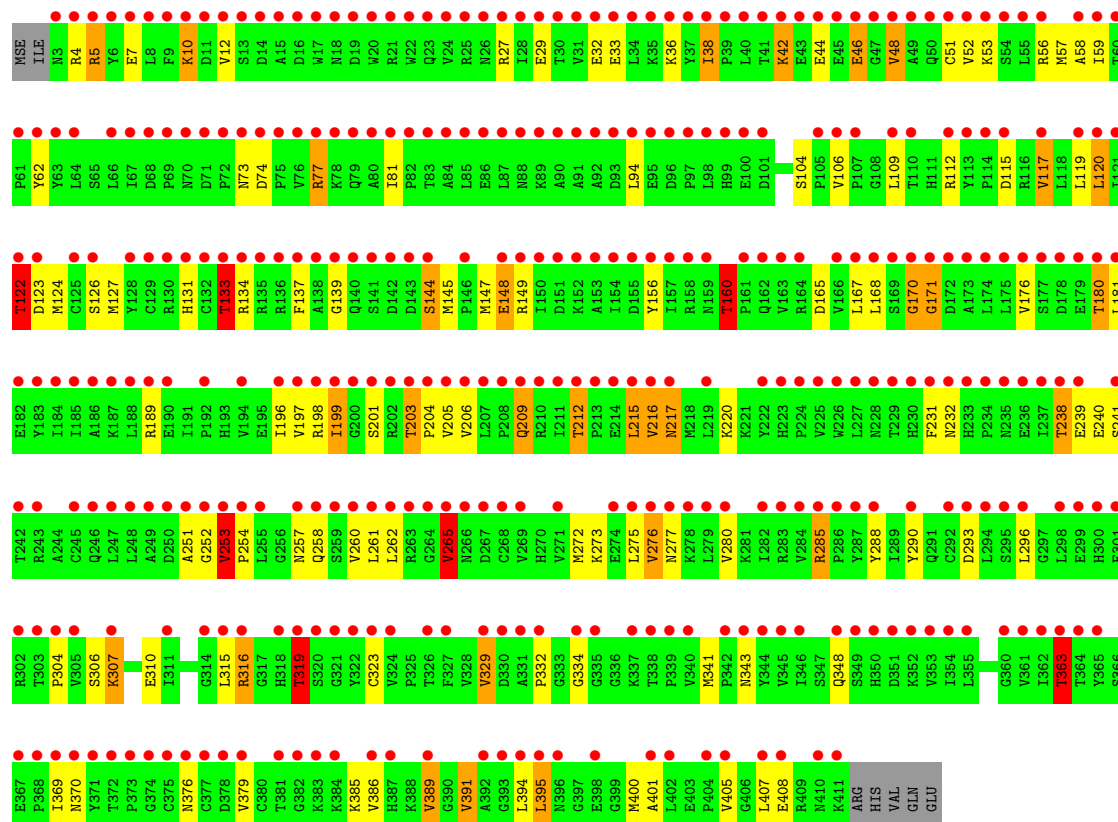
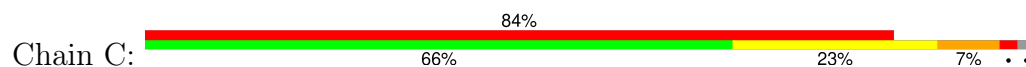
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 8	Fe 4	S 4	0	0
7	B	1	Total 8	Fe 4	S 4	0	0
7	C	1	Total 8	Fe 4	S 4	0	0
7	D	1	Total 8	Fe 4	S 4	0	0

- Molecule 8 is water.

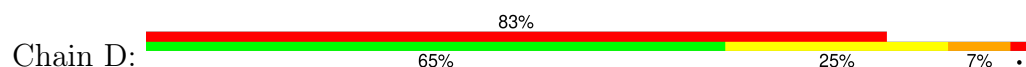
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	135	Total 135	O 135	0	0
8	B	116	Total 116	O 116	0	0
8	C	183	Total 183	O 183	0	0
8	D	174	Total 174	O 174	0	0



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



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



Y365	T303	T242	E182	T122	P61	MSE
S366	P304	R243	Y183	D123	Y62	ILE
E367	V305	A244	I184	M124	Y63	N3
P368	S306	C245	I185	C125	L64	R4
K369	K307	Q246	A186	S126	S65	R5
N370	G308	L247	K187	M127	L66	Y6
Y371	I309	L248	I188	Y128	I67	E7
T372	E310	A249	R189	C129	D68	L8
P373	I311	D250	E190	A130	P69	F9
G374	I312	A251	I191	H131	N70	K10
C375	E313	G252	P192	C132	D71	D11
N376	G314	V253	H193	T133	P72	V12
C377	L315	P254	V194	R134	N73	S13
D378	R316	L255	E195	R135	D74	D14
V379	T319	G256	I196	F136	P75	A15
C380	S320	N257	V197	F137	P76	D16
T381	G321	Q258	R198	A138	R77	W17
G382	S322	S259	I199	G139	K78	N18
K383	Y322	V260	G200	Q140	Q79	D19
K384	C323	L261	S201	S141	A80	W20
K385	V324	L262	R202	D142	Y81	R21
V386	P325	R263	T203	D143	P82	W22
H387	T326	G264	P204	S144	T83	Q23
K388	F327	V265	V205	M145	A84	V24
V389	V328	N266	V206	P146	L85	R25
G390	V329	D267	L207	M147	E86	N26
V391	D330	C268	P208	E148	L87	R27
A392	A331	V269	Q209	R149	N88	I28
G393	P332	H270	R210	I150	K89	E29
L394	G333	V271	I211	D151	A90	T30
L395	G334	N272	T212	K152	A91	V31
K396	G335	K273	P213	A153	A92	E32
G397	G336	E274	E214	I154	D93	E33
E398	K337	L275	L215	D155	L94	K34
G399	V340	V276	V216	Y156	E95	K35
M400	N277	N278	N217	I157	D96	K36
A401	K278	L279	N218	R158	P97	Y37
L402	P342	V280	L219	N159	L98	I38
E403	N343	K281	K220	T160	H99	P39
V405	V344	L282	K221	P161	E100	L40
G406	I346	V285	Y222	Q162	D101	T41
L407	S347	P286	H223	V163	K42	K42
E408	Q348	T287	P224	R164	E43	E43
R409	S349	V288	V225	D165	E44	E44
N410	H350	L289	V226	V166	E45	E45
K411	D351	V290	L227	L167	E46	E46
R412	K352	Q291	N228	L168	G47	G47
VAL	V353	C292	T229	S169	V48	V48
GLN	I354	D293	H230	G170	T110	A49
GLU	L355	L294	F231	G171	H111	Q50
	R356	S295	N232	D172	R112	C51
	N357	F358	H233	A173	Y113	V52
	E359	G360	P234	L174	P114	K53
	G360	L298	N235	L175	D115	S54
	V361	E299	E236	V176	R116	L55
	I362	H300	T237	S177	V117	R56
	T363	F301	T238	D178	L118	H57
	T364	R302	E240	E179	L119	A58
			S241	T180	L120	I59
				L181	I121	T60

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	27582 reflections (9.17%)	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: SO4, PLP, SF4, SAM, 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	1.22	7/3391 (0.2%)	1.37	31/4590 (0.7%)
1	B	1.23	7/3388 (0.2%)	1.27	23/4586 (0.5%)
1	C	1.13	10/3380 (0.3%)	1.28	30/4576 (0.7%)
1	D	1.23	9/3402 (0.3%)	1.29	24/4604 (0.5%)
All	All	1.20	33/13561 (0.2%)	1.30	108/18356 (0.6%)

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 (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	408	GLU	CD-OE2	30.07	1.82	1.25
1	A	148	GLU	CG-CD	29.07	2.24	1.52
1	B	408	GLU	CD-OE1	-25.44	0.77	1.25
1	A	33	GLU	CG-CD	-23.23	0.94	1.52
1	D	42	LYS	CG-CD	20.91	2.15	1.52
1	A	46	GLU	CG-CD	-19.50	1.03	1.52
1	D	408	GLU	CD-OE1	17.08	1.57	1.25
1	B	46	GLU	CG-CD	-14.48	1.15	1.52
1	C	46	GLU	CG-CD	-13.61	1.18	1.52
1	D	385	LYS	CG-CD	12.91	1.91	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	408	GLU	CD-OE2	-11.34	1.03	1.25
1	D	148	GLU	CG-CD	11.13	1.79	1.52
1	C	148	GLU	CG-CD	9.46	1.75	1.52
1	C	239	GLU	CG-CD	9.04	1.74	1.52
1	B	385	LYS	CG-CD	8.14	1.76	1.52
1	A	43	GLU	CB-CG	-7.91	1.28	1.52
1	C	104	SER	C-O	-7.69	1.18	1.25
1	C	253	VAL	CA-CB	7.50	1.61	1.53
1	D	253	VAL	CA-CB	7.25	1.61	1.53
1	D	391	VAL	CA-CB	6.94	1.64	1.54
1	A	42	LYS	CG-CD	-6.92	1.31	1.52
1	C	385	LYS	CG-CD	-6.69	1.32	1.52
1	A	253	VAL	CA-CB	6.54	1.60	1.53
1	B	239	GLU	CG-CD	6.31	1.67	1.52
1	C	42	LYS	CG-CD	6.23	1.71	1.52
1	C	389	VAL	CA-CB	6.23	1.61	1.54
1	B	405	VAL	CA-CB	6.19	1.60	1.54
1	C	265	VAL	CA-CB	5.65	1.61	1.55
1	C	57	MSE	SE-CE	-5.65	1.78	1.95
1	D	203	THR	CA-C	5.50	1.59	1.52
1	B	253	VAL	CA-CB	5.40	1.59	1.53
1	D	405	VAL	CA-CB	5.37	1.59	1.54
1	A	287	TYR	CA-C	5.04	1.56	1.52

