



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 12:40 AM BST

PDB ID : 5XT5  
Title : SufS-SufU complex from Bacillus subtilis  
Authors : Fujishiro, T.; Takahashi, Y.  
Deposited on : 2017-06-17  
Resolution : 2.34 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 : 2.13.1  
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) : 2.13.1

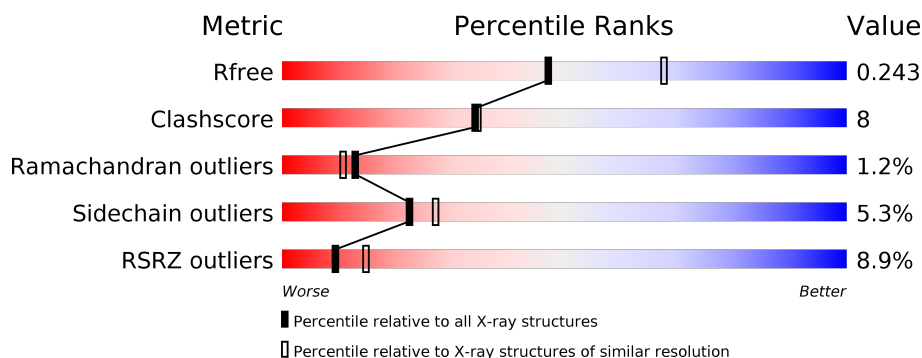
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.34 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	C	155	<div> <div>15%</div> <div>54%</div> <div>32%</div> <div>13%</div> </div>
1	D	155	<div> <div>25%</div> <div>49%</div> <div>28%</div> <div>10%</div> <div>12%</div> </div>
2	A	419	<div> <div>4%</div> <div>86%</div> <div>10%</div> <div>•</div> </div>
2	B	419	<div> <div>4%</div> <div>82%</div> <div>13%</div> <div>• •</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8619 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 Zinc-dependent sulfurtransferase SufU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	137	Total	C	N	O	S	0	0	0
			1050	651	178	209	12			
1	C	135	Total	C	N	O	S	0	0	0
			1036	642	175	207	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	148	LEU	-	expression tag	UNP O32163
D	149	GLU	-	expression tag	UNP O32163
D	150	HIS	-	expression tag	UNP O32163
D	151	HIS	-	expression tag	UNP O32163
D	152	HIS	-	expression tag	UNP O32163
D	153	HIS	-	expression tag	UNP O32163
D	154	HIS	-	expression tag	UNP O32163
D	155	HIS	-	expression tag	UNP O32163
C	148	LEU	-	expression tag	UNP O32163
C	149	GLU	-	expression tag	UNP O32163
C	150	HIS	-	expression tag	UNP O32163
C	151	HIS	-	expression tag	UNP O32163
C	152	HIS	-	expression tag	UNP O32163
C	153	HIS	-	expression tag	UNP O32163
C	154	HIS	-	expression tag	UNP O32163
C	155	HIS	-	expression tag	UNP O32163

- Molecule 2 is a protein called Cysteine desulfurase SufS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	405	Total	C	N	O	S	0	1	0
			3160	2002	538	606	14			
2	B	405	Total	C	N	O	S	0	0	0
			3152	1997	536	606	13			

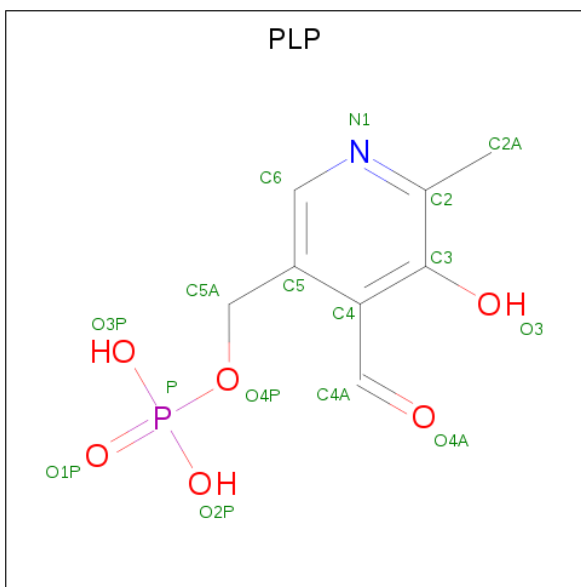
There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP O32164
A	-1	GLY	-	expression tag	UNP O32164
A	0	HIS	-	expression tag	UNP O32164
A	407	VAL	-	expression tag	UNP O32164
A	408	ASP	-	expression tag	UNP O32164
A	409	LEU	-	expression tag	UNP O32164
A	410	GLU	-	expression tag	UNP O32164
A	411	HIS	-	expression tag	UNP O32164
A	412	HIS	-	expression tag	UNP O32164
A	413	HIS	-	expression tag	UNP O32164
A	414	HIS	-	expression tag	UNP O32164
A	415	HIS	-	expression tag	UNP O32164
A	416	HIS	-	expression tag	UNP O32164
B	-2	MET	-	expression tag	UNP O32164
B	-1	GLY	-	expression tag	UNP O32164
B	0	HIS	-	expression tag	UNP O32164
B	407	VAL	-	expression tag	UNP O32164
B	408	ASP	-	expression tag	UNP O32164
B	409	LEU	-	expression tag	UNP O32164
B	410	GLU	-	expression tag	UNP O32164
B	411	HIS	-	expression tag	UNP O32164
B	412	HIS	-	expression tag	UNP O32164
B	413	HIS	-	expression tag	UNP O32164
B	414	HIS	-	expression tag	UNP O32164
B	415	HIS	-	expression tag	UNP O32164
B	416	HIS	-	expression tag	UNP O32164

