



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:20 am GMT

PDB ID : 2BWO
Title : 5-Aminolevulinate Synthase from Rhodobacter capsulatus in complex with succinyl-CoA
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 : 2.80 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

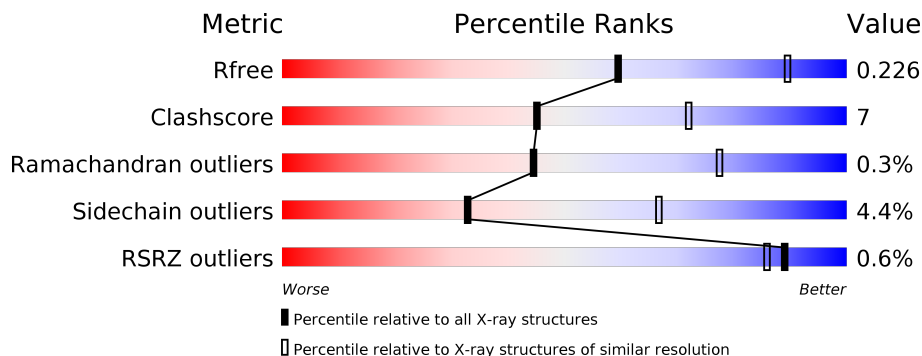
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12602 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	398	Total	C	N	O	S	0	0	0
			3048	1936	539	558	15			
1	B	399	Total	C	N	O	S	0	0	0
			3059	1942	543	559	15			
1	D	397	Total	C	N	O	S	0	0	0
			3043	1933	538	557	15			
1	E	399	Total	C	N	O	S	0	0	0
			3059	1942	543	559	15			

There are 24 discrepancies between the modelled and reference sequences:

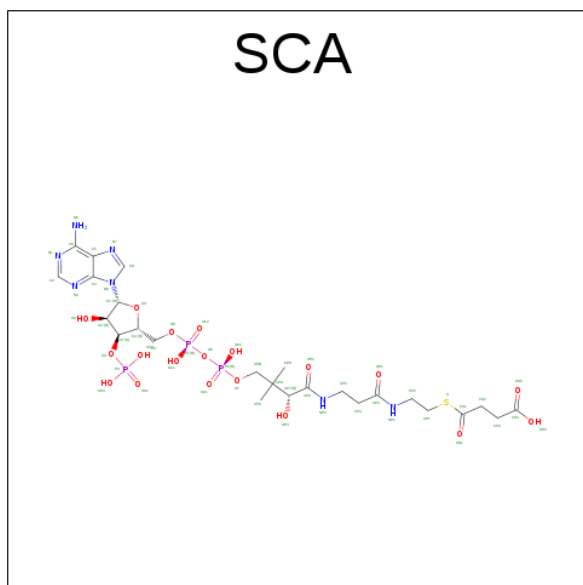
Chain	Residue	Modelled	Actual	Comment	Reference
A	102	GLY	ASP	VARIANT	UNP P18079
A	105	GLN	GLY	VARIANT	UNP P18079
A	117	ASN	ILE	VARIANT	UNP P18079
A	128	VAL	LEU	VARIANT	UNP P18079
A	205	GLU	ASP	VARIANT	UNP P18079
A	262	ARG	LYS	VARIANT	UNP P18079
B	102	GLY	ASP	VARIANT	UNP P18079
B	105	GLN	GLY	VARIANT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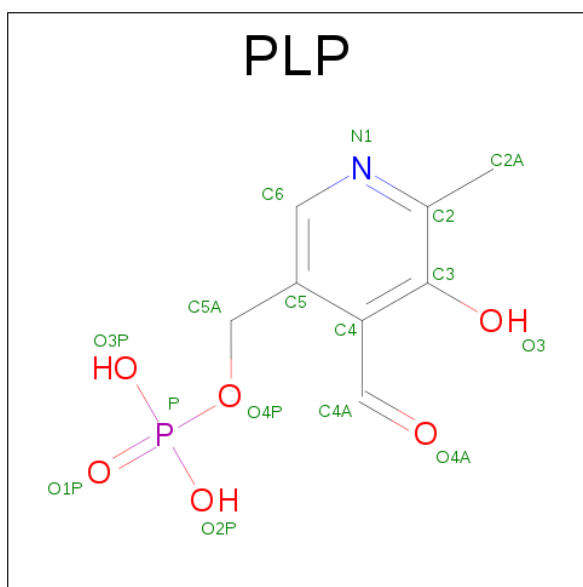
Chain	Residue	Modelled	Actual	Comment	Reference
E	128	VAL	LEU	VARIANT	UNP P18079
E	205	GLU	ASP	VARIANT	UNP P18079
E	262	ARG	LYS	VARIANT	UNP P18079

