



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:21 am GMT

PDB ID : 2BWN  
Title : 5-Aminolevulinate Synthase from Rhodobacter capsulatus  
Authors : Astner, I.; Schulze, J.O.; van den Heuvel, J.J.; Jahn, D.; Schubert, W.-D.; Heinz, D.W.  
Deposited on : 2005-07-15  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

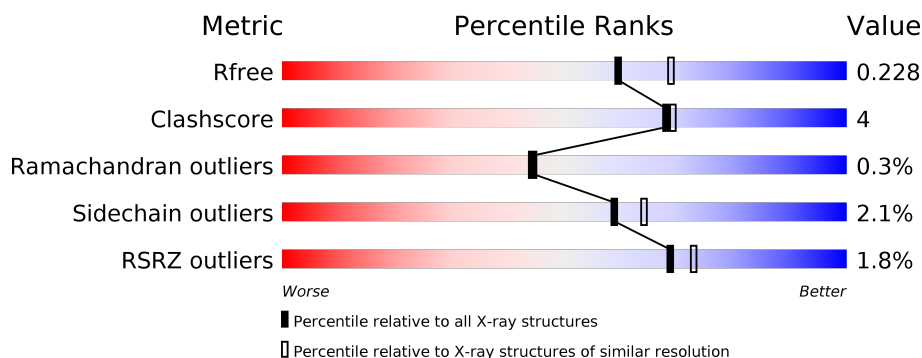
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (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  $\geq 3$ , 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  $\leq 5\%$ . 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	401	
1	B	401	
1	D	401	
1	E	401	

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	SIN	A	1398	-	-	-	X
3	SIN	D	1399	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13428 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 5-AMINOLEVULINATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	11	0
			3125	1982	557	569	17			
1	B	395	Total	C	N	O	S	0	17	0
			3171	2008	569	577	17			
1	D	397	Total	C	N	O	S	0	22	0
			3220	2041	574	588	17			
1	E	398	Total	C	N	O	S	0	24	0
			3248	2060	580	592	16			

There are 24 discrepancies between the modelled and reference sequences:

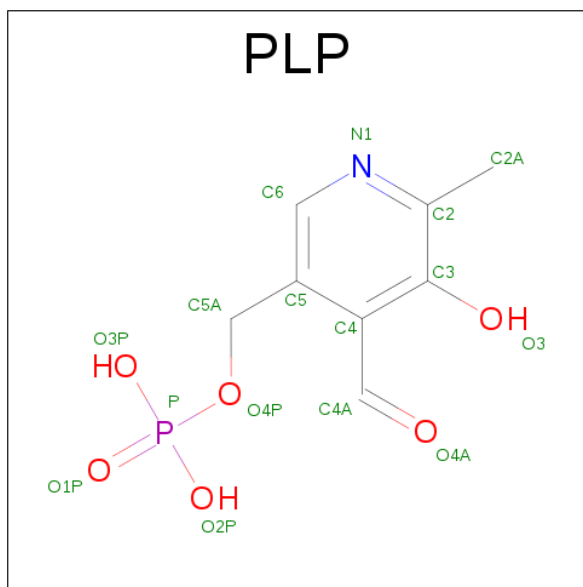
Chain	Residue	Modelled	Actual	Comment	Reference
A	102	GLY	ASP	VARIANT	UNP P18079
A	105	GLN	GLY	VARIANT	UNP P18079
A	117	ASN	ILE	VARIANT	UNP P18079
A	128	VAL	LEU	VARIANT	UNP P18079
A	205	GLU	ASP	VARIANT	UNP P18079
A	262	ARG	LYS	VARIANT	UNP P18079
B	102	GLY	ASP	VARIANT	UNP P18079
B	105	GLN	GLY	VARIANT	UNP P18079
B	117	ASN	ILE	VARIANT	UNP P18079
B	128	VAL	LEU	VARIANT	UNP P18079
B	205	GLU	ASP	VARIANT	UNP P18079
B	262	ARG	LYS	VARIANT	UNP P18079
D	102	GLY	ASP	VARIANT	UNP P18079
D	105	GLN	GLY	VARIANT	UNP P18079
D	117	ASN	ILE	VARIANT	UNP P18079
D	128	VAL	LEU	VARIANT	UNP P18079
D	205	GLU	ASP	VARIANT	UNP P18079
D	262	ARG	LYS	VARIANT	UNP P18079
E	102	GLY	ASP	VARIANT	UNP P18079
E	105	GLN	GLY	VARIANT	UNP P18079
E	117	ASN	ILE	VARIANT	UNP P18079

