



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:01 AM UTC

PDB ID : 1TZK / pdb_00001tzk
Title : Crystal structure of 1-aminocyclopropane-1-carboxylate-deaminase complexed with alpha-keto-butyrate
Authors : Karthikeyan, S.; Zhou, Q.; Zhao, Z.; Kao, C.L.; Tao, Z.; Robinson, H.; Liu, H.W.; Zhang, H.
Deposited on : 2004-07-10
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

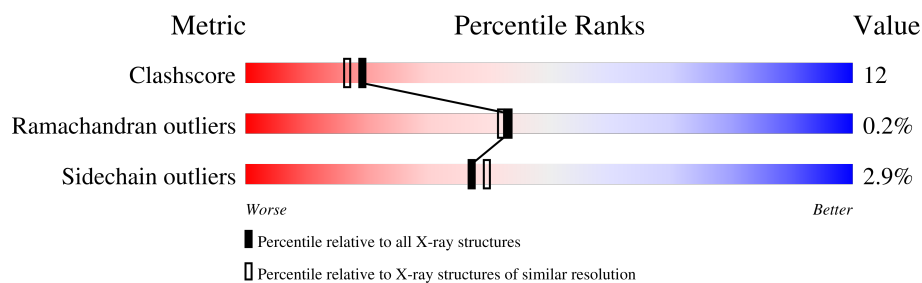
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	338	70% 24% . .
1	B	338	76% 20% . .
1	C	338	75% 23% ..
1	D	338	75% 20% . .

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	2KT	A	501	-	-	X	-
3	2KT	C	502	-	X	X	-

2 Entry composition [i](#)

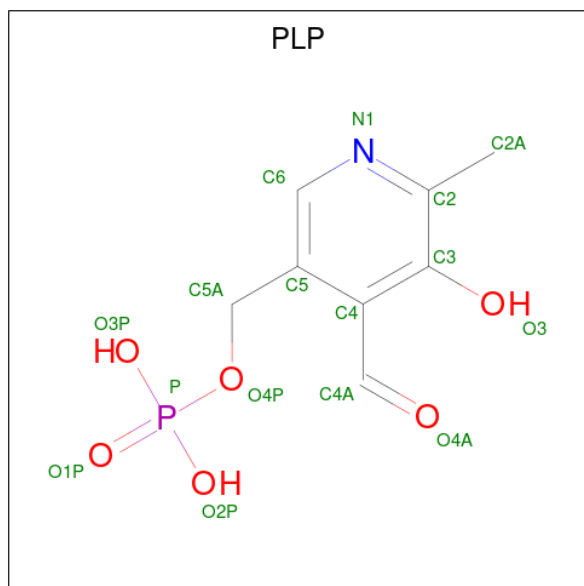
There are 5 unique types of molecules in this entry. The entry contains 10661 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1-aminocyclopropane-1-carboxylate deaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2514	1576	451	472	15			
1	B	329	Total	C	N	O	S	0	0	0
			2499	1567	449	468	15			
1	C	335	Total	C	N	O	S	0	0	0
			2554	1600	461	478	15			
1	D	329	Total	C	N	O	S	0	0	0
			2495	1565	449	466	15			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



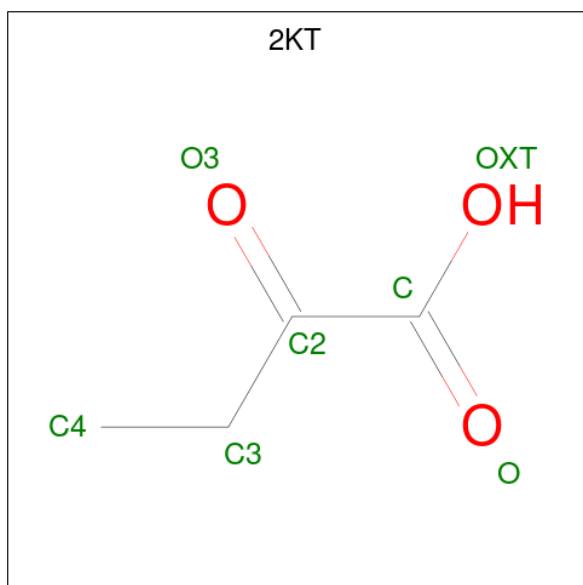
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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

- Molecule 3 is 2-KETOBUTYRIC ACID (CCD ID: 2KT) (formula: $C_4H_6O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	131	Total	O	0	0
			131	131		
5	B	118	Total	O	0	0
			118	118		
5	C	144	Total	O	0	0
			144	144		
5	D	122	Total	O	0	0
			122	122		