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

- Molecule 4 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
4	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
4	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

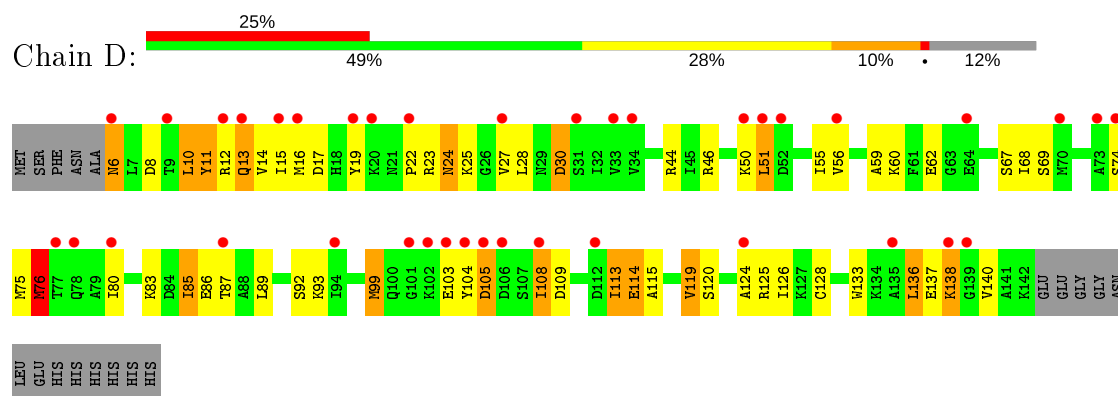
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	3	Total	O	0	0
			3	3		
5	A	97	Total	O	0	0
			97	97		
5	B	82	Total	O	0	0
			82	82		
5	C	7	Total	O	0	0
			7	7		

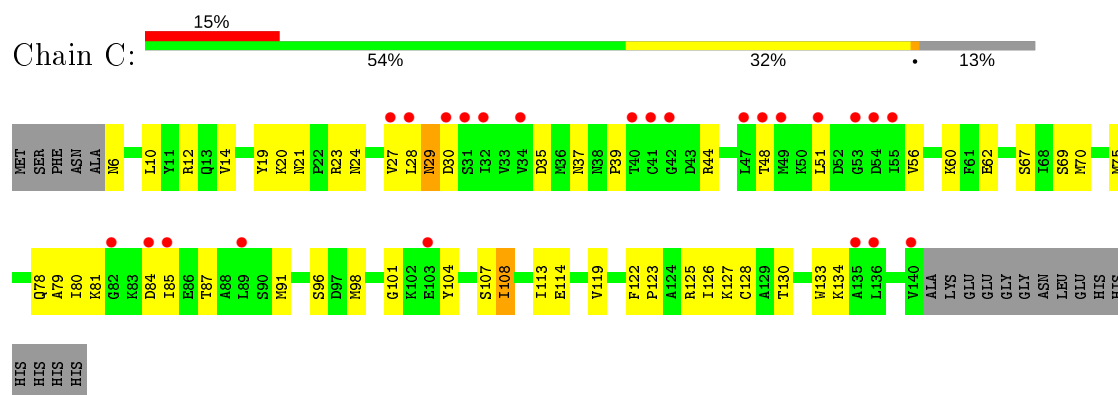
### 3 Residue-property plots [i](#)

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 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.