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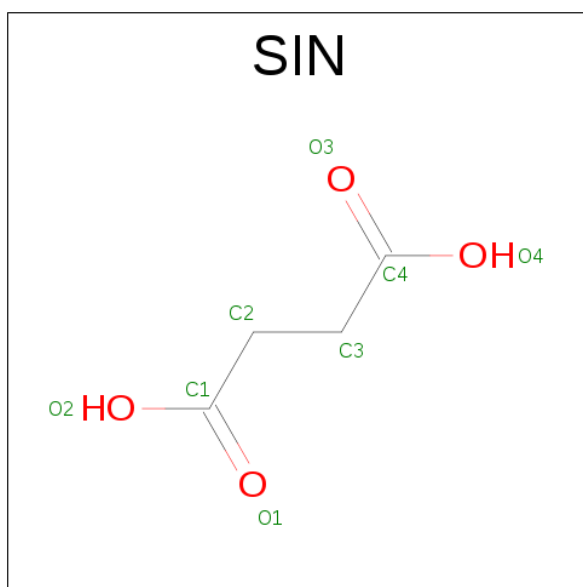
Chain	Residue	Modelled	Actual	Comment	Reference
E	128	VAL	LEU	VARIANT	UNP P18079
E	205	GLU	ASP	VARIANT	UNP P18079
E	262	ARG	LYS	VARIANT	UNP P18079

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).



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		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is SUCCINIC ACID (three-letter code: SIN) (formula:  $C_4H_6O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	4	4		
3	D	1	Total	C	O	0	0
			8	4	4		
3	E	1	Total	C	O	0	0
			8	4	4		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

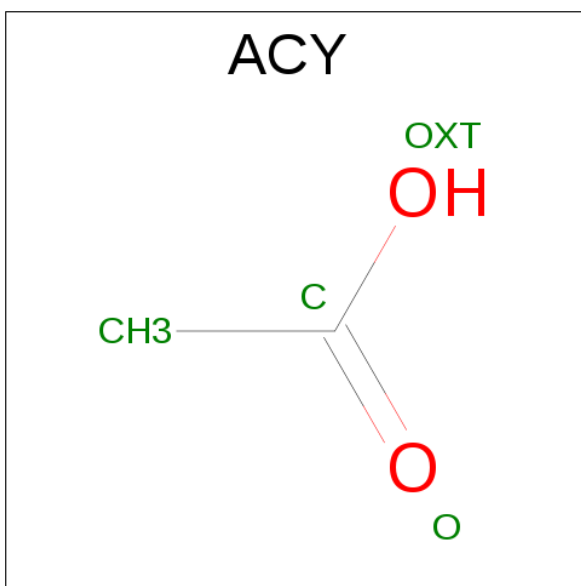
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	E	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



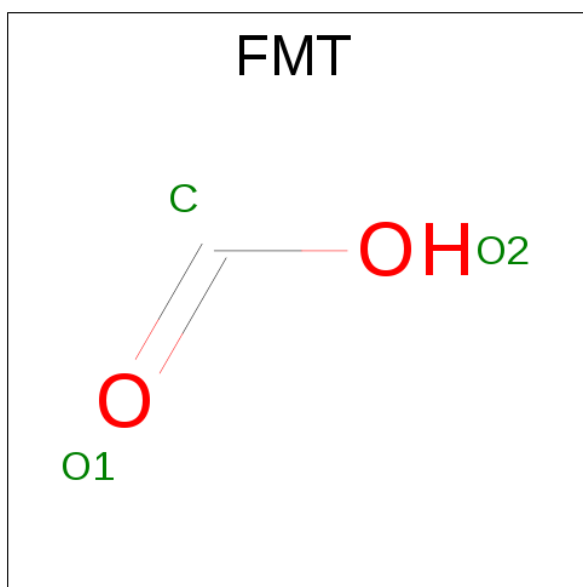
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is ACETIC ACID (three-letter code: ACY) (formula:  $C_2H_4O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is FORMIC ACID (three-letter code: FMT) (formula:  $CH_2O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	C	O	0	0
			3	1	2		

- Molecule 8 is water.

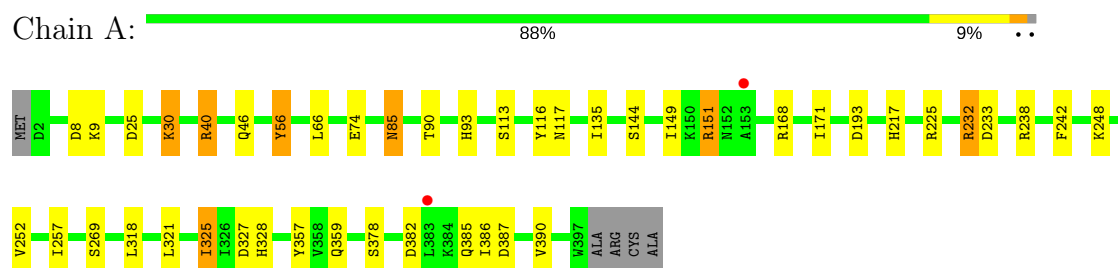
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	181	Total	O	0	0
			181	181		
8	B	137	Total	O	0	0
			137	137		
8	D	110	Total	O	0	0
			110	110		
8	E	134	Total	O	0	0
			134	134		



