



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 07:18 am BST

PDB ID : 1TZJ  
Title : Crystal Structure of 1-aminocyclopropane-1-carboxylate deaminase complexed with d-vinyl glycine  
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 : 1.99 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

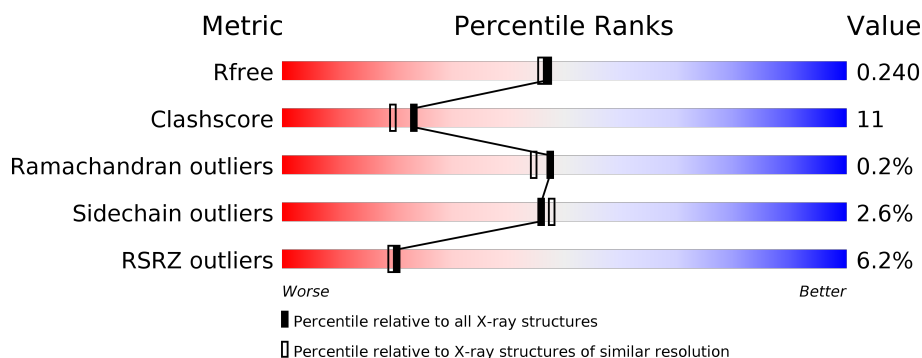
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.99 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	338	<div> <div>7%</div> <div> <div></div> <div>73%</div> <div>22%</div> <div>• •</div> </div> </div>
1	B	338	<div> <div>6%</div> <div> <div></div> <div>75%</div> <div>21%</div> <div>• •</div> </div> </div>
1	C	338	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>16%</div> <div>•</div> </div> </div>
1	D	338	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>• •</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	A3B	A	501	-	-	X	-

## 2 Entry composition [i](#)

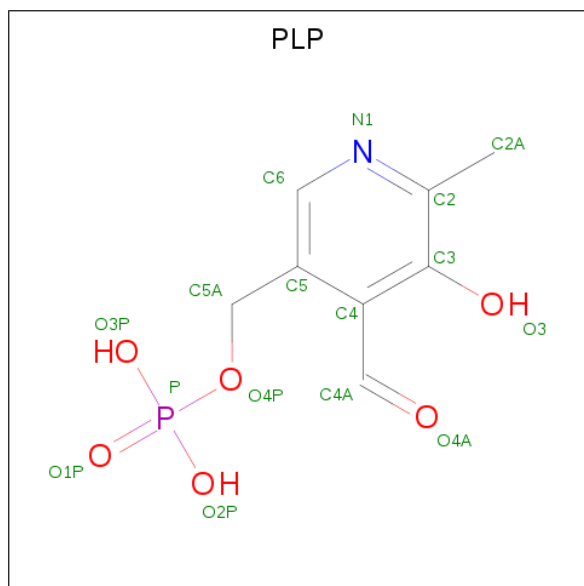
There are 5 unique types of molecules in this entry. The entry contains 10679 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	328	Total	C	N	O	S	0	0	0
			2488	1561	445	467	15			
1	C	338	Total	C	N	O	S	0	0	0
			2571	1614	461	481	15			
1	D	329	Total	C	N	O	S	0	0	0
			2495	1565	449	466	15			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



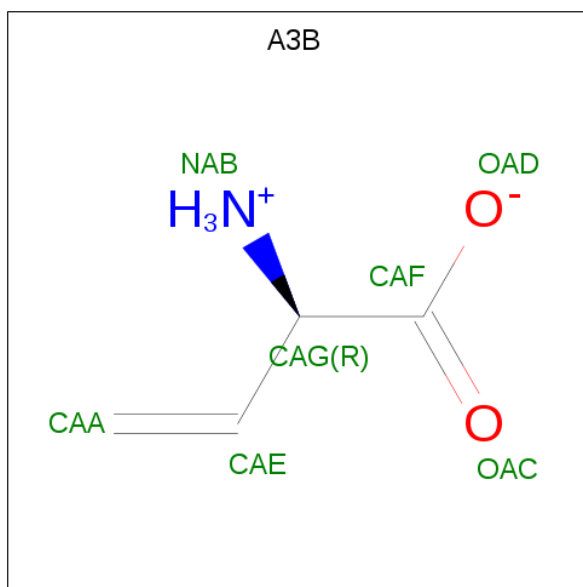
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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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 D-VINYLGLYCINE (three-letter code: A3B) (formula: C<sub>4</sub>H<sub>7</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			7	4	1	2		
3	C	1	Total	C	N	O	0	0
			7	4	1	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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		