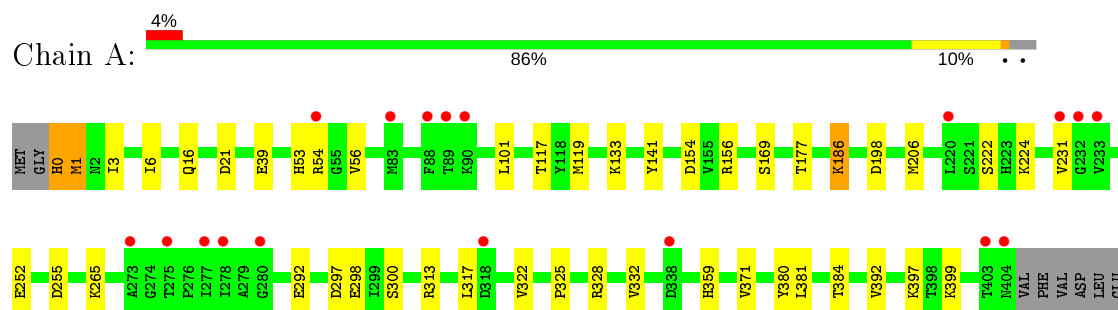
#### • Molecule 1: Zinc-dependent sulfurtransferase SufU



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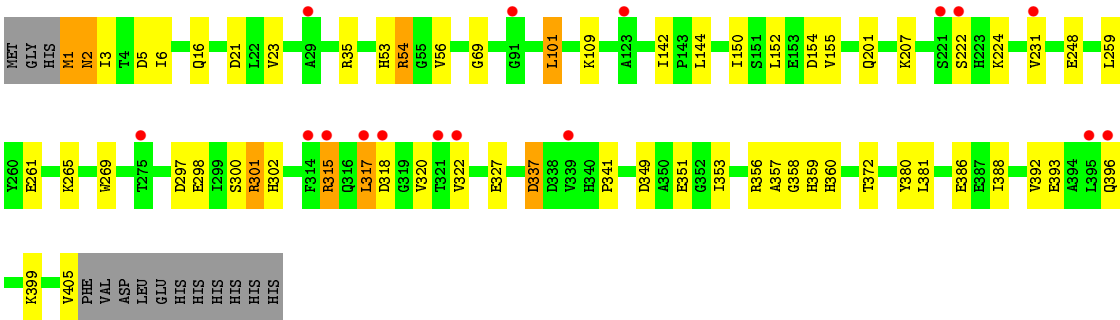
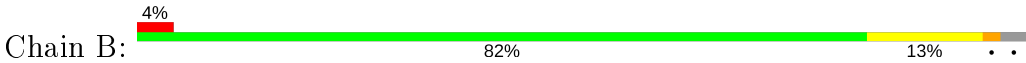


#### • Molecule 2: Cysteine desulfurase SufS



HIS  
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● Molecule 2: Cysteine desulfurase SufS



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.98Å 74.98Å 364.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	64.93 – 2.34 44.36 – 2.34	Depositor EDS
% Data completeness (in resolution range)	99.5 (64.93-2.34) 99.5 (44.36-2.34)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.199 , 0.243 0.198 , 0.243	Depositor DCC
$R_{free}$ test set	2414 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.7	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 32.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.064 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8619	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	C	0.86	0/1047	1.10	7/1403 (0.5%)
1	D	0.79	0/1061	1.09	7/1421 (0.5%)
2	A	1.05	3/3229 (0.1%)	0.97	7/4384 (0.2%)
2	B	1.06	5/3217 (0.2%)	1.01	13/4369 (0.3%)
All	All	1.00	8/8554 (0.1%)	1.02	34/11577 (0.3%)

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	C	0	1
2	B	0	1
All	All	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	261	GLU	CG-CD	9.02	1.65	1.51
2	B	248	GLU	CD-OE2	-6.45	1.18	1.25
2	A	39	GLU	CD-OE1	5.95	1.32	1.25
2	B	393	GLU	CD-OE2	5.88	1.32	1.25
2	A	39	GLU	CD-OE2	5.73	1.31	1.25
2	B	69	GLY	N-CA	5.55	1.54	1.46
2	A	292	GLU	CD-OE1	5.20	1.31	1.25
2	B	327	GLU	CG-CD	5.02	1.59	1.51

