



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 03:31 PM GMT

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

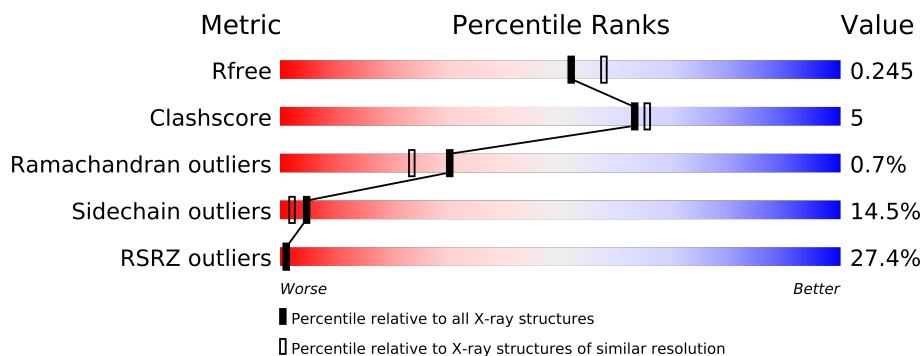
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	416	
1	B	416	
1	C	416	
1	D	416	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	A	592	-	X
3	SO4	B	495	-	X
3	SO4	C	593	-	X
3	SO4	D	494	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	SAM	C	417	-	X
5	LYS	A	420[A]	X	-
5	LYS	A	420[B]	X	-
5	LYS	B	420[A]	X	-
5	LYS	B	420[B]	X	-
5	LYS	C	420[A]	X	-
5	LYS	C	420[B]	X	-
5	LYS	D	420[A]	X	-
5	LYS	D	420[B]	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14034 atoms, of which 0 are hydrogen and 0 are deuterium.

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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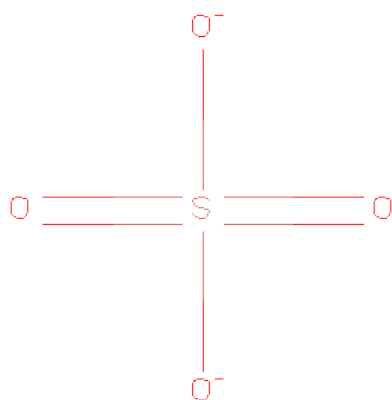
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Chain	Residue	Modelled	Actual	Comment	Reference
C	57	MSE	MET	MODIFIED RESIDUE	GB 5410603
C	124	MSE	MET	MODIFIED RESIDUE	GB 5410603
C	127	MSE	MET	MODIFIED RESIDUE	GB 5410603
C	145	MSE	MET	MODIFIED RESIDUE	GB 5410603
C	147	MSE	MET	MODIFIED RESIDUE	GB 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 (three-letter code: ZN) (formula: Zn).

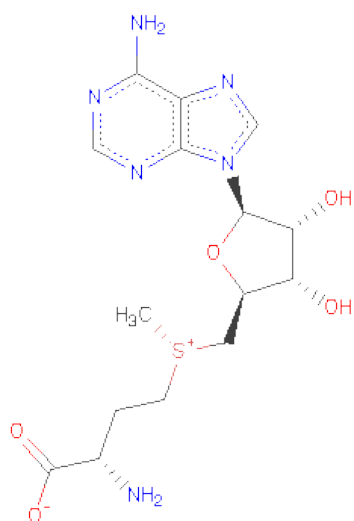
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

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



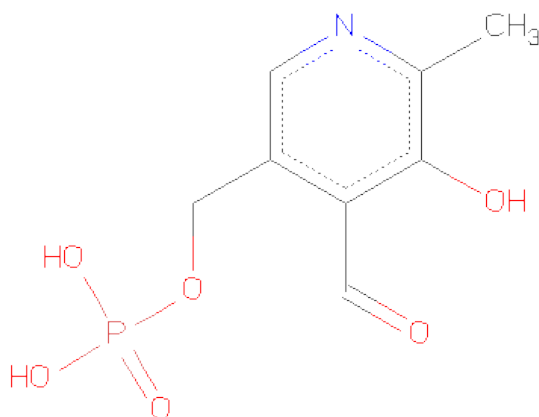
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C₁₅H₂₂N₆O₅S).



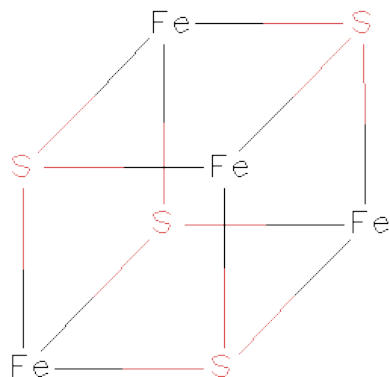
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	D	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 5 is LYSINE (three-letter code: PLP, LYS) (formula: $C_8H_{10}NO_6P$, $C_6H_{15}N_2O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	2	Total	C	N	O	P	0	1
			28	17	3	7	1		
5	B	2	Total	C	N	O	P	0	1
			28	17	3	7	1		
5	C	2	Total	C	N	O	P	0	1
			28	17	3	7	1		
5	D	2	Total	C	N	O	P	0	1
			28	17	3	7	1		

- Molecule 6 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

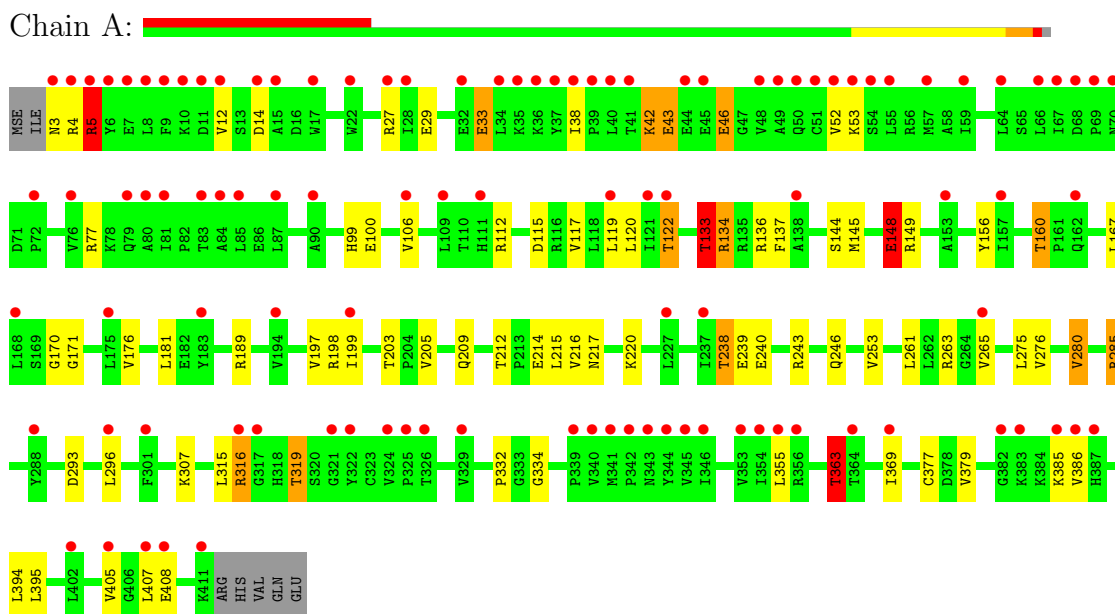
- Molecule 7 is water.