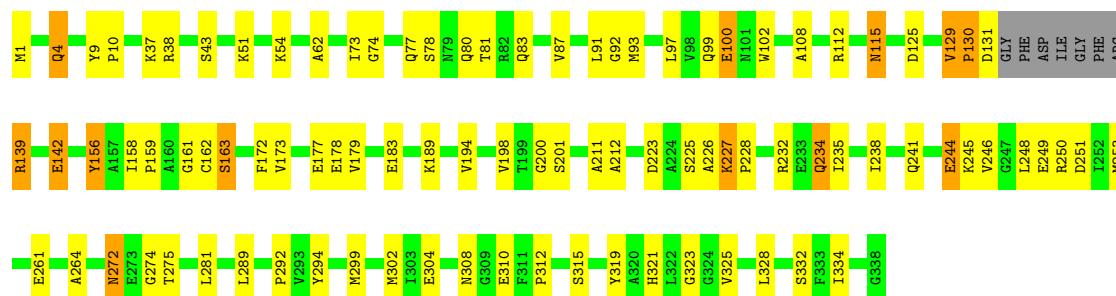
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

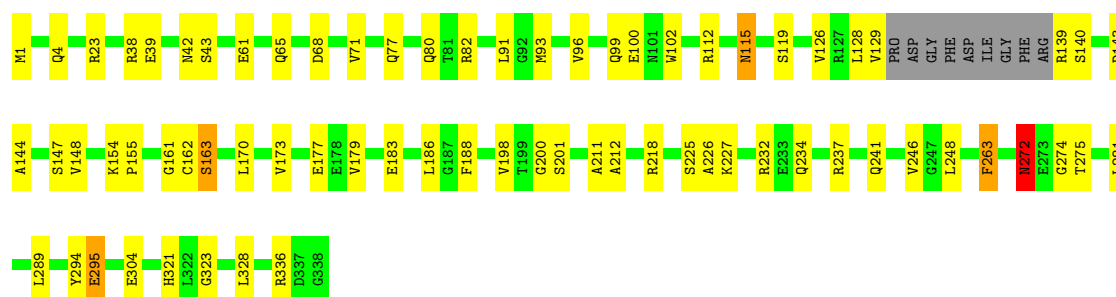
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain A: 



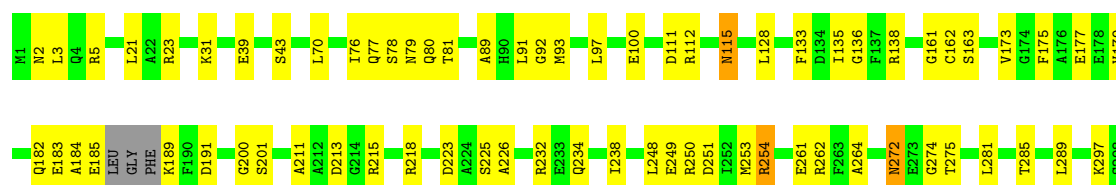
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain B: 



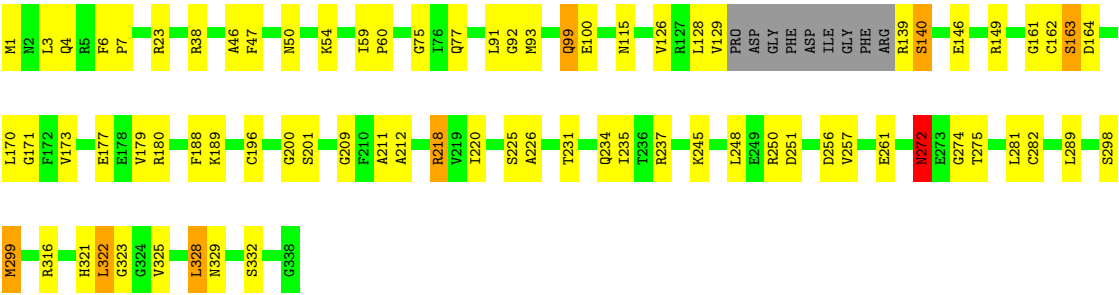
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain C: 





● Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.66 Å 68.45 Å 350.17 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.89 – 2.00	Depositor
% Data completeness (in resolution range)	99.4 (29.89-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10661	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PLP, 2KT

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	0.65	1/2561 (0.0%)	1.10	20/3461 (0.6%)
1	B	0.59	0/2545	1.07	15/3438 (0.4%)
1	C	0.61	0/2602	1.11	11/3514 (0.3%)
1	D	0.60	0/2541	1.10	12/3433 (0.3%)
All	All	0.61	1/10249 (0.0%)	1.09	58/13846 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	325	VAL	CA-CB	7.82	1.59	1.53