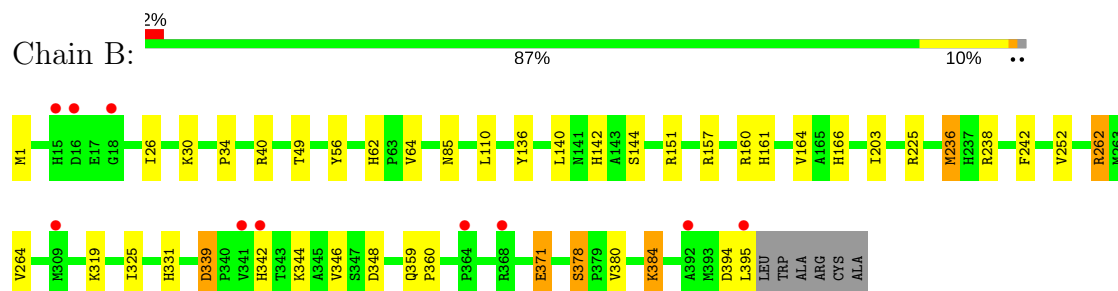
### 3 Residue-property plots

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.

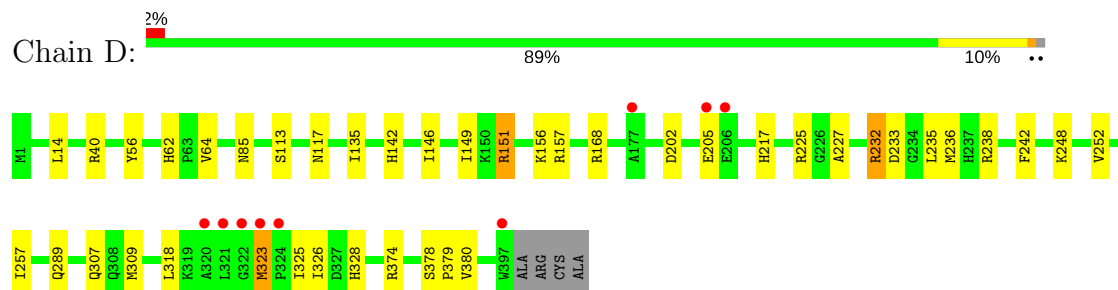
#### • Molecule 1: 5-AMINOLEVULINATE SYNTHASE



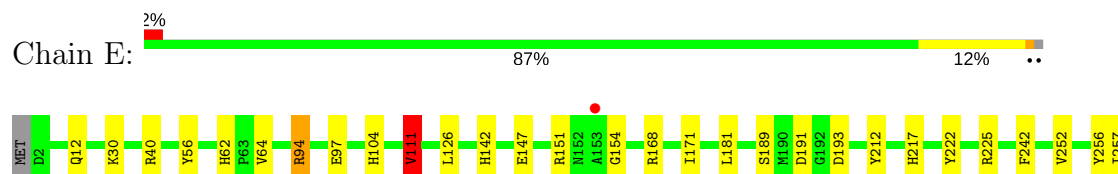
#### • Molecule 1: 5-AMINOLEVULINATE SYNTHASE

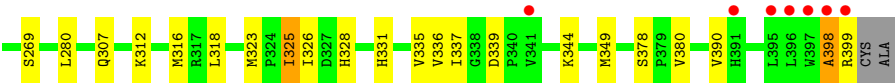


#### • Molecule 1: 5-AMINOLEVULINATE SYNTHASE



#### • Molecule 1: 5-AMINOLEVULINATE SYNTHASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.88Å 92.87Å 250.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	129.10 – 2.10 38.33 – 2.10	Depositor EDS
% Data completeness (in resolution range)	83.7 (129.10-2.10) 83.8 (38.33-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.39 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.161 , 0.217 0.173 , 0.228	Depositor DCC
$R_{free}$ test set	3874 reflections (5.21%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.2	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 55.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13428	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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: PLP, FMT, CL, SO4, ACY, SIN