- Molecule 2 is SUCCINYL-COENZYME A (three-letter code: SCA) (formula: $C_{25}H_{40}N_7O_{19}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	30	0
			55	25	7	19	3	1		
2	B	1	Total	C	N	O	P	S	25	0
			55	25	7	19	3	1		
2	D	1	Total	C	N	O	P	S	20	0
			55	25	7	19	3	1		
2	E	1	Total	C	N	O	P	S	24	0
			55	25	7	19	3	1		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
3	D	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
3	E	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

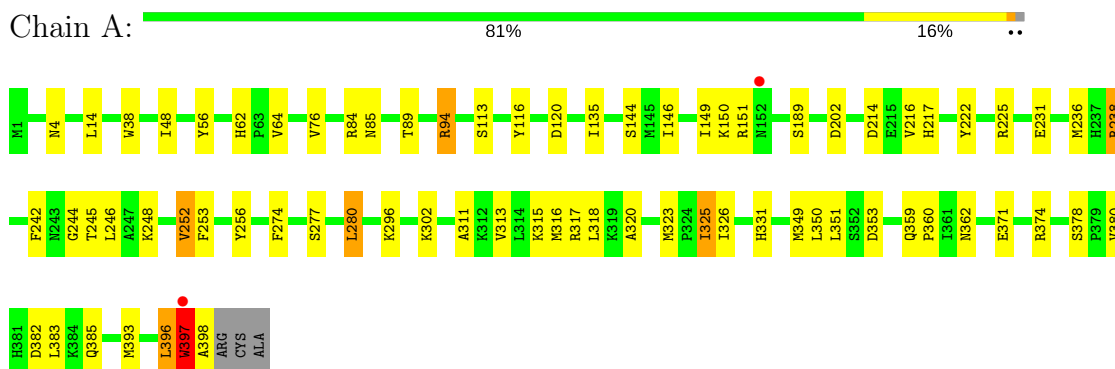
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	23	Total	O	0	0
			23	23		
4	D	30	Total	O	0	0
			30	30		
4	E	25	Total	O	0	0
			25	25		

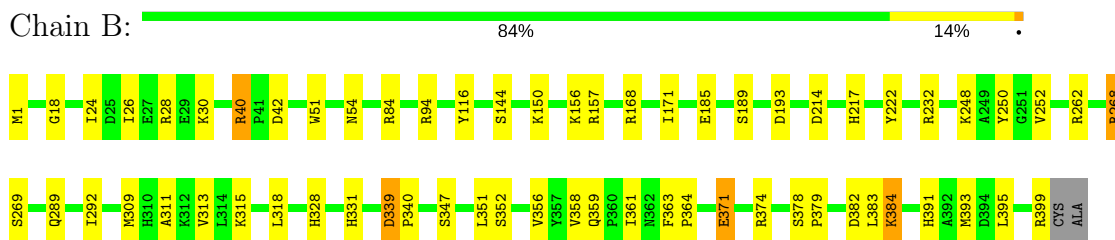
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

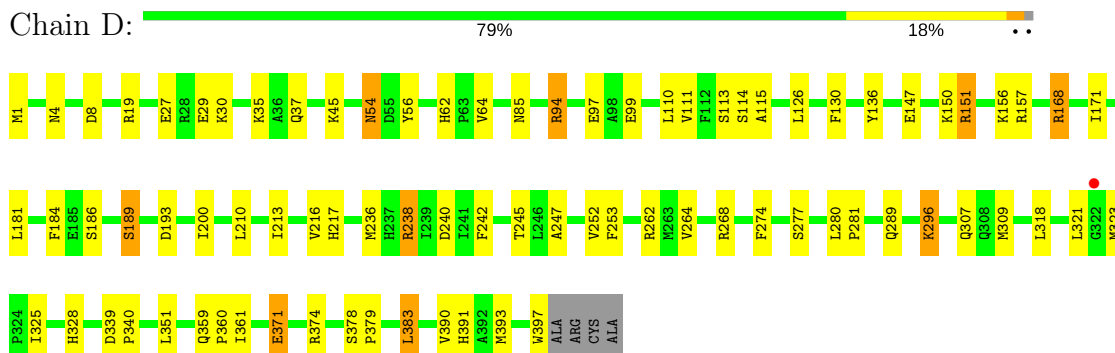
• Molecule 1: 5-AMINOLEVULINATE SYNTHASE



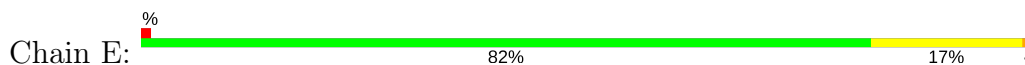
• Molecule 1: 5-AMINOLEVULINATE SYNTHASE