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

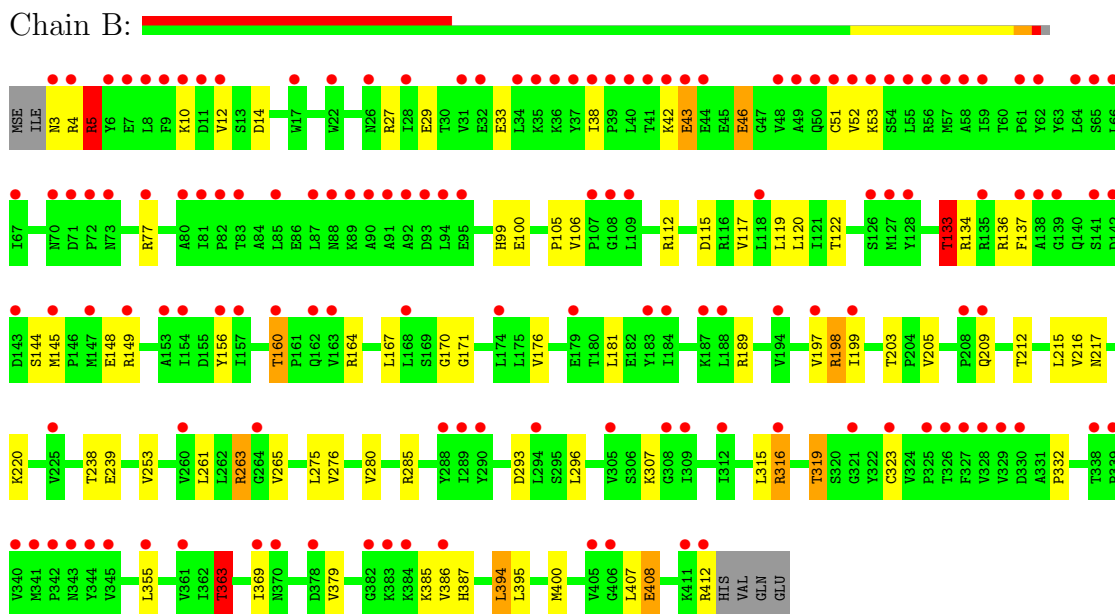
3 Residue-property plots

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

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

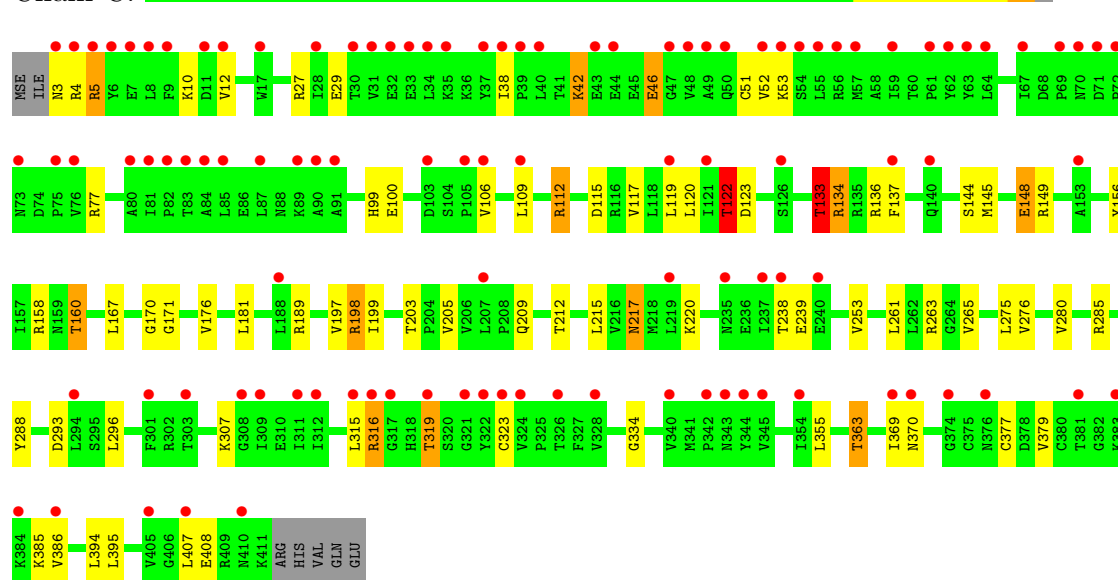


- Molecule 1: L-lysine 2,3-aminomutase



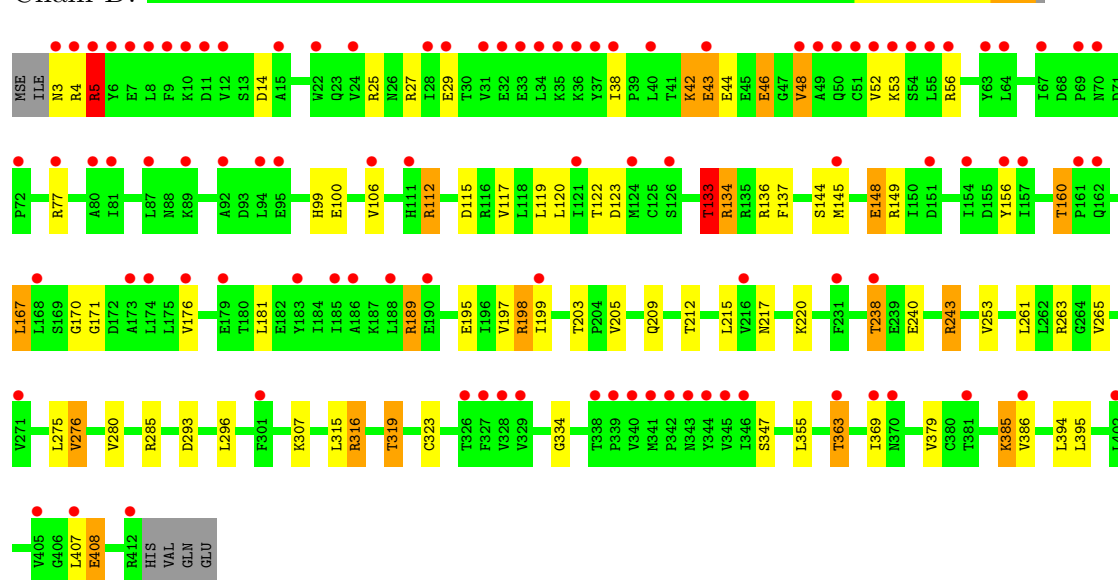
- Molecule 1: L-lysine 2,3-aminomutase

Chain C:



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

Chain D:



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 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
$\langle I/\sigma(I) \rangle$ ¹	5.65 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.184 , 0.225 0.204 , 0.245	Depositor DCC
R_{free} test set	8171 reflections (9.41%)	DCC
Wilson B-factor (Å ²)	50.2	Xtriage
Anisotropy	1.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 11.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 76379 reflections (0.003%)	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.*

¹Intensities estimated from amplitudes.