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	173	VAL	N-CA-C	-13.56	97.67	110.82
1	C	200	GLY	N-CA-C	12.81	132.73	114.67
1	A	200	GLY	N-CA-C	12.28	129.69	115.08
1	B	173	VAL	N-CA-C	-12.24	98.35	110.72
1	D	200	GLY	N-CA-C	12.05	129.91	114.25
1	B	200	GLY	N-CA-C	11.79	129.58	114.25
1	D	173	VAL	N-CA-C	-11.21	99.40	110.72
1	D	163	SER	N-CA-C	10.75	123.00	111.28
1	B	163	SER	N-CA-C	10.49	122.41	110.97
1	A	173	VAL	N-CA-C	-9.50	100.64	111.00
1	A	163	SER	N-CA-C	8.17	120.10	111.03
1	A	38	ARG	N-CA-C	7.57	121.43	109.39
1	A	227	LYS	CA-C-N	7.03	128.63	119.84
1	A	227	LYS	C-N-CA	7.03	128.63	119.84
1	D	38	ARG	N-CA-C	6.98	120.48	109.39
1	C	21	LEU	N-CA-C	-6.84	102.03	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ALA	N-CA-C	-6.81	103.86	111.28
1	B	211	ALA	N-CA-C	-6.74	103.93	111.28
1	C	254	ARG	N-CA-C	-6.65	104.11	111.82
1	C	262	ARG	N-CA-C	6.54	120.52	112.54
1	D	211	ALA	N-CA-C	-6.31	104.41	111.28
1	C	76	ILE	N-CA-C	6.30	116.97	110.36
1	D	322	LEU	N-CA-C	6.20	120.68	113.18
1	C	115	ASN	N-CA-C	6.18	117.69	111.07
1	D	299	MET	N-CA-C	-6.17	104.63	111.36
1	D	218	ARG	N-CA-C	-6.12	105.85	113.38
1	B	248	LEU	N-CA-C	-6.02	101.37	110.28
1	B	272	ASN	N-CA-C	-5.96	101.38	110.14
1	B	38	ARG	N-CA-C	5.90	118.79	108.52
1	A	235	ILE	N-CA-C	-5.68	104.79	110.30
1	B	227	LYS	N-CA-C	-5.67	99.12	108.75
1	A	172	PHE	N-CA-C	5.65	120.03	113.20
1	C	43	SER	N-CA-C	5.58	117.33	108.79
1	C	299	MET	N-CA-C	-5.55	105.31	111.36
1	B	39	GLU	N-CA-C	-5.53	105.41	111.82
1	C	211	ALA	N-CA-C	-5.51	105.28	111.28
1	A	272	ASN	N-CA-C	-5.50	102.02	109.95
1	A	156	TYR	N-CA-C	-5.44	99.65	108.52
1	D	257	VAL	N-CA-C	5.43	115.60	107.51
1	A	43	SER	N-CA-C	5.41	117.29	109.07
1	B	43	SER	N-CA-C	5.32	117.16	108.76
1	B	170	LEU	N-CA-C	5.29	117.04	111.28
1	D	179	VAL	N-CA-C	5.21	115.99	110.72
1	A	129	VAL	CA-C-N	5.17	126.31	119.84
1	A	129	VAL	C-N-CA	5.17	126.31	119.84
1	A	125	ASP	N-CA-C	-5.14	98.94	107.99
1	A	37	LYS	N-CA-C	-5.13	100.36	108.73
1	B	263	PHE	N-CA-C	5.13	120.17	112.94
1	B	42	ASN	N-CA-C	5.13	119.40	113.20
1	B	115	ASN	N-CA-C	5.11	116.53	111.07
1	A	332	SER	N-CA-C	5.09	117.57	111.71
1	C	324	GLY	N-CA-C	5.09	122.13	115.36
1	B	295	GLU	N-CA-C	5.08	116.81	111.28
1	A	115	ASN	N-CA-C	5.06	116.48	111.07
1	D	332	SER	N-CA-C	5.05	116.87	111.36
1	A	108	ALA	N-CA-C	5.05	117.44	111.33
1	A	299	MET	N-CA-C	-5.04	105.86	111.36
1	D	272	ASN	N-CA-C	-5.02	102.72	109.95

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2514	0	2486	75	0
1	B	2499	0	2474	46	0
1	C	2554	0	2526	63	0
1	D	2495	0	2471	54	0
2	A	15	0	7	1	0
2	B	15	0	7	1	0
2	C	15	0	7	0	0
2	D	15	0	7	0	0
3	A	7	0	5	7	0
3	C	7	0	5	5	0
4	B	5	0	0	1	0
4	D	5	0	0	0	0
5	A	131	0	0	9	0
5	B	118	0	0	1	0
5	C	144	0	0	9	0
5	D	122	0	0	5	0
All	All	10661	0	9995	235	0

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 12.