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	1.02	7/3194 (0.2%)	0.92	11/4321 (0.3%)
1	B	0.97	0/3240	0.86	6/4386 (0.1%)
1	D	0.97	1/3291 (0.0%)	0.88	12/4452 (0.3%)
1	E	0.93	1/3326 (0.0%)	0.87	9/4503 (0.2%)
All	All	0.97	9/13051 (0.1%)	0.88	38/17662 (0.2%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	111	VAL	CB-CG1	-6.52	1.39	1.52
1	A	56	TYR	CD2-CE2	-6.08	1.30	1.39
1	D	248	LYS	CD-CE	5.96	1.66	1.51
1	A	248	LYS	CD-CE	5.38	1.64	1.51
1	A	225	ARG	CG-CD	-5.29	1.38	1.51
1	A	85	ASN	CB-CG	5.28	1.63	1.51
1	A	74	GLU	CD-OE2	5.25	1.31	1.25
1	A	225	ARG	CZ-NH2	-5.19	1.26	1.33
1	A	269	SER	CB-OG	5.05	1.48	1.42

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	225	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	E	40	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	E	94	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	A	225	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	E	40	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	A	40	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	B	262	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	A	238	ARG	NE-CZ-NH2	-6.80	116.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	E	225	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	E	94	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	B	40	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	D	225	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	B	225	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	D	232	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	D	151	ARG	CG-CD-NE	-6.07	99.05	111.80
1	A	9	LYS	CD-CE-NZ	5.93	125.35	111.70
1	A	387	ASP	CB-CA-C	-5.79	98.81	110.40
1	A	248	LYS	CD-CE-NZ	5.78	125.00	111.70
1	B	238	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	232	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	40	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	E	225	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	D	151	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	B	225	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	D	40	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	A	327	ASP	CB-CG-OD1	5.41	123.17	118.30
1	E	398	ALA	N-CA-C	-5.31	96.67	111.00
1	D	40	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	E	191	ASP	CB-CG-OD1	5.19	122.97	118.30
1	B	238	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	D	238	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	25	ASP	CB-CG-OD1	5.09	122.88	118.30
1	D	248	LYS	CD-CE-NZ	5.07	123.35	111.70
1	D	157[A]	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	D	157[B]	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	E	325	ILE	CB-CA-C	-5.01	101.57	111.60
1	D	374	ARG	NE-CZ-NH1	5.00	122.80	120.30

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	3125	0	3106	22	0
1	B	3171	0	3151	29	0
1	D	3220	0	3206	27	0
1	E	3248	0	3205	44	0
2	A	15	0	6	1	0
2	B	15	0	6	2	0
2	D	15	0	6	2	0
2	E	15	0	6	3	0
3	A	8	0	4	0	0
3	D	8	0	4	0	0
3	E	8	0	4	0	0
4	A	1	0	0	0	0
4	E	1	0	0	0	0
5	B	5	0	0	0	0
6	B	4	0	3	0	0
6	D	4	0	3	0	0
7	E	3	0	1	0	0
8	A	181	0	0	1	0
8	B	137	0	0	2	0
8	D	110	0	0	1	0
8	E	134	0	0	5	0
All	All	13428	0	12711	114	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 4.