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, ZN, SF4, SAM, PLP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.47	7/3391 (0.2%)	1.17	35/4590 (0.8%)
1	B	1.50	8/3388 (0.2%)	1.14	25/4586 (0.5%)
1	C	1.05	6/3380 (0.2%)	1.18	34/4576 (0.7%)
1	D	1.19	7/3402 (0.2%)	1.15	35/4604 (0.8%)
All	All	1.32	28/13561 (0.2%)	1.16	129/18356 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

All (28) bond length outliers are listed below:

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

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

All (129) bond angle outliers are listed below:

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

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

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

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

There are no chirality outliers.

All (8) planarity outliers are listed below:

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

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3285	0	0	18	0
1	B	3288	0	0	20	0
1	C	3280	0	0	20	0
1	D	3297	0	0	25	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	0	0	0
4	B	27	0	0	0	0
4	C	27	0	0	0	0
4	D	27	0	0	0	0
5	A	28	0	0	0	0
5	B	28	0	0	1	0
5	C	28	0	0	0	0
5	D	28	0	0	1	0
6	A	8	0	0	0	0
6	B	8	0	0	0	0
6	C	8	0	0	0	0
6	D	8	0	0	0	0
7	A	135	0	0	2	0
7	B	116	0	0	3	0
7	C	183	0	0	5	1
7	D	174	0	0	3	0
All	All	14034	0	0	73	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (73) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:285[B]:ARG:CD	1:D:285[B]:ARG:CD	2.09	1.31
1:A:214:GLU:OE1	7:A:713:HOH:O	1.68	1.10
1:C:27[B]:ARG:NH2	1:C:29:GLU:OE2	2.13	0.81
1:C:285[B]:ARG:CD	1:D:285[B]:ARG:NE	2.45	0.79
1:D:243[A]:ARG:CD	7:D:578:HOH:O	2.31	0.78
1:B:27[B]:ARG:NH2	1:B:29:GLU:OE2	2.18	0.76
1:A:27[B]:ARG:NH2	1:A:29:GLU:OE2	2.19	0.75
1:D:137:PHE:CE2	1:D:145:MSE:CE	2.71	0.74
1:C:137:PHE:CE2	1:C:145:MSE:CE	2.73	0.72
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:B:137:PHE:CE2	1:B:145:MSE:CE	2.75	0.69
1:B:400:MSE:CE	7:C:744:HOH:O	2.40	0.69
1:C:370:ASN:ND2	7:C:775:HOH:O	2.27	0.67
1:C:122:THR:CG2	7:C:732:HOH:O	2.43	0.66
1:C:217:ASN:ND2	7:C:661:HOH:O	2.28	0.65
1:A:133:THR:CG2	1:A:293:ASP:OD2	2.45	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: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:285[B]:ARG:NE	1:D:285[B]:ARG:CD	2.64	0.59
1:A:156:TYR:O	1:A:160:THR:CG2	2.52	0.58
1:A:5[A]:ARG:NH1	1:A:14:ASP:OD1	2.36	0.58
1:B:133:THR:CG2	1:B:293:ASP:OD2	2.51	0.58
1:D:25:ARG:NH1	7:D:624:HOH:O	2.38	0.57
1:A:122:THR:CG2	7:A:633:HOH:O	2.55	0.55
1:D:133:THR:CG2	1:D:293:ASP:OD2	2.55	0.55
1:B:100:GLU:OE1	1:B:136:ARG:NH1	2.41	0.54
1:D:5[A]:ARG:NH2	7:D:623:HOH:O	2.40	0.53
1:D:5[A]:ARG:NH1	1:D:14:ASP:OD1	2.41	0.53
1:B:387:HIS:NE2	1:C:408:GLU:OE1	2.41	0.53
1:B:5[A]:ARG:NH2	1:B:12:VAL:O	2.42	0.53
1:A:100:GLU:OE1	1:A:136:ARG:NH1	2.43	0.52
1:D:137:PHE:CZ	1:D:145:MSE:CE	2.93	0.52
1:C:133:THR:CG2	1:C:293:ASP:OD2	2.57	0.52
1:C:319:THR:CG2	1:D:115:ASP:OD1	2.60	0.50
1:D:189:ARG:NH2	1:D:195:GLU:O	2.45	0.50
1:C:100:GLU:OE1	1:C:136:ARG:NH1	2.46	0.49
1:C:145:MSE:CE	1:C:149:ARG:NH2	2.76	0.48
1:A:145:MSE:CE	1:A:149:ARG:NH2	2.76	0.48
1:B:112:ARG:CD	7:B:501:HOH:O	2.61	0.48
1:A:243[B]:ARG:NH1	1:A:246:GLN:OE1	2.47	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:100:GLU:OE1	1:D:136:ARG:NH1	2.47	0.47
1:B:198:ARG:NH2	5:B:419:PLP:O1P	2.47	0.47
1:A:115:ASP:OD1	1:B:319:THR:CG2	2.63	0.46
1:B:164:ARG:NH1	7:B:516:HOH:O	2.47	0.46
1:A:319:THR:CG2	1:B:115:ASP:OD1	2.63	0.46
1:C:158:ARG:NH1	7:C:747:HOH:O	2.50	0.45
1:C:112:ARG:CD	1:C:334:GLY:O	2.65	0.45
1:D:145:MSE:CE	1:D:149:ARG:NH2	2.80	0.45
1:B:263:ARG:NH2	7:B:599:HOH:O	2.49	0.45
1:A:112:ARG:CD	1:A:334:GLY:O	2.65	0.45
1:D:198:ARG:NH2	5:D:419:PLP:O1P	2.50	0.44
1:C:115:ASP:OD1	1:D:319:THR:CG2	2.65	0.44
1:C:5[A]:ARG:NH2	1:C:12:VAL:O	2.50	0.43
1:D:123:ASP:C	1:D:123:ASP:OD1	2.56	0.43
1:C:123:ASP:OD1	1:C:123:ASP:C	2.57	0.43
1:B:145:MSE:CE	1:B:149:ARG:NH2	2.83	0.42
1:D:112:ARG:CD	1:D:334:GLY:O	2.67	0.42
1:A:332:PRO:O	1:B:363:THR:CG2	2.67	0.42
1:D:43:GLU:CG	1:D:44:GLU:N	2.82	0.42
1:A:5[A]:ARG:NH2	1:A:12:VAL:O	2.53	0.42
1:D:238:THR:CG2	1:D:240:GLU:OE1	2.68	0.42
1:A:363:THR:CG2	1:B:332:PRO:O	2.68	0.41
1:D:44:GLU:O	1:D:48:VAL:CG1	2.68	0.41
1:B:137:PHE:CZ	1:B:145:MSE:CE	3.03	0.41
1:A:238:THR:CG2	1:A:240:GLU:OE1	2.69	0.41