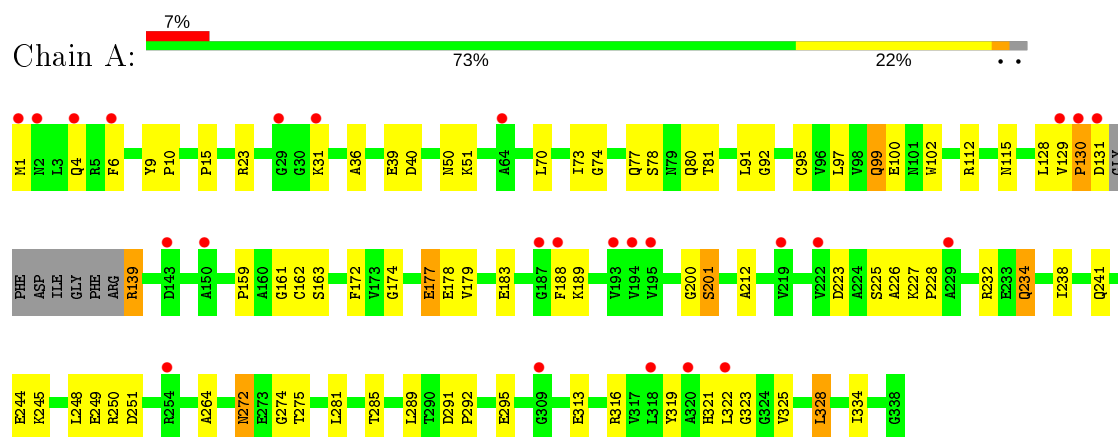
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	119	Total	O	0	0
			119	119		
5	B	124	Total	O	0	0
			124	124		
5	C	148	Total	O	0	0
			148	148		
5	D	136	Total	O	0	0
			136	136		

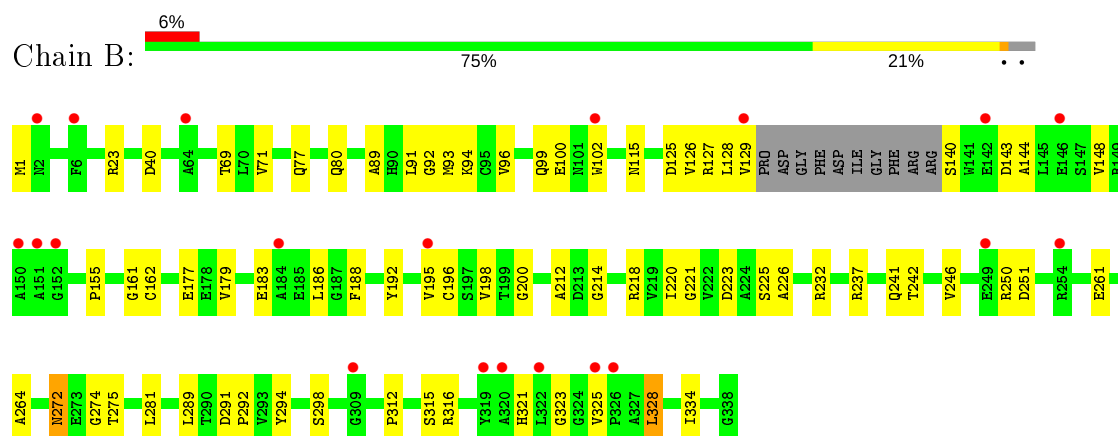
### 3 Residue-property plots

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

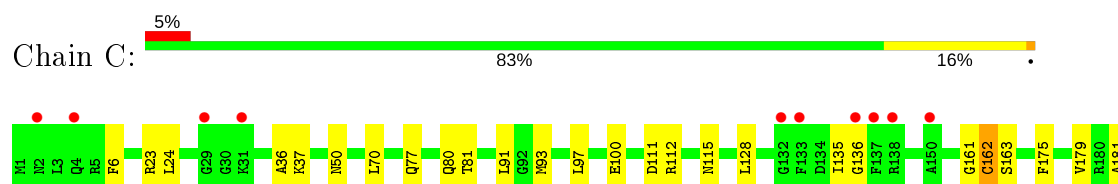
- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

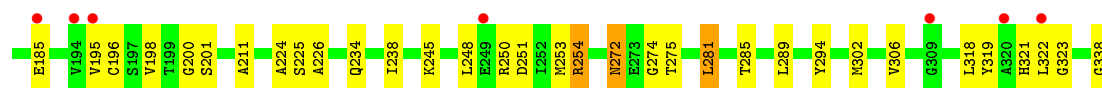


- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

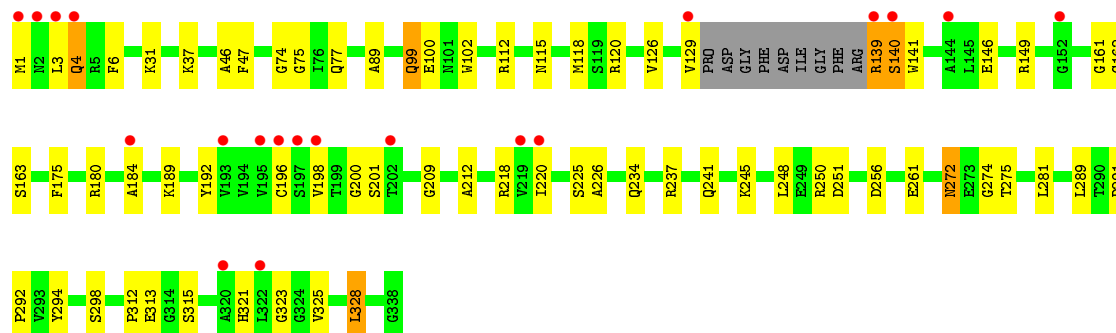
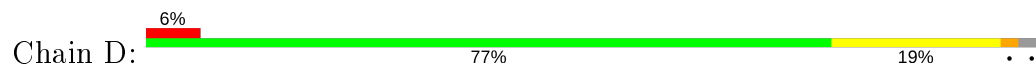


- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase





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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.67Å 68.42Å 350.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 1.99 29.88 – 1.99	Depositor EDS
% Data completeness (in resolution range)	98.1 (29.88-1.99) 97.7 (29.88-1.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 1.98Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.213 , 0.251 0.204 , 0.240	Depositor DCC
$R_{free}$ test set	5544 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.2	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.039 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10679	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A3B, SO4, 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	0.50	0/2561	0.71	2/3461 (0.1%)
1	B	0.46	0/2534	0.70	1/3424 (0.0%)
1	C	0.52	0/2621	0.75	1/3542 (0.0%)
1	D	0.50	0/2541	0.72	1/3433 (0.0%)
All	All	0.50	0/10257	0.72	5/13860 (0.0%)

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	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	200	GLY	N-CA-C	7.73	132.42	113.10
1	B	200	GLY	N-CA-C	6.73	129.91	113.10
1	D	200	GLY	N-CA-C	6.22	128.66	113.10
1	A	200	GLY	N-CA-C	6.09	128.33	113.10
1	A	112	ARG	NE-CZ-NH1	-5.29	117.65	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	172	PHE	Sidechain

## 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	71	0
1	B	2488	0	2462	55	0
1	C	2571	0	2539	47	0
1	D	2495	0	2471	60	0
2	A	15	0	7	1	0
2	B	15	0	7	0	0
2	C	15	0	7	0	0
2	D	15	0	7	0	0
3	A	7	0	7	8	0
3	C	7	0	7	1	0
4	B	5	0	0	1	0
4	D	5	0	0	0	0
5	A	119	0	0	8	0
5	B	124	0	0	3	0
5	C	148	0	0	6	0
5	D	136	0	0	4	0
All	All	10679	0	10000	228	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 11.