All (235) 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:D:1:MET:HE3	1:D:212:ALA:HB2	1.31	1.12
1:B:1:MET:HE3	1:B:212:ALA:HB2	1.38	1.05
1:A:131:ASP:HB3	5:A:961:HOH:O	1.68	0.92
1:A:272:ASN:HD22	1:A:274:GLY:H	1.19	0.85
1:D:1:MET:CE	1:D:212:ALA:HB2	2.06	0.85
1:C:272:ASN:HD22	1:C:274:GLY:H	1.24	0.83
1:C:78:SER:OG	3:C:502:2KT:H31	1.78	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:MET:HE1	1:A:319:TYR:HB2	1.62	0.80
1:A:100:GLU:OE1	1:A:129:VAL:HG11	1.83	0.78
3:C:502:2KT:H32	5:C:805:HOH:O	1.85	0.77
1:D:100:GLU:HB3	5:D:970:HOH:O	1.83	0.77
1:B:272:ASN:HD22	1:B:274:GLY:H	1.32	0.76
1:A:228:PRO:HG3	5:A:955:HOH:O	1.85	0.76
1:C:272:ASN:HD22	1:C:274:GLY:N	1.84	0.74
1:A:161:GLY:O	1:A:162:CYS:HB2	1.86	0.73
1:B:1:MET:CE	1:B:212:ALA:HB2	2.17	0.73
1:B:77:GLN:HE22	1:B:115:ASN:H	1.37	0.73
1:C:182:GLN:O	1:C:185:GLU:HG2	1.91	0.71
1:D:180:ARG:NH2	1:D:209:GLY:O	2.23	0.71
1:A:142:GLU:HG3	5:A:946:HOH:O	1.90	0.70
1:D:7:PRO:O	1:D:60:PRO:HG2	1.91	0.70
1:C:191:ASP:O	1:C:218:ARG:HD2	1.92	0.69
1:C:80:GLN:HG2	5:C:805:HOH:O	1.91	0.69
1:A:178:GLU:HG3	5:A:1052:HOH:O	1.94	0.68
1:D:77:GLN:HE22	1:D:115:ASN:H	1.40	0.68
1:A:272:ASN:HD22	1:A:274:GLY:N	1.92	0.67
1:C:91:LEU:CD1	1:C:93:MET:HE2	2.25	0.66
1:C:251:ASP:HB2	1:C:253:MET:HE1	1.76	0.66
1:D:1:MET:HE3	1:D:212:ALA:CB	2.20	0.66
1:D:272:ASN:HD22	1:D:274:GLY:H	1.43	0.66
1:C:272:ASN:ND2	1:C:275:THR:H	1.92	0.66
1:C:77:GLN:HE22	1:C:115:ASN:H	1.43	0.66
1:B:321:HIS:HD2	1:B:323:GLY:H	1.42	0.65
1:A:77:GLN:HE22	1:A:115:ASN:H	1.44	0.65
1:B:289:LEU:O	1:B:321:HIS:HE1	1.80	0.65
1:A:251:ASP:O	1:A:253:MET:HE2	1.97	0.65
1:A:251:ASP:HB2	1:A:253:MET:HE1	1.79	0.65
1:A:241:GLN:NE2	1:A:245:LYS:HD3	2.12	0.64
1:B:161:GLY:O	1:B:162:CYS:HB2	1.97	0.64
1:A:234:GLN:O	1:A:238:ILE:HG13	1.97	0.64
1:A:272:ASN:ND2	1:A:274:GLY:H	1.95	0.63
1:A:308:ASN:HB2	1:A:310:GLU:HG3	1.81	0.63
1:C:311:PHE:HB2	5:C:1030:HOH:O	1.98	0.63
1:D:234:GLN:HG2	1:D:237:ARG:NH2	2.14	0.63
1:C:112:ARG:HD3	5:D:954:HOH:O	1.98	0.62
1:A:81:THR:HB	1:A:97:LEU:HD13	1.81	0.62
1:D:99:GLN:HB2	1:D:128:LEU:HD23	1.81	0.62
1:C:183:GLU:C	1:C:185:GLU:H	2.08	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:GLY:O	1:D:162:CYS:HB2	2.00	0.61
1:C:183:GLU:CD	1:C:189:LYS:HD3	2.25	0.61
1:C:161:GLY:O	1:C:162:CYS:HB2	2.00	0.61
1:B:272:ASN:HD22	1:B:274:GLY:N	1.98	0.61
3:C:502:2KT:H42	5:C:1163:HOH:O	1.99	0.61
1:D:188:PHE:HB2	1:D:316:ARG:NH1	2.15	0.61
1:A:91:LEU:CD1	1:A:93:MET:HE2	2.29	0.61
1:C:175:PHE:O	1:C:179:VAL:HG23	2.01	0.60
1:A:289:LEU:O	1:A:321:HIS:HE1	1.83	0.60