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	Distance(Å)	Clash(Å)
7:C:764:HOH:O	7:C:764:HOH:O[2_454]	1.88	0.32

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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%)	30	23
1	B	416/416 (100%)	398 (96%)	15 (4%)	3 (1%)	30	23
1	C	415/416 (100%)	397 (96%)	15 (4%)	3 (1%)	30	23
1	D	417/416 (100%)	397 (95%)	17 (4%)	3 (1%)	30	23
All	All	1664/1664 (100%)	1592 (96%)	60 (4%)	12 (1%)	30	23

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 ⓘ

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%)	4	2
1	B	374/362 (103%)	315 (84%)	59 (16%)	4	1
1	C	373/362 (103%)	320 (86%)	53 (14%)	5	2
1	D	375/362 (104%)	318 (85%)	57 (15%)	4	2
All	All	1496/1448 (103%)	1269 (85%)	227 (15%)	5	2

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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$
4	SAM	A	417	6	26,29,29	2.49	6 (23%)	38,42,42	2.17	11 (28%)
6	SF4	A	418	1,4	12,12,12	25.52	11 (91%)	0,24,24	0.00	-
5	PLP	A	419	5	14,15,16	1.33	1 (7%)	20,22,23	1.27	4 (20%)
5	LYS	A	420[A]	-	2,2,9	7.49	2 (100%)	0,1,10	0.00	-
5	LYS	A	420[B]	-	2,2,9	6.28	2 (100%)	0,1,10	0.00	-
3	SO4	A	592	-	4,4,4	0.18	0	6,6,6	0.19	0
4	SAM	B	417	6	26,29,29	2.34	7 (26%)	38,42,42	2.05	13 (34%)
6	SF4	B	418	1,4	12,12,12	23.20	11 (91%)	0,24,24	0.00	-
5	PLP	B	419	5	14,15,16	1.26	1 (7%)	20,22,23	1.01	0
5	LYS	B	420[A]	-	2,2,9	4.90	2 (100%)	0,1,10	0.00	-
5	LYS	B	420[B]	-	2,2,9	4.72	2 (100%)	0,1,10	0.00	-
3	SO4	B	495	-	4,4,4	0.26	0	6,6,6	0.26	0
4	SAM	C	417	6	26,29,29	2.52	6 (23%)	38,42,42	1.91	10 (26%)
6	SF4	C	418	1,4	12,12,12	22.66	12 (100%)	0,24,24	0.00	-
5	PLP	C	419	5	14,15,16	1.19	1 (7%)	20,22,23	0.98	0
5	LYS	C	420[A]	-	2,2,9	3.97	2 (100%)	0,1,10	0.00	-
5	LYS	C	420[B]	-	2,2,9	4.34	2 (100%)	0,1,10	0.00	-
3	SO4	C	593	-	4,4,4	0.20	0	6,6,6	0.39	0
4	SAM	D	417	6	26,29,29	2.37	5 (19%)	38,42,42	2.28	11 (28%)
6	SF4	D	418	1,4	12,12,12	23.29	12 (100%)	0,24,24	0.00	-
5	PLP	D	419	5	14,15,16	1.36	2 (14%)	20,22,23	1.03	2 (10%)
5	LYS	D	420[A]	-	2,2,9	5.31	2 (100%)	0,1,10	0.00	-
5	LYS	D	420[B]	-	2,2,9	4.90	2 (100%)	0,1,10	0.00	-
3	SO4	D	494	-	4,4,4	0.24	0	6,6,6	0.41	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
4	SAM	A	417	6	-	0/13/33/33	0/1/3/3
6	SF4	A	418	1,4	-	0/0/48/48	0/0/5/5
5	PLP	A	419	5	-	0/6/6/8	0/1/1/1
5	LYS	A	420[A]	-	-	0/0/0/9	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LYS	A	420[B]	-	-	0/0/0/9	0/0/0/0
3	SO4	A	592	-	-	0/0/0/0	0/0/0/0
4	SAM	B	417	6	-	0/13/33/33	0/1/3/3
6	SF4	B	418	1,4	-	0/0/48/48	0/0/5/5
5	PLP	B	419	5	-	0/6/6/8	0/1/1/1
5	LYS	B	420[A]	-	-	0/0/0/9	0/0/0/0
5	LYS	B	420[B]	-	-	0/0/0/9	0/0/0/0
3	SO4	B	495	-	-	0/0/0/0	0/0/0/0
4	SAM	C	417	6	-	0/13/33/33	0/1/3/3
6	SF4	C	418	1,4	-	0/0/48/48	0/0/5/5
5	PLP	C	419	5	-	0/6/6/8	0/1/1/1
5	LYS	C	420[A]	-	-	0/0/0/9	0/0/0/0
5	LYS	C	420[B]	-	-	0/0/0/9	0/0/0/0
3	SO4	C	593	-	-	0/0/0/0	0/0/0/0
4	SAM	D	417	6	-	0/13/33/33	0/1/3/3
6	SF4	D	418	1,4	-	0/0/48/48	0/0/5/5
5	PLP	D	419	5	-	0/6/6/8	0/1/1/1
5	LYS	D	420[A]	-	-	0/0/0/9	0/0/0/0
5	LYS	D	420[B]	-	-	0/0/0/9	0/0/0/0
3	SO4	D	494	-	-	0/0/0/0	0/0/0/0

