Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:23 AM 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 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

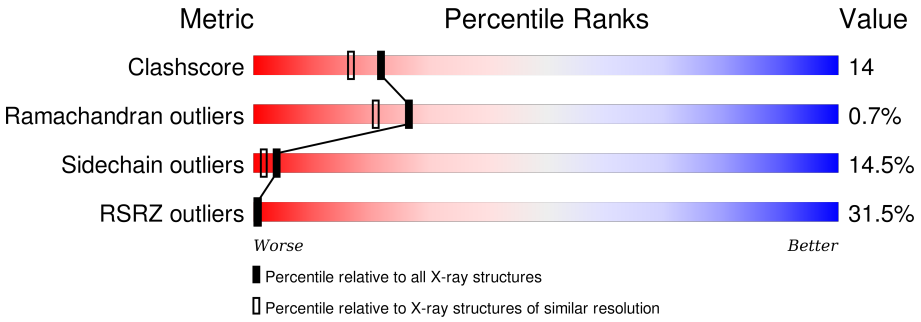
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	416	31% 68% 22% 7%
1	B	416	42% 67% 24% 6%
1	C	416	24% 67% 23% 7%
1	D	416	24% 66% 24% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	592	-	-	-	X
3	SO4	B	495	-	-	-	X
3	SO4	C	593	-	-	-	X
3	SO4	D	494	-	-	-	X
4	SAM	C	417	-	-	-	X

2 Entry composition (i)

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

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

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

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

There are 40 discrepancies between the modelled and reference sequences:

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

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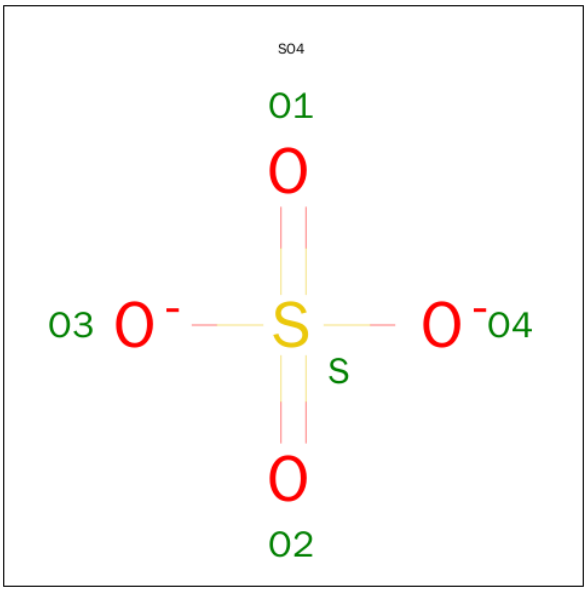
Chain	Residue	Modelled	Actual	Comment	Reference
C	57	MSE	MET	MODIFIED RESIDUE	GB 5410603
C	124	MSE	MET	MODIFIED RESIDUE	GB 5410603
C	127	MSE	MET	MODIFIED RESIDUE	GB 5410603
C	145	MSE	MET	MODIFIED RESIDUE	GB 5410603
C	147	MSE	MET	MODIFIED RESIDUE	GB 5410603
C	218	MSE	MET	MODIFIED RESIDUE	GB 5410603
C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

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

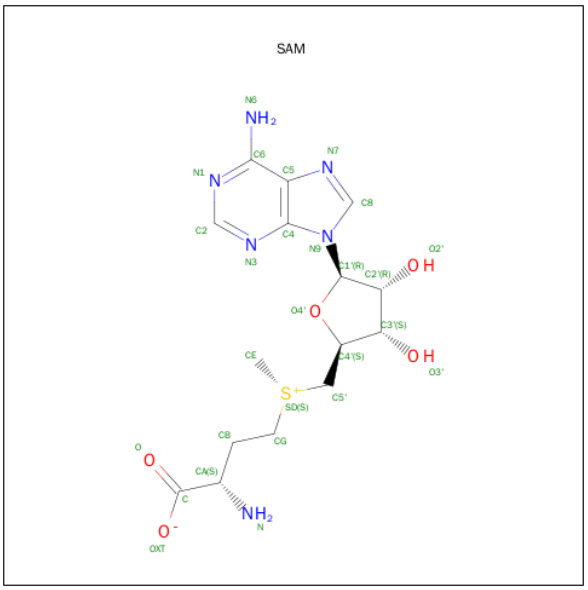
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

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



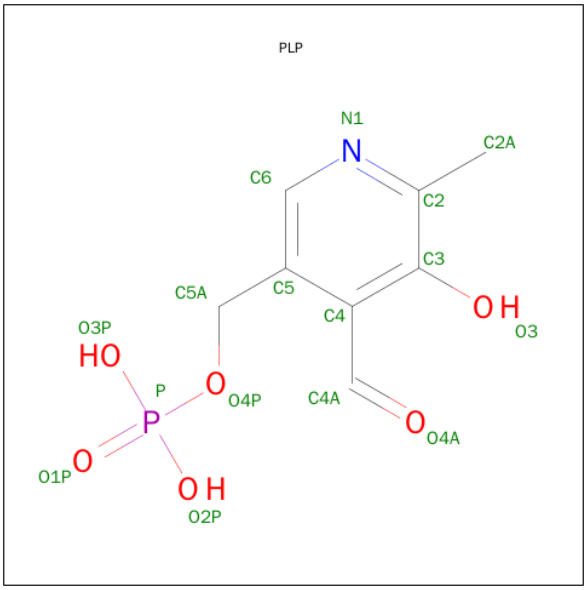
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

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



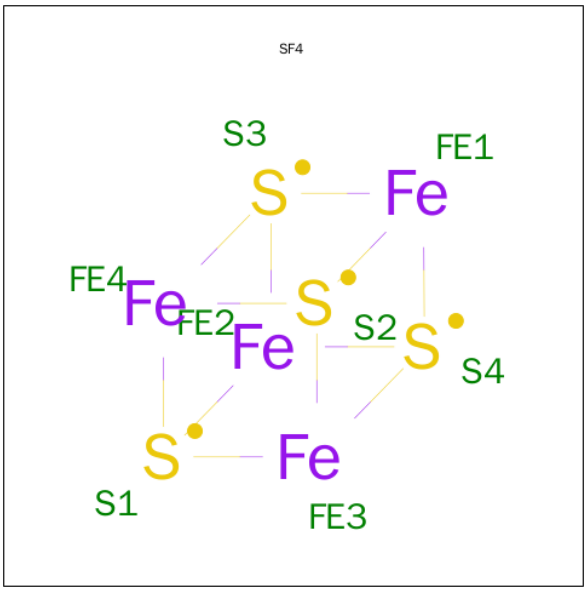
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	D	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 5 is LYSINE (three-letter code: 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 8 4 4	0	0
6	B	1	Total Fe S 8 4 4	0	0
6	C	1	Total Fe S 8 4 4	0	0
6	D	1	Total Fe S 8 4 4	0	0

- Molecule 7 is water.