1:A:80:GLN:HG2	3:A:501:2KT:H43	1.83	0.60
1:A:129:VAL:HG23	1:A:129:VAL:O	2.00	0.59
1:B:91:LEU:HD13	1:B:93:MET:HE3	1.84	0.59
1:C:321:HIS:HD2	1:C:323:GLY:H	1.50	0.59
1:B:234:GLN:CD	1:B:237:ARG:HH22	2.08	0.59
1:D:91:LEU:HD13	1:D:93:MET:HE2	1.85	0.59
1:D:272:ASN:HD22	1:D:274:GLY:N	2.00	0.59
1:C:111:ASP:O	1:C:112:ARG:HG2	2.02	0.59
1:A:74:GLY:HA2	1:A:102:TRP:CH2	2.39	0.58
1:D:1:MET:HE2	1:D:248:LEU:HD13	1.85	0.58
1:B:100:GLU:HB2	1:B:102:TRP:NE1	2.19	0.58
1:C:91:LEU:HD12	1:C:93:MET:HE2	1.86	0.58
1:A:1:MET:CE	1:A:212:ALA:HB2	2.33	0.57
1:D:139:ARG:HH11	1:D:140:SER:HB3	1.68	0.57
1:A:100:GLU:HB2	1:A:102:TRP:CD1	2.40	0.57
1:B:144:ALA:O	1:B:147:SER:HB3	2.05	0.57
1:D:4:GLN:O	1:D:4:GLN:NE2	2.38	0.57
1:D:234:GLN:HG2	1:D:237:ARG:HH21	1.70	0.57
1:C:289:LEU:O	1:C:321:HIS:HE1	1.89	0.56
1:A:161:GLY:H	3:A:501:2KT:H42	1.71	0.56
1:A:302:MET:HE1	1:A:319:TYR:CB	2.35	0.56
1:D:321:HIS:HD2	1:D:323:GLY:H	1.51	0.56
1:A:321:HIS:HD2	1:A:323:GLY:H	1.52	0.56
1:B:100:GLU:HB2	1:B:102:TRP:CD1	2.41	0.55
1:B:179:VAL:O	1:B:183:GLU:HG3	2.06	0.54
1:B:100:GLU:HA	1:B:129:VAL:HG22	1.88	0.54
1:D:6:PHE:CZ	1:D:245:LYS:HG2	2.43	0.54
1:B:80:GLN:HB3	4:B:601:SO4:O2	2.08	0.54
1:A:91:LEU:HD13	1:A:93:MET:HE2	1.89	0.54
1:C:232:ARG:NH2	1:C:261:GLU:OE2	2.40	0.54
1:C:111:ASP:C	1:C:112:ARG:HG2	2.32	0.54
1:B:186:LEU:HD13	1:B:188:PHE:CZ	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:ARG:HD2	1:D:251:ASP:O	2.07	0.53
1:A:251:ASP:C	1:A:253:MET:HE2	2.33	0.53
1:A:78:SER:OG	3:A:501:2KT:H32	2.09	0.52
1:D:99:GLN:HG3	1:D:126:VAL:HG13	1.91	0.52
1:B:91:LEU:HD13	1:B:93:MET:CE	2.39	0.52
1:C:213:ASP:OD1	1:C:215:ARG:HG3	2.10	0.52
1:B:198:VAL:HG21	1:B:294:TYR:HE1	1.75	0.52
1:C:248:LEU:CD1	1:C:250:ARG:HB3	2.40	0.52
1:D:289:LEU:O	1:D:321:HIS:HE1	1.93	0.52
1:B:99:GLN:HG3	1:B:126:VAL:HG13	1.92	0.51
1:C:78:SER:HG	3:C:502:2KT:H31	1.74	0.51
1:C:91:LEU:HD13	1:C:93:MET:HE2	1.91	0.51
1:C:112:ARG:CD	5:D:954:HOH:O	2.54	0.51
1:C:81:THR:HB	1:C:97:LEU:HD13	1.92	0.51
1:D:231:THR:O	1:D:235:ILE:HG13	2.10	0.51
1:A:161:GLY:H	3:A:501:2KT:C4	2.24	0.51
1:A:244:GLU:OE1	1:A:244:GLU:C	2.53	0.51
1:A:1:MET:HB2	1:A:246:VAL:O	2.10	0.51
1:A:100:GLU:HA	1:A:129:VAL:HG22	1.93	0.51
1:A:112:ARG:HD3	5:C:850:HOH:O	2.11	0.51
1:B:91:LEU:CD1	1:B:93:MET:HE3	2.41	0.51
1:C:234:GLN:O	1:C:238:ILE:HG13	2.11	0.50
1:A:334:ILE:HG13	5:A:1035:HOH:O	2.10	0.50
1:A:250:ARG:HG2	1:A:251:ASP:N	2.27	0.50
1:A:223:ASP:O	1:A:264:ALA:HB2	2.11	0.50
1:D:282:CYS:SG	1:D:299:MET:HE3	2.52	0.49
1:D:1:MET:HE2	1:D:248:LEU:CD1	2.42	0.49