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	418	SF4	S1-FE4	-30.64	2.12	2.33
6	A	418	SF4	S1-FE2	-30.22	2.12	2.33
6	B	418	SF4	S3-FE1	-30.08	2.13	2.33
6	A	418	SF4	S4-FE3	-30.03	2.13	2.33
6	D	418	SF4	S3-FE4	-29.60	2.13	2.33
6	A	418	SF4	S1-FE4	-29.08	2.13	2.33
6	A	418	SF4	S1-FE3	-29.04	2.13	2.33
6	D	418	SF4	S4-FE1	-28.74	2.13	2.33
6	C	418	SF4	S1-FE4	-28.58	2.14	2.33
6	A	418	SF4	S4-FE2	-28.17	2.14	2.33
6	C	418	SF4	S4-FE1	-27.90	2.14	2.33
6	C	418	SF4	S3-FE4	-27.63	2.14	2.33
6	B	418	SF4	S1-FE2	-27.57	2.14	2.33
6	B	418	SF4	S1-FE3	-26.96	2.15	2.33
6	A	418	SF4	S3-FE4	-26.87	2.15	2.33
6	C	418	SF4	S4-FE2	-26.82	2.15	2.33
6	A	418	SF4	S2-FE4	-26.55	2.15	2.33
6	D	418	SF4	S1-FE4	-25.88	2.15	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	418	SF4	S3-FE1	-25.75	2.15	2.33
6	B	418	SF4	S4-FE2	-25.50	2.16	2.33
6	B	418	SF4	S4-FE1	-24.95	2.16	2.33
6	D	418	SF4	S4-FE3	-24.62	2.16	2.33
6	D	418	SF4	S1-FE3	-24.61	2.16	2.33
6	C	418	SF4	S4-FE3	-24.52	2.16	2.33
6	C	418	SF4	S3-FE1	-24.27	2.16	2.33
6	B	418	SF4	S3-FE4	-24.25	2.16	2.33
6	A	418	SF4	S4-FE1	-24.25	2.16	2.33
6	D	418	SF4	S1-FE2	-24.13	2.17	2.33
6	C	418	SF4	S1-FE3	-23.99	2.17	2.33
6	C	418	SF4	S1-FE2	-23.96	2.17	2.33
6	D	418	SF4	S3-FE1	-23.42	2.17	2.33
6	A	418	SF4	S3-FE2	-23.12	2.17	2.33
6	D	418	SF4	S3-FE2	-22.29	2.18	2.33
6	D	418	SF4	S4-FE2	-21.57	2.18	2.33
6	B	418	SF4	S4-FE3	-21.32	2.18	2.33
6	C	418	SF4	S3-FE2	-20.50	2.19	2.33
6	B	418	SF4	S3-FE2	-19.26	2.20	2.33
6	D	418	SF4	S2-FE3	-19.08	2.20	2.33
6	B	418	SF4	S2-FE4	-17.72	2.21	2.33
6	A	418	SF4	S2-FE3	-17.56	2.21	2.33
6	D	418	SF4	S2-FE1	17.40	2.45	2.33
6	C	418	SF4	S2-FE4	-14.45	2.23	2.33
6	D	418	SF4	S2-FE4	-12.96	2.24	2.33
6	B	418	SF4	S2-FE3	-11.20	2.25	2.33
6	C	418	SF4	S2-FE3	-9.93	2.26	2.33
4	D	417	SAM	CG-SD	9.35	1.99	1.80
4	C	417	SAM	CG-SD	9.29	1.99	1.80
4	A	417	SAM	CG-SD	8.92	1.98	1.80
5	A	420[A]	LYS	CG-CD	-8.92	1.51	1.55
4	B	417	SAM	CG-SD	8.54	1.97	1.80
5	A	420[B]	LYS	CG-CD	-7.19	1.52	1.55
5	D	420[A]	LYS	CG-CD	-6.13	1.52	1.55
4	C	417	SAM	C5'-SD	5.74	1.98	1.81
5	A	420[A]	LYS	CE-CD	-5.73	1.52	1.55
4	A	417	SAM	C5'-SD	5.55	1.98	1.81
5	B	420[A]	LYS	CG-CD	-5.31	1.53	1.55
5	D	420[B]	LYS	CG-CD	-5.31	1.53	1.55
5	A	420[B]	LYS	CE-CD	-5.20	1.53	1.55
5	B	420[B]	LYS	CE-CD	-4.74	1.53	1.55
4	B	417	SAM	C5'-SD	4.72	1.95	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	420[B]	LYS	CG-CD	-4.71	1.53	1.55
5	C	420[B]	LYS	CE-CD	-4.60	1.53	1.55
5	B	420[A]	LYS	CE-CD	-4.46	1.53	1.55
5	D	420[B]	LYS	CE-CD	-4.44	1.53	1.55
5	D	420[A]	LYS	CE-CD	-4.34	1.53	1.55
5	C	420[B]	LYS	CG-CD	-4.07	1.53	1.55
5	C	420[A]	LYS	CE-CD	-4.04	1.53	1.55
4	D	417	SAM	C5'-SD	3.92	1.93	1.81
5	C	420[A]	LYS	CG-CD	-3.90	1.53	1.55
4	A	417	SAM	C4-N9	-3.79	1.32	1.37
6	C	418	SF4	S2-FE1	3.79	2.35	2.33
4	C	417	SAM	C5-C4	3.53	1.48	1.40
4	D	417	SAM	C4-N9	-3.49	1.32	1.37
4	A	417	SAM	C5-C4	3.45	1.48	1.40
4	B	417	SAM	C4-N9	-3.43	1.32	1.37
4	D	417	SAM	C5-C4	3.18	1.47	1.40
4	B	417	SAM	C5-C4	3.12	1.47	1.40
5	D	419	PLP	P-O2P	-3.11	1.43	1.54
4	D	417	SAM	CE-SD	2.79	1.98	1.78
4	A	417	SAM	C2-N3	2.78	1.37	1.32
4	C	417	SAM	C4-N9	-2.60	1.33	1.37
4	A	417	SAM	CE-SD	2.56	1.97	1.78
5	C	419	PLP	P-O2P	-2.47	1.45	1.54
4	B	417	SAM	CE-SD	2.46	1.96	1.78
5	A	419	PLP	P-O2P	-2.46	1.45	1.54
4	C	417	SAM	CE-SD	2.34	1.95	1.78
4	C	417	SAM	CG-CB	2.24	1.55	1.52
4	B	417	SAM	O4'-C1'	2.20	1.44	1.41
4	B	417	SAM	CG-CB	2.18	1.55	1.52
5	D	419	PLP	C3-C2	2.10	1.42	1.40
5	B	419	PLP	P-O2P	-2.00	1.47	1.54