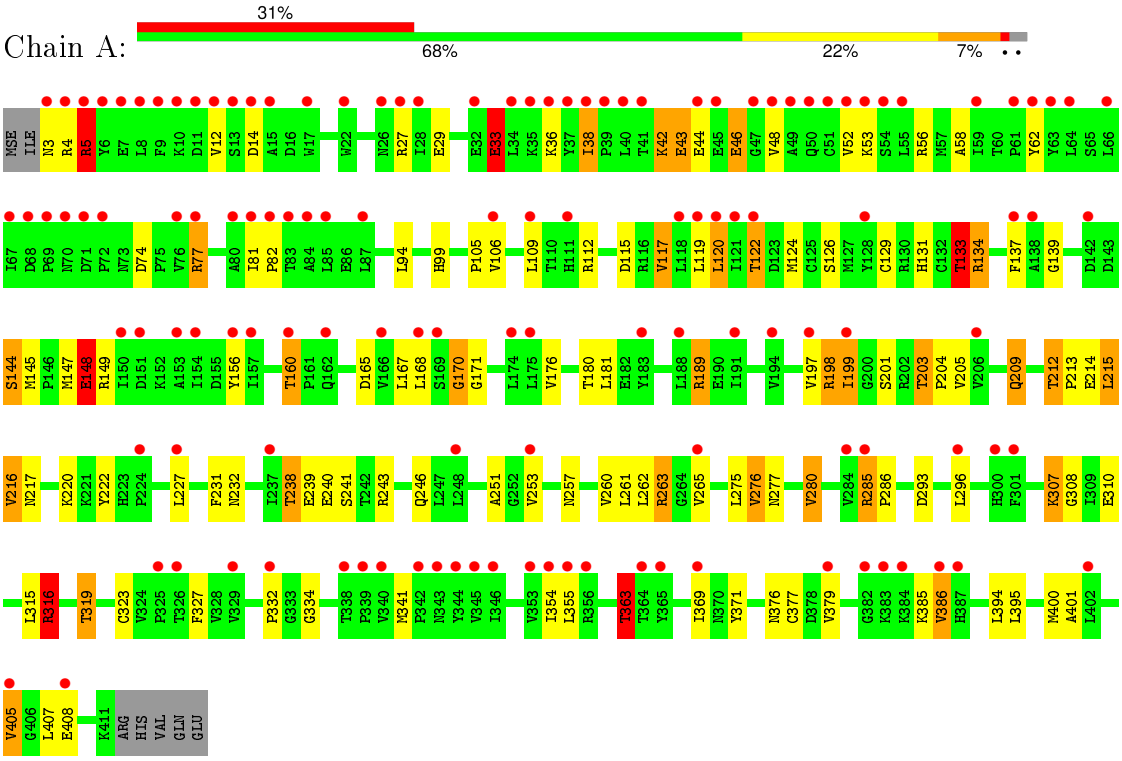
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	135	Total O 135 135	0	0
7	B	116	Total O 116 116	0	0
7	C	183	Total O 183 183	0	0
7	D	174	Total O 174 174	0	0

3 Residue-property plots (i)

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.

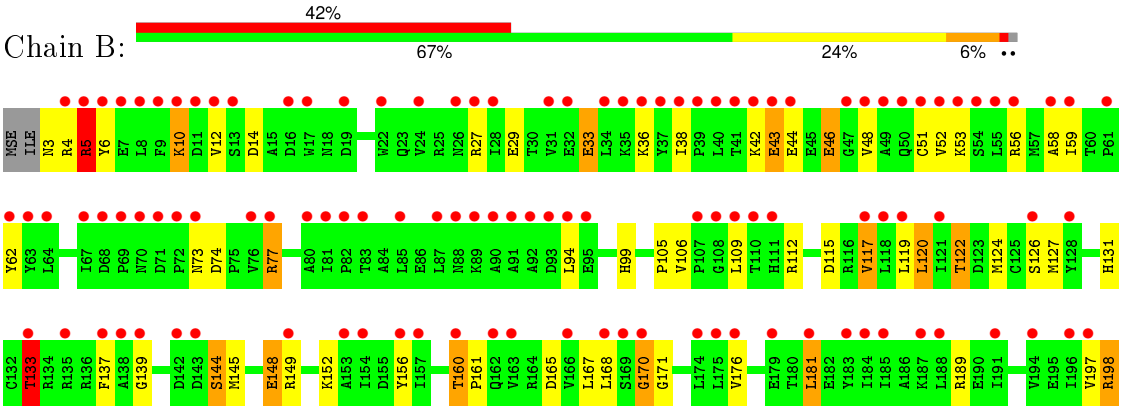
- Molecule 1: L-lysine 2,3-aminomutase

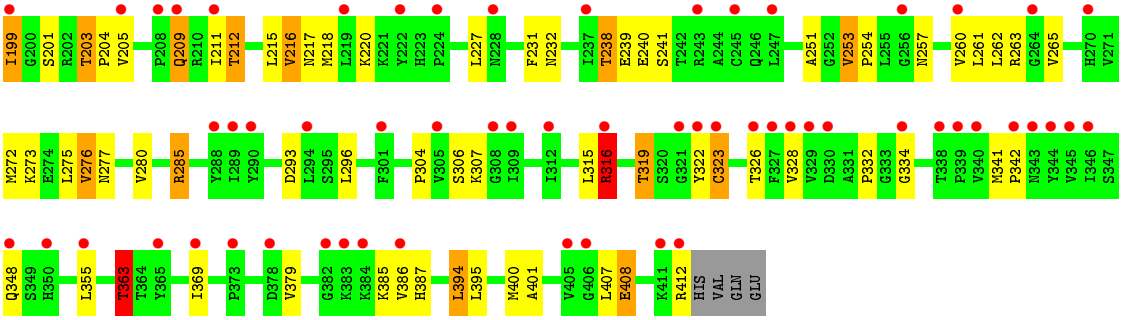
Chain A:



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

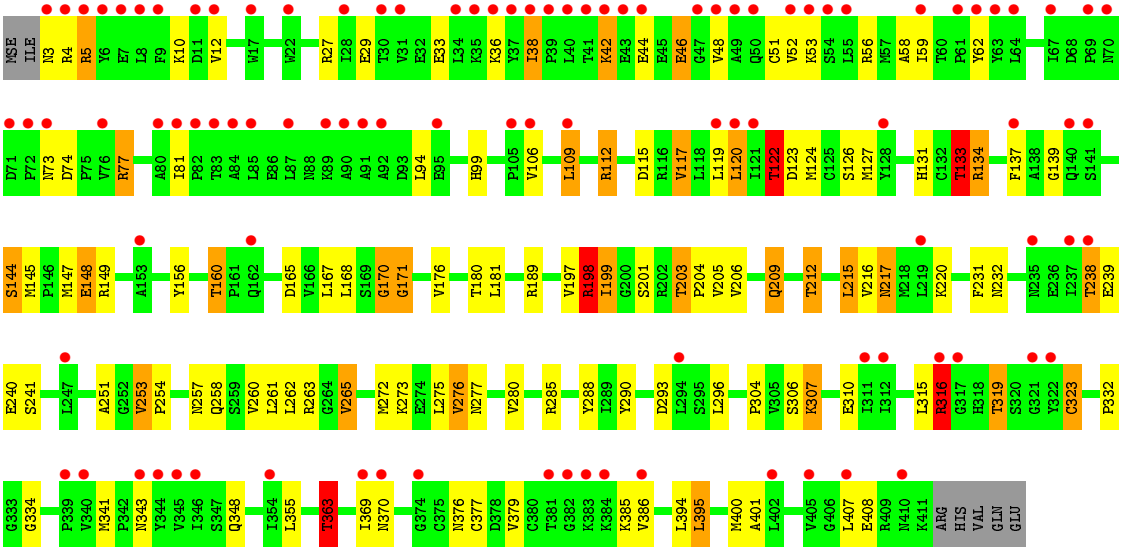
Chain B:





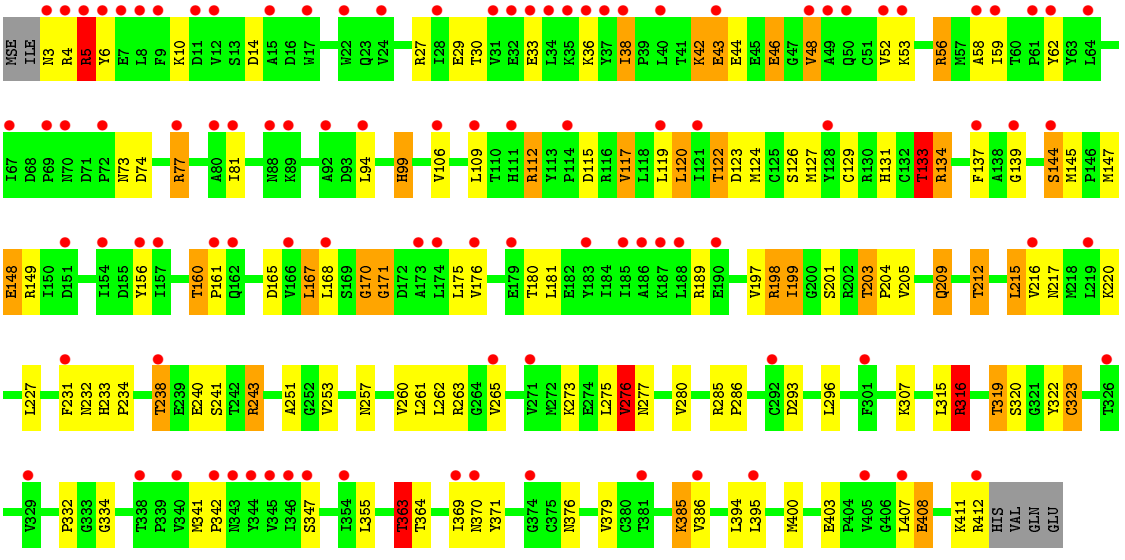
• Molecule 1: L-lysine 2,3-aminomutase

Chain C:



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

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	118.89Å 92.93Å 177.74Å 90.00° 96.74° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 46.61 – 3.00	Depositor EDS
% Data completeness (in resolution range)	81.5 (50.00-2.10) 96.8 (46.61-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	5.65 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.184 , 0.225 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å^2)	50.2	Xtriage
Anisotropy	1.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 48.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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(^{o})	Ideal(^{o})
1	B	408	GLU	CG-CD-OE2	-25.33	67.64	118.30
1	A	33	GLU	CB-CG-CD	19.16	165.93	114.20
1	D	408	GLU	CG-CD-OE1	-16.68	84.94	118.30
1	B	408	GLU	CG-CD-OE1	15.71	149.73	118.30
1	B	263	ARG	NE-CZ-NH2	15.03	127.81	120.30
1	A	408	GLU	OE1-CD-OE2	13.73	139.77	123.30
1	A	148	GLU	CG-CD-OE2	-13.15	91.99	118.30
1	A	33	GLU	CG-CD-OE2	-12.69	92.93	118.30
1	C	4	ARG	NE-CZ-NH2	-12.49	114.06	120.30
1	C	5[A]	ARG	NE-CZ-NH2	-12.36	114.12	120.30
1	C	5[B]	ARG	NE-CZ-NH2	-12.36	114.12	120.30
1	D	4	ARG	NE-CZ-NH2	12.29	126.44	120.30
1	A	33	GLU	CG-CD-OE1	12.10	142.50	118.30
1	C	4	ARG	NE-CZ-NH1	11.82	126.21	120.30
1	D	4	ARG	NE-CZ-NH1	-11.69	114.45	120.30
1	C	5[A]	ARG	NE-CZ-NH1	11.11	125.86	120.30
1	C	5[B]	ARG	NE-CZ-NH1	11.11	125.86	120.30
1	D	42	LYS	CB-CG-CD	-10.93	83.19	111.60
1	A	4	ARG	NE-CZ-NH2	10.86	125.73	120.30
1	B	263	ARG	NE-CZ-NH1	-10.46	115.07	120.30

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

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

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

There are no chirality outliers.

All (8) planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3285	0	3300	99	0
1	B	3288	0	3306	91	0
1	C	3280	0	3295	112	0
1	D	3297	0	3313	121	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	27	0	21	0	0
4	B	27	0	21	0	0
4	C	27	0	21	0	0
4	D	27	0	21	0	0
5	A	28	0	28	0	0
5	B	28	0	28	0	0
5	C	28	0	28	0	0
5	D	28	0	28	0	0
6	A	8	0	0	0	0
6	B	8	0	0	0	0
6	C	8	0	0	1	0
6	D	8	0	0	1	0
7	A	135	0	0	7	0
7	B	116	0	0	3	0
7	C	183	0	0	10	1
7	D	174	0	0	8	0
All	All	14034	0	13410	376	1