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	ARG	NE-CZ-NH2	10.85	125.72	120.30
2	B	315	ARG	NE-CZ-NH1	8.24	124.42	120.30
2	A	156	ARG	NE-CZ-NH1	8.05	124.33	120.30
2	B	356	ARG	NE-CZ-NH2	7.50	124.05	120.30
2	A	154	ASP	CB-CG-OD1	7.48	125.03	118.30
2	B	154	ASP	CB-CG-OD2	-7.23	111.79	118.30
2	A	206	MET	CG-SD-CE	7.18	111.69	100.20
1	C	125	ARG	NE-CZ-NH2	7.18	123.89	120.30
2	B	317	LEU	CB-CG-CD2	-6.64	99.72	111.00
1	C	51	LEU	CA-CB-CG	6.36	129.92	115.30
2	A	328	ARG	NE-CZ-NH2	-6.24	117.18	120.30
2	B	297	ASP	CB-CG-OD1	6.19	123.87	118.30
2	B	154	ASP	CB-CG-OD1	6.09	123.78	118.30
1	D	76	MET	CG-SD-CE	-6.03	90.56	100.20
1	D	125	ARG	NE-CZ-NH2	-6.01	117.29	120.30
2	A	255	ASP	CB-CG-OD2	-5.94	112.96	118.30
2	A	206	MET	CA-CB-CG	5.92	123.36	113.30
2	A	313	ARG	NE-CZ-NH2	5.88	123.24	120.30
2	B	349	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	D	108	ILE	N-CA-C	-5.81	95.31	111.00
2	B	337	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	C	23	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	D	51	LEU	CA-CB-CG	5.59	128.15	115.30
1	C	134	LYS	CD-CE-NZ	5.54	124.44	111.70
2	B	35	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	D	105	ASP	CB-CG-OD1	5.50	123.25	118.30
1	D	11	TYR	CA-CB-CG	5.36	123.59	113.40
1	C	12	ARG	NE-CZ-NH1	-5.31	117.65	120.30
2	B	356	ARG	NE-CZ-NH1	-5.22	117.69	120.30
2	B	248	GLU	CG-CD-OE1	5.18	128.66	118.30
1	C	70	MET	CG-SD-CE	5.17	108.47	100.20
2	B	101	LEU	CB-CG-CD2	5.10	119.67	111.00
1	D	99	MET	CG-SD-CE	5.08	108.32	100.20
1	C	29	ASN	N-CA-C	5.00	124.51	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	54	ARG	Peptide
1	C	101	GLY	Peptide

## 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	C	1036	0	1038	25	0
1	D	1050	0	1056	61	0
2	A	3160	0	3115	29	0
2	B	3152	0	3108	30	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	15	0	6	2	0
4	B	15	0	6	2	0
5	A	97	0	0	2	0
5	B	82	0	0	0	0
5	C	7	0	0	0	0
5	D	3	0	0	0	0
All	All	8619	0	8329	141	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 8.