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	417	SAM	O4'-C1'-N9	7.01	114.96	108.44
4	A	417	SAM	O4'-C1'-N9	6.73	114.70	108.44
4	B	417	SAM	N3-C2-N1	-5.45	124.15	128.71
4	D	417	SAM	N3-C4-N9	5.18	134.79	125.43
4	D	417	SAM	N3-C2-N1	-5.16	124.39	128.71
4	A	417	SAM	N3-C4-N9	5.13	134.69	125.43
4	C	417	SAM	N3-C4-N9	5.01	134.47	125.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	417	SAM	N3-C2-N1	-4.68	124.79	128.71
4	B	417	SAM	N3-C4-N9	4.61	133.76	125.43
4	B	417	SAM	C8-N9-C4	4.43	110.28	106.90
4	C	417	SAM	N3-C2-N1	-4.23	125.17	128.71
4	C	417	SAM	C4'-O4'-C1'	-4.04	105.36	109.75
4	B	417	SAM	O4'-C1'-N9	4.00	112.16	108.44
4	D	417	SAM	C8-N9-C4	3.91	109.89	106.90
4	C	417	SAM	C8-N9-C4	3.33	109.44	106.90
4	A	417	SAM	C8-N9-C4	3.25	109.38	106.90
4	A	417	SAM	CB-CA-N	3.10	119.73	110.67
4	D	417	SAM	C4-C5-N7	-3.09	106.87	109.52
4	A	417	SAM	C5'-SD-CG	-3.03	93.65	102.90
4	B	417	SAM	C4-C5-N7	-2.99	106.96	109.52
4	C	417	SAM	C5'-SD-CG	-2.96	93.85	102.90
4	C	417	SAM	C4-C5-N7	-2.90	107.04	109.52
4	D	417	SAM	C3'-C2'-C1'	2.77	105.25	100.91
4	D	417	SAM	CB-CA-N	2.73	118.66	110.67
4	D	417	SAM	C5-C4-N3	-2.71	119.79	125.70
5	A	419	PLP	O4P-P-O1P	-2.62	99.02	106.71
4	B	417	SAM	C3'-C2'-C1'	2.62	105.01	100.91
4	B	417	SAM	CB-CA-N	2.60	118.28	110.67
4	A	417	SAM	C5-C4-N3	-2.57	120.11	125.70
4	C	417	SAM	C5-C4-N3	-2.52	120.22	125.70
4	A	417	SAM	C4'-O4'-C1'	-2.51	107.02	109.75
5	A	419	PLP	O2P-P-O4P	2.51	113.56	106.65
4	B	417	SAM	C4'-O4'-C1'	-2.50	107.03	109.75
4	C	417	SAM	C1'-N9-C4	-2.46	122.38	126.64
4	B	417	SAM	C1'-N9-C4	-2.40	122.50	126.64
4	D	417	SAM	CB-CA-C	-2.36	107.88	111.44
4	C	417	SAM	CG-CB-CA	2.34	115.67	112.22
4	B	417	SAM	C5-C4-N3	-2.30	120.70	125.70
5	D	419	PLP	C3-C4-C5	-2.21	117.10	121.29
4	A	417	SAM	C4-C5-N7	-2.21	107.63	109.52
4	B	417	SAM	C2'-C1'-N9	-2.21	107.59	113.27
4	C	417	SAM	C2'-C1'-N9	-2.21	107.60	113.27
4	A	417	SAM	CG-CB-CA	2.18	115.42	112.22
5	D	419	PLP	O3-C3-C2	2.18	121.47	117.61
4	D	417	SAM	C2'-C1'-N9	-2.13	107.79	113.27
5	A	419	PLP	O3P-P-O1P	2.13	117.40	110.44
4	D	417	SAM	C2-N3-C4	2.04	119.82	114.01
5	A	419	PLP	C3-C4-C5	-2.04	117.43	121.29
4	B	417	SAM	CG-CB-CA	2.03	115.20	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	417	SAM	C3'-C2'-C1'	2.02	104.07	100.91
4	B	417	SAM	CB-CA-C	-2.00	108.42	111.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	409/416 (98%)	1.45	106 (25%) 1 1	18, 39, 61, 72	9 (2%)
1	B	410/416 (98%)	1.73	140 (34%) 1 1	20, 44, 79, 98	7 (1%)
1	C	409/416 (98%)	1.47	107 (26%) 1 1	16, 32, 59, 73	7 (1%)
1	D	410/416 (98%)	1.44	98 (23%) 1 1	15, 33, 55, 69	6 (1%)
All	All	1638/1664 (98%)	1.52	451 (27%) 1 1	15, 36, 65, 98	29 (1%)