1:A:163:SER:HA	1:A:201:SER:HB3	1.94	0.49
1:A:73:ILE:O	3:A:501:2KT:H41	2.12	0.49
1:B:321:HIS:CD2	1:B:323:GLY:H	2.28	0.48
1:B:71:VAL:HG22	1:B:96:VAL:HB	1.94	0.48
1:D:188:PHE:HB2	1:D:316:ARG:HH12	1.77	0.48
1:D:189:LYS:HE2	5:D:1169:HOH:O	2.14	0.48
1:D:91:LEU:CD1	1:D:93:MET:HE2	2.42	0.48
1:B:99:GLN:HB2	1:B:128:LEU:HD23	1.94	0.48
1:B:198:VAL:HG21	1:B:294:TYR:CE1	2.49	0.48
1:C:163:SER:HA	1:C:201:SER:HB3	1.96	0.48
1:A:302:MET:CE	1:A:319:TYR:HB2	2.40	0.48
1:B:112:ARG:HD3	5:D:1080:HOH:O	2.13	0.48
1:D:272:ASN:ND2	1:D:275:THR:H	2.11	0.48
1:A:225:SER:O	1:A:226:ALA:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ARG:HD2	5:A:1096:HOH:O	2.13	0.48
1:B:163:SER:HA	1:B:201:SER:HB3	1.94	0.48
1:C:248:LEU:HD13	1:C:250:ARG:HB3	1.94	0.48
1:C:297:LYS:HG2	5:C:817:HOH:O	2.12	0.48
1:C:183:GLU:C	1:C:185:GLU:N	2.72	0.47
1:C:312:PRO:O	1:C:315:SER:OG	2.29	0.47
1:C:70:LEU:HD21	1:C:93:MET:HE1	1.96	0.47
1:C:78:SER:CB	3:C:502:2KT:H31	2.45	0.47
1:D:146:GLU:HA	1:D:149:ARG:NH1	2.30	0.47
1:A:91:LEU:HD12	1:A:93:MET:HE2	1.96	0.47
1:B:225:SER:O	1:B:226:ALA:HB3	2.15	0.47
1:C:100:GLU:OE1	1:C:135:ILE:HG12	2.14	0.47
1:A:272:ASN:ND2	1:A:274:GLY:N	2.58	0.47
1:B:139:ARG:O	1:B:143:ASP:OD2	2.33	0.47
1:B:218:ARG:NH1	1:B:218:ARG:HG3	2.29	0.47
1:C:249:GLU:HG2	5:C:1012:HOH:O	2.14	0.46
1:D:139:ARG:NH1	1:D:140:SER:HB3	2.30	0.46
1:A:4:GLN:HE21	1:A:4:GLN:HA	1.81	0.46
1:C:92:GLY:HA2	1:D:23:ARG:CZ	2.45	0.46
1:A:227:LYS:N	1:A:228:PRO:HD3	2.30	0.46
1:D:6:PHE:HZ	1:D:245:LYS:HG2	1.81	0.46
1:A:250:ARG:HD2	5:A:1173:HOH:O	2.15	0.46
1:B:336:ARG:HG2	1:B:336:ARG:HH11	1.79	0.46
1:C:23:ARG:NH1	1:D:92:GLY:HA2	2.31	0.46
1:B:148:VAL:HG11	1:B:155:PRO:HB3	1.98	0.45
1:A:1:MET:HE3	1:A:212:ALA:HB2	1.98	0.45
1:A:92:GLY:HA2	1:B:23:ARG:CZ	2.46	0.45
1:C:272:ASN:ND2	1:C:274:GLY:N	2.59	0.45
1:C:250:ARG:HG2	1:C:251:ASP:N	2.32	0.45
1:D:321:HIS:CD2	1:D:323:GLY:H	2.33	0.45
1:A:272:ASN:ND2	1:A:275:THR:H	2.15	0.45
1:D:218:ARG:O	1:D:220:ILE:HD12	2.17	0.45
1:A:179:VAL:O	1:A:183:GLU:HG3	2.16	0.45
1:D:46:ALA:O	1:D:47:PHE:HB2	2.16	0.45
1:D:163:SER:HA	1:D:201:SER:HB3	1.98	0.45
1:B:272:ASN:ND2	1:B:275:THR:H	2.15	0.44
1:C:23:ARG:HD3	1:C:285:THR:O	2.17	0.44
1:D:225:SER:O	1:D:226:ALA:HB3	2.18	0.44
1:C:2:ASN:ND2	1:C:5:ARG:HB2	2.32	0.44
1:B:61:GLU:O	1:B:65:GLN:HG3	2.17	0.44
1:C:31:LYS:HB3	1:C:313:GLU:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:MET:O	1:C:306:VAL:HG23	2.17	0.44
1:D:54:LYS:HD3	1:D:162:CYS:HB2	1.98	0.44
1:A:289:LEU:O	1:A:321:HIS:CE1	2.68	0.44
1:C:302:MET:SD	1:C:319:TYR:HB2	2.57	0.44