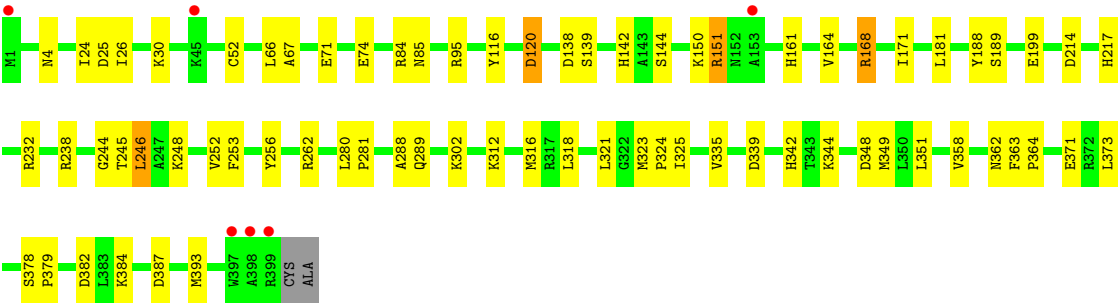


• Molecule 1: 5-AMINOLEVULINATE SYNTHASE



• 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, α , β , γ	67.94Å 91.36Å 247.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.52 – 2.80 29.78 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (119.52-2.80) 99.5 (29.78-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.160 , 0.224 0.164 , 0.226	Depositor DCC
R_{free} test set	1876 reflections (5.12%)	DCC
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12602	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: SCA, 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	0.86	1/3118 (0.0%)	0.79	6/4225 (0.1%)
1	B	0.85	0/3129	0.78	3/4239 (0.1%)
1	D	0.88	2/3113 (0.1%)	0.81	2/4218 (0.0%)
1	E	0.86	0/3129	0.78	2/4239 (0.0%)
All	All	0.86	3/12489 (0.0%)	0.79	13/16921 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	27	GLU	CG-CD	7.30	1.62	1.51
1	A	248	LYS	CE-NZ	5.24	1.62	1.49
1	D	130	PHE	CE1-CZ	5.13	1.47	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	ALA	N-CA-C	6.16	127.64	111.00
1	D	19	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	374	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	D	168	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	E	120	ASP	CB-CG-OD1	5.62	123.36	118.30
1	B	268	ARG	NE-CZ-NH2	-5.62	117.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	397	TRP	C-N-CA	5.51	135.47	121.70
1	A	397	TRP	O-C-N	-5.44	113.99	122.70
1	B	232	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	268	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	E	25	ASP	CB-CG-OD2	-5.07	113.73	118.30
1	A	120	ASP	CB-CG-OD1	5.03	122.82	118.30
1	A	374	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	396	LEU	Peptide
1	A	397	TRP	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	A	3048	0	3028	44	0
1	B	3059	0	3043	42	0
1	D	3043	0	3025	54	0
1	E	3059	0	3043	56	0
2	A	55	0	31	0	0
2	B	55	0	31	1	0
2	D	55	0	35	1	0
2	E	55	0	31	0	0
3	A	15	0	6	0	0
3	B	16	0	8	3	0
3	D	16	0	8	3	0
3	E	16	0	8	1	0
4	A	32	0	0	0	0
4	B	23	0	0	0	0
4	D	30	0	0	1	0
4	E	25	0	0	2	0
All	All	12602	0	12297	183	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 7.