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

All (376) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285[B]:ARG:CD	1:D:285[B]:ARG:HD2	1.54	1.37
1:C:285[B]:ARG:CD	1:D:285[B]:ARG:CD	2.09	1.31
1:C:285[B]:ARG:HD2	1:D:285[B]:ARG:CD	1.65	1.23
1:C:285[B]:ARG:HD2	1:D:285[B]:ARG:NE	1.62	1.14
1:D:243[A]:ARG:HD2	7:D:578:HOH:O	1.48	1.11
1:A:214:GLU:OE1	7:A:713:HOH:O	1.68	1.10
1:C:285[B]:ARG:HD3	1:D:285[B]:ARG:HD2	1.33	1.06
1:B:231:PHE:H	1:B:257:ASN:HD21	1.08	0.97
1:D:212:THR:HG22	1:D:215:LEU:H	1.30	0.95
1:A:231:PHE:H	1:A:257:ASN:HD21	1.16	0.94
1:C:231:PHE:H	1:C:257:ASN:HD21	1.15	0.93
1:C:285[B]:ARG:NE	1:D:285[B]:ARG:HD2	1.83	0.93
1:A:212:THR:HG22	1:A:215:LEU:H	1.32	0.92
1:C:285[B]:ARG:HD3	1:D:285[B]:ARG:CD	1.93	0.92
1:D:137:PHE:CZ	1:D:145:MSE:HE2	2.04	0.91
1:B:112:ARG:HD3	7:B:501:HOH:O	1.69	0.91
1:A:216:VAL:HG13	1:A:251:ALA:HB2	1.53	0.90
1:D:112:ARG:HD2	1:D:334:GLY:O	1.70	0.90
1:B:216:VAL:HG13	1:B:251:ALA:HB2	1.54	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:D:44:GLU:O	1:D:48:VAL:HG13	1.73	0.89
1:C:212:THR:HG22	1:C:215:LEU:H	1.36	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:D:212:THR:HG21	7:D:626:HOH:O	1.77	0.85
1:C:44:GLU:O	1:C:48:VAL:HG13	1.76	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:C:27[B]:ARG:NH2	1:C:29:GLU:OE2	2.13	0.81
1:A:332:PRO:O	1:B:363:THR:HG21	1.80	0.81
1:B:137:PHE:CZ	1:B:145:MSE:HE2	2.15	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	7:D:500:HOH:O	1.83	0.78
1:D:122:THR:HG23	1:D:144:SER:HA	1.66	0.78
1:C:216:VAL:HG13	1:C:251:ALA:HB2	1.64	0.77
1:B:168:LEU:HB2	1:B:199[B]:ILE:HG22	1.66	0.77
1:B:145:MSE:HE3	1:B:149:ARG:NH2	1.99	0.77
1:B:122:THR:HG23	1:B:144:SER:HA	1.67	0.77
1:D:168:LEU:HB2	1:D:199[B]:ILE:HG22	1.67	0.76
1:C:276:VAL:HG13	1:C:323:CYS:HB3	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:D:137:PHE:CE2	1:D:145:MSE:CE	2.71	0.74
1:B:137:PHE:CE2	1:B:145:MSE:HE2	2.23	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	7:D:654:HOH:O	1.88	0.71
1:C:316[A]:ARG:HG2	1:C:316[A]:ARG:HH11	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1:B:316[A]:ARG:HG2	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:B:400:MSE:CE	7:C:744:HOH:O	2.40	0.69
1:C:343:ASN:HB3	7:C:615:HOH:O	1.92	0.69
1:A:94:LEU:HD11	1:D:400:MSE:HE1	1.73	0.69
1:C:112:ARG:HD3	7: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:D:137:PHE:HE2	1:D:145:MSE:CE	2.09	0.66
1:C:156:TYR:O	1:C:160:THR:HG23	1.95	0.66
1:A:122:THR:HG21	7:A:633:HOH:O	1.95	0.66
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: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:C:156:TYR:O	1:C:160:THR:CG2	2.45	0.64
1:B:156:TYR:O	1:B: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:D:137:PHE:HE2	1:D:145:MSE:HE1	1.63	0.63
1:C:203:THR:HG22	1:C:204:PRO:HD3	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:341:MSE:HG2	1:D:341:MSE:HE2	1.82	0.61
1:C:332:PRO:O	1:D:363:THR:HG21	2.00	0.61
1:B:131:HIS:CD2	1:B:260[A]:VAL:HG11	2.35	0.61
1:A:212:THR:HG21	7:A:683:HOH:O	2.01	0.61
1:A:319:THR:HG22	1:B:115:ASP:OD1	2.00	0.60
1:A:137:PHE:HE2	1:A:145:MSE:CE	2.13	0.60
1:D:43:GLU:HG2	1:D:44:GLU:N	2.14	0.60
1:C:137:PHE:HE2	1:C:145:MSE:HE1	1.65	0.60
1:D:131:HIS:CD2	1:D:260[A]:VAL:HG11	2.37	0.60
1:C:56:ARG:HD2	1:C:139:GLY:O	2.02	0.60
1:C:307:LYS:HE3	1:C:310:GLU:OE1	2.01	0.60
1:A:209:GLN:H	1:A:209:GLN:NE2	2.00	0.59
1:A:112:ARG:HD3	7: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:C:216:VAL:HG13	1:C:251:ALA:CB	2.34	0.58
1:B:133:THR:CG2	1:B:293:ASP:OD2	2.51	0.58
1:D:363:THR:HG22	1:D:364:THR:H	1.69	0.58
1:A:263:ARG:HD3	7:A:629:HOH:O	2.03	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:C:231:PHE:N	1:C:257:ASN:HD21	1.93	0.56
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:D:238:THR:HG23	1:D:240:GLU:OE1	2.05	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:B:148:GLU:OE2	1:B:152:LYS:HE3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243[A]:ARG:HG3	1:D:243[A]:ARG:NH1	2.10	0.56
1:D:238:THR:HG22	1:D:241:SER:H	1.71	0.56
1:C:277:ASN:OD1	1:C:319:THR:HG21	2.06	0.55
1:C:238:THR:HG22	1:C:241:SER:H	1.72	0.55
1:D:232:ASN:HD21	1:D:260[B]:VAL:H	1.54	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:C:77:ARG:HD3	7:C:727:HOH:O	2.07	0.55
1:D:109:LEU:HD21	1:D:117:VAL:CG1	2.36	0.55
1:C:122:THR:HG21	7: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
7: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	7:D:649:HOH:O	1.91	0.53
1:D:109:LEU:HD21	1:D:117:VAL:HG11	1.90	0.53
1:C:285[B]:ARG:HD3	1:D:285[B]:ARG:HD3	1.82	0.53
1:C:133:THR:HG23	1:C:293:ASP:HB2	1.89	0.53
1:B:5[A]:ARG:NH2	1:B:12:VAL:O	2.42	0.53
1:D:232:ASN:HD21	1:D:260[A]:VAL:H	1.55	0.53
1:A:156:TYR:O	1:A:160:THR:HG23	2.07	0.53
1:C:376:ASN:CG	1:D:73:ASN:HD22	2.11	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:CG	2.39	0.52
1:B:74:ASP:HB3	1:B:77:ARG:HG2	1.92	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:NE2	1:B:209:GLN:H	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:231:PHE:N	1:B:257:ASN:HD21	1.92	0.52
1:B:27[A]:ARG:NH1	1:B:124:MSE:HE2	2.25	0.52
1:C:133:THR:CG2	1:C:293:ASP:OD2	2.57	0.52
1:B:120:LEU:HD12	1:B:170:GLY:HA2	1.90	0.52
1:B:216:VAL:CG1	1:B:251:ALA:HB2	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:PHE:HE2	1:A:145:MSE:HE1	1.75	0.52
1:D:341:MSE:HB2	1:D:342:PRO:CD	2.40	0.52
1:C:74:ASP:HB3	1:C:77:ARG:CG	2.39	0.52
1:C:122:THR:HG23	7:C:732:HOH:O	2.08	0.51
1:B:277:ASN:OD1	1:B:319:THR:HG21	2.09	0.51
1:D:5[A]:ARG:NH2	7:D:623:HOH:O	2.40	0.51
1:D:5[A]:ARG:NH1	1:D:14:ASP:OD1	2.41	0.51
1:A:260[B]:VAL:HG22	1:A:262:LEU:HG	1.92	0.51
1:A:308:GLY:HA3	1:A:327:PHE:CE2	2.45	0.51
1:A:401:ALA:HB2	1:C:363:THR:HG23	1.93	0.51
1:D:145:MSE:HE3	1:D:149:ARG:HH22	1.71	0.51
1:A:376:ASN:CG	1:B:73:ASN:HD22	2.14	0.51
1:D:411:LYS:O	1:D:412:ARG:HG3	2.11	0.51
1:A:122:THR:CG2	7: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:C:285[B]:ARG:CZ	1:D:285[B]:ARG:HD2	2.40	0.50
1:A:199[B]:ILE:HG13	1:A:227:LEU:HD12	1.93	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	6: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	7: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:NE2	1:D:209:GLN:H	2.10	0.49
1:A:232:ASN:ND2	1:A:260[B]:VAL:H	2.10	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:232:ASN:ND2	1:B:260[A]:VAL:H	2.11	0.49
1:A:203:THR:HG22	1:A:204:PRO:HD3	1.96	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:B:59:ILE:HA	1:B:127:MSE:HG2	1.95	0.48
1:C:73:ASN:HD22	1:D:376:ASN:CG	2.17	0.48
1:B:109:LEU:HD21	1:B:117:VAL:CG1	2.43	0.48
1:A:276:VAL:HG22	1:A:286:PRO:CG	2.43	0.48
1:D:277:ASN:OD1	1:D:319:THR:HG21	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:273:LYS:HZ2	1:D:277:ASN:HD21	1.61	0.47
1:D:233:HIS:CG	1:D:234:PRO:HD2	2.48	0.47
1:C:137:PHE:HZ	1:C:145:MSE:HE2	1.78	0.47
1:A:260[A]:VAL:HG13	1:A:262:LEU:HG	1.94	0.47
1:A:109:LEU:HD21	1:A:117:VAL:HG11	1.94	0.47
1:A:276:VAL:HG22	1:A:286:PRO:HG2	1.96	0.47
1:C:74:ASP:HB3	1:C:77:ARG:HG2	1.97	0.47
1:B:238:THR:HG23	1:B:240:GLU:OE1	2.15	0.47
1:C:133:THR:HG21	1:C:293:ASP:OD2	2.14	0.47
1:B:203:THR:HG22	1:B:204:PRO:CD	2.40	0.47
1:B:232:ASN:HD21	1:B:260[B]:VAL:H	1.63	0.47
1:D:6:TYR:O	1:D:10:LYS:HB3	2.15	0.47
1:B:232:ASN:ND2	1:B:260[B]:VAL:H	2.12	0.47
1:A:147:MSE:HE1	1:A:180:THR:HG23	1.97	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:D:243[A]:ARG:CD	7:D:578:HOH:O	2.31	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: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:D:203:THR:HG22	1:D:204:PRO:HD3	1.98	0.46
1:A:308:GLY:HA3	1:A:327:PHE:CZ	2.50	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:D:276:VAL:HG22	1:D:286:PRO:HG2	1.98	0.46
1:C:260[B]:VAL:HG22	1:C:262:LEU:HG	1.96	0.46
1:A:115:ASP:OD1	1:B:319:THR:CG2	2.63	0.46
1:A:386:VAL:HG21	7: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	7:C:775:HOH:O	2.17	0.45
1:D:124:MSE:SE	1:D:175:LEU:HD12	2.66	0.45
1:A:232:ASN:HD21	1:A:260[B]:VAL:H	1.64	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:320:SER:HB3	1:D:322:TYR:CE1	2.52	0.45
1:D:74:ASP:HB3	1:D:77:ARG:CG	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ILE:HD11	1:A:81:ILE:HD11	1.97	0.45
1:D:212:THR:CG2	1:D:215:LEU:H	2.15	0.45
1:A:145:MSE:HE3	1:A:149:ARG:HH22	1.79	0.45
1:D:122:THR:HG21	7:D:621:HOH:O	2.17	0.45
1:C:109:LEU:HD21	1:C:117:VAL:CG1	2.48	0.45
1:D:120:LEU:HD12	1:D:170:GLY:HA2	1.98	0.45
1:B:348:GLN:HG3	1:C:306:SER:HB2	1.99	0.45
1:D:30:THR:OG1	1:D:33:GLU:HB2	2.17	0.44
1:C:59:ILE:HA	1:C:127:MSE:HG2	1.98	0.44
1:A:156:TYR:O	1:A:160:THR:HG22	2.17	0.44
1:A:232:ASN:HD21	1:A:260[A]:VAL:H	1.65	0.44
1:B:253:VAL:HA	1:B:254:PRO:HD3	1.91	0.44
1:A:48:VAL:HG12	1:A:82:PRO:HD2	1.99	0.44
1:C:27[A]:ARG:NH1	1:C:124:MSE:HE2	2.33	0.44
1:A:129:CYS:HB3	1:A:131:HIS:CE1	2.53	0.44
1:D:133:THR:HG23	1:D:293:ASP:HB2	1.98	0.44
1:A:363:THR:HG23	1:C:401:ALA:HB2	2.00	0.44
1:B:273:LYS:NZ	1:B:277:ASN:HD21	2.15	0.44
1:C:5[A]:ARG:NH2	1:C:12:VAL:O	2.50	0.43
1:D:123:ASP:OD1	1:D:123:ASP:C	2.56	0.43
1:D:59:ILE:HA	1:D:127:MSE:HG2	2.00	0.43
1:C:206:VAL:HG21	7: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:C:123:ASP:OD1	1:C:123:ASP:C	2.57	0.43
1:B:122:THR:HG22	1:B:124:MSE:H	1.83	0.43
1:D:160:THR:HA	1:D:161:PRO:HD3	1.65	0.43
1:C:109:LEU:CD2	1:C:117:VAL:HG13	2.49	0.43
1:B:285:ARG:HD3	1:B:322:TYR:O	2.18	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: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:C:120:LEU:HD12	1:C:170:GLY:HA2	2.01	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: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: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:A:109:LEU:HD21	1:A:117:VAL:HG13	1.99	0.42
1:D:171:GLY:HA2	6:D:418:SF4:S4	2.60	0.42
1:D:38:ILE:HD11	1:D:81:ILE:HD11	2.01	0.42
1:D:199[A]:ILE:HD11	1:D:201:SER:HB2	2.01	0.42
1:B:145:MSE:HE3	1:B:149:ARG:HH22	1.82	0.42
1:A:5[A]:ARG:NH2	1:A:12:VAL:O	2.53	0.42
1:C:109:LEU:HD21	1:C:117:VAL:HG11	2.02	0.42
1:A:189:ARG:HD2	1:A:222:TYR:O	2.20	0.42
1:D:216:VAL:CG1	1:D:251:ALA:HB2	2.40	0.41
1:D:122:THR:HG22	1:D:124:MSE:H	1.84	0.41
1:C:253:VAL:HA	1:C:254:PRO:HD3	1.91	0.41
1:A:105:PRO:HG2	1:A:109:LEU:HD12	2.01	0.41
1:C:273:LYS:HZ2	1:C:319:THR:HG23	1.84	0.41
1:A:238:THR:HG22	1:A:240:GLU:N	2.35	0.41
1:C:147:MSE:HE1	1:C:180:THR:HG23	2.02	0.41
1:B:137:PHE:CE2	1:B:145:MSE:HE1	2.46	0.41
1:B:181:LEU:HD13	1:B:218:MSE:HE1	2.02	0.41
1:C:307:LYS:HD3	1:C:307:LYS:O	2.20	0.41
1:D:238:THR:CG2	1:D:240:GLU:OE1	2.68	0.41
1:C:156:TYR:O	1:C:160:THR:HG22	2.18	0.41
1:A:354:ILE:HD11	1:C:395:LEU:HD13	2.02	0.41
1:B:203:THR:CG2	1:B:211:ILE:HD11	2.51	0.41
1:A:238:THR:CG2	1:A:240:GLU:OE1	2.69	0.41
1:B:260[A]:VAL:HG13	1:B:262:LEU:HG	2.02	0.41
1:C:304:PRO:HD3	1:D:371:TYR:CG	2.56	0.41
1:A:260[A]:VAL:HG13	1:A:262:LEU:CG	2.51	0.41
1:A:405:VAL:HG13	1:D:403:GLU:O	2.20	0.41
1:B:27[B]:ARG:HH21	1:B:58:ALA:HB1	1.86	0.40
1:D:147:MSE:HE1	1:D:180:THR:HG23	2.03	0.40
1:B:260[A]:VAL:HG13	1:B:262:LEU:CD1	2.51	0.40
1:A:243[B]:ARG:NH1	1:A:246:GLN:OE1	2.47	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)
7:C:764:HOH:O	7: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%)	26	21
1	B	416/416 (100%)	398 (96%)	15 (4%)	3 (1%)	26	21
1	C	415/416 (100%)	397 (96%)	15 (4%)	3 (1%)	26	21
1	D	417/416 (100%)	397 (95%)	17 (4%)	3 (1%)	26	21
All	All	1664/1664 (100%)	1592 (96%)	60 (4%)	12 (1%)	26	21