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	GLU	CB-CG-CD	31.37	165.93	112.60
1	B	408	GLU	CG-CD-OE2	-22.07	67.64	118.40
1	A	46	GLU	CB-CG-CD	17.54	142.41	112.60
1	B	46	GLU	CB-CG-CD	15.27	138.56	112.60
1	D	408	GLU	CG-CD-OE1	-14.55	84.94	118.40
1	C	46	GLU	CB-CG-CD	14.37	137.03	112.60
1	B	408	GLU	CG-CD-OE1	13.62	149.73	118.40
1	D	42	LYS	CB-CG-CD	-12.22	83.19	111.30
1	A	42	LYS	CG-CD-CE	-11.65	84.49	111.30
1	B	133	THR	CB-CA-C	-11.51	91.11	110.68
1	A	148	GLU	CG-CD-OE2	-11.48	91.99	118.40
1	A	133	THR	CB-CA-C	-11.48	91.74	110.79
1	C	133	THR	CB-CA-C	-11.38	91.90	110.79
1	A	33	GLU	CG-CD-OE2	-11.07	92.93	118.40
1	D	133	THR	CB-CA-C	-11.01	92.51	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	THR	CA-C-N	10.81	130.59	119.56
1	A	160	THR	C-N-CA	10.81	130.59	119.56
1	C	253	VAL	N-CA-C	10.55	117.16	107.56
1	A	33	GLU	CG-CD-OE1	10.48	142.50	118.40
1	A	385	LYS	CG-CD-CE	-9.74	88.90	111.30
1	B	263	ARG	NE-CZ-NH2	9.57	127.81	119.20
1	D	160	THR	CA-C-N	9.46	129.09	119.82
1	D	160	THR	C-N-CA	9.46	129.09	119.82
1	A	42	LYS	CB-CG-CD	8.60	131.08	111.30
1	A	408	GLU	CG-CD-OE1	-8.42	99.03	118.40
1	A	285[A]	ARG	CB-CA-C	8.20	121.18	109.38
1	A	285[B]	ARG	CB-CA-C	8.20	121.18	109.38
1	C	385	LYS	CG-CD-CE	-8.06	92.76	111.30
1	D	4	ARG	NE-CZ-NH2	8.05	126.44	119.20
1	C	160	THR	CA-C-N	7.89	127.61	119.56
1	C	160	THR	C-N-CA	7.89	127.61	119.56
1	D	363	THR	CB-CA-C	-7.43	95.50	111.11
1	B	160	THR	CA-C-N	7.42	127.13	119.56
1	B	160	THR	C-N-CA	7.42	127.13	119.56
1	D	46	GLU	CB-CG-CD	7.39	125.17	112.60
1	D	253	VAL	N-CA-C	7.31	115.14	107.76
1	A	4	ARG	NE-CZ-NH2	7.25	125.73	119.20
1	D	385	LYS	CG-CD-CE	7.25	127.97	111.30
1	D	4	ARG	NE-CZ-NH1	-7.05	114.45	121.50
1	A	408	GLU	OE1-CD-OE2	7.03	139.77	122.90
1	B	363	THR	CB-CA-C	-6.91	96.59	111.11
1	C	104	SER	CA-C-N	6.80	126.40	119.19
1	C	104	SER	C-N-CA	6.80	126.40	119.19
1	C	363	THR	CB-CA-C	-6.79	96.86	110.30
1	B	191	ILE	CA-C-N	6.71	126.97	119.32
1	B	191	ILE	C-N-CA	6.71	126.97	119.32
1	D	122	THR	CB-CA-C	-6.71	98.14	110.62
1	A	363	THR	CB-CA-C	-6.61	97.24	111.11
1	B	263	ARG	NE-CZ-NH1	-6.43	115.07	121.50
1	A	4	ARG	NE-CZ-NH1	-6.42	115.08	121.50
1	D	46	GLU	CG-CD-OE1	-6.14	104.28	118.40
1	C	285[A]	ARG	CB-CA-C	5.96	116.93	110.08
1	C	285[B]	ARG	CB-CA-C	5.96	116.93	110.08
1	C	385	LYS	CB-CG-CD	5.85	124.76	111.30
1	C	265	VAL	CB-CA-C	5.84	116.99	111.44
1	D	385	LYS	CB-CG-CD	-5.81	97.93	111.30
1	B	319	THR	CB-CA-C	-5.81	99.48	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	252	GLY	CA-C-N	-5.81	118.65	122.60
1	C	252	GLY	C-N-CA	-5.81	118.65	122.60
1	B	253	VAL	N-CA-C	5.75	113.57	107.76
1	C	122	THR	CB-CA-C	-5.75	98.08	110.45
1	C	196	ILE	CA-C-N	-5.74	115.69	123.10
1	C	196	ILE	C-N-CA	-5.74	115.69	123.10
1	C	4	ARG	NE-CZ-NH2	-5.71	114.06	119.20
1	A	252	GLY	CA-C-N	-5.66	118.51	122.59
1	A	252	GLY	C-N-CA	-5.66	118.51	122.59
1	C	148	GLU	CB-CG-CD	5.62	122.16	112.60
1	A	191	ILE	CA-C-N	5.60	125.26	119.05
1	A	191	ILE	C-N-CA	5.60	125.26	119.05
1	D	148	GLU	CB-CG-CD	5.58	122.09	112.60
1	C	5[A]	ARG	NE-CZ-NH2	-5.57	114.19	119.20
1	C	5[B]	ARG	NE-CZ-NH2	-5.57	114.19	119.20
1	A	319	THR	CB-CA-C	-5.55	100.01	111.22
1	D	276	VAL	CB-CA-C	5.54	119.86	112.22
1	A	329	VAL	CB-CA-C	5.52	118.54	110.98
1	D	148	GLU	CG-CD-OE2	-5.45	105.87	118.40
1	D	53	LYS	N-CA-C	-5.43	99.24	110.80
1	D	319	THR	CB-CA-C	-5.42	100.27	111.22
1	A	43	GLU	CA-CB-CG	5.39	124.88	114.10
1	B	265	VAL	CB-CA-C	5.37	115.83	111.05
1	D	238	THR	N-CA-CB	-5.36	102.70	111.66
1	B	276	VAL	CB-CA-C	5.36	119.62	112.22
1	D	205	VAL	CB-CA-C	5.35	118.68	111.94
1	B	205	VAL	CB-CA-C	5.34	117.69	111.55
1	A	171	GLY	N-CA-C	-5.30	100.62	113.18
1	A	148	GLU	CG-CD-OE1	5.28	130.55	118.40
1	B	391	VAL	N-CA-C	5.28	116.06	110.72
1	C	180	THR	N-CA-C	-5.28	105.44	111.14
1	C	160	THR	CB-CA-C	5.28	120.75	111.20
1	A	122	THR	CB-CA-C	-5.27	99.12	110.45
1	C	4	ARG	CD-NE-CZ	5.24	131.74	124.40
1	A	104	SER	CA-C-N	5.24	124.74	119.19
1	A	104	SER	C-N-CA	5.24	124.74	119.19
1	C	10	LYS	CB-CG-CD	5.22	123.31	111.30
1	A	253	VAL	CB-CA-C	5.21	116.29	110.71
1	C	329	VAL	CB-CA-C	5.21	118.12	110.98
1	C	253	VAL	N-CA-CB	5.16	116.93	111.20
1	D	148	GLU	CG-CD-OE1	5.13	130.19	118.40
1	D	280	VAL	CB-CA-C	5.12	120.56	112.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	391	VAL	N-CA-CB	5.12	118.26	110.58
1	C	148	GLU	CG-CD-OE2	-5.12	106.64	118.40
1	D	319	THR	N-CA-CB	5.11	118.58	110.87
1	B	319	THR	N-CA-CB	5.09	118.55	110.87
1	C	319	THR	CB-CA-C	-5.06	100.49	111.11
1	B	238	THR	N-CA-CB	-5.03	103.26	111.66
1	B	370	ASN	N-CA-C	5.03	118.52	111.74
1	B	196	ILE	CA-C-N	-5.01	116.98	123.19
1	B	196	ILE	C-N-CA	-5.01	116.98	123.19

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	101	0
1	B	3288	0	3306	97	0
1	C	3280	0	3295	114	0
1	D	3297	0	3313	123	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	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	386	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 (386) 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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:376:ASN:CG	1:D:73:ASN:HD22	2.11	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
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:A:376:ASN:CG	1:B:73:ASN:HD22	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:73:ASN:HD22	1:D:376:ASN:CG	2.17	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:134:ARG:CZ	4:B:417:SAM:HE3	2.43	0.48
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:D:123:ASP:C	1:D:123:ASP:OD1	2.56	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
1:C:123:ASP:OD1	1:C:123:ASP:C	2.57	0.48
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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:123:ASP:C	1:A:123:ASP:OD1	2.60	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:73:ASN:HD22	1:B:376:ASN:CG	2.26	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:B:29:GLU:C	1:B:57:MSE:HE3	2.43	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:C:273:LYS:HZ2	1:C:319:THR:HG23	1.82	0.43
1:C:391:VAL:HG22	1:D:313:GLU:CD	2.43	0.43
1:D:59:ILE:HA	1:D:127:MSE:HG2	2.00	0.43
1:B:123:ASP:OD1	1:B:123:ASP:C	2.60	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: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:134:ARG:NH2	4:B:417:SAM:HE3	2.33	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:307:LYS:HD3	1:C:307:LYS:C	2.44	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%)	18	15
1	B	416/416 (100%)	398 (96%)	15 (4%)	3 (1%)	18	15
1	C	415/416 (100%)	397 (96%)	15 (4%)	3 (1%)	18	15
1	D	417/416 (100%)	397 (95%)	17 (4%)	3 (1%)	18	15
All	All	1664/1664 (100%)	1592 (96%)	60 (4%)	12 (1%)	18	15

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%)	314 (84%)	60 (16%)	2	1
1	B	374/362 (103%)	313 (84%)	61 (16%)	2	1
1	C	373/362 (103%)	316 (85%)	57 (15%)	3	1
1	D	375/362 (104%)	314 (84%)	61 (16%)	2	1
All	All	1496/1448 (103%)	1257 (84%)	239 (16%)	3	1

All (239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5[A]	ARG
1	A	5[B]	ARG
1	A	32	GLU
1	A	33	GLU
1	A	38	ILE
1	A	42	LYS
1	A	43	GLU
1	A	46	GLU
1	A	48	VAL
1	A	77	ARG
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	189	ARG
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

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Mol	Chain	Res	Type
1	A	220	LYS
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	329	VAL
1	A	363	THR
1	A	369	ILE
1	A	379	VAL
1	A	386	VAL
1	A	389	VAL
1	A	391	VAL
1	A	394	LEU
1	A	395	LEU
1	A	405	VAL
1	A	407	LEU
1	B	5[A]	ARG
1	B	5[B]	ARG
1	B	10	LYS
1	B	32	GLU
1	B	38	ILE
1	B	42	LYS
1	B	43	GLU
1	B	46	GLU
1	B	48	VAL
1	B	51	CYS
1	B	77	ARG
1	B	106	VAL
1	B	117	VAL
1	B	119	LEU
1	B	120	LEU

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Mol	Chain	Res	Type
1	B	122	THR
1	B	133	THR
1	B	144	SER
1	B	160	THR
1	B	167	LEU
1	B	176	VAL
1	B	181	LEU
1	B	189	ARG
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	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	329	VAL
1	B	363	THR
1	B	369	ILE
1	B	379	VAL
1	B	385	LYS
1	B	386	VAL
1	B	389	VAL
1	B	391	VAL
1	B	394	LEU

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Mol	Chain	Res	Type
1	B	395	LEU
1	B	405	VAL
1	B	407	LEU
1	B	412	ARG
1	C	7	GLU
1	C	10	LYS
1	C	32	GLU
1	C	38	ILE
1	C	42	LYS
1	C	46	GLU
1	C	48	VAL
1	C	51	CYS
1	C	77	ARG
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	189	ARG
1	C	197	VAL
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	216	VAL
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

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Mol	Chain	Res	Type
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
1	C	316[B]	ARG
1	C	319	THR
1	C	329	VAL
1	C	363	THR
1	C	369	ILE
1	C	379	VAL
1	C	386	VAL
1	C	389	VAL
1	C	391	VAL
1	C	394	LEU
1	C	395	LEU
1	C	405	VAL
1	C	407	LEU
1	D	5[A]	ARG
1	D	5[B]	ARG
1	D	32	GLU
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	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	187	LYS
1	D	189	ARG