All (228) 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:A:272:ASN:HD22	1:A:274:GLY:H	1.29	0.79
1:B:1:MET:HE3	1:B:212:ALA:HB2	1.63	0.79
1:D:77:GLN:HE22	1:D:115:ASN:H	1.35	0.74
1:D:146:GLU:HA	1:D:149:ARG:NH1	2.02	0.73
1:B:77:GLN:HE22	1:B:115:ASN:H	1.33	0.73
1:B:214:GLY:HA2	5:B:1169:HOH:O	1.89	0.73
1:D:1:MET:CE	1:D:212:ALA:HB2	2.18	0.72
1:A:131:ASP:HB3	5:A:983:HOH:O	1.89	0.71
1:B:321:HIS:HD2	1:B:323:GLY:H	1.38	0.71
5:C:1067:HOH:O	1:D:112:ARG:HD3	1.91	0.70
1:B:1:MET:CE	1:B:212:ALA:HB2	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ARG:HD2	5:A:1039:HOH:O	1.89	0.69
1:D:139:ARG:HH11	1:D:140:SER:HB3	1.59	0.68
1:D:272:ASN:HD22	1:D:274:GLY:H	1.41	0.68
1:D:1:MET:HE3	1:D:212:ALA:HB2	1.76	0.68
1:D:321:HIS:HD2	1:D:323:GLY:H	1.41	0.67
1:A:161:GLY:H	3:A:501:A3B:HAA1	1.59	0.67
1:A:272:ASN:HD22	1:A:274:GLY:N	1.92	0.67
1:B:272:ASN:HD22	1:B:274:GLY:H	1.41	0.67
1:A:1:MET:HE3	1:A:212:ALA:HB2	1.78	0.66
1:C:111:ASP:C	1:C:112:ARG:HG2	2.17	0.65
1:C:91:LEU:HD13	1:C:93:MET:HE2	1.78	0.65
1:B:100:GLU:HA	1:B:129:VAL:HG22	1.79	0.65
1:C:77:GLN:HE22	1:C:115:ASN:H	1.43	0.64
1:C:161:GLY:O	1:C:162:CYS:HB2	1.97	0.64
1:D:234:GLN:HG2	1:D:237:ARG:NH2	2.14	0.63
1:D:6:PHE:CZ	1:D:245:LYS:HG2	2.33	0.63
1:D:234:GLN:HG2	1:D:237:ARG:HH21	1.62	0.63
1:A:4:GLN:H	1:A:4:GLN:CD	2.02	0.63
1:D:220:ILE:N	1:D:220:ILE:HD12	2.15	0.62
1:D:139:ARG:HH11	1:D:141:TRP:H	1.48	0.62
1:A:250:ARG:HD2	5:A:1153:HOH:O	1.99	0.62
1:C:272:ASN:HD22	1:C:274:GLY:H	1.45	0.62
1:A:80:GLN:HB3	3:A:501:A3B:CAE	2.30	0.61
1:A:161:GLY:N	3:A:501:A3B:HAA1	2.15	0.61
1:A:73:ILE:O	3:A:501:A3B:HAA2	2.00	0.61
1:C:234:GLN:O	1:C:238:ILE:HG13	2.01	0.61
1:C:272:ASN:ND2	1:C:275:THR:H	1.97	0.61
1:A:161:GLY:O	1:A:162:CYS:HB2	2.00	0.61
1:A:78:SER:OG	3:A:501:A3B:HAE	2.01	0.61
1:C:23:ARG:HD2	5:C:1004:HOH:O	2.01	0.60
1:B:289:LEU:O	1:B:321:HIS:HE1	1.84	0.60
1:D:289:LEU:O	1:D:321:HIS:HE1	1.85	0.60
1:D:272:ASN:HD22	1:D:274:GLY:N	1.99	0.60
1:D:139:ARG:NH1	1:D:140:SER:HB3	2.16	0.59
1:C:135:ILE:HG13	1:C:136:GLY:N	2.17	0.59
1:A:234:GLN:O	1:A:238:ILE:HG13	2.03	0.59
1:C:272:ASN:HD22	1:C:274:GLY:N	2.01	0.59
1:C:91:LEU:CD1	1:C:93:MET:HE2	2.34	0.58
1:A:1:MET:CE	1:A:212:ALA:HB2	2.34	0.58
1:D:250:ARG:HD2	1:D:251:ASP:O	2.02	0.58
1:D:1:MET:HE2	1:D:212:ALA:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:ARG:HH11	1:D:218:ARG:HG3	1.68	0.57
1:D:272:ASN:ND2	1:D:275:THR:H	2.01	0.57
1:B:148:VAL:HG11	1:B:155:PRO:HB3	1.86	0.57
1:A:163:SER:HA	1:A:201:SER:HB3	1.87	0.57
1:A:334:ILE:HG13	5:A:1015:HOH:O	2.05	0.56
1:B:161:GLY:O	1:B:162:CYS:HB2	2.05	0.56
1:A:139:ARG:HG3	1:A:139:ARG:HH11	1.71	0.56
1:B:179:VAL:O	1:B:183:GLU:HG3	2.06	0.56
1:D:163:SER:HA	1:D:201:SER:HB3	1.87	0.56
1:B:186:LEU:HD13	1:B:188:PHE:CZ	2.41	0.56
1:A:100:GLU:OE1	1:A:129:VAL:HG11	2.06	0.56
1:B:99:GLN:HG3	1:B:126:VAL:HG13	1.87	0.55
1:C:181:ALA:O	1:C:185:GLU:HG2	2.07	0.55
1:D:31:LYS:HD2	1:D:313:GLU:HG3	1.88	0.55
1:A:241:GLN:NE2	1:A:245:LYS:HE2	2.21	0.55
1:D:100:GLU:HB3	5:D:1094:HOH:O	2.06	0.55
1:D:180:ARG:NH2	1:D:209:GLY:O	2.37	0.55
1:D:198:VAL:HG21	1:D:294:TYR:CE1	2.42	0.55
1:B:237:ARG:O	1:B:241:GLN:HG3	2.06	0.55
1:B:272:ASN:HD22	1:B:274:GLY:N	2.04	0.55
1:D:321:HIS:CD2	1:D:323:GLY:H	2.24	0.55
1:D:198:VAL:HG21	1:D:294:TYR:HE1	1.71	0.54
1:D:189:LYS:HD3	5:D:933:HOH:O	2.08	0.54