All (12) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	374/362 (103%)	316 (84%)	58 (16%)	3 1
1	B	374/362 (103%)	315 (84%)	59 (16%)	3 1
1	C	373/362 (103%)	320 (86%)	53 (14%)	4 2
1	D	375/362 (104%)	318 (85%)	57 (15%)	3 1
All	All	1496/1448 (103%)	1269 (85%)	227 (15%)	4 1

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

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

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

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

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

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

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

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

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

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no 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	21,29,29	2.20	4 (19%)	17,42,42	2.22	7 (41%)
6	SF4	A	418	1,4	0,12,12	0.00	-	0,24,24	0.00	-
5	PLP	A	419	5	15,15,16	2.67	2 (13%)	21,22,23	1.24	3 (14%)
5	LYS	A	420[A]	-	6,9,9	0.39	0	4,10,10	0.68	0
5	LYS	A	420[B]	-	6,9,9	0.38	0	4,10,10	0.70	0
3	SO4	A	592	-	4,4,4	0.19	0	6,6,6	0.18	0
4	SAM	B	417	6	21,29,29	2.15	5 (23%)	17,42,42	2.38	6 (35%)
6	SF4	B	418	1,4	0,12,12	0.00	-	0,24,24	0.00	-
5	PLP	B	419	5	15,15,16	2.69	2 (13%)	21,22,23	0.92	0
5	LYS	B	420[A]	-	6,9,9	0.40	0	4,10,10	1.17	0
5	LYS	B	420[B]	-	6,9,9	0.40	0	4,10,10	1.10	0
3	SO4	B	495	-	4,4,4	0.26	0	6,6,6	0.27	0
4	SAM	C	417	6	21,29,29	2.29	5 (23%)	17,42,42	2.21	5 (29%)
6	SF4	C	418	1,4	0,12,12	0.00	-	0,24,24	0.00	-
5	PLP	C	419	5	15,15,16	2.74	3 (20%)	21,22,23	0.97	1 (4%)
5	LYS	C	420[A]	-	6,9,9	0.45	0	4,10,10	1.20	0
5	LYS	C	420[B]	-	6,9,9	0.44	0	4,10,10	1.11	0
3	SO4	C	593	-	4,4,4	0.21	0	6,6,6	0.39	0
4	SAM	D	417	6	21,29,29	2.20	3 (14%)	17,42,42	2.30	5 (29%)
6	SF4	D	418	1,4	0,12,12	0.00	-	0,24,24	0.00	-
5	PLP	D	419	5	15,15,16	2.84	3 (20%)	21,22,23	1.21	2 (9%)
5	LYS	D	420[A]	-	6,9,9	0.34	0	4,10,10	1.04	0
5	LYS	D	420[B]	-	6,9,9	0.36	0	4,10,10	0.93	0
3	SO4	D	494	-	4,4,4	0.24	0	6,6,6	0.43	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	-	0/8/33/33	0/3/3/3
6	SF4	A	418	1,4	-	0/0/48/48	0/6/5/5
5	PLP	A	419	5	-	0/6/6/8	0/1/1/1
5	LYS	A	420[A]	-	-	0/5/9/9	0/0/0/0
5	LYS	A	420[B]	-	-	0/5/9/9	0/0/0/0