All (183) 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:94:ARG:HG2	1:D:94:ARG:HH11	1.21	1.03
1:D:383:LEU:H	1:D:383:LEU:HD23	1.21	1.03
1:A:94:ARG:HH11	1:A:94:ARG:CG	1.73	1.00
1:A:94:ARG:HH11	1:A:94:ARG:HG3	1.34	0.91
1:E:151:ARG:HH11	1:E:151:ARG:CB	1.85	0.90
1:D:94:ARG:CG	1:D:94:ARG:HH11	1.91	0.83
1:D:383:LEU:H	1:D:383:LEU:CD2	1.94	0.80
1:E:67:ALA:O	1:E:71:GLU:HG2	1.81	0.80
1:D:238:ARG:HH11	1:D:238:ARG:HG2	1.45	0.80
1:A:222:TYR:OH	1:A:331:HIS:HD2	1.66	0.78
1:D:85:ASN:HB2	4:E:2005:HOH:O	1.82	0.78
1:E:151:ARG:HH11	1:E:151:ARG:CG	1.96	0.77
1:D:383:LEU:N	1:D:383:LEU:HD23	1.99	0.76
1:A:94:ARG:NH1	1:A:94:ARG:HG3	1.97	0.74
1:D:8:ASP:OD1	1:E:262:ARG:HD3	1.88	0.73
1:A:94:ARG:HH11	1:A:94:ARG:HG2	1.54	0.72
1:D:383:LEU:CD2	1:D:383:LEU:N	2.54	0.70
1:B:378:SER:HB2	1:B:379:PRO:HD2	1.74	0.70
1:B:94:ARG:HG2	1:B:94:ARG:HH11	1.58	0.69
1:E:318:LEU:HD21	1:E:393:MET:HE3	1.75	0.68
1:A:94:ARG:NH1	1:A:94:ARG:CG	2.43	0.67
1:D:54:ASN:HD21	1:D:374:ARG:HH22	1.40	0.67
1:A:225:ARG:HG3	1:A:231:GLU:OE2	1.96	0.66
1:E:189:SER:HB3	1:E:217:HIS:NE2	2.11	0.66
1:D:97:GLU:HG2	1:D:111:VAL:HG23	1.81	0.62
1:D:189:SER:HB3	1:D:217:HIS:NE2	2.14	0.62
1:A:393:MET:O	1:A:397:TRP:HB2	1.99	0.61
1:B:248:LYS:CE	3:B:600:PLP:H4A	2.30	0.61
1:E:189:SER:HB3	1:E:217:HIS:CD2	2.35	0.61
1:E:318:LEU:HB3	1:E:325:ILE:HD11	1.83	0.60
1:A:14:LEU:HD11	1:B:269:SER:HB3	1.82	0.60
1:D:236:MET:HG3	1:D:242:PHE:CZ	2.36	0.60
1:A:56:TYR:O	1:A:378:SER:HB2	2.02	0.59
1:B:189:SER:HB3	1:B:217:HIS:NE2	2.17	0.59
1:D:378:SER:HB2	1:D:379:PRO:HD2	1.85	0.59
1:A:116:TYR:CD2	1:A:144:SER:HB3	2.38	0.58
1:B:150:LYS:HD3	2:B:500:SCA:O4'	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:SER:OG	1:A:380:VAL:HG22	2.03	0.58
1:B:248:LYS:NZ	3:B:600:PLP:H4A	2.17	0.58
1:B:168:ARG:HA	1:B:171:ILE:HG22	1.85	0.58
1:E:363:PHE:CD1	1:E:364:PRO:HA	2.38	0.57
1:A:84:ARG:HG3	1:A:274:PHE:CZ	2.39	0.57
1:B:248:LYS:HE3	3:B:600:PLP:H4A	1.85	0.57
1:D:110:LEU:HB2	1:D:264:VAL:HG13	1.87	0.57
1:A:362:ASN:HA	1:A:371:GLU:HG3	1.86	0.57
1:A:4:ASN:HB3	1:B:262:ARG:HH11	1.70	0.57
1:E:151:ARG:HH11	1:E:151:ARG:HB3	1.66	0.56
1:E:151:ARG:HG2	1:E:151:ARG:HH11	1.69	0.56
1:B:156:LYS:O	1:B:157:ARG:HD3	2.05	0.56
1:E:95:ARG:HB3	1:E:289:GLN:NE2	2.21	0.56
1:D:359:GLN:HG3	1:D:360:PRO:HD2	1.88	0.56
1:E:318:LEU:CB	1:E:325:ILE:HD11	2.36	0.56
1:D:236:MET:HG3	1:D:242:PHE:HZ	1.71	0.55
1:B:384:LYS:HD3	1:B:384:LYS:H	1.71	0.55
1:D:262:ARG:NH1	1:E:4:ASN:HB3	2.22	0.54
1:D:321:LEU:HD11	1:D:390:VAL:HG13	1.89	0.54
1:A:146:ILE:O	1:A:150:LYS:HG2	2.07	0.54
1:D:186:SER:HB3	1:D:213:ILE:HD11	1.90	0.53
1:D:216:VAL:HG13	1:D:245:THR:CG2	2.39	0.53
1:E:168:ARG:HA	1:E:171:ILE:HG22	1.89	0.53
1:E:151:ARG:HH11	1:E:151:ARG:CA	2.21	0.53
1:A:313:VAL:O	1:A:317:ARG:HG2	2.09	0.53
1:E:151:ARG:HG2	1:E:151:ARG:NH1	2.22	0.53
1:D:126:LEU:HD13	1:D:181:LEU:HD13	1.90	0.52
1:A:382:ASP:OD1	1:A:385:GLN:HB2	2.09	0.52
1:D:359:GLN:O	1:D:361:ILE:HD12	2.09	0.52