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Mol	Chain	Res	Type
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	216	VAL
1	D	217	ASN
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	329	VAL
1	D	363	THR
1	D	369	ILE
1	D	379	VAL
1	D	385	LYS
1	D	386	VAL
1	D	389	VAL
1	D	391	VAL
1	D	394	LEU
1	D	395	LEU
1	D	405	VAL
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	209	GLN
1	A	232	ASN
1	A	257	ASN
1	A	343	ASN
1	A	348	GLN
1	B	3	ASN
1	B	88	ASN
1	B	159	ASN
1	B	209	GLN
1	B	232	ASN
1	B	257	ASN
1	B	370	ASN
1	C	3	ASN
1	C	88	ASN
1	C	99	HIS
1	C	159	ASN
1	C	209	GLN
1	C	217	ASN
1	C	257	ASN
1	C	370	ASN
1	D	3	ASN
1	D	88	ASN
1	D	99	HIS
1	D	159	ASN
1	D	209	GLN
1	D	232	ASN
1	D	257	ASN
1	D	343	ASN
1	D	350	HIS
1	D	370	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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
7	SF4	A	418	4,1	0,12,12	-	-	-		
5	LYS	B	420[A]	-	8,9,9	0.74	0	7,10,10	1.02	1 (14%)
6	PLP	A	419	5	15,15,16	2.72	2 (13%)	21,22,23	1.18	2 (9%)
5	LYS	C	420[B]	-	8,9,9	1.02	0	7,10,10	0.90	0
3	SO4	B	495	-	4,4,4	0.25	0	6,6,6	0.31	0
5	LYS	A	420[B]	-	8,9,9	0.85	1 (12%)	7,10,10	1.05	0
7	SF4	C	418	4,1	0,12,12	-	-	-		
5	LYS	D	420[B]	-	8,9,9	0.94	1 (12%)	7,10,10	1.12	1 (14%)
4	SAM	B	417	7	27,29,29	1.86	6 (22%)	34,42,42	2.01	12 (35%)
5	LYS	B	420[B]	-	8,9,9	0.75	0	7,10,10	0.99	1 (14%)
4	SAM	D	417	7	27,29,29	1.74	6 (22%)	34,42,42	2.25	14 (41%)
6	PLP	C	419	5	15,15,16	2.80	3 (20%)	21,22,23	0.97	0
4	SAM	C	417	7	27,29,29	1.87	6 (22%)	34,42,42	1.99	11 (32%)
7	SF4	D	418	4,1	0,12,12	-	-	-		
3	SO4	D	494	-	4,4,4	0.31	0	6,6,6	0.34	0
3	SO4	A	592	-	4,4,4	0.30	0	6,6,6	0.22	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
5	LYS	C	420[A]	-	8,9,9	1.03	0	7,10,10	0.94	0
7	SF4	B	418	4,1	0,12,12	-	-	-		
4	SAM	A	417	7	27,29,29	1.87	8 (29%)	34,42,42	2.09	9 (26%)
5	LYS	A	420[A]	-	8,9,9	0.85	1 (12%)	7,10,10	1.04	0
5	LYS	D	420[A]	-	8,9,9	0.94	1 (12%)	7,10,10	1.17	1 (14%)
6	PLP	B	419	5	15,15,16	2.76	2 (13%)	21,22,23	0.93	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
7	SF4	A	418	4,1	-	-	0/6/5/5
5	LYS	B	420[A]	-	-	1/9/9/9	-
6	PLP	A	419	5	-	1/6/6/8	0/1/1/1
5	LYS	C	420[B]	-	-	1/9/9/9	-
5	LYS	A	420[B]	-	-	1/9/9/9	-
7	SF4	C	418	4,1	-	-	0/6/5/5
5	LYS	D	420[B]	-	-	1/9/9/9	-
4	SAM	B	417	7	-	2/17/33/33	0/3/3/3
5	LYS	B	420[B]	-	-	1/9/9/9	-
4	SAM	D	417	7	-	2/17/33/33	0/3/3/3
6	PLP	C	419	5	-	0/6/6/8	0/1/1/1
4	SAM	C	417	7	-	3/17/33/33	0/3/3/3
7	SF4	D	418	4,1	-	-	0/6/5/5
6	PLP	D	419	5	-	0/6/6/8	0/1/1/1
5	LYS	C	420[A]	-	-	1/9/9/9	-
7	SF4	B	418	4,1	-	-	0/6/5/5
4	SAM	A	417	7	-	2/17/33/33	0/3/3/3
5	LYS	A	420[A]	-	-	1/9/9/9	-
5	LYS	D	420[A]	-	-	1/9/9/9	-
6	PLP	B	419	5	-	0/6/6/8	0/1/1/1

All (39) 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	C	417	SAM	C5-C4	5.26	1.48	1.39
4	A	417	SAM	C5-C4	5.15	1.48	1.39
4	B	417	SAM	OXT-C	5.04	1.46	1.30
4	D	417	SAM	C5-C4	4.82	1.47	1.39
4	A	417	SAM	OXT-C	4.78	1.45	1.30
4	B	417	SAM	C5-C4	4.74	1.47	1.39
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	D	417	SAM	C5-C6	3.29	1.50	1.41
4	D	417	SAM	CE-SD	3.17	1.98	1.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	419	PLP	P-O2P	-3.08	1.43	1.54
4	C	417	SAM	C5-C6	2.95	1.49	1.41
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	B	417	SAM	C5-C6	2.79	1.48	1.41
4	A	417	SAM	C5-C6	2.69	1.48	1.41
4	C	417	SAM	CE-SD	2.65	1.95	1.78
4	A	417	SAM	C4-N9	-2.63	1.32	1.37
6	C	419	PLP	P-O2P	-2.46	1.45	1.54
6	A	419	PLP	P-O2P	-2.44	1.45	1.54
4	D	417	SAM	C4-N9	-2.42	1.32	1.37
4	A	417	SAM	C5-N7	-2.40	1.34	1.39
4	C	417	SAM	C8-N7	2.39	1.36	1.31
4	B	417	SAM	C4-N9	-2.38	1.32	1.37
4	B	417	SAM	C8-N7	2.32	1.36	1.31
4	D	417	SAM	C5-N7	-2.24	1.35	1.39
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
6	B	419	PLP	C6-C5	2.14	1.42	1.37
4	A	417	SAM	C2-N3	2.11	1.37	1.33
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
4	C	417	SAM	C5-N7	-2.06	1.35	1.39
4	A	417	SAM	C8-N7	2.05	1.35	1.31

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	417	SAM	C5-C4-N3	-5.03	119.79	126.72
4	A	417	SAM	C5-C4-N3	-4.80	120.11	126.72
4	C	417	SAM	C5-C4-N3	-4.72	120.22	126.72
4	D	417	SAM	N3-C4-N9	4.48	134.79	127.17
4	A	417	SAM	N3-C4-N9	4.42	134.69	127.17
4	B	417	SAM	C5-C4-N3	-4.37	120.70	126.72
4	B	417	SAM	C4-N9-C8	4.32	110.28	105.74
4	C	417	SAM	N3-C4-N9	4.30	134.47	127.17
4	A	417	SAM	CG-SD-C5'	-4.00	93.65	103.43
4	D	417	SAM	C4-N9-C8	3.95	109.89	105.74
4	C	417	SAM	CG-SD-C5'	-3.92	93.85	103.43
4	B	417	SAM	N3-C4-N9	3.87	133.76	127.17
4	A	417	SAM	CB-CA-N	3.69	119.73	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	417	SAM	O4'-C1'-N9	3.58	114.96	108.09
4	C	417	SAM	C4-N9-C8	3.53	109.44	105.74
4	A	417	SAM	C4-N9-C8	3.47	109.38	105.74
4	A	417	SAM	O4'-C1'-N9	3.44	114.70	108.09
4	D	417	SAM	CB-CA-N	3.28	118.66	110.12
4	D	417	SAM	C5-N7-C8	3.27	108.59	103.45
4	D	417	SAM	C2-N3-C4	3.27	119.82	111.83
4	D	417	SAM	N9-C8-N7	-3.25	109.33	113.94
4	D	417	SAM	C4-C5-N7	-3.24	106.87	110.58
4	B	417	SAM	C4-C5-N7	-3.17	106.96	110.58
4	B	417	SAM	CB-CA-N	3.13	118.28	110.12
4	B	417	SAM	C2-N3-C4	3.11	119.44	111.83
4	C	417	SAM	C4-C5-N7	-3.10	107.04	110.58
4	C	417	SAM	C2-N3-C4	3.08	119.36	111.83
4	B	417	SAM	N3-C2-N1	-2.93	124.15	128.58
4	A	417	SAM	C2-N3-C4	2.92	118.97	111.83
6	D	419	PLP	C4A-C4-C5	2.81	123.83	120.94
4	B	417	SAM	N9-C8-N7	-2.80	109.97	113.94
4	D	417	SAM	N3-C2-N1	-2.77	124.39	128.58
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	D	417	SAM	C6-C5-N7	2.63	137.15	132.09
4	C	417	SAM	C6-C5-N7	2.61	137.12	132.09
4	A	417	SAM	C4-C5-N7	-2.58	107.63	110.58
4	A	417	SAM	N3-C2-N1	-2.50	124.79	128.58
4	B	417	SAM	C5-N7-C8	2.42	107.26	103.45
4	C	417	SAM	C5-N7-C8	2.40	107.22	103.45
4	B	417	SAM	C6-C5-N7	2.31	136.54	132.09
4	B	417	SAM	C2'-C1'-N9	-2.30	107.59	113.30
4	C	417	SAM	C2'-C1'-N9	-2.30	107.60	113.30
4	C	417	SAM	N3-C2-N1	-2.25	125.17	128.58
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	D	417	SAM	C2'-C1'-N9	-2.22	107.79	113.30
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
4	B	417	SAM	O4'-C1'-N9	2.12	112.16	108.09
4	C	417	SAM	N9-C8-N7	-2.07	110.99	113.94
4	D	417	SAM	C3'-C2'-C1'	2.00	105.25	101.46

There are no chirality outliers.

All (18) torsion outliers are listed below:

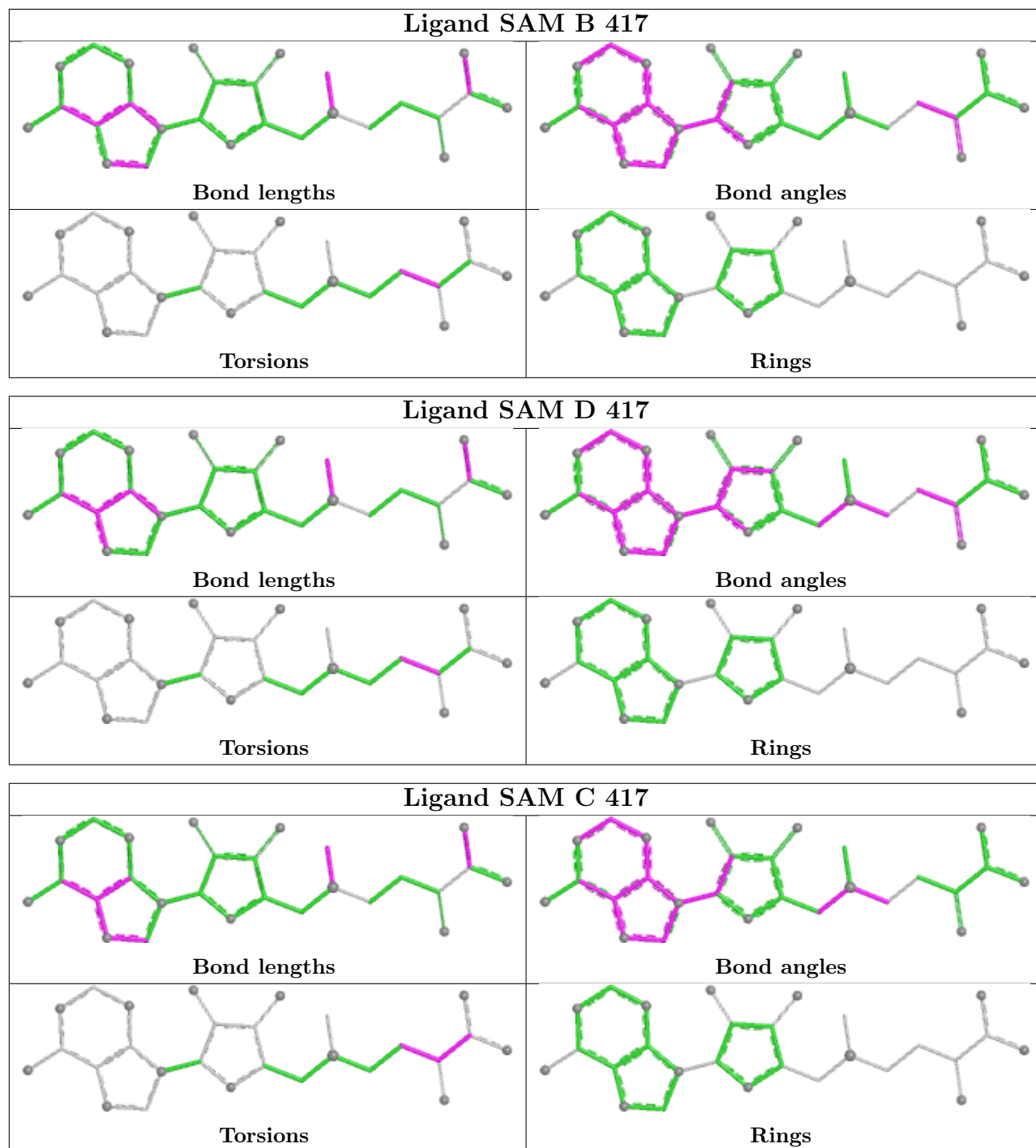
Mol	Chain	Res	Type	Atoms
4	C	417	SAM	N-CA-CB-CG
4	D	417	SAM	N-CA-CB-CG
4	A	417	SAM	C-CA-CB-CG
4	B	417	SAM	C-CA-CB-CG
4	C	417	SAM	C-CA-CB-CG
4	D	417	SAM	C-CA-CB-CG
4	A	417	SAM	N-CA-CB-CG
4	B	417	SAM	N-CA-CB-CG
6	A	419	PLP	C5A-O4P-P-O1P
5	A	420[A]	LYS	OXT-C-CA-N
5	A	420[B]	LYS	OXT-C-CA-N
4	C	417	SAM	O-C-CA-N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