1:A:248:LEU:C	1:A:250:ARG:H	2.26	0.44
1:A:194:VAL:HB	1:A:302:MET:CE	2.48	0.44
1:D:54:LYS:NZ	1:D:161:GLY:O	2.45	0.44
1:D:75:GLY:HA2	1:D:100:GLU:O	2.17	0.44
1:B:82:ARG:HA	1:B:119:SER:OG	2.19	0.43
1:C:184:ALA:O	1:C:185:GLU:CD	2.62	0.43
1:A:129:VAL:O	1:A:129:VAL:CG2	2.65	0.43
1:B:295:GLU:OE2	2:B:401:PLP:N1	2.51	0.43
1:A:226:ALA:C	1:A:228:PRO:HD3	2.43	0.43
1:C:223:ASP:O	1:C:264:ALA:HB2	2.19	0.43
1:C:89:ALA:O	1:D:23:ARG:NH1	2.52	0.43
1:A:198:VAL:HG21	1:A:294:TYR:CE1	2.54	0.43
1:C:135:ILE:HG13	1:C:136:GLY:N	2.33	0.43
1:D:188:PHE:CB	1:D:316:ARG:NH1	2.82	0.43
1:D:196:CYS:HB2	1:D:298:SER:HB3	2.01	0.43
1:A:304:GLU:HG3	5:A:1213:HOH:O	2.19	0.42
1:C:161:GLY:C	1:C:163:SER:H	2.27	0.42
1:A:80:GLN:CB	3:A:501:2KT:H43	2.50	0.42
1:C:272:ASN:ND2	1:C:275:THR:N	2.65	0.42
1:A:158:ILE:HA	1:A:159:PRO:HD2	1.91	0.42
1:B:68:ASP:OD1	1:B:154:LYS:N	2.50	0.42
1:D:325:VAL:O	1:D:328:LEU:HB2	2.19	0.42
1:D:4:GLN:O	1:D:4:GLN:CD	2.62	0.42
1:C:225:SER:O	1:C:226:ALA:HB3	2.20	0.42
1:A:62:ALA:HA	1:A:156:TYR:CD1	2.54	0.42
1:D:50:ASN:HB3	1:D:322:LEU:HD22	2.01	0.42
1:B:234:GLN:CD	1:B:237:ARG:NH2	2.78	0.42
1:B:263:PHE:HE1	1:B:304:GLU:HG2	1.84	0.42
1:C:3:LEU:C	1:C:5:ARG:N	2.76	0.42
1:A:198:VAL:HG21	1:A:294:TYR:HE1	1.85	0.42
1:D:250:ARG:NH1	1:D:256:ASP:OD2	2.47	0.42
1:C:39:GLU:HB2	1:C:321:HIS:O	2.20	0.42
1:B:234:GLN:HE21	1:B:234:GLN:HB2	1.64	0.41
1:B:237:ARG:O	1:B:241:GLN:HG3	2.20	0.41
1:A:161:GLY:N	3:A:501:2KT:H42	2.34	0.41
1:A:312:PRO:HD2	1:A:315:SER:OG	2.21	0.41
1:C:79:ASN:OD1	1:C:324:GLY:HA2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:GLN:O	1:B:154:LYS:NZ	2.52	0.41
1:C:133:PHE:CE1	1:C:138:ARG:NH1	2.88	0.41
1:D:59:ILE:HD12	1:D:91:LEU:CD1	2.50	0.41
1:B:232:ARG:NE	5:B:1004:HOH:O	2.25	0.41
1:D:139:ARG:CD	1:D:139:ARG:C	2.93	0.41
1:A:100:GLU:HB2	1:A:102:TRP:NE1	2.36	0.41
1:A:9:TYR:HA	1:A:10:PRO:HD3	1.91	0.41
1:A:54:LYS:NZ	2:A:401:PLP:O2P	2.41	0.41
1:A:244:GLU:OE1	1:A:245:LYS:N	2.54	0.41
1:B:1:MET:HB2	1:B:246:VAL:O	2.21	0.41
1:C:272:ASN:ND2	1:C:274:GLY:H	2.04	0.41
1:C:316:ARG:NE	5:C:1112:HOH:O	2.53	0.41
1:A:51:LYS:HD2	1:A:80:GLN:OE1	2.20	0.41
1:A:139:ARG:HB3	1:A:142:GLU:HB2	2.04	0.40
1:A:292:PRO:HD3	1:A:328:LEU:HD23	2.02	0.40
1:A:83:GLN:O	1:A:87:VAL:HG23	2.22	0.40
1:A:189:LYS:HE2	5:A:1013:HOH:O	2.21	0.40
1:C:91:LEU:HD12	1:C:93:MET:CE	2.51	0.40
1:C:254:ARG:HD3	5:C:1088:HOH:O	2.22	0.40
1:C:329:ASN:CG	1:D:329:ASN:CG	2.89	0.40
1:A:139:ARG:HA	1:A:139:ARG:HD3	1.94	0.40
1:D:170:LEU:O	1:D:171:GLY:C	2.63	0.40
1:B:91:LEU:CB	1:B:93:MET:HE3	2.52	0.40