1:D:156:LYS:O	1:D:157:ARG:HD3	2.10	0.52
1:D:37:GLN:NE2	1:D:45:LYS:HD2	2.25	0.52
1:D:94:ARG:CG	1:D:94:ARG:NH1	2.61	0.52
1:A:4:ASN:HB3	1:B:262:ARG:NH1	2.25	0.52
1:A:135:ILE:HG21	1:A:149:ILE:HG12	1.91	0.52
1:D:189:SER:HB3	1:D:217:HIS:CD2	2.45	0.52
1:D:94:ARG:HG2	1:D:94:ARG:NH1	2.02	0.51
1:B:222:TYR:OH	1:B:331:HIS:HD2	1.93	0.51
1:D:168:ARG:HA	1:D:171:ILE:HG22	1.92	0.51
1:E:339:ASP:OD2	1:E:342:HIS:HB2	2.11	0.51
1:E:30:LYS:HE3	1:E:66:LEU:HD13	1.93	0.50
1:D:99:GLU:OE2	1:D:296:LYS:NZ	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:391:HIS:CE1	4:D:2025:HOH:O	2.65	0.50
1:E:382:ASP:OD1	1:E:384:LYS:HB3	2.11	0.50
1:D:340:PRO:N	1:D:371:GLU:HG3	2.25	0.50
1:D:115:ALA:HB3	3:D:600:PLP:O4P	2.10	0.50
1:D:147:GLU:CD	1:E:151:ARG:HH21	2.15	0.50
1:B:54:ASN:HD21	1:B:374:ARG:HH12	1.58	0.50
1:E:246:LEU:HG	1:E:288:ALA:HB1	1.93	0.50
1:B:391:HIS:O	1:B:395:LEU:HG	2.12	0.49
1:D:281:PRO:HG3	1:E:253:PHE:HB2	1.94	0.49
1:E:116:TYR:CD2	1:E:144:SER:HB3	2.47	0.49
1:A:331:HIS:CD2	1:A:331:HIS:H	2.30	0.49
1:B:193:ASP:HB3	1:B:328:HIS:CG	2.48	0.49
1:A:202:ASP:OD1	1:A:238:ARG:NH2	2.46	0.49
1:E:362:ASN:HA	1:E:371:GLU:HG3	1.94	0.49
1:B:383:LEU:H	1:B:383:LEU:HD22	1.78	0.48
1:D:113:SER:HA	1:D:280:LEU:HD13	1.96	0.48
1:A:244:GLY:HA3	1:A:256:TYR:CZ	2.49	0.48
1:D:151:ARG:NH2	1:E:120:ASP:OD2	2.47	0.48
1:D:29:GLU:OE1	1:D:35:LYS:HE2	2.14	0.48
1:B:339:ASP:C	1:B:371:GLU:HG3	2.35	0.47
1:D:184:PHE:CE1	1:D:200:ILE:HG21	2.49	0.47
1:A:252:VAL:HG12	1:A:253:PHE:N	2.29	0.47
1:A:62:HIS:ND1	1:A:64:VAL:HG22	2.29	0.47
1:E:358:VAL:HG13	1:E:373:LEU:HD22	1.96	0.47
1:D:193:ASP:HB3	1:D:328:HIS:CG	2.50	0.47
1:E:151:ARG:NH1	1:E:151:ARG:CG	2.62	0.47
1:B:185:GLU:HG2	1:B:214:ASP:HB3	1.97	0.47
1:B:363:PHE:CD1	1:B:364:PRO:HA	2.49	0.46
1:E:378:SER:HB2	1:E:379:PRO:HD2	1.95	0.46
1:E:24:ILE:HG22	1:E:26:ILE:HG23	1.96	0.46
1:E:363:PHE:CG	1:E:364:PRO:HA	2.51	0.46
1:B:94:ARG:HG2	1:B:94:ARG:NH1	2.27	0.46
1:D:238:ARG:NH1	1:D:238:ARG:HG2	2.23	0.46
1:B:189:SER:HB3	1:B:217:HIS:CD2	2.51	0.46
1:B:24:ILE:HG22	1:B:26:ILE:HG23	1.97	0.46
1:E:164:VAL:HG11	1:E:199:GLU:HB3	1.98	0.46
1:D:216:VAL:HG21	3:D:600:PLP:C6	2.46	0.46
1:D:210:LEU:HA	1:D:240:ASP:OD2	2.16	0.45
1:E:384:LYS:HB2	1:E:384:LYS:HE3	1.75	0.45
1:A:222:TYR:OH	1:A:331:HIS:CD2	2.58	0.45
1:A:311:ALA:O	1:A:315:LYS:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ARG:O	1:A:320:ALA:HB3	2.17	0.45
1:E:151:ARG:CB	1:E:151:ARG:NH1	2.68	0.45
1:D:247:ALA:HB2	1:D:253:PHE:HA	1.99	0.45
1:B:250:TYR:CE1	1:B:292:ILE:HA	2.52	0.44
1:E:312:LYS:HE2	1:E:316:MET:CE	2.47	0.44
1:B:309:MET:O	1:B:313:VAL:HG23	2.17	0.44
1:D:253:PHE:HB2	1:E:281:PRO:HG3	1.99	0.44
1:A:396:LEU:HD12	1:A:396:LEU:HA	1.88	0.44
1:E:30:LYS:HE3	1:E:66:LEU:CD1	2.48	0.44
1:D:4:ASN:HD22	1:D:4:ASN:HA	1.58	0.44
1:A:85:ASN:OD1	1:B:359:GLN:NE2	2.51	0.44
1:E:150:LYS:HB2	1:E:150:LYS:HE3	1.69	0.43
1:A:189:SER:HB3	1:A:217:HIS:NE2	2.33	0.43