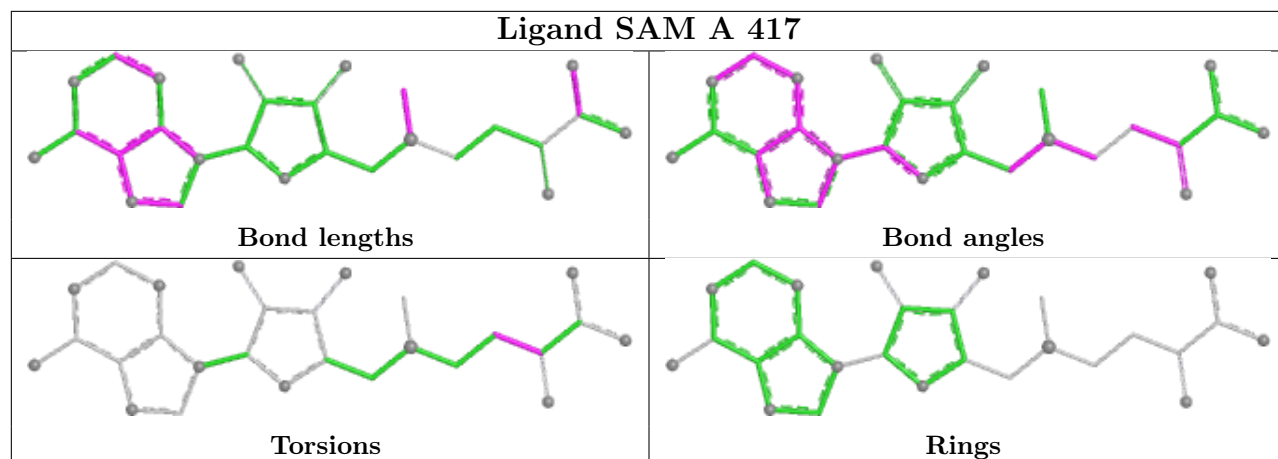
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	418	SF4	1	0
4	B	417	SAM	2	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 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%)	3.79	366 (91%)  	12, 38, 60, 72	18 (4%)
1	B	401/416 (96%)	4.27	381 (95%)  	13, 42, 78, 98	15 (3%)
1	C	400/416 (96%)	3.61	349 (87%)  	11, 32, 58, 73	15 (3%)
1	D	401/416 (96%)	3.40	345 (86%)  	9, 32, 54, 69	15 (3%)
All	All	1602/1664 (96%)	3.77	1441 (89%)  	9, 36, 64, 98	63 (3%)

All (1441) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	47	GLY	13.6
1	D	52	VAL	12.6
1	A	48	VAL	12.3
1	B	31	VAL	11.8
1	A	46	GLU	10.0
1	A	90	ALA	9.9
1	B	138	ALA	9.9
1	B	81	ILE	9.8
1	C	38	ILE	9.5
1	A	52	VAL	9.5
1	B	48	VAL	9.1
1	C	48	VAL	9.0
1	B	66	LEU	9.0
1	B	176	VAL	8.9
1	B	88	ASN	8.8
1	C	30	THR	8.7
1	C	369	ILE	8.6
1	B	4	ARG	8.6
1	A	34	LEU	8.5
1	B	30	THR	8.5
1	A	206	VAL	8.2

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Mol	Chain	Res	Type	RSRZ
1	B	6	TYR	8.2
1	B	38	ILE	8.2
1	D	34	LEU	8.2
1	B	64	LEU	8.2
1	B	92	ALA	8.2
1	C	52	VAL	8.2
1	D	48	VAL	8.1
1	C	153	ALA	8.1
1	B	175	LEU	8.1
1	C	31	VAL	8.0
1	B	14	ASP	7.9
1	D	92	ALA	7.9
1	B	55	LEU	7.9
1	B	8	LEU	7.8
1	A	53	LYS	7.8
1	B	12	VAL	7.7
1	C	51	CYS	7.6
1	B	35	LYS	7.6
1	B	32	GLU	7.5
1	D	43	GLU	7.5
1	A	120	LEU	7.5
1	C	12	VAL	7.5
1	D	128	TYR	7.5
1	A	406	GLY	7.5
1	B	93	ASP	7.5
1	C	175	LEU	7.4
1	A	368	PRO	7.4
1	D	40	LEU	7.4
1	A	10	LYS	7.3
1	A	38	ILE	7.3
1	B	22	TRP	7.3
1	B	98	LEU	7.3
1	D	120	LEU	7.2
1	C	73	ASN	7.2
1	B	369	ILE	7.2
1	B	95	GLU	7.1
1	B	37	TYR	7.1
1	A	51	CYS	7.1
1	A	174	LEU	7.1
1	B	229	THR	7.1
1	D	55	LEU	7.1
1	C	53	LYS	7.1

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Mol	Chain	Res	Type	RSRZ
1	D	33	GLU	7.0
1	C	62	TYR	7.0
1	B	119	LEU	7.0
1	B	181	LEU	7.0
1	C	11	ASP	7.0
1	D	254	PRO	7.0
1	B	139	GLY	6.9
1	B	59	ILE	6.9
1	B	40	LEU	6.9
1	A	89	LYS	6.9
1	A	92	ALA	6.8
1	C	58	ALA	6.8
1	A	117	VAL	6.8
1	D	46	GLU	6.8
1	B	47	GLY	6.7
1	C	7	GLU	6.7
1	D	35	LYS	6.7
1	A	31	VAL	6.7
1	C	128	TYR	6.7
1	B	239	GLU	6.7
1	A	395	LEU	6.7
1	B	50	GLN	6.7
1	C	90	ALA	6.6
1	A	128	TYR	6.6
1	C	81	ILE	6.6
1	C	59	ILE	6.6
1	B	10	LYS	6.6
1	B	211	ILE	6.6
1	A	85	LEU	6.6
1	B	264	GLY	6.6
1	B	87	LEU	6.5
1	A	47	GLY	6.5
1	D	265	VAL	6.5
1	A	28	ILE	6.5
1	A	40	LEU	6.5
1	A	369	ILE	6.5
1	D	31	VAL	6.5
1	D	29	GLU	6.5
1	D	69	PRO	6.4
1	B	128	TYR	6.4
1	D	49	ALA	6.4
1	C	95	GLU	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	71	ASP	6.4
1	C	37	TYR	6.4
1	A	55	LEU	6.4
1	B	34	LEU	6.4
1	A	9	PHE	6.4
1	B	126	SER	6.4
1	A	37	TYR	6.3
1	A	87	LEU	6.4
1	B	9	PHE	6.3
1	D	334	GLY	6.3
1	A	91	ALA	6.3
1	A	66	LEU	6.3
1	C	241	SER	6.3
1	C	253	VAL	6.3
1	B	39	PRO	6.3
1	B	75	PRO	6.2
1	B	143	ASP	6.2
1	D	84	ALA	6.2
1	C	54	SER	6.2
1	B	140	GLN	6.2
1	D	38	ILE	6.2
1	B	254	PRO	6.2
1	B	44	GLU	6.2
1	B	24	VAL	6.1
1	B	63	TYR	6.1
1	A	258	GLN	6.1
1	D	54	SER	6.1
1	B	260[A]	VAL	6.1
1	A	84	ALA	6.1
1	B	94	LEU	6.1
1	B	154	ILE	6.1
1	D	47	GLY	6.1
1	B	76	VAL	6.1
1	B	203	THR	6.1
1	B	246	GLN	6.0
1	B	89	LYS	6.0
1	A	188	LEU	6.0
1	B	83	THR	6.0
1	A	362	ILE	6.0
1	B	28	ILE	6.0
1	B	52	VAL	6.0
1	B	227	LEU	6.0

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Mol	Chain	Res	Type	RSRZ
1	B	58	ALA	6.0
1	B	296	LEU	6.0
1	C	40	LEU	6.0
1	C	10	LYS	6.0
1	B	13	SER	5.9
1	D	51	CYS	5.9
1	D	196	ILE	5.9
1	B	85	LEU	5.9
1	B	160	THR	5.9
1	B	134	ARG	5.9
1	B	53	LYS	5.9
1	D	53	LYS	5.9
1	C	9	PHE	5.9
1	C	6	TYR	5.8
1	B	69	PRO	5.8
1	B	135	ARG	5.8
1	C	56	ARG	5.8
1	D	39	PRO	5.8
1	D	381	THR	5.8
1	C	8	LEU	5.8
1	C	55	LEU	5.8
1	A	346[A]	ILE	5.8
1	C	22	TRP	5.8
1	B	46	GLU	5.7
1	C	170	GLY	5.7
1	B	54	SER	5.7
1	B	184	ILE	5.7
1	B	334	GLY	5.7
1	A	166	VAL	5.7
1	A	49	ALA	5.7
1	A	119	LEU	5.7
1	B	137	PHE	5.7
1	C	137	PHE	5.7
1	A	69	PRO	5.7
1	B	121	ILE	5.7
1	C	176	VAL	5.7
1	A	199[A]	ILE	5.7
1	D	96	ASP	5.6
1	B	247	LEU	5.6
1	B	262	LEU	5.6
1	D	369	ILE	5.6
1	B	3	ASN	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	386	VAL	5.6
1	B	389	VAL	5.6
1	C	64	LEU	5.6
1	D	190	GLU	5.6
1	B	370	ASN	5.6
1	C	389	VAL	5.6
1	A	146	PRO	5.6
1	A	296	LEU	5.6
1	B	146	PRO	5.6
1	B	231	PHE	5.6
1	D	56	ARG	5.6
1	C	32	GLU	5.6
1	D	382	GLY	5.6
1	C	370	ASN	5.6
1	A	62	TYR	5.6
1	B	33	GLU	5.5
1	B	11	ASP	5.5
1	C	171	GLY	5.5
1	B	26	ASN	5.5
1	D	83	THR	5.5
1	A	205	VAL	5.5
1	B	276	VAL	5.5
1	D	122	THR	5.5
1	D	412	ARG	5.5
1	B	82	PRO	5.5
1	C	119	LEU	5.5
1	C	408	GLU	5.5
1	B	73	ASN	5.5
1	A	263	ARG	5.5
1	B	27[A]	ARG	5.5
1	D	185	ILE	5.5
1	A	186	ALA	5.5
1	A	6	TYR	5.5
1	C	152	LYS	5.5
1	A	191	ILE	5.4
1	B	84	ALA	5.4
1	A	12	VAL	5.4
1	B	156	TYR	5.4
1	A	95	GLU	5.4
1	A	214	GLU	5.4
1	A	311	ILE	5.4
1	B	157	ILE	5.4