All (141) 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:27:VAL:HG12	1:D:46:ARG:HH12	1.25	1.01
2:A:117:THR:CG2	2:A:119:MET:HG2	1.91	1.00
2:B:315:ARG:NH1	2:B:322:VAL:HG11	1.77	0.97
1:D:113:ILE:HD12	1:D:114:GLU:H	1.30	0.96
2:A:117:THR:HG21	2:A:119:MET:HG2	1.50	0.92
1:D:113:ILE:O	1:D:115:ALA:N	2.04	0.90
2:A:117:THR:HG22	2:A:119:MET:H	1.35	0.89
1:D:99:MET:HE1	1:D:119:VAL:HG22	1.56	0.87
1:D:27:VAL:HG12	1:D:46:ARG:NH1	1.95	0.81
1:D:76:MET:O	1:D:80:ILE:CD1	2.29	0.81
1:D:76:MET:O	1:D:80:ILE:HD12	1.83	0.79
1:D:89:LEU:HD11	1:D:140:VAL:HG21	1.65	0.77
1:D:80:ILE:HA	1:D:83:LYS:HG2	1.64	0.77
1:C:27:VAL:HA	1:C:48:THR:HG21	1.66	0.77
1:D:27:VAL:CG1	1:D:46:ARG:HH12	1.97	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:LEU:HD13	1:D:60:LYS:CB	2.18	0.73
1:C:28:LEU:HD13	1:C:60:LYS:HD2	1.71	0.73
1:D:44:ARG:HH12	1:D:46:ARG:HB2	1.54	0.72
1:D:99:MET:CE	1:D:119:VAL:HG22	2.20	0.71
1:D:12:ARG:HG3	1:D:115:ALA:HB1	1.73	0.71
1:C:87:THR:O	1:C:91:MET:HG3	1.91	0.70
2:B:317:LEU:CD2	2:B:320:VAL:HG23	2.23	0.69
1:D:24:ASN:C	1:D:60:LYS:HD3	2.13	0.69
1:C:75:MET:HE3	1:C:113:ILE:HA	1.76	0.68
1:D:56:VAL:HG11	1:D:59:ALA:HB2	1.77	0.67
1:D:133:TRP:HA	1:D:136:LEU:HD23	1.78	0.66
1:C:78:GLN:HA	1:C:81:LYS:HE3	1.77	0.65
1:D:99:MET:HB3	1:D:126:ILE:HD12	1.80	0.64
2:A:141:TYR:CE1	2:B:259:LEU:HB3	2.32	0.64
2:A:117:THR:HG22	2:A:119:MET:N	2.11	0.64
1:D:113:ILE:CD1	1:D:114:GLU:H	2.06	0.64
2:A:169:SER:HB3	5:A:620:HOH:O	1.99	0.61
2:A:117:THR:HG22	2:A:119:MET:HG2	1.77	0.61
1:D:76:MET:O	1:D:80:ILE:HD13	1.99	0.61
2:B:54:ARG:HH21	2:B:54:ARG:HG3	1.65	0.60
1:D:28:LEU:HD13	1:D:60:LYS:HB2	1.83	0.60
2:B:142:ILE:HD13	2:B:155:VAL:HG12	1.83	0.60
1:D:28:LEU:HD13	1:D:60:LYS:HB3	1.83	0.60
1:D:83:LYS:HA	1:D:83:LYS:HE2	1.84	0.60
1:C:75:MET:CE	1:C:113:ILE:HA	2.32	0.59
2:B:317:LEU:CD2	2:B:320:VAL:CG2	2.81	0.58
2:B:317:LEU:HD23	2:B:320:VAL:HG23	1.86	0.58
1:D:80:ILE:HA	1:D:83:LYS:CG	2.32	0.58
1:D:15:ILE:HA	1:D:75:MET:CE	2.33	0.58
2:B:358:GLY:O	2:B:360:HIS:N	2.34	0.58
1:D:13:GLN:HE21	1:D:13:GLN:HA	1.71	0.56
2:B:315:ARG:NH1	2:B:322:VAL:CG1	2.62	0.55
1:D:24:ASN:O	1:D:60:LYS:HD3	2.07	0.54
1:C:123:PRO:HA	1:C:126:ILE:HG13	1.90	0.54
1:D:6:ASN:N	1:D:6:ASN:HD22	2.06	0.54
1:D:92:SER:OG	1:D:137:GLU:OE2	2.25	0.53
1:D:124:ALA:HB1	2:A:56:VAL:HA	1.89	0.53
1:D:51:LEU:HB2	1:D:55:ILE:O	2.09	0.53
1:D:8:ASP:O	1:D:11:TYR:HD2	1.92	0.52
1:D:85:ILE:HG13	1:D:87:THR:H	1.75	0.52
2:B:1:MET:HE2	2:B:6:ILE:HG12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:LEU:HD23	1:D:10:LEU:N	2.25	0.52
2:A:0:HIS:HB2	2:A:298:GLU:CD	2.31	0.51
2:A:1:MET:CE	2:A:6:ILE:HG13	2.41	0.51
1:D:113:ILE:HD12	1:D:114:GLU:N	2.13	0.51
2:B:54:ARG:HD2	1:C:39:PRO:O	2.11	0.51
1:D:67:SER:OG	1:D:68:ILE:HD12	2.10	0.51
2:A:1:MET:HG3	2:A:298:GLU:HG3	1.92	0.51
1:D:24:ASN:N	1:D:24:ASN:OD1	2.43	0.51
1:D:69:SER:HA	1:D:128:CYS:O	2.11	0.50
1:D:99:MET:CE	1:D:119:VAL:CG2	2.87	0.50
1:D:133:TRP:O	1:D:136:LEU:HG	2.11	0.50
1:D:17:ASP:OD2	1:D:23:ARG:NH1	2.45	0.49
2:B:152:LEU:HA	2:B:155:VAL:HG22	1.93	0.49
1:C:28:LEU:CD1	1:C:60:LYS:HD2	2.40	0.49
1:D:30:ASP:O	1:D:50:LYS:HG2	2.13	0.49
1:D:16:MET:HG3	2:B:405:VAL:HG21	1.94	0.49
2:B:298:GLU:OE1	2:B:301:ARG:NH2	2.29	0.49
2:B:317:LEU:HD21	2:B:320:VAL:CG2	2.43	0.49