1:E:321:LEU:HD23	1:E:323:MET:HE2	2.00	0.43
1:E:142:HIS:HB2	3:E:600:PLP:H2A3	2.00	0.43
1:B:311:ALA:O	1:B:315:LYS:HG3	2.18	0.43
1:B:359:GLN:O	1:B:361:ILE:HD12	2.18	0.43
1:D:307:GLN:HB2	1:D:379:PRO:HD3	2.00	0.43
1:E:244:GLY:HA3	1:E:256:TYR:CZ	2.54	0.43
1:D:30:LYS:HD2	1:E:74:GLU:O	2.19	0.43
1:A:349:MET:O	1:A:353:ASP:HB2	2.19	0.43
1:B:371:GLU:HG2	1:B:371:GLU:H	1.52	0.43
1:B:40:ARG:HB2	1:B:42:ASP:OD1	2.18	0.43
1:B:84:ARG:HA	1:B:84:ARG:HD2	1.75	0.43
1:B:382:ASP:OD1	1:B:382:ASP:C	2.57	0.43
1:E:138:ASP:OD1	1:E:161:HIS:HA	2.19	0.43
1:A:216:VAL:HG13	1:A:245:THR:CG2	2.49	0.43
1:D:318:LEU:O	1:D:323:MET:HG2	2.19	0.43
1:E:245:THR:HG21	1:E:248:LYS:HG3	2.01	0.42
1:E:52:CYS:SG	1:E:358:VAL:HA	2.60	0.42
1:A:325:ILE:HG12	1:A:325:ILE:O	2.17	0.42
1:E:256:TYR:C	1:E:256:TYR:CD1	2.92	0.42
1:A:359:GLN:HG3	1:A:360:PRO:HD2	2.02	0.42
1:E:324:PRO:O	1:E:335:VAL:HA	2.20	0.42
1:D:136:TYR:CZ	1:D:171:ILE:HG13	2.55	0.42
1:A:236:MET:HG3	1:A:242:PHE:CZ	2.55	0.41
1:A:350:LEU:HD23	1:A:350:LEU:HA	1.91	0.41
1:E:84:ARG:HD2	1:E:84:ARG:HA	1.89	0.41
1:A:38:TRP:HB2	1:A:48:ILE:HD13	2.01	0.41
1:B:54:ASN:HB3	1:B:248:LYS:HG2	2.02	0.41
1:E:52:CYS:HB3	1:E:358:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:SER:HB2	1:B:379:PRO:CD	2.48	0.41
1:D:110:LEU:HD11	1:D:274:PHE:CE2	2.55	0.41
1:A:214:ASP:C	1:A:214:ASP:OD1	2.59	0.41
2:D:500:SCA:OS4	1:E:85:ASN:HB3	2.20	0.41
1:E:344:LYS:NZ	1:E:348:ASP:OD2	2.51	0.41
1:B:18:GLY:O	1:B:340:PRO:HB2	2.20	0.41
1:A:113:SER:HA	1:A:280:LEU:HD13	2.01	0.41
1:A:76:VAL:HG12	1:B:28:ARG:O	2.21	0.41
1:D:56:TYR:O	1:D:378:SER:HB2	2.20	0.41
1:E:151:ARG:HB3	1:E:151:ARG:NH1	2.33	0.41
1:A:84:ARG:HH21	1:A:89:THR:HG23	1.86	0.41
1:E:312:LYS:HE2	1:E:316:MET:HE2	2.02	0.41
1:A:14:LEU:CD1	1:B:269:SER:HB3	2.50	0.40
1:B:116:TYR:CD2	1:B:144:SER:HB3	2.56	0.40
1:B:318:LEU:HA	1:B:318:LEU:HD23	1.81	0.40
1:A:318:LEU:HD22	1:A:323:MET:HG3	2.04	0.40
1:B:347:SER:OG	1:B:358:VAL:O	2.39	0.40
1:D:62:HIS:CE1	1:D:64:VAL:HG22	2.56	0.40
1:E:161:HIS:HE1	1:E:188:TYR:CD1	2.39	0.40
1:E:280:LEU:HB2	4:E:2021:HOH:O	2.21	0.40
1:B:51:TRP:CD1	1:B:356:VAL:HG13	2.55	0.40
1:D:114:SER:HB2	3:D:600:PLP:O3P	2.22	0.40
1:E:214:ASP:OD1	1:E:214:ASP:C	2.59	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	396/401 (99%)	380 (96%)	15 (4%)	1 (0%)	44 77
1	B	397/401 (99%)	384 (97%)	12 (3%)	1 (0%)	44 77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	395/401 (98%)	380 (96%)	14 (4%)	1 (0%)	44	77
1	E	397/401 (99%)	382 (96%)	14 (4%)	1 (0%)	44	77
All	All	1585/1604 (99%)	1526 (96%)	55 (4%)	4 (0%)	44	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	VAL
1	D	252	VAL
1	E	252	VAL
1	B	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	311/313 (99%)	298 (96%)	13 (4%)	34	68
1	B	312/313 (100%)	300 (96%)	12 (4%)	38	72
1	D	311/313 (99%)	292 (94%)	19 (6%)	22	53
1	E	312/313 (100%)	301 (96%)	11 (4%)	41	75
All	All	1246/1252 (100%)	1191 (96%)	55 (4%)	33	67