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Mol	Chain	Res	Type	RSRZ
1	C	121	ILE	5.4
1	C	237	ILE	5.4
1	A	167	LEU	5.4
1	C	34	LEU	5.4
1	D	106	VAL	5.4
1	A	122	THR	5.4
1	A	138	ALA	5.4
1	B	80	ALA	5.4
1	C	279	LEU	5.4
1	D	64	LEU	5.4
1	B	186	ALA	5.3
1	A	298	LEU	5.3
1	D	181	LEU	5.3
1	D	89	LYS	5.3
1	B	150	ILE	5.3
1	B	192	PRO	5.3
1	C	35	LYS	5.3
1	A	319	THR	5.3
1	B	207	LEU	5.3
1	B	7	GLU	5.3
1	D	50	GLN	5.3
1	A	157	ILE	5.3
1	D	36	LYS	5.3
1	C	15	ALA	5.3
1	C	84	ALA	5.3
1	C	138	ALA	5.3
1	A	64	LEU	5.3
1	B	412	ARG	5.2
1	C	43	GLU	5.2
1	D	154	ILE	5.2
1	D	199[A]	ILE	5.2
1	B	153	ALA	5.2
1	C	299	GLU	5.2
1	A	350	HIS	5.2
1	C	346[A]	ILE	5.2
1	A	126	SER	5.2
1	A	7	GLU	5.2
1	B	294	LEU	5.2
1	D	117	VAL	5.2
1	B	17	TRP	5.2
1	A	181	LEU	5.2
1	B	230	HIS	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	216	VAL	5.2
1	B	61	PRO	5.1
1	B	86	GLU	5.1
1	B	183	TYR	5.1
1	D	226	TRP	5.1
1	B	19	ASP	5.1
1	D	87	LEU	5.1
1	B	65	SER	5.1
1	B	252	GLY	5.1
1	D	9	PHE	5.1
1	B	149	ARG	5.1
1	B	298	LEU	5.1
1	A	50	GLN	5.1
1	C	72	PRO	5.1
1	A	156	TYR	5.1
1	B	56	ARG	5.1
1	B	199[A]	ILE	5.1
1	B	49	ALA	5.1
1	A	98	LEU	5.1
1	A	207	LEU	5.0
1	C	181	LEU	5.0
1	D	171	GLY	5.0
1	A	121	ILE	5.0
1	C	235	ASN	5.0
1	C	248	LEU	5.0
1	C	36	LYS	5.0
1	C	75	PRO	5.0
1	B	91	ALA	5.0
1	D	150	ILE	5.0
1	A	245	CYS	5.0
1	C	375	CYS	5.0
1	C	24	VAL	5.0
1	D	260[A]	VAL	5.0
1	D	45	GLU	5.0
1	D	399	GLY	5.0
1	B	90	ALA	5.0
1	B	315	LEU	5.0
1	C	296	LEU	5.0
1	B	103	ASP	4.9
1	D	126	SER	4.9
1	C	373	PRO	4.9
1	A	22	TRP	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	90	ALA	4.9
1	D	91	ALA	4.9
1	B	180	THR	4.9
1	A	54	SER	4.9
1	B	141	SER	4.9
1	A	76	VAL	4.9
1	B	271	VAL	4.9
1	C	374	GLY	4.9
1	A	73	ASN	4.9
1	C	20	TRP	4.9
1	A	43	GLU	4.9
1	B	174	LEU	4.9
1	C	315	LEU	4.9
1	D	41	THR	4.9
1	B	301	PHE	4.9
1	A	208	PRO	4.9
1	C	383	LYS	4.9
1	B	360	GLY	4.9
1	B	397	GLY	4.9
1	B	329	VAL	4.9
1	D	197	VAL	4.9
1	C	33	GLU	4.8
1	A	8	LEU	4.8
1	A	109	LEU	4.8
1	B	282	ILE	4.8
1	A	254	PRO	4.8
1	A	399	GLY	4.8
1	C	260[A]	VAL	4.8
1	D	58	ALA	4.8
1	B	109	LEU	4.8
1	B	224	PRO	4.8
1	B	368	PRO	4.8
1	A	260[A]	VAL	4.8
1	A	79	GLN	4.8
1	B	25	ARG	4.8
1	B	373	PRO	4.8
1	C	89	LYS	4.8
1	B	122	THR	4.8
1	A	150	ILE	4.7
1	C	154	ILE	4.7
1	D	311	ILE	4.7
1	B	72	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	332	PRO	4.7
1	B	281	LYS	4.7
1	D	280	VAL	4.7
1	B	349	SER	4.7
1	C	376	ASN	4.7
1	D	229	THR	4.7
1	D	362	ILE	4.7
1	A	82	PRO	4.7
1	D	27[A]	ARG	4.7
1	D	379	VAL	4.7
1	C	46	GLU	4.7
1	B	232	ASN	4.7
1	D	88	ASN	4.7
1	C	66	LEU	4.7
1	D	294	LEU	4.7
1	C	4	ARG	4.7
1	C	252	GLY	4.7
1	A	352	LYS	4.7
1	B	70	ASN	4.7
1	A	212	THR	4.7
1	A	300	HIS	4.7
1	D	11	ASP	4.7
1	D	301	PHE	4.6
1	A	24	VAL	4.6
1	C	379	VAL	4.6
1	D	78	LYS	4.6
1	A	67	ILE	4.6
1	A	29	GLU	4.6
1	D	142	ASP	4.6
1	D	143	ASP	4.6
1	D	130	ARG	4.6
1	A	60	THR	4.6
1	A	110	THR	4.6
1	B	200	GLY	4.6
1	C	139	GLY	4.6
1	A	94	LEU	4.6
1	A	402	LEU	4.6
1	D	148	GLU	4.6
1	A	27[A]	ARG	4.6
1	A	137	PHE	4.6
1	C	144	SER	4.6
1	A	83	THR	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	41	THR	4.6
1	D	22	TRP	4.6
1	B	97	PRO	4.6
1	C	87	LEU	4.6
1	A	159	ASN	4.6
1	D	86	GLU	4.5
1	A	197	VAL	4.5
1	A	171	GLY	4.5
1	B	20	TRP	4.5
1	C	17	TRP	4.5
1	B	378	ASP	4.5
1	A	63	TYR	4.5
1	B	275	LEU	4.5
1	C	402	LEU	4.5
1	B	278	LYS	4.5
1	B	144	SER	4.5
1	C	301	PHE	4.5
1	C	212	THR	4.5
1	A	389	VAL	4.5
1	B	305	VAL	4.5
1	B	51	CYS	4.5
1	C	204	PRO	4.5
1	B	168	LEU	4.5
1	B	36	LYS	4.5
1	A	44	GLU	4.5
1	A	30	THR	4.5
1	B	133	THR	4.5
1	C	133	THR	4.5
1	A	334	GLY	4.5
1	C	360	GLY	4.5
1	B	166	VAL	4.5
1	B	206	VAL	4.5
1	B	265	VAL	4.5
1	B	244	ALA	4.5
1	B	255	LEU	4.5
1	A	371	TYR	4.5
1	B	287	TYR	4.5
1	A	237	ILE	4.5
1	C	150	ILE	4.5
1	D	32	GLU	4.5
1	D	121	ILE	4.5
1	C	27[A]	ARG	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	68	ASP	4.5
1	B	381	THR	4.5
1	C	151	ASP	4.5
1	B	171	GLY	4.5
1	C	264	GLY	4.5
1	A	107	PRO	4.5
1	C	92	ALA	4.5
1	A	343	ASN	4.5
1	C	94	LEU	4.5
1	C	131	HIS	4.5
1	D	129	CYS	4.5
1	D	296	LEU	4.5
1	D	376	ASN	4.5
1	A	226	TRP	4.4
1	B	297	GLY	4.4
1	C	106	VAL	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	A	196	ILE	4.4
1	A	17	TRP	4.4
1	A	382	GLY	4.4
1	B	43	GLU	4.4
1	D	24	VAL	4.4
1	C	130	ARG	4.4
1	D	402	LEU	4.4
1	C	50	GLN	4.4
1	B	187	LYS	4.4
1	A	160	THR	4.4
1	A	135	ARG	4.4
1	A	243[A]	ARG	4.4
1	C	109	LEU	4.4
1	D	94	LEU	4.4
1	A	411	LYS	4.4
1	A	309	ILE	4.4
1	C	157	ILE	4.4
1	B	62	TYR	4.3
1	C	113	TYR	4.3
1	B	170	GLY	4.3
1	C	41	THR	4.3
1	C	382	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	20	TRP	4.3
1	B	158	ARG	4.3
1	B	376	ASN	4.3
1	A	39	PRO	4.3
1	A	224	PRO	4.3
1	D	251	ALA	4.3
1	B	42	LYS	4.3
1	C	125	CYS	4.3
1	B	191	ILE	4.3
1	D	157	ILE	4.3
1	A	133	THR	4.3
1	B	21	ARG	4.3
1	C	3	ASN	4.3
1	A	35	LYS	4.3
1	A	153	ALA	4.3
1	B	104	SER	4.3
1	B	194	VAL	4.3
1	C	205	VAL	4.3
1	B	274	GLU	4.3
1	D	377	CYS	4.3
1	D	28	ILE	4.3
1	A	297	GLY	4.3
1	D	156	TYR	4.3
1	C	13	SER	4.3
1	B	331	ALA	4.3
1	D	244	ALA	4.3
1	A	194	VAL	4.3
1	A	248	LEU	4.3
1	C	276	VAL	4.3
1	C	211	ILE	4.3
1	D	217	ASN	4.3
1	D	319	THR	4.3
1	D	10	LYS	4.3
1	B	195	GLU	4.3
1	B	299	GLU	4.3
1	C	80	ALA	4.2
1	A	136	ARG	4.2
1	D	389	VAL	4.2
1	A	200	GLY	4.2
1	C	311	ILE	4.2
1	A	33	GLU	4.2
1	B	45	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	69	PRO	4.2
1	C	126	SER	4.2
1	B	243	ARG	4.2
1	A	80	ALA	4.2
1	D	206	VAL	4.2
1	D	386	VAL	4.2
1	B	384	LYS	4.2
1	B	190	GLU	4.2
1	D	155	ASP	4.2
1	A	230	HIS	4.2
1	B	280	VAL	4.2
1	C	410	ASN	4.2
1	B	108	GLY	4.2
1	D	363	THR	4.2
1	D	141	SER	4.2
1	C	63	TYR	4.2
1	A	45	GLU	4.2
1	A	86	GLU	4.2
1	C	206	VAL	4.2
1	D	110	THR	4.1
1	A	349	SER	4.1
1	A	111	HIS	4.1
1	C	258	GLN	4.1
1	C	88	ASN	4.1
1	D	222	TYR	4.1
1	B	219	LEU	4.1
1	D	17	TRP	4.1
1	B	286	PRO	4.1
1	D	107	PRO	4.1
1	A	70	ASN	4.1
1	A	376	ASN	4.1
1	A	244	ALA	4.1
1	A	322	TYR	4.1
1	B	120	LEU	4.1
1	B	279	LEU	4.1
1	D	85	LEU	4.1
1	D	207	LEU	4.1
1	D	365	TYR	4.1
1	C	231	PHE	4.1
1	C	329	VAL	4.1
1	B	142	ASP	4.1
1	C	362	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	191	ILE	4.1
1	B	253	VAL	4.1
1	B	411	LYS	4.1
1	C	91	ALA	4.0
1	D	173	ALA	4.0
1	A	262	LEU	4.0
1	D	221	LYS	4.0
1	D	411	LYS	4.0
1	A	163	VAL	4.0
1	A	358	PHE	4.0
1	B	367	GLU	4.0
1	A	3	ASN	4.0
1	A	375	CYS	4.0
1	B	217	ASN	4.0
1	B	380	CYS	4.0
1	C	29	GLU	4.0
1	C	86	GLU	4.0
1	C	247	LEU	4.0
1	D	100	GLU	4.0
1	D	119	LEU	4.0
1	A	104	SER	4.0
1	B	212	THR	4.0
1	C	322	TYR	4.0
1	D	37	TYR	4.0
1	D	62	TYR	4.0
1	D	82	PRO	4.0
1	A	26	ASN	4.0
1	A	139	GLY	4.0
1	A	172	ASP	4.0
1	A	378	ASP	4.0
1	C	115	ASP	4.0
1	A	149	ARG	4.0
1	A	407	LEU	4.0
1	B	372	THR	4.0
1	D	6	TYR	4.0
1	D	3	ASN	4.0
1	A	154	ILE	4.0
1	A	36	LYS	4.0
1	C	78	LYS	4.0
1	C	129	CYS	4.0
1	A	190	GLU	4.0
1	B	151	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	374	GLY	4.0
1	C	134	ARG	4.0
1	D	25	ARG	4.0
1	B	248	LEU	3.9
1	D	8	LEU	3.9
1	C	141	SER	3.9
1	C	229	THR	3.9
1	A	269	VAL	3.9
1	A	353	VAL	3.9
1	A	379	VAL	3.9
1	C	197	VAL	3.9
1	B	266	ASN	3.9
1	C	224	PRO	3.9
1	B	383	LYS	3.9
1	C	209	GLN	3.9
1	A	240	GLU	3.9
1	B	354	ILE	3.9
1	B	285	ARG	3.9
1	C	316[A]	ARG	3.9
1	B	394	LEU	3.9
1	C	98	LEU	3.9
1	C	207	LEU	3.9
1	C	255	LEU	3.9
1	D	174	LEU	3.9
1	D	30	THR	3.9
1	D	372	THR	3.9
1	C	76	VAL	3.9
1	B	78	LYS	3.9
1	C	39	PRO	3.9
1	C	146	PRO	3.9
1	D	7	GLU	3.9
1	B	131	HIS	3.9
1	C	354	ILE	3.9
1	C	19	ASP	3.9
1	B	375	CYS	3.9
1	B	167	LEU	3.9
1	C	215	LEU	3.9
1	B	235	ASN	3.9
1	C	266	ASN	3.9
1	A	383	LYS	3.9
1	A	97	PRO	3.9
1	B	106	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	225	VAL	3.9
1	C	230	HIS	3.9
1	C	71	ASP	3.9
1	D	170	GLY	3.9
1	B	348	GLN	3.9
1	C	398	GLU	3.9
1	A	373	PRO	3.9
1	B	107	PRO	3.9
1	A	253	VAL	3.8
1	B	353	VAL	3.8
1	B	379	VAL	3.8
1	A	327	PHE	3.8
1	B	16	ASP	3.8
1	B	123	ASP	3.8
1	B	351	ASP	3.8
1	C	314	GLY	3.8
1	D	59	ILE	3.8
1	C	45	GLU	3.8
1	D	152	LYS	3.8
1	A	247	LEU	3.8
1	A	275	LEU	3.8
1	A	285[A]	ARG	3.8
1	C	407	LEU	3.8
1	A	213	PRO	3.8
1	D	99	HIS	3.8
1	A	276	VAL	3.8
1	C	345	VAL	3.8
1	C	378	ASP	3.8
1	A	390	GLY	3.8
1	A	385	LYS	3.8
1	D	42	LYS	3.8
1	C	201	SER	3.8
1	C	202	ARG	3.8
1	A	227	LEU	3.8
1	A	255	LEU	3.8
1	D	175	LEU	3.8
1	C	61	PRO	3.8
1	C	82	PRO	3.8
1	A	96	ASP	3.8
1	B	340	VAL	3.8
1	B	382	GLY	3.8
1	C	337	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	312	ILE	3.8
1	A	287	TYR	3.8
1	B	222	TYR	3.8
1	B	228	ASN	3.8
1	B	277	ASN	3.8
1	B	173	ALA	3.8
1	D	401	ALA	3.8
1	D	61	PRO	3.8
1	D	75	PRO	3.8
1	A	225	VAL	3.8
1	A	367	GLU	3.8
1	B	328	VAL	3.8
1	C	140	GLN	3.8
1	C	335	GLY	3.8
1	A	131	HIS	3.7
1	C	387	HIS	3.7
1	B	60	THR	3.7
1	C	83	THR	3.7
1	B	118	LEU	3.7
1	C	85	LEU	3.7
1	A	398	GLU	3.7
1	C	214	GLU	3.7
1	B	162	GLN	3.7
1	B	302	ARG	3.7
1	B	205	VAL	3.7
1	B	196	ILE	3.7
1	D	282	ILE	3.7
1	B	226	TRP	3.7
1	B	110	THR	3.7
1	C	60	THR	3.7
1	A	132	CYS	3.7
1	C	68	ASP	3.7
1	C	120	LEU	3.7
1	C	172	ASP	3.7
1	C	292	CYS	3.7
1	D	403	GLU	3.7
1	A	286	PRO	3.7
1	C	136	ARG	3.7
1	C	404	PRO	3.7
1	D	136	ARG	3.7
1	D	176	VAL	3.7
1	A	295	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	366	SER	3.7
1	D	137	PHE	3.7
1	C	67	ILE	3.7
1	C	199[A]	ILE	3.7
1	A	78	LYS	3.7
1	B	15	ALA	3.7
1	D	138	ALA	3.7
1	A	189	ARG	3.7
1	B	112	ARG	3.7
1	D	158	ARG	3.7
1	A	118	LEU	3.7
1	A	348	GLN	3.7
1	C	262	LEU	3.7
1	C	217	ASN	3.7
1	B	284	VAL	3.7
1	B	345	VAL	3.7
1	C	340	VAL	3.7
1	C	282	ILE	3.7
1	C	14	ASP	3.7
1	B	251	ALA	3.7
1	C	377	CYS	3.6
1	D	349	SER	3.6
1	A	81	ILE	3.6
1	B	74	ASP	3.6
1	C	142	ASP	3.6
1	D	160	THR	3.6
1	A	72	PRO	3.6
1	B	215[A]	LEU	3.6
1	D	98	LEU	3.6
1	D	407	LEU	3.6
1	D	73	ASN	3.6
1	B	29	GLU	3.6
1	A	176	VAL	3.6
1	D	12	VAL	3.6
1	A	19	ASP	3.6
1	A	184	ILE	3.6
1	B	67	ILE	3.6
1	A	105	PRO	3.6
1	B	188	LEU	3.6
1	D	298	LEU	3.6
1	A	183	TYR	3.6
1	A	222	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	132	CYS	3.6
1	B	233	HIS	3.6
1	A	32	GLU	3.6
1	A	169	SER	3.6
1	C	278	LYS	3.6
1	D	320	SER	3.6
1	A	155	ASP	3.6
1	C	117	VAL	3.6
1	C	163	VAL	3.6
1	D	178	ASP	3.6
1	B	237	ILE	3.6
1	C	174	LEU	3.6
1	D	255	LEU	3.6
1	A	88	ASN	3.6
1	A	387	HIS	3.6
1	C	228	ASN	3.6
1	A	170	GLY	3.6
1	A	360	GLY	3.6
1	A	11	ASP	3.5
1	D	172	ASP	3.5
1	D	194	VAL	3.5
1	C	122	THR	3.5
1	D	67	ILE	3.5
1	B	387	HIS	3.5
1	C	105	PRO	3.5
1	A	13	SER	3.5
1	D	169	SER	3.5
1	D	151	ASP	3.5
1	A	329	VAL	3.5
1	A	299	GLU	3.5
1	A	408	GLU	3.5
1	B	214	GLU	3.5
1	C	44	GLU	3.5
1	C	77	ARG	3.5
1	A	211	ILE	3.5
1	B	327	PHE	3.5
1	A	114	PRO	3.5
1	B	213	PRO	3.5
1	D	373	PRO	3.5
1	D	247	LEU	3.5
1	A	333	GLY	3.5
1	D	333	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	172	ASP	3.5
1	B	245	CYS	3.5
1	B	148	GLU	3.5
1	B	164	ARG	3.5
1	A	216	VAL	3.5
1	A	271	VAL	3.5
1	B	391	VAL	3.5
1	D	205	VAL	3.5
1	A	246	GLN	3.5
1	C	277	ASN	3.5
1	A	279	LEU	3.5
1	A	294	LEU	3.5
1	A	393	GLY	3.5
1	D	295	SER	3.5
1	B	330	ASP	3.5
1	D	330	ASP	3.5
1	A	164	ARG	3.5
1	B	310	GLU	3.5
1	B	371	TYR	3.5
1	B	408	GLU	3.5
1	D	322	TYR	3.5
1	A	220	LYS	3.5
1	D	350	HIS	3.5
1	A	284	VAL	3.5
1	B	386	VAL	3.5
1	C	353	VAL	3.5
1	A	102	THR	3.5
1	A	75	PRO	3.4
1	B	114	PRO	3.4
1	A	142	ASP	3.4
1	C	189	ARG	3.4
1	A	187	LYS	3.4
1	B	216	VAL	3.4
1	C	242	THR	3.4
1	C	386	VAL	3.4
1	A	330	ASP	3.4
1	C	298	LEU	3.4
1	D	66	LEU	3.4
1	D	44	GLU	3.4
1	A	388	LYS	3.4
1	D	246	GLN	3.4
1	A	61	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	68	ASP	3.4
1	D	200	GLY	3.4
1	D	374	GLY	3.4
1	C	49	ALA	3.4
1	C	173	ALA	3.4
1	C	355	LEU	3.4
1	C	268	CYS	3.4
1	A	41	THR	3.4
1	B	113	TYR	3.4
1	D	60	THR	3.4
1	A	77	ARG	3.4
1	C	25	ARG	3.4
1	D	274	GLU	3.4
1	D	353	VAL	3.4
1	A	374	GLY	3.4
1	B	169	SER	3.4
1	D	16	ASP	3.4
1	D	97	PRO	3.4
1	D	259	SER	3.4
1	A	152	LYS	3.4
1	A	173	ALA	3.4
1	A	168	LEU	3.4
1	A	215	LEU	3.4
1	B	358	PHE	3.4
1	B	257	ASN	3.3
1	B	268	CYS	3.3
1	A	4	ARG	3.3
1	A	100	GLU	3.3
1	D	95	GLU	3.3
1	C	261	LEU	3.3
1	D	395	LEU	3.3
1	C	5[A]	ARG	3.3
1	C	238	THR	3.3
1	B	241	SER	3.3
1	D	144	SER	3.3
1	B	325	PRO	3.3
1	C	23	GLN	3.3
1	D	368	PRO	3.3
1	A	290	TYR	3.3
1	B	361	VAL	3.3
1	D	163	VAL	3.3
1	D	329	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	282	ILE	3.3
1	C	233	HIS	3.3
1	A	175	LEU	3.3
1	A	410	ASN	3.3
1	B	198	ARG	3.3
1	C	42	LYS	3.3
1	A	14	ASP	3.3
1	B	125	CYS	3.3
1	B	326	THR	3.3
1	C	381	THR	3.3
1	A	252	GLY	3.3
1	A	264	GLY	3.3
1	D	114	PRO	3.3
1	D	183	TYR	3.3
1	B	362	ILE	3.3
1	C	196	ILE	3.3
1	B	189	ARG	3.3
1	D	149	ARG	3.3
1	C	148	GLU	3.3
1	B	96	ASP	3.3
1	A	229	THR	3.2
1	B	363	THR	3.2
1	A	129	CYS	3.2
1	B	350	HIS	3.2
1	A	134	ARG	3.2
1	D	164	ARG	3.2
1	C	28	ILE	3.2
1	D	168	LEU	3.2
1	D	188	LEU	3.2
1	A	103	ASP	3.2
1	A	178	ASP	3.2
1	A	381	THR	3.2
1	A	256	GLY	3.2
1	C	321	GLY	3.2
1	A	130	ARG	3.2
1	B	136	ARG	3.2
1	B	210	ARG	3.2
1	B	234	PRO	3.2
1	C	182	GLU	3.2
1	D	214	GLU	3.2
1	A	257	ASN	3.2
1	D	220	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	183	TYR	3.2
1	C	275	LEU	3.2
1	C	112	ARG	3.2
1	D	303	THR	3.2
1	B	182	GLU	3.2
1	C	107	PRO	3.2
1	C	339	PRO	3.2
1	D	195	GLU	3.2
1	A	221	LYS	3.2
1	C	18	ASN	3.2
1	C	26	ASN	3.2
1	D	277	ASN	3.2
1	A	58	ALA	3.2
1	B	261	LEU	3.2
1	B	365	TYR	3.2
1	A	231	PHE	3.2
1	B	263	ARG	3.2
1	B	316[A]	ARG	3.2
1	A	182	GLU	3.2
1	A	363	THR	3.2
1	C	200	GLY	3.2
1	B	220	LYS	3.2
1	B	18	ASN	3.2
1	B	377	CYS	3.2
1	C	70	ASN	3.2
1	D	257	ASN	3.2
1	B	23	GLN	3.2
1	D	140	GLN	3.2
1	B	269	VAL	3.1
1	A	59	ILE	3.1
1	D	167	LEU	3.1
1	D	211	ILE	3.1
1	D	250	ASP	3.1
1	A	5[A]	ARG	3.1
1	C	283	ARG	3.1
1	D	287	TYR	3.1
1	B	152	LYS	3.1
1	B	352	LYS	3.1
1	C	208	PRO	3.1
1	B	209	GLN	3.1
1	D	380	CYS	3.1
1	A	202	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	405	VAL	3.1
1	C	263	ARG	3.1
1	C	219	LEU	3.1
1	D	193	HIS	3.1
1	C	371	TYR	3.1
1	D	281	LYS	3.1
1	C	203	THR	3.1
1	B	79	GLN	3.1
1	C	114	PRO	3.1
1	D	72	PRO	3.1
1	B	130	ARG	3.1
1	A	143	ASP	3.1
1	B	197	VAL	3.1
1	B	236	GLU	3.1
1	A	219	LEU	3.1
1	D	109	LEU	3.1
1	D	118	LEU	3.1
1	B	346[A]	ILE	3.1
1	B	295	SER	3.1
1	D	13	SER	3.1
1	A	113	TYR	3.1
1	A	288	TYR	3.1
1	C	393	GLY	3.1
1	D	393	GLY	3.1
1	B	238	THR	3.1
1	D	204	PRO	3.1
1	D	404	PRO	3.1
1	D	134	ARG	3.1
1	A	99	HIS	3.1
1	A	265	VAL	3.1
1	C	352	LYS	3.1
1	B	185	ILE	3.1
1	B	344	TYR	3.0
1	A	372	THR	3.0
1	B	410	ASN	3.0
1	C	396	ASN	3.0
1	D	26	ASN	3.0
1	A	301	PHE	3.0
1	A	101	ASP	3.0
1	C	351	ASP	3.0
1	A	324	VAL	3.0
1	D	76	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	328	VAL	3.0
1	B	314	GLY	3.0
1	B	335	GLY	3.0
1	C	290	TYR	3.0
1	C	332	PRO	3.0
1	C	293	ASP	3.0
1	D	293	ASP	3.0
1	D	351	ASP	3.0
1	C	411	LYS	3.0
1	A	251	ALA	3.0
1	C	394	LEU	3.0
1	D	391	VAL	3.0
1	B	283	ARG	3.0
1	D	346[A]	ILE	3.0
1	C	334	GLY	3.0
1	D	321	GLY	3.0
1	A	180	THR	3.0
1	C	363	THR	3.0
1	D	304	PRO	3.0
1	C	156	TYR	3.0
1	C	384	LYS	3.0
1	A	23	GLN	3.0
1	C	79	GLN	3.0
1	B	249	ALA	3.0
1	B	401	ALA	3.0
1	D	4	ARG	3.0
1	D	15	ALA	3.0
1	D	77	ARG	3.0
1	A	377	CYS	3.0
1	A	217	ASN	3.0
1	B	179	GLU	3.0
1	C	185	ILE	3.0
1	B	204	PRO	3.0
1	D	14	ASP	3.0
1	C	100	GLU	2.9
1	C	186	ALA	2.9
1	D	186	ALA	2.9
1	D	219	LEU	2.9
1	D	370	ASN	2.9
1	D	216	VAL	2.9
1	A	108	GLY	2.9
1	C	184	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	309	ILE	2.9
1	B	337	LYS	2.9
1	A	203	THR	2.9
1	B	71	ASP	2.9
1	D	233	HIS	2.9
1	D	21	ARG	2.9
1	D	285[A]	ARG	2.9
1	D	231	PHE	2.9
1	D	367	GLU	2.9
1	A	401	ALA	2.9
1	B	159	ASN	2.9
1	A	384	LYS	2.9
1	D	352	LYS	2.9
1	A	193	HIS	2.9
1	C	250	ASP	2.9
1	D	101	ASP	2.9
1	D	238	THR	2.9
1	A	161	PRO	2.9
1	A	144	SER	2.9
1	A	273	LYS	2.9
1	A	278	LYS	2.9
1	D	273	LYS	2.9
1	C	294	LEU	2.9
1	C	123	ASP	2.9
1	D	230	HIS	2.9
1	C	284	VAL	2.9
1	B	312	ILE	2.9
1	C	149	ARG	2.9
1	C	97	PRO	2.9
1	B	240	GLU	2.9
1	C	295	SER	2.9
1	C	251	ALA	2.9
1	D	139	GLY	2.9
1	A	140	GLN	2.8
1	C	162	GLN	2.8
1	C	188	LEU	2.8
1	D	315	LEU	2.8
1	A	391	VAL	2.8
1	D	340	VAL	2.8
1	B	319	THR	2.8
1	C	364	THR	2.8
1	C	372	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	81	ILE	2.8
1	A	234	PRO	2.8
1	C	254	PRO	2.8
1	C	304	PRO	2.8
1	D	325	PRO	2.8
1	D	187	LYS	2.8
1	A	228	ASN	2.8
1	A	370	ASN	2.8
1	C	343	ASN	2.8
1	D	104	SER	2.8
1	B	308	GLY	2.8
1	B	355	LEU	2.8
1	D	355	LEU	2.8
1	D	133	THR	2.8
1	D	234	PRO	2.8
1	A	210	ARG	2.8
1	A	302	ARG	2.8
1	B	409	ARG	2.8
1	C	158	ARG	2.8
1	C	246	GLN	2.8
1	D	23	GLN	2.8
1	D	223	HIS	2.8
1	A	151	ASP	2.8
1	B	290	TYR	2.8
1	A	261	LEU	2.8
1	A	394	LEU	2.8
1	A	125	CYS	2.8
1	B	323	CYS	2.8
1	C	405	VAL	2.8
1	D	20	TRP	2.8
1	D	271	VAL	2.8
1	A	281	LYS	2.8
1	B	177	SER	2.8
1	B	291	GLN	2.8
1	C	143	ASP	2.8
1	C	267	ASP	2.8
1	C	367	GLU	2.8
1	A	321	GLY	2.8
1	D	256	GLY	2.8
1	B	288	TYR	2.8
1	C	288	TYR	2.8
1	D	113	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	192	PRO	2.8
1	D	105	PRO	2.8
1	A	106	VAL	2.8
1	D	276	VAL	2.8
1	D	237	ILE	2.8
1	A	396	ASN	2.7
1	B	201	SER	2.7
1	C	190	GLU	2.7
1	D	290	TYR	2.7
1	B	202	ARG	2.7
1	C	368	PRO	2.7
1	D	192	PRO	2.7
1	B	117	VAL	2.7
1	B	163	VAL	2.7
1	C	159	ASN	2.7
1	C	245	CYS	2.7
1	D	125	CYS	2.7
1	B	320	SER	2.7
1	A	397	GLY	2.7
1	B	321	GLY	2.7
1	A	392	ALA	2.7
1	C	135	ARG	2.7
1	C	227	LEU	2.7
1	D	135	ARG	2.7
1	D	409	ARG	2.7
1	C	319	THR	2.7
1	D	180	THR	2.7
1	B	404	PRO	2.7
1	C	280	VAL	2.7
1	C	155	ASP	2.7
1	D	93	ASP	2.7
1	A	198	ARG	2.7
1	C	302	ARG	2.7
1	C	327	PHE	2.7
1	A	238	THR	2.7
1	D	242	THR	2.7
1	C	179	GLU	2.7
1	D	70	ASN	2.7
1	A	185	ILE	2.7
1	C	265	VAL	2.7
1	B	273	LYS	2.7
1	A	359	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	223	HIS	2.6
1	B	395	LEU	2.6
1	B	407	LEU	2.6
1	D	300	HIS	2.6
1	D	410	ASN	2.6
1	B	322	TYR	2.6
1	C	330	ASP	2.6
1	A	405	VAL	2.6
1	B	311	ILE	2.6
1	D	225	VAL	2.6
1	C	180	THR	2.6
1	D	159	ASN	2.6
1	B	208	PRO	2.6
1	D	248	LEU	2.6
1	B	115	ASP	2.6
1	B	385	LYS	2.6
1	D	189	ARG	2.6
1	C	132	CYS	2.6
1	D	299	GLU	2.6
1	B	300	HIS	2.6
1	C	300	HIS	2.6
1	A	235	ASN	2.6
1	D	235	ASN	2.6
1	A	328	VAL	2.6
1	A	345	VAL	2.6
1	C	194	VAL	2.6
1	C	365	TYR	2.6
1	D	288	TYR	2.6
1	C	236	GLU	2.6
1	D	337	LYS	2.6
1	A	112	ARG	2.6
1	C	93	ASP	2.6
1	C	213	PRO	2.6
1	D	263	ARG	2.6
1	C	167	LEU	2.6
1	D	262	LEU	2.6
1	D	358	PHE	2.5
1	A	340	VAL	2.5
1	B	129	CYS	2.5
1	A	18	ASN	2.5
1	D	383	LYS	2.5
1	A	21	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	303	THR	2.5
1	B	303	THR	2.5
1	D	74	ASP	2.5
1	D	326	THR	2.5
1	C	259	SER	2.5
1	C	168	LEU	2.5
1	C	269	VAL	2.5
1	D	166	VAL	2.5
1	D	264	GLY	2.5
1	D	324	VAL	2.5
1	D	361	VAL	2.5
1	A	233	HIS	2.5
1	D	131	HIS	2.5
1	A	337	LYS	2.5
1	A	365	TYR	2.5
1	C	210	ARG	2.5
1	B	267	ASP	2.5
1	B	293	ASP	2.5
1	B	242	THR	2.5
1	A	15	ALA	2.5
1	C	331	ALA	2.5
1	C	349	SER	2.5
1	D	275	LEU	2.5
1	D	279	LEU	2.5
1	A	42	LYS	2.5
1	D	397	GLY	2.5
1	A	361	VAL	2.5
1	C	285[A]	ARG	2.5
1	D	269	VAL	2.5
1	D	289	ILE	2.5
1	B	357	ASN	2.5
1	D	343	ASN	2.5
1	D	63	TYR	2.5
1	C	16	ASP	2.5
1	A	241	SER	2.5
1	B	259	SER	2.5
1	D	347	SER	2.5
1	A	249	ALA	2.5
1	A	331	ALA	2.5
1	D	80	ALA	2.5
1	C	164	ARG	2.5
1	C	318	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	343	ASN	2.5
1	D	239	GLU	2.4
1	A	323	CYS	2.4
1	C	338	THR	2.4
1	C	249	ALA	2.4
1	D	331	ALA	2.4
1	B	221	LYS	2.4
1	A	25	ARG	2.4
1	D	198	ARG	2.4
1	A	336	GLY	2.4
1	B	333	GLY	2.4
1	D	360	GLY	2.4
1	D	18	ASN	2.4
1	B	258	GLN	2.4
1	B	178	ASP	2.4
1	C	226	TRP	2.4
1	C	401	ALA	2.4
1	D	385	LYS	2.4
1	B	111	HIS	2.4
1	C	257	ASN	2.4
1	D	123	ASP	2.4
1	B	292	CYS	2.4
1	C	323	CYS	2.4
1	A	344	TYR	2.4
1	C	344	TYR	2.4
1	A	315	LEU	2.4
1	D	227	LEU	2.4
1	C	232	ASN	2.4
1	D	406	GLY	2.4
1	C	166	VAL	2.4
1	D	184	ILE	2.4
1	A	158	ARG	2.4
1	A	259	SER	2.4
1	C	169	SER	2.4
1	C	350	HIS	2.4
1	C	222	TYR	2.3
1	D	252	GLY	2.3
1	D	335	GLY	2.3
1	C	187	LYS	2.3
1	C	243	ARG	2.3
1	C	271	VAL	2.3
1	C	361	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	201	SER	2.3
1	B	270	HIS	2.3
1	D	387	HIS	2.3
1	B	105	PRO	2.3
1	C	239	GLU	2.3
1	D	146	PRO	2.3
1	D	323	CYS	2.3
1	D	308	GLY	2.3
1	C	99	HIS	2.3
1	A	274	GLU	2.3
1	C	324	VAL	2.3
1	B	102	THR	2.3
1	C	303	THR	2.3
1	D	203	THR	2.3
1	C	392	ALA	2.3
1	A	16	ASP	2.3
1	D	165	ASP	2.3
1	D	261	LEU	2.3
1	A	177	SER	2.3
1	B	193	HIS	2.3
1	B	318	HIS	2.3
1	D	253	VAL	2.3
1	B	161	PRO	2.3
1	C	326	THR	2.3
1	A	165	ASP	2.3
1	C	96	ASP	2.3
1	C	307	LYS	2.3
1	D	378	ASP	2.3
1	B	402	LEU	2.3
1	A	148	GLU	2.2
1	B	359	GLU	2.2
1	C	320	SER	2.2
1	A	289	ILE	2.2
1	D	354	ILE	2.2
1	A	242	THR	2.2
1	A	304	PRO	2.2
1	D	305	VAL	2.2
1	C	198	ARG	2.2
1	D	5[A]	ARG	2.2
1	D	243[A]	ARG	2.2
1	D	316[A]	ARG	2.2
1	B	165	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	74	ASP	2.2
1	A	380	CYS	2.2
1	D	314	GLY	2.2
1	C	395	LEU	2.2
1	A	204	PRO	2.2
1	A	307	LYS	2.2
1	A	325	PRO	2.2
1	A	332	PRO	2.2
1	D	307	LYS	2.2
1	D	345	VAL	2.2
1	B	406	GLY	2.2
1	D	398	GLU	2.2
1	D	394	LEU	2.2
1	A	141	SER	2.2
1	D	278	LYS	2.2
1	A	277	ASN	2.2
1	A	326	THR	2.2
1	A	342	PRO	2.2
1	C	234	PRO	2.2
1	C	286	PRO	2.2
1	D	342	PRO	2.2
1	C	178	ASP	2.2
1	D	71	ASP	2.2
1	C	225	VAL	2.2
1	A	403	GLU	2.2
1	D	408	GLU	2.2
1	A	292	CYS	2.2
1	C	287	TYR	2.2
1	A	232	ASN	2.2
1	B	101	ASP	2.2
1	B	250	ASP	2.2
1	B	364	THR	2.2
1	D	332	PRO	2.1
1	C	274	GLU	2.1
1	C	305	VAL	2.1
1	D	153	ALA	2.1
1	A	116	ARG	2.1
1	D	292	CYS	2.1
1	A	366	SER	2.1
1	C	177	SER	2.1
1	B	396	ASN	2.1
1	D	396	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	155	ASP	2.1
1	C	110	THR	2.1
1	C	342	PRO	2.1
1	C	348	GLN	2.1
1	A	280	VAL	2.1
1	A	335	GLY	2.1
1	B	99	HIS	2.1
1	B	336	GLY	2.1
1	D	249	ALA	2.1
1	D	268	CYS	2.1
1	D	228	ASN	2.1
1	A	93	ASP	2.1
1	B	256	GLY	2.1
1	D	108	GLY	2.1
1	D	215	LEU	2.1
1	D	132	CYS	2.1
1	A	404	PRO	2.1
1	B	339	PRO	2.1
1	C	161	PRO	2.1
1	C	192	PRO	2.1
1	C	223	HIS	2.1
1	B	309	ILE	2.1
1	B	388	LYS	2.1
1	A	201	SER	2.1
1	A	310	GLU	2.0
1	C	101	ASP	2.0
1	D	348	GLN	2.0
1	A	305	VAL	2.0
1	D	291	GLN	2.0
1	A	351	ASP	2.0
1	D	267	ASP	2.0
1	A	356[A]	ARG	2.0
1	A	409	ARG	2.0
1	D	212	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