All (114) 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:E:398:ALA:O	1:E:399:ARG:HG2	1.47	1.12
1:D:323[B]:MET:O	1:D:325[B]:ILE:HD12	1.50	1.11
1:E:398:ALA:O	1:E:399:ARG:CG	2.04	1.05
1:D:323[B]:MET:CB	1:D:325[B]:ILE:HD11	1.87	1.04
1:D:323[B]:MET:HB2	1:D:325[B]:ILE:HD11	1.04	1.01
1:D:323[B]:MET:HB2	1:D:325[B]:ILE:CD1	1.95	0.96
1:E:312[B]:LYS:HE3	1:E:316[B]:MET:CE	2.08	0.84
1:E:398:ALA:C	1:E:399:ARG:HG2	2.06	0.76
1:E:312[B]:LYS:HE3	1:E:316[B]:MET:HE3	1.67	0.74
1:B:359[A]:GLN:HE21	1:B:360:PRO:HD2	1.56	0.70
1:B:1:MET:N	8:B:2001:HOH:O	2.27	0.67
1:E:318[B]:LEU:HD13	1:E:390[B]:VAL:HG22	1.77	0.67
1:D:323[B]:MET:C	1:D:325[B]:ILE:HD12	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:HIS:HD2	1:E:64:VAL:H	1.43	0.64
1:E:312[B]:LYS:HE3	1:E:316[B]:MET:HE1	1.80	0.64
1:E:398:ALA:O	1:E:399:ARG:HG3	1.96	0.62
1:E:217[A]:HIS:NE2	2:E:1248:PLP:O3	2.30	0.61
1:A:113:SER:HB2	1:A:117:ASN:HD22	1.66	0.60
1:B:339:ASP:OD2	1:B:342:HIS:ND1	2.35	0.60
1:D:323[B]:MET:CB	1:D:325[B]:ILE:CD1	2.70	0.60
1:A:151:ARG:HH12	1:B:151:ARG:HA	1.67	0.59
1:E:344:LYS:NZ	8:E:2124:HOH:O	2.35	0.58
1:D:217:HIS:NE2	2:D:1248:PLP:O3	2.35	0.58
1:E:142[A]:HIS:HB2	2:E:1248:PLP:H2A3	1.88	0.56
1:A:357:TYR:OH	1:A:359:GLN:NE2	2.39	0.55
1:D:323[B]:MET:O	1:D:325[B]:ILE:CD1	2.41	0.55
1:B:164[B]:VAL:HG22	1:B:203:ILE:HD11	1.88	0.54
1:D:227:ALA:HB1	1:D:236[B]:MET:HE1	1.90	0.54
1:E:142[B]:HIS:HB2	2:E:1248:PLP:H2A3	1.90	0.54
1:D:56:TYR:O	1:D:378:SER:HB2	2.09	0.53
1:E:326:ILE:HD12	1:E:336[A]:VAL:HG21	1.89	0.53
1:E:326:ILE:HD12	1:E:336[B]:VAL:HG21	1.89	0.53
1:D:135:ILE:HG21	1:D:149:ILE:HG12	1.90	0.52
1:E:62:HIS:CD2	1:E:64:VAL:HG22	2.45	0.52
1:A:232:ARG:HD2	1:A:233:ASP:OD1	2.10	0.52
1:B:236:MET:HG3	1:B:242:PHE:CZ	2.45	0.52
1:D:62:HIS:ND1	1:D:64:VAL:HG22	2.25	0.52
1:A:217:HIS:NE2	2:A:1248:PLP:O3	2.34	0.52
1:A:151:ARG:NH1	1:B:151:ARG:HA	2.24	0.52
1:E:181[B]:LEU:HD21	1:E:212:TYR:HB2	1.91	0.51
1:E:325:ILE:HD13	1:E:335:VAL:HG22	1.91	0.51
1:E:126:LEU:HD23	1:E:181[A]:LEU:CD1	2.41	0.51
1:D:378:SER:OG	1:D:380:VAL:HG22	2.09	0.50
1:E:56:TYR:O	1:E:378:SER:HB2	2.12	0.50
1:E:312[B]:LYS:CE	1:E:316[B]:MET:HE1	2.42	0.50
1:B:142[B]:HIS:HB2	2:B:1248:PLP:H2A3	1.93	0.50
1:B:142[A]:HIS:HB2	2:B:1248:PLP:H2A3	1.93	0.50
1:B:62:HIS:ND1	1:B:64:VAL:HG22	2.27	0.49
1:B:339:ASP:CA	1:B:371:GLU:HG3	2.42	0.49
1:A:40:ARG:HE	1:A:46:GLN:HE21	1.61	0.48
1:E:312[B]:LYS:CE	1:E:316[B]:MET:CE	2.89	0.48
1:E:318[A]:LEU:HB3	1:E:325:ILE:HD11	1.95	0.48
1:D:318[B]:LEU:HD22	1:D:323[B]:MET:HG3	1.94	0.48
1:E:318[A]:LEU:HD13	1:E:325:ILE:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:HIS:HB2	2:D:1248:PLP:H2A3	1.95	0.47
1:A:386:ILE:O	1:A:390:VAL:HG23	2.14	0.47
1:D:235[B]:LEU:O	1:D:236[B]:MET:C	2.53	0.47
1:E:318[B]:LEU:CD1	1:E:390[B]:VAL:HG22	2.43	0.47