1:C:19:TYR:CD1	1:C:67:SER:HA	2.48	0.49
1:D:15:ILE:HA	1:D:75:MET:HE2	1.95	0.49
2:B:317:LEU:HD21	2:B:320:VAL:HG23	1.96	0.48
2:A:252:GLU:O	2:A:265:LYS:HE2	2.13	0.48
2:A:56:VAL:HG12	2:A:56:VAL:O	2.13	0.48
1:D:22:PRO:HB2	1:D:25:LYS:HG3	1.95	0.48
2:A:1:MET:HE2	2:A:6:ILE:HG13	1.94	0.48
2:B:341:PRO:HB2	2:B:357:ALA:HB1	1.96	0.48
1:C:119:VAL:CG2	1:C:119:VAL:O	2.62	0.47
1:C:69:SER:HA	1:C:128:CYS:O	2.14	0.47
1:D:60:LYS:HE2	1:D:60:LYS:HB2	1.59	0.47
1:C:20:LYS:HG2	1:C:21:ASN:OD1	2.14	0.47
2:A:117:THR:HG21	2:A:119:MET:CG	2.35	0.47
1:C:84:ASP:OD1	1:C:85:ILE:N	2.48	0.47
2:A:297:ASP:HB2	5:A:671:HOH:O	2.15	0.46
1:D:19:TYR:CD1	1:D:67:SER:HA	2.50	0.46
2:A:3:ILE:HG21	2:A:384:THR:HG22	1.97	0.46
2:A:186:LYS:HE3	2:A:186:LYS:HB2	1.45	0.46
2:A:322:VAL:HG13	2:A:332:VAL:HG13	1.97	0.46
2:A:177:THR:HG22	2:A:325:PRO:HG3	1.98	0.46
2:A:317:LEU:HD11	2:A:392:VAL:HG13	1.97	0.46
2:B:388:ILE:O	2:B:392:VAL:HG13	2.16	0.46
2:B:224:LYS:NZ	4:B:501:PLP:O3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:381:LEU:H	2:B:381:LEU:HD23	1.80	0.45
2:B:201:GLN:HG2	4:B:501:PLP:O3	2.16	0.45
2:A:16:GLN:NE2	2:A:21:ASP:OD1	2.46	0.45
1:D:15:ILE:HG22	1:D:16:MET:HE3	1.99	0.45
2:B:265:LYS:HD3	2:B:269:TRP:HB2	1.99	0.45
2:A:222:SER:CB	2:A:231:VAL:HG13	2.46	0.44
1:D:28:LEU:CD1	1:D:60:LYS:HB2	2.47	0.44
1:D:6:ASN:N	1:D:6:ASN:ND2	2.65	0.44
1:D:133:TRP:O	1:D:137:GLU:HG3	2.17	0.44
2:A:56:VAL:CG1	2:A:56:VAL:O	2.66	0.44
2:B:265:LYS:CD	2:B:269:TRP:HB2	2.47	0.44
1:D:133:TRP:CE3	1:D:136:LEU:CD2	3.01	0.44
2:B:23:VAL:HB	2:B:353:ILE:HG12	1.99	0.43
1:C:113:ILE:HD13	1:C:133:TRP:HZ2	1.84	0.43
2:B:16:GLN:NE2	2:B:21:ASP:OD1	2.49	0.43
1:C:56:VAL:HG23	1:C:56:VAL:O	2.17	0.43
1:C:27:VAL:CA	1:C:48:THR:HG21	2.45	0.43
2:A:198:ASP:OD2	4:A:501:PLP:N1	2.51	0.43
2:A:117:THR:CG2	2:A:119:MET:H	2.19	0.42
1:C:107:SER:O	1:C:108:ILE:HB	2.18	0.42
1:D:133:TRP:CE3	1:D:136:LEU:HD21	2.54	0.42
1:D:44:ARG:NH1	1:D:46:ARG:HB2	2.26	0.42
2:B:3:ILE:HD13	2:B:302:HIS:CE1	2.55	0.42
1:C:79:ALA:HB3	1:C:113:ILE:HD11	2.01	0.42
1:D:138:LYS:HD2	1:D:138:LYS:HA	1.89	0.42
1:C:10:LEU:HB2	1:C:122:PHE:CE1	2.54	0.42
1:C:37:ASN:OD1	1:C:44:ARG:HG3	2.20	0.42
1:C:56:VAL:CG2	1:C:80:ILE:O	2.68	0.42
1:D:23:ARG:HA	1:D:23:ARG:HD3	1.82	0.42
2:B:144:LEU:HD23	2:B:150:ILE:HD13	2.01	0.41
2:A:381:LEU:HD23	2:A:381:LEU:H	1.85	0.41
2:B:2:ASN:O	2:B:5:ASP:HB2	2.19	0.41
1:C:107:SER:O	1:C:108:ILE:CB	2.68	0.41
1:D:136:LEU:HD12	1:D:136:LEU:C	2.40	0.41
1:D:105:ASP:OD2	1:D:108:ILE:HD11	2.21	0.41
1:D:23:ARG:HG2	1:D:74:SER:OG	2.20	0.41
2:B:222:SER:CB	2:B:231:VAL:HG13	2.51	0.41
1:D:75:MET:CB	1:D:113:ILE:HG22	2.51	0.41
1:D:103:GLU:HG3	1:D:104:TYR:N	2.36	0.40
1:C:27:VAL:C	1:C:28:LEU:HD12	2.41	0.40
2:A:1:MET:HG3	2:A:298:GLU:CG	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:224:LYS:NZ	4:A:501:PLP:O3	2.54	0.40
2:B:54:ARG:NH2	2:B:54:ARG:HG3	2.34	0.40
1:C:24:ASN:HB3	1:C:60:LYS:HA	2.04	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	C	133/155 (86%)	122 (92%)	7 (5%)	4 (3%)	4	2
1	D	135/155 (87%)	114 (84%)	15 (11%)	6 (4%)	2	1
2	A	404/419 (96%)	391 (97%)	12 (3%)	1 (0%)	47	55
2	B	403/419 (96%)	393 (98%)	8 (2%)	2 (0%)	29	31
All	All	1075/1148 (94%)	1020 (95%)	42 (4%)	13 (1%)	13	11