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

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	419	PLP	C4A-C4	-9.72	1.31	1.51
5	C	419	PLP	C4A-C4	-9.45	1.32	1.51
5	B	419	PLP	C4A-C4	-9.28	1.32	1.51
5	A	419	PLP	C4A-C4	-8.92	1.33	1.51
5	D	419	PLP	P-O2P	-3.16	1.43	1.54
5	C	419	PLP	P-O2P	-2.52	1.45	1.54
5	A	419	PLP	P-O2P	-2.50	1.45	1.54
5	B	419	PLP	P-O2P	-2.04	1.47	1.54
5	C	419	PLP	O4P-C5A	2.00	1.53	1.44
5	D	419	PLP	C3-C2	2.17	1.42	1.40
4	B	417	SAM	CG-CB	2.18	1.55	1.52
4	C	417	SAM	CG-CB	2.24	1.55	1.52
4	C	417	SAM	CE-SD	2.41	1.95	1.78
4	C	417	SAM	O4'-C1'	2.48	1.44	1.41
4	B	417	SAM	CE-SD	2.53	1.96	1.78
4	A	417	SAM	CE-SD	2.63	1.97	1.78
4	B	417	SAM	O4'-C1'	2.78	1.44	1.41
4	D	417	SAM	CE-SD	2.87	1.98	1.78
4	A	417	SAM	C2-N3	3.10	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	417	SAM	C5-C4	3.12	1.47	1.40
4	D	417	SAM	C5-C4	3.18	1.47	1.40
4	A	417	SAM	C5-C4	3.45	1.48	1.40
4	C	417	SAM	C5-C4	3.53	1.48	1.40
4	B	417	SAM	CG-SD	7.69	1.97	1.80
4	A	417	SAM	CG-SD	8.03	1.98	1.80
4	C	417	SAM	CG-SD	8.36	1.99	1.80
4	D	417	SAM	CG-SD	8.42	1.99	1.80

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	417	SAM	N3-C2-N1	-6.20	124.15	128.89
4	D	417	SAM	N3-C2-N1	-5.88	124.39	128.89
4	A	417	SAM	N3-C2-N1	-5.36	124.79	128.89
4	C	417	SAM	N3-C2-N1	-4.86	125.17	128.89
4	B	417	SAM	C2'-C1'-N9	-4.39	107.59	114.29
4	C	417	SAM	C2'-C1'-N9	-4.38	107.60	114.29
4	D	417	SAM	C2'-C1'-N9	-4.25	107.79	114.29
4	C	417	SAM	C4'-O4'-C1'	-3.97	105.36	109.72
4	A	417	SAM	C2'-C1'-N9	-3.71	108.62	114.29
5	A	419	PLP	O4P-P-O1P	-3.19	99.02	107.14
4	C	417	SAM	C1'-N9-C4	-3.02	122.38	126.94
4	B	417	SAM	C1'-N9-C4	-2.95	122.50	126.94
4	D	417	SAM	C4-C5-N7	-2.83	106.87	109.48
4	B	417	SAM	C4-C5-N7	-2.74	106.96	109.48
4	C	417	SAM	C4-C5-N7	-2.65	107.04	109.48
4	A	417	SAM	C4'-O4'-C1'	-2.46	107.02	109.72
4	B	417	SAM	C4'-O4'-C1'	-2.44	107.03	109.72
4	A	417	SAM	C1'-N9-C4	-2.34	123.41	126.94
5	C	419	PLP	C5A-C5-C4	-2.19	118.75	121.65
4	A	417	SAM	C4-C5-N7	-2.01	107.63	109.48
5	A	419	PLP	O3P-P-O1P	2.12	117.40	110.58
5	D	419	PLP	O3-C3-C2	2.19	121.47	117.66
5	A	419	PLP	O2P-P-O4P	2.43	113.56	106.56
4	B	417	SAM	CB-CA-N	2.73	118.28	110.52
5	D	419	PLP	C4A-C4-C5	2.83	123.83	120.88
4	D	417	SAM	CB-CA-N	2.86	118.66	110.52
4	A	417	SAM	O4'-C1'-N9	3.15	114.70	108.10
4	A	417	SAM	CB-CA-N	3.24	119.73	110.52
4	D	417	SAM	O4'-C1'-N9	3.28	114.96	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	400/416 (96%)	1.71	130 (32%)	1	1	18, 39, 61, 72	9 (2%)
1	B	401/416 (96%)	1.99	173 (43%)	0	0	20, 43, 79, 98	7 (1%)
1	C	400/416 (96%)	1.50	100 (25%)	1	1	16, 32, 59, 73	7 (1%)
1	D	401/416 (96%)	1.45	101 (25%)	1	1	15, 32, 55, 69	6 (1%)
All	All	1602/1664 (96%)	1.66	504 (31%)	1	1	15, 36, 65, 98	29 (1%)

All (504) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	48	VAL	11.1
1	B	22	TRP	8.4
1	C	64	LEU	7.6
1	B	38	ILE	7.5
1	B	54	SER	6.9
1	B	85	LEU	6.9
1	D	6	TYR	6.7
1	B	81	ILE	6.6
1	C	40	LEU	6.6
1	C	369	ILE	6.6
1	B	139	GLY	6.4
1	C	8	LEU	6.3
1	D	9	PHE	6.2
1	B	40	LEU	6.2
1	C	85	LEU	6.2
1	B	48	VAL	6.2
1	C	38	ILE	6.0
1	B	126	SER	6.0
1	A	6	TYR	5.9
1	B	53	LYS	5.8
1	B	90	ALA	5.8