All (451) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	38	ILE	8.6
1	A	48	VAL	8.0
1	C	40	LEU	7.5
1	B	85	LEU	7.3
1	C	64	LEU	7.0
1	D	9	PHE	6.7
1	D	6	TYR	6.6
1	C	31	VAL	6.6
1	B	48	VAL	6.5
1	C	369	ILE	6.4
1	C	8	LEU	6.2
1	B	40	LEU	6.2
1	B	81	ILE	6.0
1	A	49	ALA	6.0
1	C	70	ASN	5.8
1	C	9	PHE	5.7
1	C	38	ILE	5.7
1	A	6	TYR	5.6
1	D	386	VAL	5.6
1	B	22	TRP	5.6
1	D	52	VAL	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	37	TYR	5.3
1	A	51	CYS	5.3
1	D	8	LEU	5.3
1	B	59	ILE	5.2
1	C	67	ILE	5.2
1	A	52	VAL	5.2
1	B	143	ASP	5.2
1	B	54	SER	5.1
1	B	90	ALA	5.0
1	C	37	TYR	5.0
1	A	38	ILE	5.0
1	B	31	VAL	4.9
1	D	38	ILE	4.8
1	B	8	LEU	4.8
1	B	92	ALA	4.8
1	C	84	ALA	4.7
1	D	40	LEU	4.7
1	B	126	SER	4.7
1	B	328	VAL	4.6
1	A	37	TYR	4.6
1	A	15	ALA	4.6
1	A	17	TRP	4.6
1	C	85	LEU	4.6
1	C	6	TYR	4.5
1	D	4	ARG	4.5
1	C	386	VAL	4.5
1	B	53	LYS	4.5
1	B	70	ASN	4.5
1	A	12	VAL	4.5
1	B	28	ILE	4.4
1	D	49	ALA	4.4
1	C	80	ALA	4.3
1	C	4	ARG	4.3
1	A	11	ASP	4.3
1	D	34	LEU	4.2
1	C	54	SER	4.2
1	D	67	ILE	4.2
1	A	85	LEU	4.2
1	C	43	GLU	4.1
1	D	369	ILE	4.1
1	C	7	GLU	4.1
1	B	326	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	50	GLN	4.1
1	B	139	GLY	4.0
1	B	9	PHE	4.0
1	C	49	ALA	4.0
1	A	70	ASN	4.0
1	D	11	ASP	4.0
1	A	40	LEU	4.0
1	B	87	LEU	4.0
1	B	312	ILE	4.0
1	B	142	ASP	3.9
1	B	6	TYR	3.9
1	B	4	ARG	3.9
1	C	53	LYS	3.9
1	A	80	ALA	3.9
1	C	90	ALA	3.9
1	A	9	PHE	3.9
1	A	45	GLU	3.9
1	B	108	GLY	3.8
1	B	94	LEU	3.8
1	A	81	ILE	3.8
1	D	106	VAL	3.8
1	C	87	LEU	3.8
1	B	88	ASN	3.8
1	C	106	VAL	3.8
1	D	156	TYR	3.8
1	D	162	GLN	3.8
1	D	190	GLU	3.8
1	B	156	TYR	3.7
1	C	343	ASN	3.7
1	B	71	ASP	3.7
1	D	37	TYR	3.7
1	B	80	ALA	3.7
1	B	95	GLU	3.7
1	C	383	LYS	3.7
1	C	73	ASN	3.7
1	A	84	ALA	3.6
1	B	83	THR	3.6
1	B	147	MSE	3.6
1	C	81	ILE	3.6
1	D	157	ILE	3.6
1	A	345	VAL	3.6
1	C	69	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	54	SER	3.6
1	C	39	PRO	3.6
1	D	69	PRO	3.5
1	D	340	VAL	3.5
1	B	35	LYS	3.5
1	D	412	ARG	3.5
1	D	173	ALA	3.4
1	A	369	ILE	3.4
1	A	22	TRP	3.4
1	A	346[A]	ILE	3.4
1	B	329	VAL	3.4
1	B	51	CYS	3.4
1	D	53	LYS	3.3
1	B	39	PRO	3.3
1	B	10	LYS	3.3
1	D	154	ILE	3.3
1	B	72	PRO	3.3
1	B	91	ALA	3.3
1	B	12	VAL	3.3
1	C	3	ASN	3.3
1	D	87	LEU	3.3
1	D	405	VAL	3.2
1	A	36	LYS	3.2
1	C	52	VAL	3.2
1	D	81	ILE	3.2
1	C	89	LYS	3.2
1	C	17	TRP	3.2
1	A	14	ASP	3.2
1	A	59	ILE	3.2
1	A	57	MSE	3.2
1	B	145	MSE	3.2
1	D	342	PRO	3.2
1	D	188	LEU	3.2
1	B	49	ALA	3.2
1	D	33	GLU	3.2
1	D	111	HIS	3.2
1	A	72	PRO	3.2
1	B	386	VAL	3.2
1	D	48	VAL	3.2
1	B	127	MSE	3.1
1	B	343	ASN	3.1
1	C	62	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	63	TYR	3.1
1	B	138	ALA	3.1
1	A	3	ASN	3.1
1	B	340	VAL	3.1
1	B	341	MSE	3.1
1	A	53	LYS	3.1
1	B	41	THR	3.1
1	B	55	LEU	3.1
1	B	58	ALA	3.1
1	B	153	ALA	3.1
1	A	194	VAL	3.1
1	C	344	TYR	3.1
1	B	11	ASP	3.1
1	D	94	LEU	3.1
1	B	209	GLN	3.1
1	A	10	LYS	3.0
1	D	36	LYS	3.0
1	A	354	ILE	3.0
1	A	27[A]	ARG	3.0
1	C	384	LYS	3.0
1	B	339	PRO	3.0
1	B	93	ASP	3.0
1	C	410	ASN	3.0
1	B	7	GLU	3.0
1	C	321	GLY	3.0
1	D	179	GLU	3.0
1	A	387	HIS	3.0
1	D	345	VAL	3.0
1	D	370	ASN	3.0
1	C	374	GLY	3.0
1	C	61	PRO	2.9
1	B	327	PHE	2.9
1	A	199[A]	ILE	2.9
1	D	185	ILE	2.9
1	D	326	THR	2.9
1	D	77	ARG	2.9
1	D	3	ASN	2.9
1	B	128	TYR	2.9
1	A	340	VAL	2.9
1	B	32	GLU	2.9
1	D	32	GLU	2.9
1	A	4	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	64	LEU	2.9
1	C	381	THR	2.9
1	A	39	PRO	2.9
1	A	342	PRO	2.9
1	B	52	VAL	2.9
1	C	48	VAL	2.9
1	D	301	PHE	2.9
1	C	34	LEU	2.9
1	C	237	ILE	2.9
1	A	8	LEU	2.8
1	B	355	LEU	2.8
1	A	69	PRO	2.8
1	B	382	GLY	2.8
1	C	345	VAL	2.8
1	D	12	VAL	2.8
1	C	235	ASN	2.8
1	B	309	ILE	2.8
1	D	183	TYR	2.8
1	B	34	LEU	2.8
1	D	5[A]	ARG	2.8
1	A	343	ASN	2.8
1	D	22	TRP	2.8
1	A	175	LEU	2.8
1	C	119	LEU	2.8
1	B	289	ILE	2.8
1	C	121	ILE	2.8
1	B	82	PRO	2.7
1	B	342	PRO	2.7
1	C	72	PRO	2.7
1	A	35	LYS	2.7
1	B	187	LYS	2.7
1	D	80	ALA	2.7
1	B	36	LYS	2.7
1	B	338	THR	2.7
1	B	26	ASN	2.7
1	D	343	ASN	2.7
1	A	32	GLU	2.7
1	D	89	LYS	2.7
1	B	107	PRO	2.7
1	D	72	PRO	2.7
1	C	11	ASP	2.7
1	A	411	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	64	LEU	2.7
1	A	383	LYS	2.7
1	C	57	MSE	2.7
1	C	47	GLY	2.7
1	A	405	VAL	2.7
1	A	64	LEU	2.7
1	A	408	GLU	2.6
1	C	126	SER	2.6
1	B	308	GLY	2.6
1	B	168	LEU	2.6
1	D	168	LEU	2.6
1	B	160	THR	2.6
1	D	407	LEU	2.6
1	B	162	GLN	2.6
1	D	238	THR	2.6
1	B	157	ILE	2.6
1	A	341	MSE	2.6
1	A	301	PHE	2.6
1	A	5[A]	ARG	2.6
1	A	339	PRO	2.6
1	C	55	LEU	2.6
1	C	30	THR	2.6
1	A	28	ILE	2.6
1	B	57	MSE	2.6
1	B	67	ILE	2.6
1	B	199[A]	ILE	2.6
1	D	151	ASP	2.6
1	B	149	ARG	2.6
1	B	50	GLN	2.6
1	D	29	GLU	2.6
1	A	168	LEU	2.6
1	A	321	GLY	2.6
1	A	157	ILE	2.6
1	D	43	GLU	2.6
1	B	62	TYR	2.6
1	A	386	VAL	2.6
1	B	370	ASN	2.6
1	D	15	ALA	2.6
1	D	145	MSE	2.5
1	A	227	LEU	2.5
1	B	77	ARG	2.5
1	B	412	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	50	GLN	2.5
1	A	83	THR	2.5
1	A	344	TYR	2.5
1	B	66	LEU	2.5
1	B	174	LEU	2.5
1	B	288	TYR	2.5
1	B	135	ARG	2.5
1	C	71	ASP	2.5
1	A	34	LEU	2.5
1	B	344	TYR	2.5
1	D	126	SER	2.5
1	D	51	CYS	2.5
1	B	369	ILE	2.5
1	B	197	VAL	2.5
1	C	405	VAL	2.5
1	C	5[A]	ARG	2.5
1	A	121	ILE	2.5
1	C	105	PRO	2.5
1	A	66	LEU	2.5
1	D	174	LEU	2.5
1	B	405	VAL	2.5
1	D	344	TYR	2.5
1	B	321	GLY	2.4
1	B	383	LYS	2.4
1	B	411	LYS	2.4
1	B	316[A]	ARG	2.4
1	D	55	LEU	2.4
1	A	353	VAL	2.4
1	A	7	GLU	2.4
1	D	28	ILE	2.4
1	C	316[A]	ARG	2.4
1	B	73	ASN	2.4
1	B	264	GLY	2.4
1	A	326	THR	2.4
1	C	238	THR	2.4
1	D	56	ARG	2.4
1	B	89	LYS	2.4
1	A	355	LEU	2.4
1	C	407	LEU	2.4
1	D	70	ASN	2.4
1	B	290	TYR	2.4
1	D	24	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	328	VAL	2.4
1	D	381	THR	2.4
1	B	44	GLU	2.4
1	C	153	ALA	2.4
1	B	141	SER	2.3
1	A	265	VAL	2.3
1	D	31	VAL	2.3
1	D	338	THR	2.3
1	B	3	ASN	2.3
1	C	91	ALA	2.3
1	D	231	PHE	2.3
1	D	199[A]	ILE	2.3
1	D	54	SER	2.3
1	A	325	PRO	2.3
1	B	305	VAL	2.3
1	C	370	ASN	2.3
1	B	17	TRP	2.3
1	B	56	ARG	2.3
1	A	67	ILE	2.3
1	C	76	VAL	2.3
1	C	28	ILE	2.3
1	C	207	LEU	2.3
1	D	339	PRO	2.3
1	B	323	CYS	2.3
1	A	76	VAL	2.3
1	D	50	GLN	2.3
1	D	341	MSE	2.3
1	B	43	GLU	2.3
1	C	319	THR	2.3
1	C	328	VAL	2.3
1	A	153	ALA	2.3
1	C	63	TYR	2.3
1	C	322	TYR	2.3
1	A	402	LEU	2.3
1	B	65	SER	2.2
1	B	163	VAL	2.2
1	A	90	ALA	2.2
1	C	33	GLU	2.2
1	A	296	LEU	2.2
1	B	118	LEU	2.2
1	B	208	PRO	2.2
1	B	194	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	41	THR	2.2
1	A	87	LEU	2.2
1	A	109	LEU	2.2
1	C	109	LEU	2.2
1	D	346[A]	ILE	2.2
1	A	324	VAL	2.2
1	C	324	VAL	2.2
1	A	288	TYR	2.2
1	A	356[A]	ARG	2.2
1	B	109	LEU	2.2
1	D	161	PRO	2.2
1	A	138	ALA	2.2
1	C	340	VAL	2.2
1	A	382	GLY	2.2
1	D	186	ALA	2.2
1	B	260[A]	VAL	2.2
1	D	329	VAL	2.2
1	B	42	LYS	2.2
1	C	83	THR	2.2
1	C	326	THR	2.2
1	A	44	GLU	2.2
1	A	322	TYR	2.2
1	D	95	GLU	2.2
1	B	61	PRO	2.2
1	C	75	PRO	2.2
1	A	119	LEU	2.2
1	B	188	LEU	2.2
1	C	312	ILE	2.2
1	D	92	ALA	2.2
1	A	329	VAL	2.2
1	D	216	VAL	2.2
1	C	311	ILE	2.1
1	C	354	ILE	2.1
1	A	106	VAL	2.1
1	B	183	TYR	2.1
1	C	240	GLU	2.1
1	A	237	ILE	2.1
1	B	325	PRO	2.1
1	A	364	THR	2.1
1	B	406	GLY	2.1
1	B	345	VAL	2.1
1	B	137	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	140	GLN	2.1
1	C	188	LEU	2.1
1	C	303	THR	2.1
1	A	68	ASP	2.1
1	B	225	VAL	2.1
1	C	56	ARG	2.1
1	D	176	VAL	2.1
1	A	183	TYR	2.1
1	B	179	GLU	2.1
1	C	219	LEU	2.1
1	C	315	LEU	2.1
1	C	308	GLY	2.1
1	C	317	GLY	2.1
1	D	121	ILE	2.1
1	A	316[A]	ARG	2.1
1	D	10	LYS	2.1
1	C	32	GLU	2.1
1	B	294	LEU	2.1
1	A	122	THR	2.1
1	A	385	LYS	2.1
1	A	79	GLN	2.1
1	B	184	ILE	2.1
1	C	309	ILE	2.1
1	D	7	GLU	2.1
1	C	301	PHE	2.1
1	C	342	PRO	2.1
1	D	271	VAL	2.1
1	D	327	PHE	2.1
1	A	162	GLN	2.0
1	A	407	LEU	2.0
1	C	44	GLU	2.0
1	C	294	LEU	2.0
1	B	154	ILE	2.0
1	C	59	ILE	2.0
1	C	323	CYS	2.0
1	A	111	HIS	2.0
1	C	82	PRO	2.0
1	D	35	LYS	2.0
1	C	12	VAL	2.0
1	A	55	LEU	2.0
1	C	376	ASN	2.0
1	B	361	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	137	PHE	2.0
1	B	384	LYS	2.0
1	C	35	LYS	2.0
1	D	363	THR	2.0
1	D	402	LEU	2.0
1	B	330	ASP	2.0
1	B	378	ASP	2.0
1	C	103	ASP	2.0
1	D	124	MSE	2.0
1	A	317	GLY	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SO4	C	593	5/5	0.48	7.35	79,80,81,81	0
3	SO4	B	495	5/5	0.41	3.04	101,101,101,101	0
3	SO4	D	494	5/5	0.51	2.87	88,88,88,89	0
3	SO4	A	592	5/5	0.31	2.68	98,98,99,99	0
4	SAM	C	417	27/27	0.21	2.17	21,23,25,31	1
5	LYS	C	420[B]	3/10	0.18	1.95	23,23,23,23	3
4	SAM	B	417	27/27	0.25	1.66	32,34,39,43	1
5	LYS	C	420[A]	3/10	0.18	1.64	23,23,23,23	3
5	LYS	D	420[A]	3/10	0.21	1.08	24,24,25,25	3
4	SAM	A	417	27/27	0.19	0.94	25,27,31,36	1
5	LYS	D	420[B]	3/10	0.21	0.52	24,24,25,25	3