1:A:272:ASN:ND2	1:A:274:GLY:H	2.03	0.54
1:A:77:GLN:HE22	1:A:115:ASN:H	1.54	0.54
1:A:250:ARG:HG2	1:A:251:ASP:N	2.23	0.54
1:B:272:ASN:ND2	1:B:275:THR:H	2.07	0.53
1:C:225:SER:O	1:C:226:ALA:HB3	2.08	0.53
1:D:4:GLN:NE2	1:D:4:GLN:O	2.41	0.53
1:C:248:LEU:HD13	1:C:250:ARG:HB3	1.91	0.52
1:A:321:HIS:HD2	1:A:323:GLY:H	1.57	0.52
1:D:225:SER:O	1:D:226:ALA:HB3	2.10	0.52
1:A:39:GLU:HB2	1:A:321:HIS:O	2.08	0.52
1:B:232:ARG:NH2	1:B:261:GLU:OE2	2.42	0.52
1:A:250:ARG:HG2	1:A:251:ASP:H	1.74	0.52
1:B:140:SER:N	5:B:991:HOH:O	2.42	0.52
1:C:175:PHE:O	1:C:179:VAL:HG23	2.10	0.52
1:D:31:LYS:HD2	1:D:313:GLU:CD	2.30	0.51
1:C:195:VAL:HG23	1:C:322:LEU:HD11	1.93	0.51
1:D:250:ARG:NH1	1:D:256:ASP:OD2	2.38	0.51
1:A:289:LEU:O	1:A:321:HIS:HE1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:SER:O	1:A:226:ALA:HB3	2.11	0.50
1:B:223:ASP:O	1:B:264:ALA:HB2	2.11	0.50
1:B:99:GLN:HB2	1:B:128:LEU:HD23	1.93	0.50
1:A:6:PHE:CZ	1:A:245:LYS:HG3	2.46	0.50
1:D:99:GLN:HG3	1:D:126:VAL:HG13	1.94	0.50
1:D:325:VAL:O	1:D:328:LEU:HB2	2.11	0.50
1:D:218:ARG:HH11	1:D:218:ARG:CG	2.23	0.50
1:A:161:GLY:H	3:A:501:A3B:CAA	2.23	0.50
1:D:139:ARG:HD3	1:D:140:SER:N	2.27	0.50
1:A:4:GLN:N	1:A:4:GLN:CD	2.66	0.49
1:C:321:HIS:HD2	1:C:323:GLY:H	1.60	0.49
1:A:92:GLY:HA2	1:B:23:ARG:CZ	2.42	0.49
1:B:80:GLN:HB3	4:B:601:SO4:O2	2.13	0.49
1:B:292:PRO:HD3	1:B:328:LEU:CD1	2.43	0.49
1:B:69:THR:OG1	1:B:94:LYS:HB2	2.13	0.49
1:D:218:ARG:O	1:D:220:ILE:HD12	2.12	0.49
1:D:161:GLY:O	1:D:162:CYS:HB2	2.12	0.49
1:D:6:PHE:HZ	1:D:245:LYS:HG2	1.78	0.49
1:B:100:GLU:HB2	1:B:102:TRP:NE1	2.28	0.48
1:C:111:ASP:O	1:C:112:ARG:HG2	2.12	0.48
1:A:272:ASN:ND2	1:A:275:THR:H	2.11	0.48
1:D:100:GLU:HA	1:D:129:VAL:HG22	1.95	0.48
1:A:272:ASN:ND2	1:A:274:GLY:N	2.59	0.48
1:B:292:PRO:HD3	1:B:328:LEU:HD13	1.95	0.48
1:A:31:LYS:HB3	1:A:313:GLU:HG3	1.95	0.47
1:D:312:PRO:HG2	1:D:315:SER:OG	2.14	0.47
1:A:23:ARG:NH1	1:B:92:GLY:HA2	2.29	0.47
1:C:250:ARG:HG2	1:C:251:ASP:N	2.29	0.47
1:A:50:ASN:HB3	1:A:322:LEU:HB3	1.97	0.47
1:B:321:HIS:CD2	1:B:323:GLY:H	2.26	0.47
1:C:100:GLU:OE1	1:C:135:ILE:HG12	2.15	0.47
1:D:291:ASP:HB2	1:D:292:PRO:HD2	1.96	0.47
1:A:74:GLY:HA2	1:A:102:TRP:CH2	2.50	0.47
1:B:186:LEU:HB3	1:B:188:PHE:CE2	2.50	0.47
1:D:237:ARG:O	1:D:241:GLN:HG3	2.15	0.47
1:D:46:ALA:O	1:D:47:PHE:HB2	2.14	0.47
1:A:223:ASP:O	1:A:264:ALA:HB2	2.15	0.47
1:A:139:ARG:HD3	1:A:139:ARG:C	2.35	0.47
1:D:146:GLU:HA	1:D:149:ARG:HH11	1.78	0.47
1:D:31:LYS:HD2	1:D:313:GLU:CG	2.44	0.47
1:C:289:LEU:O	1:C:321:HIS:HE1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:SER:O	1:B:226:ALA:HB3	2.15	0.46
1:B:188:PHE:CG	1:B:316:ARG:NH1	2.83	0.46
1:C:254:ARG:HD3	5:C:847:HOH:O	2.15	0.46
3:C:502:A3B:HAE	5:C:936:HOH:O	2.16	0.46
1:A:248:LEU:C	1:A:250:ARG:H	2.19	0.46
1:B:250:ARG:HG2	1:B:251:ASP:N	2.30	0.46
1:C:289:LEU:HD13	1:D:118:MET:HG2	1.97	0.46
1:C:302:MET:O	1:C:306:VAL:HG23	2.16	0.46
1:C:24:LEU:HD13	1:C:281:LEU:HD22	1.98	0.46
1:A:36:ALA:HA	1:A:319:TYR:O	2.15	0.45
1:B:334:ILE:HG13	5:B:1042:HOH:O	2.16	0.45
1:A:159:PRO:HB2	5:A:1133:HOH:O	2.15	0.45
1:A:189:LYS:HE2	5:A:1116:HOH:O	2.16	0.45
1:C:211:ALA:HB1	1:C:250:ARG:NH1	2.31	0.45
1:A:188:PHE:CE1	1:A:316:ARG:HD3	2.52	0.45
1:D:192:TYR:HB3	1:D:220:ILE:HD13	1.97	0.45
1:B:91:LEU:HD13	1:B:93:MET:CE	2.47	0.45