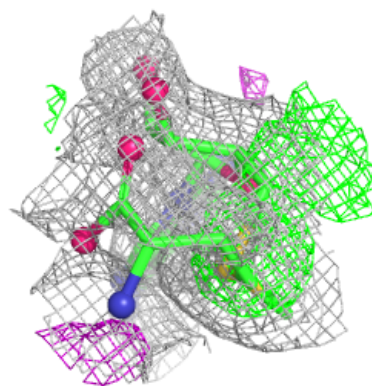
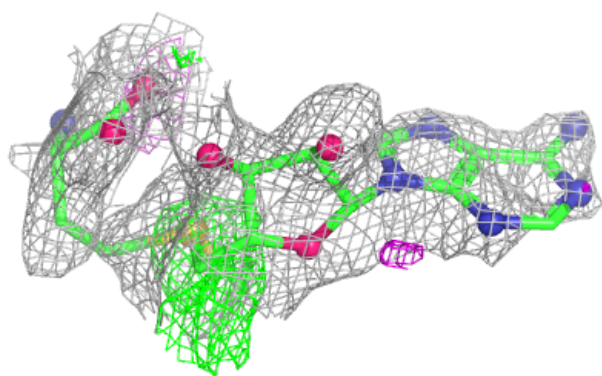
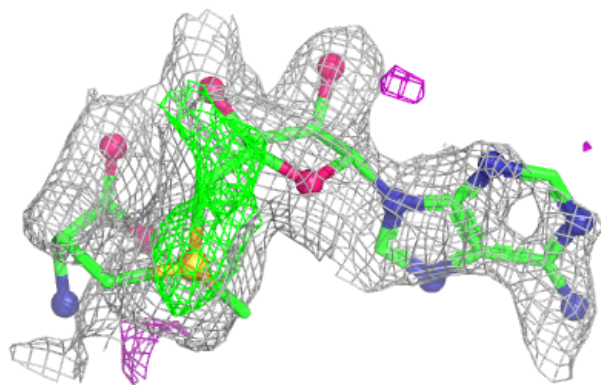
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	C	593	5/5	0.37	0.31	79,80,81,81	0
3	SO4	A	592	5/5	0.48	0.28	98,98,99,99	0
5	LYS	C	420[A]	10/10	0.51	0.28	22,24,27,27	3
5	LYS	C	420[B]	10/10	0.51	0.28	22,24,27,27	3
3	SO4	D	494	5/5	0.55	0.25	88,88,88,89	0
5	LYS	B	420[B]	10/10	0.64	0.30	32,34,39,39	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	C	419	15/16	0.90	0.16	18,24,25,26	0
6	PLP	D	419	15/16	0.90	0.14	20,27,29,30	0
2	ZN	D	421	1/1	0.90	0.08	31,31,31,31	0
7	SF4	D	418	8/8	0.90	0.08	21,22,25,26	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.