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	114	GLU
2	B	359	HIS
1	C	29	ASN
1	D	30	ASP
1	D	85	ILE
1	D	109	ASP
2	B	53	HIS
1	C	30	ASP
1	C	104	TYR
1	D	86	GLU
1	D	113	ILE
2	A	53	HIS

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Mol	Chain	Res	Type
1	C	108	ILE

### 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	C	116/132 (88%)	107 (92%)	9 (8%)	12	12
1	D	117/132 (89%)	105 (90%)	12 (10%)	7	6
2	A	337/349 (97%)	325 (96%)	12 (4%)	35	44
2	B	336/349 (96%)	321 (96%)	15 (4%)	27	34
All	All	906/962 (94%)	858 (95%)	48 (5%)	22	27

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	6	ASN
1	D	10	LEU
1	D	13	GLN
1	D	14	VAL
1	D	24	ASN
1	D	62	GLU
1	D	76	MET
1	D	93	LYS
1	D	119	VAL
1	D	120	SER
1	D	136	LEU
1	D	138	LYS
2	A	0	HIS
2	A	1	MET
2	A	54	ARG
2	A	101	LEU
2	A	133	LYS
2	A	186	LYS
2	A	300	SER
2	A	359	HIS

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Mol	Chain	Res	Type
2	A	371	VAL
2	A	380	TYR
2	A	397	LYS
2	A	399	LYS
2	B	1	MET
2	B	2	ASN
2	B	56	VAL
2	B	101	LEU
2	B	109	LYS
2	B	207	LYS
2	B	300	SER
2	B	318	ASP
2	B	337	ASP
2	B	351	GLU
2	B	372	THR
2	B	380	TYR
2	B	386	GLU
2	B	396	GLN
2	B	399	LYS
1	C	6	ASN
1	C	14	VAL
1	C	35	ASP
1	C	62	GLU
1	C	96	SER
1	C	98	MET
1	C	114	GLU
1	C	127	LYS
1	C	130	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	13	GLN
1	D	21	ASN
1	C	117	GLN

### 5.3.3 RNA ⓘ

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	PLP	A	501	2	15,15,16	2.72	4 (26%)	20,22,23	1.53	5 (25%)
4	PLP	B	501	2	15,15,16	3.09	3 (20%)	20,22,23	1.75	5 (25%)

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	PLP	A	501	2	-	1/6/6/8	0/1/1/1
4	PLP	B	501	2	-	1/6/6/8	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	PLP	C3-C2	7.97	1.48	1.40
4	B	501	PLP	C5-C4	7.63	1.48	1.40
4	B	501	PLP	C3-C2	7.43	1.48	1.40
4	A	501	PLP	C5-C4	4.41	1.45	1.40
4	B	501	PLP	C3-C4	3.74	1.47	1.40
4	A	501	PLP	C3-C4	3.12	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	PLP	C4A-C4	-2.37	1.46	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	PLP	C4A-C4-C5	4.73	125.81	120.94
4	A	501	PLP	C6-N1-C2	3.17	125.03	119.17
4	B	501	PLP	C3-C4-C5	-2.80	115.72	118.74
4	A	501	PLP	O3P-P-O4P	-2.48	100.12	106.73
4	B	501	PLP	O3P-P-O2P	2.44	116.95	107.64
4	A	501	PLP	C3-C2-N1	-2.40	117.66	120.77
4	B	501	PLP	C3-C2-N1	-2.23	117.88	120.77
4	B	501	PLP	C6-N1-C2	2.15	123.16	119.17
4	A	501	PLP	O3-C3-C2	2.15	122.18	117.49
4	A	501	PLP	C4A-C4-C5	2.14	123.14	120.94