1:B:196:CYS:HB2	1:B:298:SER:HB3	1.99	0.45
1:D:139:ARG:NH1	1:D:141:TRP:H	2.11	0.45
1:C:234:GLN:HE21	1:C:234:GLN:HB2	1.54	0.45
1:C:6:PHE:CZ	1:C:245:LYS:HD2	2.52	0.45
1:C:253:MET:HA	1:C:253:MET:HE2	1.99	0.45
1:D:75:GLY:HA2	1:D:100:GLU:O	2.16	0.45
1:A:226:ALA:C	1:A:228:PRO:HD3	2.38	0.45
1:C:248:LEU:CD1	1:C:250:ARG:HB3	2.46	0.45
1:A:234:GLN:HE21	1:A:234:GLN:HB2	1.53	0.45
1:A:295:GLU:OE2	2:A:401:PLP:N1	2.50	0.45
1:B:91:LEU:CD1	1:B:93:MET:HE3	2.46	0.44
1:B:91:LEU:HD13	1:B:93:MET:HE3	1.99	0.44
1:B:198:VAL:HG21	1:B:294:TYR:HE1	1.82	0.44
1:B:291:ASP:HB2	1:B:292:PRO:HD2	2.00	0.44
1:B:40:ASP:HB3	1:B:323:GLY:HA2	1.98	0.44
1:A:15:PRO:HA	1:A:178:GLU:OE2	2.17	0.44
1:A:51:LYS:HE2	3:A:501:A3B:NAB	2.32	0.44
1:B:242:THR:O	1:B:246:VAL:HG22	2.18	0.44
1:C:195:VAL:CG2	1:C:322:LEU:HD11	2.47	0.44
1:C:36:ALA:HA	1:C:319:TYR:O	2.17	0.44
1:A:129:VAL:HG23	1:A:129:VAL:O	2.18	0.44
1:A:291:ASP:HB2	1:A:292:PRO:HD2	2.00	0.44
1:B:195:VAL:O	1:B:221:GLY:HA2	2.18	0.43
1:A:227:LYS:N	1:A:228:PRO:HD3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:GLN:CG	1:B:126:VAL:HG13	2.47	0.43
1:A:249:GLU:HG3	5:A:1079:HOH:O	2.18	0.43
1:B:99:GLN:HG3	1:B:126:VAL:CG1	2.49	0.43
1:B:192:TYR:CD2	1:B:220:ILE:HD11	2.53	0.43
1:A:188:PHE:CE1	1:A:316:ARG:CD	3.02	0.43
1:A:74:GLY:O	1:A:99:GLN:HA	2.19	0.43
1:A:23:ARG:NH1	1:B:89:ALA:O	2.52	0.43
1:C:135:ILE:HG13	1:C:136:GLY:H	1.82	0.42
1:B:218:ARG:HG3	1:B:218:ARG:NH1	2.34	0.42
1:C:112:ARG:CD	5:D:810:HOH:O	2.67	0.42
1:A:99:GLN:HB2	1:A:128:LEU:HD23	2.01	0.42
1:B:188:PHE:CD2	1:B:316:ARG:NH1	2.87	0.42
1:D:184:ALA:HA	5:D:952:HOH:O	2.19	0.42
1:D:196:CYS:HB2	1:D:298:SER:HB3	2.01	0.42
1:A:70:LEU:O	1:A:95:CYS:HA	2.19	0.42
1:B:144:ALA:O	1:B:148:VAL:HG23	2.19	0.42
1:C:80:GLN:HG2	5:C:936:HOH:O	2.19	0.42
1:B:71:VAL:HG22	1:B:96:VAL:HB	2.01	0.42
1:C:338:GLY:HA2	1:D:120:ARG:HB3	2.01	0.42
1:A:40:ASP:CB	1:A:323:GLY:HA2	2.50	0.42
1:A:174:GLY:O	1:A:177:GLU:HB3	2.20	0.41
1:A:81:THR:HB	1:A:97:LEU:HD13	2.02	0.41
1:C:70:LEU:HD11	1:C:93:MET:HE3	2.02	0.41
1:A:292:PRO:HD3	1:A:328:LEU:HD13	2.03	0.41
1:C:196:CYS:SG	1:C:224:ALA:HB2	2.61	0.41
1:A:292:PRO:HD3	1:A:328:LEU:CD1	2.50	0.41
1:D:100:GLU:HB2	1:D:102:TRP:CD1	2.56	0.41
1:C:198:VAL:HG21	1:C:294:TYR:HE1	1.85	0.41
1:C:6:PHE:CZ	1:C:245:LYS:HG3	2.55	0.41
1:C:50:ASN:HB3	1:C:322:LEU:HB3	2.03	0.41
1:D:77:GLN:HE22	1:D:115:ASN:N	2.11	0.41
1:B:312:PRO:O	1:B:315:SER:OG	2.32	0.41
1:C:234:GLN:HG2	5:C:1009:HOH:O	2.19	0.41
1:A:9:TYR:HA	1:A:10:PRO:HD3	1.85	0.41
1:D:220:ILE:CD1	1:D:220:ILE:N	2.83	0.41
1:C:81:THR:HB	1:C:97:LEU:HD22	2.02	0.41
1:A:23:ARG:HD3	1:A:285:THR:O	2.21	0.41
1:B:140:SER:HA	1:B:143:ASP:OD2	2.20	0.41
1:C:37:LYS:HB2	1:C:318:LEU:HD11	2.03	0.41
1:D:74:GLY:O	1:D:99:GLN:HA	2.21	0.41
1:A:325:VAL:O	1:A:328:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ASP:CB	1:B:323:GLY:HA2	2.50	0.41
1:C:163:SER:HA	1:C:201:SER:HB3	2.02	0.41
1:A:174:GLY:HA3	5:A:920:HOH:O	2.19	0.40
1:B:125:ASP:OD2	1:B:127:ARG:NE	2.44	0.40
1:D:218:ARG:NH1	1:D:218:ARG:CG	2.81	0.40
1:A:51:LYS:HE2	3:A:501:A3B:HAB1	1.84	0.40
1:A:179:VAL:O	1:A:183:GLU:HG3	2.20	0.40
1:A:9:TYR:CE1	1:A:91:LEU:HD21	2.57	0.40
1:B:325:VAL:O	1:B:328:LEU:HB2	2.20	0.40
1:C:23:ARG:HD3	1:C:285:THR:O	2.21	0.40
1:D:37:LYS:HD3	1:D:175:PHE:CE2	2.57	0.40
1:C:23:ARG:NH1	1:D:89:ALA:O	2.54	0.40