1:A:90:THR:OG1	1:A:93:HIS:HD2	1.98	0.47
1:B:56:TYR:O	1:B:378:SER:HB2	2.15	0.46
1:B:342:HIS:O	1:B:346:VAL:HG23	2.15	0.46
1:A:90:THR:HA	1:B:26:ILE:O	2.16	0.46
1:A:85:ASN:O	1:B:359[B]:GLN:NE2	2.48	0.46
1:D:236[A]:MET:HG3	1:D:242:PHE:CZ	2.51	0.46
1:E:312[B]:LYS:NZ	8:E:2114:HOH:O	2.49	0.46
1:D:307:GLN:NE2	8:D:2100:HOH:O	2.48	0.46
1:D:85:ASN:HB2	8:E:2011:HOH:O	2.15	0.46
1:E:222:TYR:OH	1:E:331:HIS:HD2	2.00	0.45
1:E:378:SER:OG	1:E:380:VAL:HG22	2.17	0.45
1:B:142[A]:HIS:ND1	1:B:144:SER:OG	2.45	0.45
1:E:111:VAL:HG21	1:E:280:LEU:HD12	1.99	0.45
1:B:34:PRO:HG2	1:B:49:THR:HG23	1.98	0.45
1:D:232:ARG:HD2	1:D:233:ASP:OD1	2.17	0.45
1:B:110:LEU:HB2	1:B:264:VAL:HG13	1.98	0.45
1:E:318[A]:LEU:CB	1:E:325:ILE:HD11	2.46	0.45
1:E:318[B]:LEU:HB3	1:E:325:ILE:HD11	1.98	0.45
1:A:56:TYR:O	1:A:378:SER:HB2	2.17	0.44
1:E:339[B]:ASP:OD1	1:E:339[B]:ASP:N	2.50	0.44
1:D:326:ILE:CG2	1:D:328:HIS:CE1	3.01	0.44
1:D:113:SER:HB2	1:D:117:ASN:HD22	1.83	0.44
1:A:30:LYS:HE2	1:A:66:LEU:CD1	2.48	0.44
1:D:14:LEU:HD11	1:E:269:SER:HB3	1.99	0.43
1:B:378:SER:OG	1:B:380:VAL:HG22	2.17	0.43
1:A:168:ARG:HA	1:A:171:ILE:HG22	2.01	0.43
1:D:242:PHE:O	1:D:257:ILE:HA	2.19	0.43
1:D:151:ARG:NH2	1:E:147:GLU:HB3	2.33	0.43
1:E:104[B]:HIS:HE1	1:E:256:TYR:OH	2.02	0.43
1:B:160[A]:ARG:H	1:B:166:HIS:HD2	1.67	0.42
1:E:326:ILE:HD12	1:E:336[A]:VAL:CG2	2.49	0.42
1:B:136:TYR:CE2	1:B:157:ARG:HG3	2.53	0.42
1:A:135:ILE:HG21	1:A:149:ILE:HG12	2.01	0.42
1:B:140:LEU:HD12	1:B:161:HIS:CG	2.55	0.42
1:E:337:ILE:HG22	1:E:339[B]:ASP:OD1	2.19	0.42
1:A:8:ASP:OD2	1:B:262:ARG:NH1	2.53	0.42
1:E:154:GLY:N	8:E:2058:HOH:O	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:LYS:HG3	1:B:348:ASP:OD2	2.20	0.42
1:B:331:HIS:H	1:B:331:HIS:CD2	2.37	0.42
1:E:307:GLN:NE2	8:E:2112:HOH:O	2.53	0.42
1:A:242:PHE:O	1:A:257:ILE:HA	2.20	0.41
1:B:384:LYS:NZ	8:B:2137:HOH:O	2.53	0.41
1:E:94:ARG:HH11	1:E:94:ARG:HG2	1.86	0.41
1:A:151:ARG:HD2	1:B:151:ARG:NH1	2.35	0.41
1:D:378:SER:HB2	1:D:379:PRO:HD2	2.01	0.41
1:E:97:GLU:CG	1:E:111:VAL:HG12	2.50	0.41
1:A:193:ASP:HB3	1:A:328:HIS:CG	2.56	0.41
1:A:321:LEU:HD11	1:A:390:VAL:HG13	2.02	0.41
1:A:318:LEU:HD12	1:A:325[B]:ILE:HD11	2.03	0.41
1:E:168:ARG:HA	1:E:171:ILE:HG22	2.02	0.41
1:E:242:PHE:O	1:E:257:ILE:HA	2.21	0.41
1:E:193:ASP:HB3	1:E:328:HIS:CG	2.56	0.40
1:A:116:TYR:CD2	1:A:144:SER:HB3	2.57	0.40
1:B:319:LYS:HE2	1:B:325:ILE:HB	2.03	0.40
8:A:2009:HOH:O	1:B:85:ASN:HB2	2.22	0.40
1:D:202:ASP:O	1:D:205[B]:GLU:HG3	2.21	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	405/401 (101%)	399 (98%)	5 (1%)	1 (0%)	51	52
1	B	410/401 (102%)	399 (97%)	10 (2%)	1 (0%)	51	52
1	D	417/401 (104%)	406 (97%)	10 (2%)	1 (0%)	51	52
1	E	420/401 (105%)	411 (98%)	8 (2%)	1 (0%)	51	52
All	All	1652/1604 (103%)	1615 (98%)	33 (2%)	4 (0%)	44	52