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ARG
1	A	151	ARG
1	A	238	ARG
1	A	246	LEU
1	A	277	SER
1	A	280	LEU
1	A	296	LYS
1	A	302	LYS

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Mol	Chain	Res	Type
1	A	316	MET
1	A	325	ILE
1	A	326	ILE
1	A	351	LEU
1	A	383	LEU
1	B	1	MET
1	B	30	LYS
1	B	40	ARG
1	B	268	ARG
1	B	289	GLN
1	B	339	ASP
1	B	351	LEU
1	B	352	SER
1	B	371	GLU
1	B	384	LYS
1	B	393	MET
1	B	399	ARG
1	D	1	MET
1	D	54	ASN
1	D	94	ARG
1	D	150	LYS
1	D	151	ARG
1	D	189	SER
1	D	238	ARG
1	D	268	ARG
1	D	277	SER
1	D	289	GLN
1	D	296	LYS
1	D	309	MET
1	D	325	ILE
1	D	339	ASP
1	D	351	LEU
1	D	371	GLU
1	D	383	LEU
1	D	393	MET
1	D	397	TRP
1	E	139	SER
1	E	151	ARG
1	E	168	ARG
1	E	181	LEU
1	E	232	ARG
1	E	238	ARG

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Mol	Chain	Res	Type
1	E	246	LEU
1	E	302	LYS
1	E	349	MET
1	E	351	LEU
1	E	387	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	105	GLN
1	A	117	ASN
1	A	331	HIS
1	A	385	GLN
1	B	307	GLN
1	B	331	HIS
1	D	4	ASN
1	D	37	GLN
1	D	391	HIS
1	E	12	GLN
1	E	37	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SCA	A	500	-	47,57,57	1.79	5 (10%)	55,84,84	3.59	12 (21%)
3	PLP	A	600	1	15,15,16	2.38	3 (20%)	20,22,23	2.19	7 (35%)
2	SCA	B	500	-	47,57,57	1.46	4 (8%)	55,84,84	2.19	10 (18%)
3	PLP	B	600	-	16,16,16	1.48	3 (18%)	22,23,23	0.89	1 (4%)
2	SCA	D	500	-	47,57,57	1.30	5 (10%)	55,84,84	1.78	10 (18%)
3	PLP	D	600	-	16,16,16	1.40	2 (12%)	22,23,23	0.89	1 (4%)
2	SCA	E	500	3	47,57,57	1.43	4 (8%)	55,84,84	2.48	8 (14%)
3	PLP	E	600	2	16,16,16	1.72	3 (18%)	22,23,23	0.99	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	SCA	A	500	-	-	0/50/72/72	0/3/3/3
3	PLP	A	600	1	-	0/6/6/8	0/1/1/1
2	SCA	B	500	-	-	2/50/72/72	0/3/3/3
3	PLP	B	600	-	-	0/8/8/8	0/1/1/1
2	SCA	D	500	-	-	2/50/72/72	0/3/3/3
3	PLP	D	600	-	-	0/8/8/8	0/1/1/1
2	SCA	E	500	3	-	2/50/72/72	0/3/3/3
3	PLP	E	600	2	-	0/8/8/8	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	SCA	CS3-CS2	-9.38	1.05	1.52
2	E	500	SCA	CS3-CS2	-7.16	1.16	1.52
2	B	500	SCA	CS3-CS2	-7.03	1.17	1.52
3	A	600	PLP	O3-C3	-5.42	1.24	1.37
2	D	500	SCA	CS3-CS2	-3.20	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	500	SCA	C2-N3	2.20	1.35	1.32
3	B	600	PLP	C3-C2	2.24	1.42	1.40
2	A	500	SCA	P3-O3'	2.25	1.63	1.59
2	D	500	SCA	CS2-CS1	2.54	1.53	1.50
2	A	500	SCA	CS2-CS1	2.60	1.53	1.50
2	E	500	SCA	CS2-CS1	2.63	1.53	1.50
3	B	600	PLP	C2-N1	2.66	1.39	1.33
2	B	500	SCA	CS2-CS1	2.68	1.53	1.50
2	D	500	SCA	C5-C4	2.72	1.46	1.40
2	D	500	SCA	C2-N3	2.74	1.36	1.32
3	D	600	PLP	C4-C4A	2.91	1.53	1.46
2	B	500	SCA	C5-C4	2.98	1.47	1.40
3	A	600	PLP	C2-N1	2.99	1.40	1.33
2	B	500	SCA	O4'-C1'	3.01	1.45	1.41
3	B	600	PLP	C4-C4A	3.04	1.53	1.46
2	E	500	SCA	C5-C4	3.07	1.47	1.40
3	D	600	PLP	C2-N1	3.17	1.40	1.33
3	E	600	PLP	C2-N1	3.26	1.40	1.33
2	A	500	SCA	O4'-C1'	3.32	1.45	1.41
2	A	500	SCA	C5-C4	3.36	1.48	1.40
3	E	600	PLP	C3-C2	3.36	1.43	1.40
3	E	600	PLP	C4-C4A	3.39	1.54	1.46
2	D	500	SCA	O7-CPB	4.95	1.60	1.43
3	A	600	PLP	C3-C2	5.74	1.44	1.40