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Mol	Chain	Res	Type	RSRZ
1	C	70	ASN	5.7
1	C	84	ALA	5.7
1	A	17	TRP	5.6
1	B	37	TYR	5.6
1	C	31	VAL	5.6
1	B	59	ILE	5.4
1	D	40	LEU	5.4
1	C	9	PHE	5.4
1	A	85	LEU	5.3
1	B	12	VAL	5.2
1	D	52	VAL	5.2
1	B	80	ALA	5.2
1	A	369	ILE	5.2
1	A	22	TRP	5.2
1	A	9	PHE	5.1
1	A	49	ALA	5.1
1	A	81	ILE	5.0
1	C	67	ILE	5.0
1	A	38	ILE	5.0
1	D	67	ILE	4.9
1	D	38	ILE	4.9
1	D	8	LEU	4.9
1	C	383	LYS	4.8
1	D	4	ARG	4.8
1	D	369	ILE	4.8
1	A	15	ALA	4.8
1	B	71	ASP	4.8
1	B	31	VAL	4.7
1	B	108	GLY	4.7
1	B	138	ALA	4.7
1	C	386	VAL	4.7
1	D	386	VAL	4.6
1	B	4	ARG	4.6
1	C	4	ARG	4.6
1	A	14	ASP	4.6
1	C	69	PRO	4.5
1	B	9	PHE	4.5
1	A	51	CYS	4.5
1	A	37	TYR	4.5
1	C	3	ASN	4.5
1	D	34	LEU	4.5
1	C	43	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	40	LEU	4.4
1	D	156	TYR	4.4
1	C	106	VAL	4.4
1	D	106	VAL	4.4
1	C	80	ALA	4.3
1	C	90	ALA	4.3
1	B	87	LEU	4.3
1	C	37	TYR	4.3
1	D	69	PRO	4.2
1	A	80	ALA	4.2
1	C	50	GLN	4.2
1	D	157	ILE	4.1
1	D	154	ILE	4.1
1	A	72	PRO	4.1
1	C	81	ILE	4.1
1	C	54	SER	4.1
1	C	6	TYR	4.0
1	C	73	ASN	4.0
1	C	89	LYS	4.0
1	B	143	ASP	4.0
1	A	379	VAL	4.0
1	B	8	LEU	4.0
1	A	168	LEU	3.9
1	C	11	ASP	3.9
1	B	107	PRO	3.9
1	C	47	GLY	3.9
1	B	405	VAL	3.9
1	C	105	PRO	3.9
1	B	88	ASN	3.9
1	A	345	VAL	3.9
1	D	22	TRP	3.9
1	D	72	PRO	3.8
1	C	34	LEU	3.8
1	B	39	PRO	3.8
1	A	54	SER	3.8
1	A	84	ALA	3.8
1	A	194	VAL	3.8
1	B	6	TYR	3.8
1	B	92	ALA	3.7
1	B	142	ASP	3.7
1	C	7	GLU	3.7
1	A	27[A]	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	184	ILE	3.7
1	D	168	LEU	3.7
1	C	381	THR	3.7
1	D	12	VAL	3.7
1	B	156	TYR	3.7
1	D	11	ASP	3.7
1	D	190	GLU	3.7
1	D	37	TYR	3.7
1	D	49	ALA	3.7
1	B	197	VAL	3.6
1	B	17	TRP	3.6
1	D	183	TYR	3.6
1	B	153	ALA	3.6
1	A	109	LEU	3.6
1	D	188	LEU	3.6
1	C	343	ASN	3.6
1	B	11	ASP	3.5
1	C	374	GLY	3.5
1	A	4	ARG	3.5
1	A	387	HIS	3.5
1	B	52	VAL	3.5
1	A	59	ILE	3.5
1	D	77	ARG	3.5
1	A	36	LYS	3.5
1	D	36	LYS	3.5
1	B	93	ASP	3.5
1	A	121	ILE	3.5
1	A	45	GLU	3.4
1	A	41	THR	3.4
1	B	312	ILE	3.4
1	B	62	TYR	3.4
1	B	70	ASN	3.4
1	B	41	THR	3.4
1	A	5[A]	ARG	3.4
1	D	186	ALA	3.4
1	A	52	VAL	3.4
1	B	34	LEU	3.4
1	A	157	ILE	3.4
1	A	12	VAL	3.4
1	B	35	LYS	3.4
1	B	64	LEU	3.4
1	C	39	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	53	LYS	3.3
1	B	28	ILE	3.3
1	B	26	ASN	3.3
1	B	168	LEU	3.3
1	C	87	LEU	3.3
1	D	301	PHE	3.3
1	B	77	ARG	3.3
1	A	237	ILE	3.3
1	B	339	PRO	3.3
1	C	235	ASN	3.3
1	C	61	PRO	3.3
1	C	62	TYR	3.3
1	D	64	LEU	3.3
1	B	83	THR	3.3
1	B	199[A]	ILE	3.2
1	B	43	GLU	3.2
1	A	10	LYS	3.2
1	B	55	LEU	3.2
1	B	174	LEU	3.2
1	B	32	GLU	3.2
1	D	173	ALA	3.2
1	D	342	PRO	3.2
1	A	28	ILE	3.2
1	D	162	GLN	3.2
1	C	49	ALA	3.2
1	B	326	THR	3.2
1	B	82	PRO	3.2
1	A	408	GLU	3.2
1	A	386	VAL	3.2
1	C	407	LEU	3.2
1	B	72	PRO	3.1
1	D	28	ILE	3.1
1	D	340	VAL	3.1
1	B	121	ILE	3.1
1	B	154	ILE	3.1
1	C	384	LYS	3.1
1	D	43	GLU	3.1
1	A	70	ASN	3.1
1	A	150	ILE	3.1
1	A	346[A]	ILE	3.1
1	A	11	ASP	3.1
1	C	344	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	153	ALA	3.1
1	B	338	THR	3.1
1	A	354	ILE	3.1
1	C	35	LYS	3.1
1	B	329	VAL	3.0
1	B	67	ILE	3.0
1	A	344	TYR	3.0
1	B	89	LYS	3.0
1	B	94	LEU	3.0
1	C	109	LEU	3.0
1	B	149	ARG	3.0
1	B	95	GLU	3.0
1	C	121	ILE	3.0
1	A	119	LEU	3.0
1	B	117	VAL	3.0
1	D	3	ASN	3.0
1	D	343	ASN	3.0
1	C	91	ALA	3.0
1	C	53	LYS	3.0
1	D	53	LYS	3.0
1	D	370	ASN	3.0
1	B	412	ARG	3.0
1	B	328	VAL	3.0
1	C	63	TYR	3.0
1	B	13	SER	3.0
1	A	138	ALA	3.0
1	D	111	HIS	3.0
1	C	72	PRO	2.9
1	B	118	LEU	2.9
1	B	181	LEU	2.9
1	D	35	LYS	2.9
1	D	5[A]	ARG	2.9
1	B	334	GLY	2.9
1	B	10	LYS	2.9
1	A	199[A]	ILE	2.9
1	B	355	LEU	2.9
1	C	48	VAL	2.9
1	A	106	VAL	2.9
1	B	19	ASP	2.9
1	B	50	GLN	2.9
1	B	7	GLU	2.9
1	D	94	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	24	VAL	2.9
1	A	174	LEU	2.9
1	B	51	CYS	2.9
1	B	47	GLY	2.8
1	B	36	LYS	2.8
1	D	185	ILE	2.8
1	B	343	ASN	2.8
1	B	288	TYR	2.8
1	C	36	LYS	2.8
1	C	59	ILE	2.8
1	C	237	ILE	2.8
1	A	175	LEU	2.8
1	A	340	VAL	2.8
1	B	305	VAL	2.8
1	C	30	THR	2.8
1	C	76	VAL	2.8
1	C	405	VAL	2.8
1	A	26	ASN	2.8
1	D	412	ARG	2.8
1	A	67	ILE	2.8
1	B	44	GLU	2.8
1	B	382	GLY	2.8
1	D	405	VAL	2.8
1	B	188	LEU	2.8
1	B	128	TYR	2.8
1	B	61	PRO	2.8
1	B	309	ILE	2.8
1	B	183	TYR	2.7
1	C	17	TRP	2.7
1	B	219	LEU	2.7
1	D	174	LEU	2.7
1	A	39	PRO	2.7
1	D	238	THR	2.7
1	C	55	LEU	2.7
1	A	353	VAL	2.7
1	B	63	TYR	2.7
1	C	128	TYR	2.7
1	B	323	CYS	2.7
1	D	216	VAL	2.7
1	D	179	GLU	2.7
1	A	68	ASP	2.7
1	A	301	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	208	PRO	2.7
1	C	119	LEU	2.7
1	B	386	VAL	2.7
1	B	68	ASP	2.7
1	A	111	HIS	2.7
1	D	344	TYR	2.7
1	A	64	LEU	2.6
1	B	76	VAL	2.6
1	A	343	ASN	2.6
1	A	3	ASN	2.6
1	D	70	ASN	2.6
1	D	407	LEU	2.6
1	C	354	ILE	2.6
1	B	110	THR	2.6
1	B	135	ARG	2.6
1	A	128	TYR	2.6
1	A	120	LEU	2.6
1	B	175	LEU	2.6
1	A	35	LYS	2.6
1	B	58	ALA	2.6
1	B	342	PRO	2.6
1	C	382	GLY	2.6
1	A	44	GLU	2.6
1	D	50	GLN	2.6
1	B	316[A]	ARG	2.6
1	B	373	PRO	2.6
1	C	83	THR	2.6
1	D	59	ILE	2.6
1	D	92	ALA	2.6
1	A	329	VAL	2.6
1	B	209	GLN	2.6
1	A	66	LEU	2.6
1	A	32	GLU	2.6
1	A	62	TYR	2.5
1	A	63	TYR	2.5
1	A	156	TYR	2.5