There are no symmetry-related clashes.

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	327/338 (97%)	311 (95%)	14 (4%)	2 (1%)	21 17
1	B	325/338 (96%)	316 (97%)	9 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	331/338 (98%)	315 (95%)	16 (5%)	0	100	100
1	D	325/338 (96%)	312 (96%)	12 (4%)	1 (0%)	36	35
All	All	1308/1352 (97%)	1254 (96%)	51 (4%)	3 (0%)	43	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	PRO
1	D	140	SER
1	A	249	GLU

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	258/264 (98%)	247 (96%)	11 (4%)	26	25
1	B	256/264 (97%)	250 (98%)	6 (2%)	44	49
1	C	262/264 (99%)	258 (98%)	4 (2%)	57	64
1	D	255/264 (97%)	246 (96%)	9 (4%)	32	32
All	All	1031/1056 (98%)	1001 (97%)	30 (3%)	37	40

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	99	GLN
1	A	100	GLU
1	A	130	PRO
1	A	139	ARG
1	A	142	GLU
1	A	177	GLU
1	A	234	GLN
1	A	244	GLU

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Mol	Chain	Res	Type
1	A	261	GLU
1	A	281	LEU
1	B	4	GLN
1	B	140	SER
1	B	177	GLU
1	B	272	ASN
1	B	281	LEU
1	B	328	LEU
1	C	128	LEU
1	C	177	GLU
1	C	272	ASN
1	C	281	LEU
1	D	3	LEU
1	D	99	GLN
1	D	129	VAL
1	D	164	ASP
1	D	177	GLU
1	D	261	GLU
1	D	272	ASN
1	D	281	LEU
1	D	328	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	65	GLN
1	A	77	GLN
1	A	99	GLN
1	A	101	ASN
1	A	230	GLN
1	A	234	GLN
1	A	272	ASN
1	A	321	HIS
1	B	77	GLN
1	B	99	GLN
1	B	230	GLN
1	B	234	GLN
1	B	272	ASN
1	B	321	HIS
1	C	50	ASN
1	C	77	GLN

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Mol	Chain	Res	Type
1	C	99	GLN
1	C	230	GLN
1	C	234	GLN
1	C	272	ASN
1	C	308	ASN
1	C	321	HIS
1	D	2	ASN
1	D	4	GLN
1	D	77	GLN
1	D	99	GLN
1	D	272	ASN
1	D	321	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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	SO4	B	601	-	4,4,4	0.35	0	6,6,6	0.19	0
3	2KT	A	501	-	6,6,6	1.09	0	7,7,7	1.77	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	D	602	-	4,4,4	0.34	0	6,6,6	0.19	0
2	PLP	C	401	1	15,15,16	1.52	5 (33%)	21,22,23	1.07	1 (4%)
2	PLP	D	401	1	15,15,16	1.54	4 (26%)	21,22,23	1.04	0
3	2KT	C	502	-	6,6,6	1.09	0	7,7,7	1.89	2 (28%)
2	PLP	B	401	1	15,15,16	1.76	5 (33%)	21,22,23	0.98	0
2	PLP	A	401	1	15,15,16	1.80	4 (26%)	21,22,23	1.05	1 (4%)

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
3	2KT	A	501	-	-	4/6/6/6	-
2	PLP	C	401	1	-	0/6/6/8	0/1/1/1
2	PLP	D	401	1	-	0/6/6/8	0/1/1/1
3	2KT	C	502	-	-	6/6/6/6	-
2	PLP	B	401	1	-	0/6/6/8	0/1/1/1
2	PLP	A	401	1	-	0/6/6/8	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	PLP	C5-C4	3.82	1.44	1.40
2	B	401	PLP	C2A-C2	3.51	1.56	1.50
2	A	401	PLP	C2A-C2	3.41	1.55	1.50
2	D	401	PLP	C2A-C2	3.06	1.55	1.50
2	B	401	PLP	C5-C4	3.03	1.44	1.40
2	A	401	PLP	C3-C4	3.02	1.45	1.40
2	C	401	PLP	C5-C4	3.01	1.43	1.40
2	B	401	PLP	C3-C2	2.94	1.44	1.41
2	D	401	PLP	C5-C4	2.88	1.43	1.40
2	D	401	PLP	C3-C4	2.67	1.45	1.40
2	C	401	PLP	C3-C2	2.41	1.43	1.41
2	C	401	PLP	C6-C5	2.25	1.42	1.37
2	B	401	PLP	C4A-C4	2.24	1.56	1.51
2	A	401	PLP	C6-C5	2.23	1.42	1.37
2	B	401	PLP	C3-C4	2.14	1.44	1.40
2	C	401	PLP	C3-C4	2.13	1.44	1.40
2	D	401	PLP	C6-C5	2.05	1.41	1.37
2	C	401	PLP	C2A-C2	2.01	1.53	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	2KT	O-C-C2	-3.84	117.04	121.81
3	A	501	2KT	O-C-C2	-3.38	117.61	121.81
3	A	501	2KT	C3-C2-C	2.50	120.47	116.08
3	C	502	2KT	C3-C2-C	2.45	120.39	116.08
2	A	401	PLP	C6-N1-C2	2.10	123.01	119.20
2	C	401	PLP	C6-N1-C2	2.09	122.99	119.20

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	2KT	OXT-C-C2-C3
3	A	501	2KT	OXT-C-C2-O3
3	C	502	2KT	OXT-C-C2-C3
3	C	502	2KT	O-C-C2-C3
3	C	502	2KT	OXT-C-C2-O3
3	C	502	2KT	O-C-C2-O3
3	A	501	2KT	O-C-C2-O3
3	A	501	2KT	O-C-C2-C3
3	C	502	2KT	O3-C2-C3-C4
3	C	502	2KT	C-C2-C3-C4

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	SO4	1	0
3	A	501	2KT	7	0
3	C	502	2KT	5	0
2	B	401	PLP	1	0
2	A	401	PLP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.