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	252	VAL
1	A	252	VAL
1	D	252	VAL
1	E	252	VAL

### 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	320/313 (102%)	314 (98%)	6 (2%)	62	68
1	B	326/313 (104%)	318 (98%)	8 (2%)	53	57
1	D	331/313 (106%)	324 (98%)	7 (2%)	59	64
1	E	334/313 (107%)	326 (98%)	8 (2%)	54	59
All	All	1311/1252 (105%)	1282 (98%)	29 (2%)	59	62

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LYS
1	A	151	ARG
1	A	325[A]	ILE
1	A	325[B]	ILE
1	A	382	ASP
1	A	385	GLN
1	B	30	LYS
1	B	236	MET
1	B	339	ASP
1	B	371	GLU
1	B	378	SER
1	B	384	LYS
1	B	394	ASP
1	B	395	LEU
1	D	146	ILE
1	D	156	LYS

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Mol	Chain	Res	Type
1	D	168	ARG
1	D	289	GLN
1	D	309	MET
1	D	323[A]	MET
1	D	323[B]	MET
1	E	12[A]	GLN
1	E	12[B]	GLN
1	E	30	LYS
1	E	111	VAL
1	E	151	ARG
1	E	189	SER
1	E	323	MET
1	E	349	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	93	HIS
1	A	105	GLN
1	A	117	ASN
1	A	307	GLN
1	A	331	HIS
1	A	359	GLN
1	B	104	HIS
1	B	117	ASN
1	B	166	HIS
1	B	307	GLN
1	B	331	HIS
1	D	243	ASN
1	D	289	GLN
1	D	307	GLN
1	D	328	HIS
1	D	359	GLN
1	E	62	HIS
1	E	105	GLN
1	E	307	GLN
1	E	331	HIS
1	E	342	HIS
1	E	359	GLN

### 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 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	$\# Z  > 2$
2	PLP	A	1248	1	15,15,16	2.55	4 (26%)	20,22,23	2.03	8 (40%)
3	SIN	A	1398	-	1,7,7	0.23	0	2,8,8	1.61	0
2	PLP	B	1248	1	15,15,16	2.07	6 (40%)	20,22,23	1.60	3 (15%)
5	SO4	B	1396	-	4,4,4	0.21	0	6,6,6	0.21	0
6	ACY	B	1397	-	1,3,3	2.88	1 (100%)	0,3,3	0.00	-
2	PLP	D	1248	1	15,15,16	1.91	4 (26%)	20,22,23	1.77	5 (25%)
6	ACY	D	1398	-	1,3,3	0.98	0	0,3,3	0.00	-
3	SIN	D	1399	-	1,7,7	0.82	0	2,8,8	2.22	1 (50%)
2	PLP	E	1248	1	15,15,16	2.20	5 (33%)	20,22,23	1.47	4 (20%)
3	SIN	E	1400	-	1,7,7	0.18	0	2,8,8	3.33	1 (50%)
7	FMT	E	1401	-	0,2,2	0.00	-	0,1,1	0.00	-

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	A	1248	1	-	0/6/6/8	0/1/1/1
3	SIN	A	1398	-	-	0/1/5/5	0/0/0/0
2	PLP	B	1248	1	-	0/6/6/8	0/1/1/1
5	SO4	B	1396	-	-	0/0/0/0	0/0/0/0
6	ACY	B	1397	-	-	0/0/0/0	0/0/0/0
2	PLP	D	1248	1	-	0/6/6/8	0/1/1/1
6	ACY	D	1398	-	-	0/0/0/0	0/0/0/0
3	SIN	D	1399	-	-	0/1/5/5	0/0/0/0
2	PLP	E	1248	1	-	0/6/6/8	0/1/1/1
3	SIN	E	1400	-	-	0/1/5/5	0/0/0/0
7	FMT	E	1401	-	-	0/0/0/0	0/0/0/0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1248	PLP	O3-C3	-6.94	1.21	1.37
2	D	1248	PLP	O3-C3	-5.67	1.23	1.37
2	E	1248	PLP	O3-C3	-5.29	1.24	1.37
2	B	1248	PLP	O3-C3	-5.11	1.25	1.37
2	B	1248	PLP	P-O3P	-2.39	1.45	1.54
2	E	1248	PLP	P-O3P	-2.30	1.45	1.54
2	E	1248	PLP	P-O2P	-2.20	1.45	1.54
2	D	1248	PLP	P-O2P	-2.01	1.46	1.54
2	D	1248	PLP	C6-N1	2.02	1.38	1.34
2	D	1248	PLP	C2-N1	2.03	1.38	1.33
2	B	1248	PLP	C5-C4	2.26	1.43	1.40
2	B	1248	PLP	C2-N1	2.32	1.38	1.33
2	B	1248	PLP	C3-C2	2.32	1.42	1.40
2	A	1248	PLP	C2A-C2	2.60	1.55	1.50
2	A	1248	PLP	C4A-C4	2.69	1.57	1.51
6	B	1397	ACY	CH3-C	2.88	1.52	1.48
2	B	1248	PLP	C6-N1	2.89	1.40	1.34
2	E	1248	PLP	C6-N1	2.91	1.40	1.34
2	E	1248	PLP	C4A-C4	3.08	1.57	1.51
2	A	1248	PLP	C3-C2	4.33	1.43	1.40