1	D	17	TRP	2.5
1	A	166	VAL	2.5
1	A	253	VAL	2.5
1	D	166	VAL	2.5
1	A	285[A]	ARG	2.5
1	B	301	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	69	PRO	2.5
1	A	224	PRO	2.5
1	D	338	THR	2.5
1	A	7	GLU	2.5
1	B	327	PHE	2.5
1	C	71	ASP	2.5
1	B	109	LEU	2.5
1	B	157	ILE	2.5
1	D	271	VAL	2.5
1	A	61	PRO	2.5
1	C	42	LYS	2.5
1	B	290	TYR	2.5
1	D	80	ALA	2.5
1	A	162	GLN	2.5
1	B	56	ARG	2.5
1	B	294	LEU	2.5
1	A	383	LYS	2.5
1	B	205	VAL	2.5
1	D	48	VAL	2.5
1	A	188	LEU	2.5
1	C	321	GLY	2.5
1	B	411	LYS	2.5
1	B	119	LEU	2.4
1	B	340	VAL	2.4
1	C	22	TRP	2.4
1	B	162	GLN	2.4
1	B	163	VAL	2.4
1	D	329	VAL	2.4
1	A	342	PRO	2.4
1	C	82	PRO	2.4
1	D	62	TYR	2.4
1	D	137	PHE	2.4
1	B	160	THR	2.4
1	C	44	GLU	2.4
1	A	77	ARG	2.4
1	B	170	GLY	2.4
1	B	345	VAL	2.4
1	C	12	VAL	2.4
1	C	92	ALA	2.4
1	A	151	ASP	2.4
1	A	183	TYR	2.4
1	A	169	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	144	SER	2.4
1	B	260[A]	VAL	2.4
1	A	339	PRO	2.4
1	B	211	ILE	2.4
1	B	330	ASP	2.4
1	A	122	THR	2.4
1	A	160	THR	2.4
1	A	296	LEU	2.4
1	B	187	LYS	2.4
1	B	383	LYS	2.4
1	D	33	GLU	2.4
1	A	265	VAL	2.3
1	C	345	VAL	2.3
1	B	264	GLY	2.3
1	B	308	GLY	2.3
1	D	139	GLY	2.3
1	A	227	LEU	2.3
1	A	402	LEU	2.3
1	C	402	LEU	2.3
1	B	344	TYR	2.3
1	B	91	ALA	2.3
1	C	5[A]	ARG	2.3
1	A	405	VAL	2.3
1	D	345	VAL	2.3
1	A	154	ILE	2.3
1	B	369	ILE	2.3
1	B	321	GLY	2.3
1	C	140	GLN	2.3
1	A	118	LEU	2.3
1	D	176	VAL	2.3
1	B	73	ASN	2.3
1	B	191	ILE	2.3
1	D	81	ILE	2.3
1	D	88	ASN	2.3
1	C	316[A]	ARG	2.3
1	C	41	THR	2.3
1	D	161	PRO	2.3
1	A	355	LEU	2.3
1	D	109	LEU	2.3
1	A	137	PHE	2.3
1	A	153	ALA	2.3
1	D	374	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	194	VAL	2.3
1	B	289	ILE	2.3
1	A	325	PRO	2.3
1	C	247	LEU	2.3
1	B	270	HIS	2.3
1	A	332	PRO	2.3
1	B	224	PRO	2.3
1	B	237	ILE	2.3
1	D	89	LYS	2.3
1	D	187	LYS	2.3
1	B	350	HIS	2.3
1	C	322	TYR	2.2
1	A	197	VAL	2.2
1	A	326	THR	2.2
1	B	133	THR	2.2
1	C	238	THR	2.2
1	D	32	GLU	2.2
1	B	222	TYR	2.2
1	A	83	THR	2.2
1	A	338	THR	2.2
1	B	176	VAL	2.2
1	C	28	ILE	2.2
1	A	384	LYS	2.2
1	D	119	LEU	2.2
1	D	395	LEU	2.2
1	B	111	HIS	2.2
1	A	13	SER	2.2
1	A	382	GLY	2.2
1	A	191	ILE	2.2
1	D	151	ASP	2.2
1	A	34	LEU	2.2
1	A	87	LEU	2.2
1	C	120	LEU	2.2
1	C	219	LEU	2.2
1	C	294	LEU	2.2
1	B	169	SER	2.2
1	A	76	VAL	2.2
1	C	52	VAL	2.2
1	C	311	ILE	2.2
1	D	346[A]	ILE	2.2
1	C	370	ASN	2.2
1	B	42	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	55	LEU	2.2
1	A	50	GLN	2.2
1	B	348	GLN	2.2
1	D	326	THR	2.2
1	B	365	TYR	2.2
1	C	340	VAL	2.2
1	D	219	LEU	2.1
1	B	378	ASP	2.1
1	C	141	SER	2.1
1	C	410	ASN	2.1
1	B	24	VAL	2.1
1	C	339	PRO	2.1
1	A	248	LEU	2.1
1	B	247	LEU	2.1
1	B	245	CYS	2.1
1	A	356[A]	ARG	2.1
1	B	5[A]	ARG	2.1
1	B	27[A]	ARG	2.1
1	D	231	PHE	2.1
1	B	49	ALA	2.1
1	D	7	GLU	2.1
1	A	142	ASP	2.1
1	A	300	HIS	2.1
1	B	228	ASN	2.1
1	A	8	LEU	2.1
1	D	292	CYS	2.1
1	A	71	ASP	2.1
1	D	15	ALA	2.1
1	A	365	TYR	2.1
1	B	322	TYR	2.1
1	D	128	TYR	2.1
1	B	243	ARG	2.1
1	B	16	ASP	2.1
1	D	61	PRO	2.1
1	A	47	GLY	2.1
1	B	256	GLY	2.1
1	A	284	VAL	2.1
1	D	381	THR	2.1
1	D	354	ILE	2.1
1	B	179	GLU	2.1
1	D	58	ALA	2.1
1	B	137	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	206	VAL	2.1
1	D	31	VAL	2.1
1	C	95	GLU	2.0
1	B	185	ILE	2.0
1	C	312	ILE	2.0
1	B	69	PRO	2.0
1	C	162	GLN	2.0
1	D	114	PRO	2.0
1	D	347	SER	2.0
1	A	364	THR	2.0
1	B	166	VAL	2.0
1	B	384	LYS	2.0
1	A	82	PRO	2.0
1	B	196	ILE	2.0
1	B	346[A]	ILE	2.0
1	C	346[A]	ILE	2.0
1	D	121	ILE	2.0
1	C	137	PHE	2.0
1	D	265	VAL	2.0
1	B	406	GLY	2.0
1	C	317	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	SO4	C	593	5/5	0.89	0.59	8.81	79,80,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	SO4	B	495	5/5	0.87	0.44	4.05	101,101,101,101	0
3	SO4	A	592	5/5	0.86	0.40	3.96	98,98,99,99	0
3	SO4	D	494	5/5	0.79	0.54	3.50	88,88,88,89	0
4	SAM	C	417	27/27	0.91	0.20	2.15	21,23,25,31	1
4	SAM	B	417	27/27	0.85	0.26	1.31	32,34,39,43	1
5	LYS	D	420[B]	10/10	0.91	0.22	1.13	24,25,28,29	3
5	LYS	D	420[A]	10/10	0.91	0.22	1.13	24,25,28,29	3
5	LYS	C	420[A]	10/10	0.92	0.16	0.97	22,24,27,27	3
5	LYS	C	420[B]	10/10	0.92	0.16	0.97	22,24,27,27	3
4	SAM	A	417	27/27	0.91	0.19	0.86	25,27,31,36	1
4	SAM	D	417	27/27	0.91	0.19	0.83	21,23,26,33	1
5	LYS	B	420[B]	10/10	0.85	0.25	0.43	32,34,39,39	3
5	LYS	B	420[A]	10/10	0.85	0.25	0.43	32,34,39,39	3
5	PLP	C	419	15/16	0.95	0.16	0.24	18,24,25,26	0
5	PLP	D	419	15/16	0.95	0.19	0.14	20,27,29,30	0
5	LYS	A	420[B]	10/10	0.94	0.18	0.12	27,29,32,33	3
5	LYS	A	420[A]	10/10	0.94	0.18	-0.10	27,29,32,33	3
5	PLP	B	419	15/16	0.95	0.19	-0.72	27,34,36,37	0
5	PLP	A	419	15/16	0.95	0.18	-0.87	24,31,32,33	0
2	ZN	D	421	1/1	0.84	0.11	-1.38	31,31,31,31	0
2	ZN	B	421	1/1	0.97	0.09	-1.60	45,45,45,45	0
6	SF4	B	418	8/8	0.93	0.09	-1.74	35,38,40,40	0
2	ZN	C	421	1/1	0.81	0.09	-1.76	36,36,36,36	0
2	ZN	A	421	1/1	0.98	0.09	-1.79	36,36,36,36	0
6	SF4	C	418	8/8	0.98	0.06	-2.15	22,24,25,26	0
6	SF4	A	418	8/8	0.97	0.07	-2.82	24,27,29,29	0
6	SF4	D	418	8/8	0.96	0.08	-3.06	21,22,25,26	0

6.5 Other polymers (i)

There are no such residues in this entry.