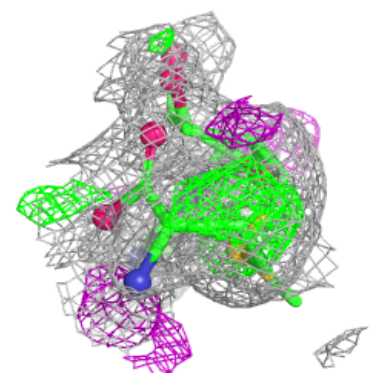
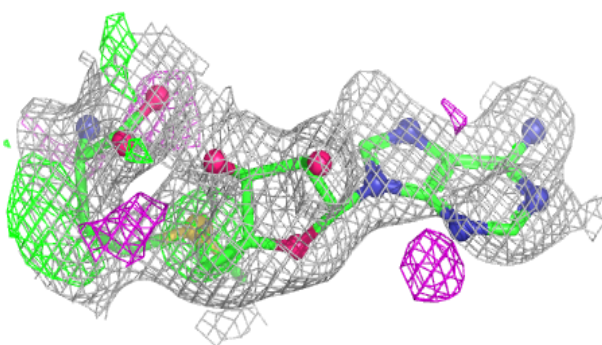
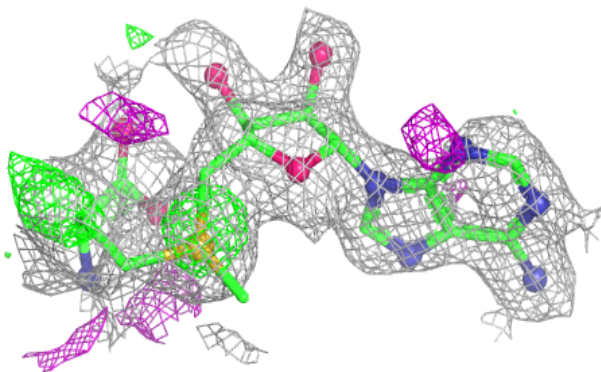
Electron density around SAM B 417:

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



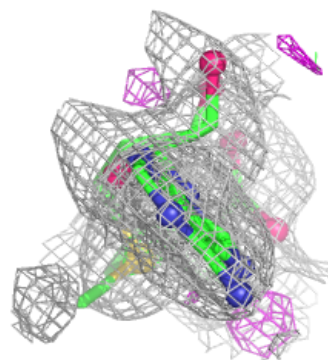
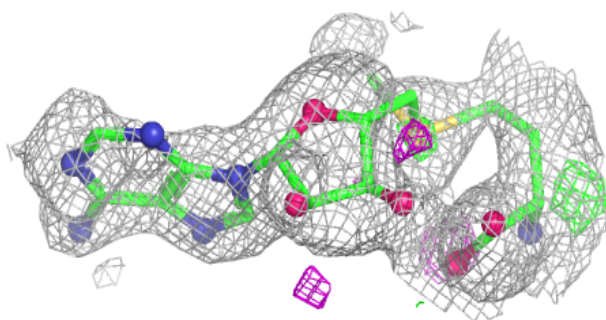
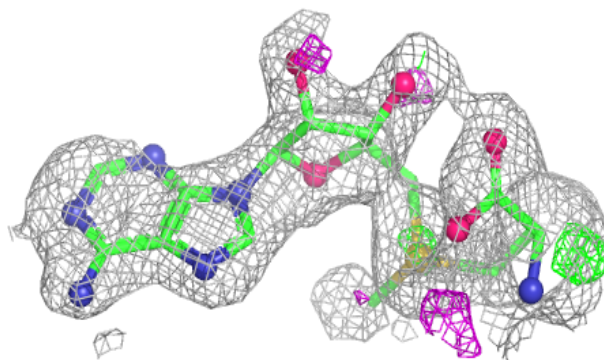
Electron density around SAM D 417:

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

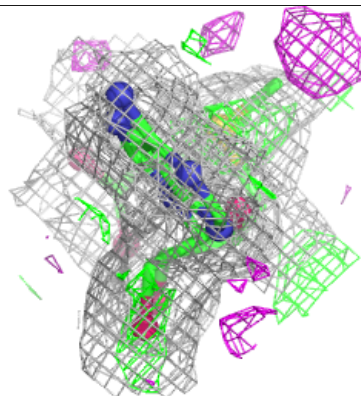
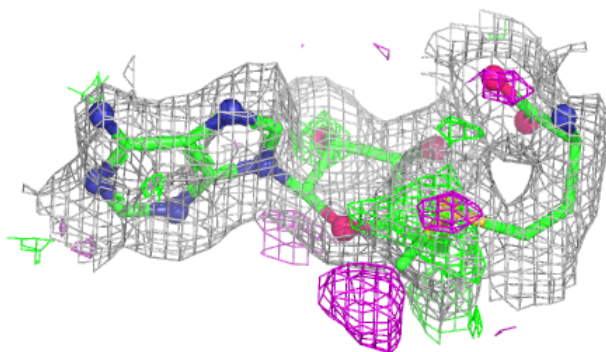
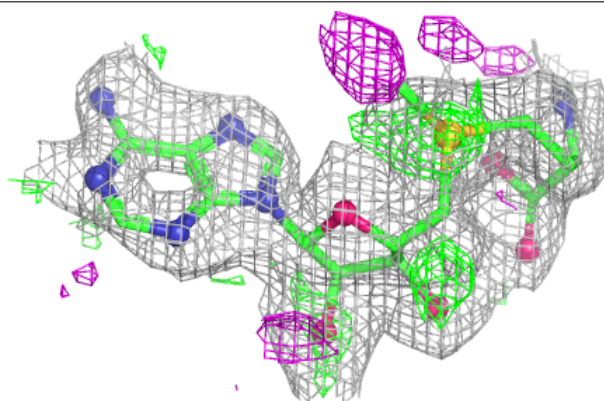


Electron density around SAM A 417:

$2mF_o-DF_c$ (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.