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1400	SIN	C2-C3-C4	-4.63	104.74	112.66
2	A	1248	PLP	C3-C4-C5	-3.30	114.89	118.63
2	B	1248	PLP	O4P-P-O1P	-3.07	97.85	106.47
3	D	1399	SIN	C2-C3-C4	-3.02	107.51	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1248	PLP	O2P-P-O4P	-2.88	99.08	106.73
2	A	1248	PLP	C3-C2-N1	-2.61	117.31	120.75
2	E	1248	PLP	O2P-P-O4P	-2.52	100.02	106.73
2	D	1248	PLP	C5-C6-N1	-2.44	119.74	123.87
2	A	1248	PLP	O2P-P-O4P	-2.22	100.84	106.73
2	D	1248	PLP	O4P-P-O1P	-2.18	100.37	106.47
2	E	1248	PLP	C5-C6-N1	-2.04	120.41	123.87
2	B	1248	PLP	C4A-C4-C5	2.43	123.31	120.86
2	A	1248	PLP	C4-C3-C2	2.47	124.13	120.06
2	A	1248	PLP	O3P-P-O1P	2.63	120.79	110.50
2	E	1248	PLP	O4P-C5A-C5	2.65	114.65	109.32
2	D	1248	PLP	C6-C5-C4	2.66	120.40	118.18
2	A	1248	PLP	O4P-C5A-C5	2.87	115.09	109.32
2	A	1248	PLP	C2A-C2-C3	2.88	124.39	120.96
2	E	1248	PLP	C6-C5-C4	3.42	121.04	118.18
2	D	1248	PLP	O4P-C5A-C5	3.76	116.88	109.32
2	A	1248	PLP	C6-C5-C4	3.98	121.50	118.18
2	B	1248	PLP	O4P-C5A-C5	4.35	118.07	109.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1248	PLP	1	0
2	B	1248	PLP	2	0
2	D	1248	PLP	2	0
2	E	1248	PLP	3	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	A	396/401 (98%)	-0.32	2 (0%) 90 92	10, 17, 31, 56	0
1	B	395/401 (98%)	-0.15	10 (2%) 58 63	8, 17, 41, 52	1 (0%)
1	D	397/401 (99%)	-0.06	9 (2%) 61 66	10, 18, 33, 57	0
1	E	398/401 (99%)	-0.11	8 (2%) 65 70	10, 17, 33, 62	3 (0%)
All	All	1586/1604 (98%)	-0.16	29 (1%) 69 73	8, 17, 36, 62	4 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	395	LEU	5.2
1	D	321	LEU	5.2
1	D	322[A]	GLY	4.5
1	E	395	LEU	4.2
1	E	341	VAL	4.1
1	D	177	ALA	4.0
1	A	383[A]	LEU	3.8
1	D	323[A]	MET	3.6
1	E	396	LEU	3.5
1	D	320	ALA	3.4
1	E	399	ARG	3.3
1	B	18	GLY	2.9
1	D	324	PRO	2.9
1	B	341	VAL	2.8
1	D	206	GLU	2.5
1	B	364	PRO	2.4
1	E	153	ALA	2.4
1	A	153	ALA	2.3
1	B	368	ARG	2.3
1	B	15	HIS	2.3
1	D	205[A]	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	392	ALA	2.3
1	E	391	HIS	2.3
1	E	397	TRP	2.2
1	B	16	ASP	2.2
1	B	342	HIS	2.2
1	E	398	ALA	2.1
1	B	309[A]	MET	2.1
1	D	397	TRP	2.1

## 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<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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	SIN	D	1399	8/8	0.82	0.20	3.84	36,44,46,54	0
3	SIN	A	1398	8/8	0.90	0.15	3.10	27,39,47,50	0
3	SIN	E	1400	8/8	0.93	0.17	1.92	29,38,42,42	0
6	ACY	B	1397	4/4	0.95	0.14	1.53	18,22,23,24	0
6	ACY	D	1398	4/4	0.97	0.11	-0.64	25,26,27,28	0
7	FMT	E	1401	3/3	0.94	0.09	-1.10	23,23,26,30	0
2	PLP	D	1248	15/16	0.97	0.10	-1.17	13,21,26,26	0
2	PLP	A	1248	15/16	0.98	0.07	-2.08	13,21,25,26	0
2	PLP	E	1248	15/16	0.98	0.08	-2.14	14,22,26,26	0
2	PLP	B	1248	15/16	0.97	0.09	-2.15	16,18,23,23	0
4	CL	E	1402	1/1	0.95	0.04	-	69,69,69,69	0
5	SO4	B	1396	5/5	0.87	0.19	-	67,68,70,70	5
4	CL	A	1399	1/1	0.84	0.07	-	65,65,65,65	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.