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SAM	D	417	27/27	0.19	0.52	21,23,26,33	1
5	LYS	B	420[B]	3/10	0.23	0.22	32,32,33,34	3
5	LYS	B	420[A]	3/10	0.23	0.22	33,33,33,34	3
5	PLP	C	419	15/16	0.16	-0.26	18,24,25,26	0
5	LYS	A	420[A]	3/10	0.18	-0.27	27,27,28,28	3
5	LYS	A	420[B]	3/10	0.18	-0.33	27,27,28,28	3
5	PLP	B	419	15/16	0.20	-0.36	27,34,36,37	0
5	PLP	D	419	15/16	0.18	-0.42	20,27,29,30	0
5	PLP	A	419	15/16	0.18	-0.65	24,31,32,33	0
2	ZN	B	421	1/1	0.09	-1.43	45,45,45,45	0
6	SF4	B	418	8/8	0.08	-1.61	35,38,40,40	0
2	ZN	C	421	1/1	0.10	-1.90	36,36,36,36	0
2	ZN	A	421	1/1	0.07	-1.99	36,36,36,36	0
2	ZN	D	421	1/1	0.09	-2.02	31,31,31,31	0
6	SF4	D	418	8/8	0.08	-2.67	21,22,25,26	0
6	SF4	C	418	8/8	0.07	-2.68	22,24,25,26	0
6	SF4	A	418	8/8	0.08	-2.69	24,27,29,29	0

6.5 Other polymers ⓘ

There are no such residues in this entry.