There are no symmetry-related clashes.

## 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	327/338 (97%)	314 (96%)	12 (4%)	1 (0%)	41	37
1	B	324/338 (96%)	311 (96%)	13 (4%)	0	100	100
1	C	336/338 (99%)	322 (96%)	14 (4%)	0	100	100
1	D	325/338 (96%)	310 (95%)	13 (4%)	2 (1%)	25	19
All	All	1312/1352 (97%)	1257 (96%)	52 (4%)	3 (0%)	47	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	PRO
1	D	140	SER
1	D	4	GLN

### 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%)	248 (96%)	10 (4%)	32	30
1	B	255/264 (97%)	251 (98%)	4 (2%)	62	67
1	C	263/264 (100%)	258 (98%)	5 (2%)	57	61
1	D	255/264 (97%)	247 (97%)	8 (3%)	40	40
All	All	1031/1056 (98%)	1004 (97%)	27 (3%)	46	48

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	130	PRO
1	A	139	ARG
1	A	177	GLU
1	A	201	SER
1	A	234	GLN
1	A	244	GLU
1	A	272	ASN
1	A	281	LEU
1	A	328	LEU
1	B	177	GLU
1	B	272	ASN
1	B	281	LEU
1	B	328	LEU
1	C	128	LEU
1	C	162	CYS
1	C	254	ARG
1	C	272	ASN
1	C	281	LEU
1	D	3	LEU
1	D	99	GLN
1	D	139	ARG
1	D	248	LEU
1	D	261	GLU

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Mol	Chain	Res	Type
1	D	272	ASN
1	D	281	LEU
1	D	328	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	99	GLN
1	A	230	GLN
1	A	234	GLN
1	A	241	GLN
1	A	272	ASN
1	A	308	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	4	GLN
1	C	77	GLN
1	C	230	GLN
1	C	272	ASN
1	C	308	ASN
1	C	321	HIS
1	D	65	GLN
1	D	77	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

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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$
2	PLP	D	401	1	15,15,16	1.91	5 (33%)	20,22,23	1.02	1 (5%)
3	A3B	A	501	-	2,6,6	1.59	0	0,7,7	0.00	-
2	PLP	C	401	1	15,15,16	2.09	4 (26%)	20,22,23	1.08	1 (5%)
2	PLP	A	401	1	15,15,16	1.76	3 (20%)	20,22,23	1.02	0
4	SO4	B	601	-	4,4,4	0.24	0	6,6,6	0.17	0
3	A3B	C	502	-	2,6,6	1.60	0	0,7,7	0.00	-
4	SO4	D	602	-	4,4,4	0.28	0	6,6,6	0.21	0
2	PLP	B	401	1	15,15,16	1.82	4 (26%)	20,22,23	1.04	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
2	PLP	D	401	1	-	0/6/6/8	0/1/1/1
3	A3B	A	501	-	-	1/1/6/6	-
2	PLP	C	401	1	-	0/6/6/8	0/1/1/1
2	PLP	A	401	1	-	0/6/6/8	0/1/1/1
3	A3B	C	502	-	-	0/1/6/6	-
2	PLP	B	401	1	-	0/6/6/8	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	PLP	C3-C2	5.44	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	PLP	C5-C4	4.06	1.45	1.40
2	B	401	PLP	C5-C4	4.01	1.44	1.40
2	B	401	PLP	C3-C2	3.90	1.44	1.40
2	D	401	PLP	C3-C2	3.80	1.44	1.40
2	D	401	PLP	C2A-C2	3.48	1.56	1.50
2	D	401	PLP	C5-C4	3.10	1.43	1.40
2	A	401	PLP	C3-C2	3.06	1.44	1.40
2	C	401	PLP	C5-C4	3.06	1.43	1.40
2	C	401	PLP	C2A-C2	2.86	1.55	1.50
2	A	401	PLP	C2A-C2	2.73	1.55	1.50
2	B	401	PLP	C2A-C2	2.57	1.54	1.50
2	D	401	PLP	C3-C4	2.28	1.44	1.40
2	D	401	PLP	C6-C5	2.19	1.42	1.37
2	C	401	PLP	C3-C4	2.04	1.44	1.40
2	B	401	PLP	C4A-C4	2.02	1.55	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	PLP	O3-C3-C2	2.18	122.25	117.49
2	C	401	PLP	O3-C3-C2	2.06	121.98	117.49