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	PLP	C5A-O4P-P-O1P
4	B	501	PLP	C5A-O4P-P-O1P

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	PLP	2	0
4	B	501	PLP	2	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 ⓘ

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	C	135/155 (87%)	0.80	24 (17%) 1 2	53, 86, 156, 224	0
1	D	137/155 (88%)	1.40	38 (27%) 0 0	78, 112, 154, 182	0
2	A	405/419 (96%)	0.09	18 (4%) 34 45	33, 51, 78, 113	0
2	B	405/419 (96%)	0.19	16 (3%) 38 49	35, 58, 111, 162	0
All	All	1082/1148 (94%)	0.38	96 (8%) 9 15	33, 61, 130, 224	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	27	VAL	6.1
1	D	104	TYR	5.3
1	D	78	GLN	4.4
1	D	50	LYS	4.1
1	D	135	ALA	4.1
1	D	103	GLU	3.8
1	C	32	ILE	3.7
1	C	30	ASP	3.6
1	C	85	ILE	3.6
1	D	27	VAL	3.6
1	C	103	GLU	3.5
1	D	51	LEU	3.5
1	D	105	ASP	3.5
2	A	231	VAL	3.4
2	A	403	THR	3.4
1	C	49	MET	3.4
2	A	273	ALA	3.4
2	A	277	ILE	3.4
1	C	41	CYS	3.4
1	C	40	THR	3.3
1	D	6	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	48	THR	3.3
2	B	91	GLY	3.3
1	D	87	THR	3.2
1	C	53	GLY	3.2
2	A	404	ASN	3.2
1	D	74	SER	3.1
1	D	106	ASP	3.1
1	D	13	GLN	3.1
2	A	338	ASP	3.1
1	C	51	LEU	3.1
1	C	136	LEU	3.1
1	C	28	LEU	3.0
1	C	47	LEU	3.0
1	C	34	VAL	3.0
1	C	89	LEU	3.0
2	A	83[A]	MET	3.0
1	D	77	THR	2.9
1	D	20	LYS	2.9
2	B	339	VAL	2.9
1	C	42	GLY	2.8
1	D	16	MET	2.8
1	D	31	SER	2.8
1	C	31	SER	2.7
2	B	315	ARG	2.7
2	B	396	GLN	2.7
1	D	80	ILE	2.7
2	A	233	VAL	2.7
1	C	54	ASP	2.6
1	D	15	ILE	2.6
2	B	321	THR	2.6
1	D	33	VAL	2.6
2	B	318	ASP	2.6
2	A	278	ILE	2.6
1	D	112	ASP	2.6
1	D	9	THR	2.6
1	D	108	ILE	2.6
2	B	322	VAL	2.6
2	A	232	GLY	2.5
2	A	88	PHE	2.5
1	D	139	GLY	2.5
1	D	12	ARG	2.4
1	C	135	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	56	VAL	2.4
2	A	275	THR	2.4
2	A	89	THR	2.3
2	A	90	LYS	2.3
1	D	102	LYS	2.3
1	D	19	TYR	2.3
1	D	124	ALA	2.3
2	B	29	ALA	2.3
1	D	34	VAL	2.3
2	B	221	SER	2.3
1	D	101	GLY	2.3
1	D	94	ILE	2.3
1	C	82	GLY	2.2
1	C	140	VAL	2.2
2	B	222	SER	2.2
2	B	395	LEU	2.2
2	B	123	ALA	2.2
2	A	220	LEU	2.2
1	D	64	GLU	2.2
1	D	138	LYS	2.2
1	C	55	ILE	2.2
2	B	231	VAL	2.2
1	D	52	ASP	2.2
2	B	314	PHE	2.2
1	D	73	ALA	2.1
2	B	317	LEU	2.1
1	D	70	MET	2.1
2	A	318	ASP	2.1
2	A	280	GLY	2.1
1	D	22	PRO	2.1
2	A	54	ARG	2.0
1	C	84	ASP	2.0
2	B	275	THR	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides 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(Å <sup>2</sup> )	Q<0.9
3	ZN	C	201	1/1	0.94	0.07	64,64,64,64	0
3	ZN	D	201	1/1	0.96	0.04	73,73,73,73	0
4	PLP	B	501	15/16	0.98	0.20	41,47,57,61	0
4	PLP	A	501	15/16	0.99	0.19	34,40,43,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.