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	A3B	CAA-CAE-CAG-CAF

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	A3B	8	0
2	A	401	PLP	1	0
4	B	601	SO4	1	0
3	C	502	A3B	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	331/338 (97%)	0.49	25 (7%)	13 13	23, 39, 59, 80	0
1	B	328/338 (97%)	0.43	20 (6%)	21 20	23, 38, 60, 69	0
1	C	338/338 (100%)	0.30	17 (5%)	28 28	22, 35, 54, 65	0
1	D	329/338 (97%)	0.42	20 (6%)	21 20	22, 37, 56, 74	0
All	All	1326/1352 (98%)	0.41	82 (6%)	20 19	22, 37, 57, 80	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	130	PRO	6.5
1	A	131	ASP	5.0
1	C	136	GLY	4.1
1	D	184	ALA	4.0
1	B	254	ARG	3.6
1	C	133	PHE	3.6
1	D	195	VAL	3.5
1	C	195	VAL	3.5
1	A	129	VAL	3.4
1	C	137	PHE	3.4
1	A	195	VAL	3.3
1	D	4	GLN	3.3
1	A	254	ARG	3.3
1	D	219	VAL	3.2
1	B	249	GLU	3.2
1	C	322	LEU	3.1
1	D	322	LEU	3.1
1	D	140	SER	3.1
1	A	219	VAL	3.1
1	D	2	ASN	3.1
1	B	309	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	194	VAL	3.0
1	A	309	GLY	3.0
1	D	152	GLY	3.0
1	B	151	ALA	3.0
1	C	132	GLY	3.0
1	D	3	LEU	3.0
1	A	29	GLY	2.9
1	D	193	VAL	2.9
1	C	31	LYS	2.8
1	D	139	ARG	2.8
1	B	64	ALA	2.8
1	D	129	VAL	2.8
1	C	2	ASN	2.8
1	D	196	CYS	2.8
1	B	129	VAL	2.8
1	A	31	LYS	2.7
1	A	322	LEU	2.7
1	D	202	THR	2.7
1	B	152	GLY	2.7
1	A	193	VAL	2.6
1	B	184	ALA	2.5
1	C	309	GLY	2.5
1	A	2	ASN	2.5
1	A	64	ALA	2.5
1	A	188	PHE	2.5
1	C	185	GLU	2.5
1	B	150	ALA	2.4
1	A	4	GLN	2.4
1	B	195	VAL	2.4
1	A	143	ASP	2.4
1	B	322	LEU	2.4
1	B	326	PRO	2.4
1	C	138	ARG	2.3
1	C	194	VAL	2.3
1	B	142	GLU	2.3
1	A	320	ALA	2.3
1	D	320	ALA	2.3
1	C	29	GLY	2.3
1	D	198	VAL	2.3
1	A	229	ALA	2.3
1	D	220	ILE	2.3
1	A	150	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	325	VAL	2.2
1	D	197	SER	2.2
1	A	1	MET	2.2
1	B	320	ALA	2.2
1	B	6	PHE	2.1
1	A	187	GLY	2.1
1	A	318	LEU	2.1
1	A	6	PHE	2.1
1	A	222	VAL	2.1
1	B	146	GLU	2.1
1	C	4	GLN	2.1
1	B	319	TYR	2.1
1	B	2	ASN	2.0
1	C	249	GLU	2.0
1	D	1	MET	2.0
1	C	150	ALA	2.0
1	C	320	ALA	2.0
1	D	144	ALA	2.0
1	B	102	TRP	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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	A3B	C	502	7/7	0.79	0.25	36,40,45,46	0
3	A3B	A	501	7/7	0.93	0.17	35,43,45,46	0
4	SO4	B	601	5/5	0.95	0.16	74,75,75,75	0
2	PLP	D	401	15/16	0.97	0.17	25,28,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PLP	A	401	15/16	0.97	0.14	31,32,37,38	0
4	SO4	D	602	5/5	0.97	0.10	60,61,61,62	0
2	PLP	C	401	15/16	0.98	0.13	24,28,29,30	0
2	PLP	B	401	15/16	0.98	0.14	26,30,31,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.