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	SCA	N3-C2-N1	-6.45	123.24	128.86
2	E	500	SCA	N3-C2-N1	-6.38	123.31	128.86
2	B	500	SCA	N3-C2-N1	-5.99	123.64	128.86
2	D	500	SCA	N3-C2-N1	-5.86	123.75	128.86
2	A	500	SCA	C5'-C4'-C3'	-4.81	97.98	114.30
2	B	500	SCA	C4-C5-N7	-4.08	105.46	109.41
2	D	500	SCA	OS1-CS1-CS2	-3.84	120.59	123.95
2	B	500	SCA	OS1-CS1-CS2	-3.70	120.71	123.95
2	A	500	SCA	OS1-CS1-CS2	-3.64	120.76	123.95
2	E	500	SCA	OS1-CS1-CS2	-3.63	120.77	123.95
2	D	500	SCA	C4-C5-N7	-3.43	106.10	109.41
2	B	500	SCA	OS1-CS1-S	-3.33	119.35	122.84
2	E	500	SCA	OS1-CS1-S	-3.31	119.37	122.84
2	A	500	SCA	OS1-CS1-S	-3.08	119.61	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	PLP	O3P-P-O4P	-3.03	98.66	106.73
2	D	500	SCA	C1'-N9-C4	-3.00	121.46	126.64
2	E	500	SCA	C4-C5-N7	-2.98	106.53	109.41
2	D	500	SCA	OS1-CS1-S	-2.92	119.78	122.84
2	A	500	SCA	C4-C5-N7	-2.83	106.67	109.41
2	A	500	SCA	O4'-C4'-C5'	-2.82	99.89	109.40
2	E	500	SCA	O3'-P3-O31	-2.73	98.57	109.26
3	A	600	PLP	C5-C6-N1	-2.40	119.81	123.87
2	D	500	SCA	O3'-P3-O31	-2.31	100.20	109.26
3	B	600	PLP	C5-C4-C4A	-2.30	117.58	122.39
3	D	600	PLP	C5-C6-N1	-2.27	120.02	123.87
2	B	500	SCA	C1'-N9-C4	-2.21	122.82	126.64
3	A	600	PLP	C5A-C5-C6	-2.00	115.89	119.33
2	D	500	SCA	O32-P3-O31	2.07	118.61	110.50
2	B	500	SCA	C2-N1-C6	2.07	122.40	118.77
2	A	500	SCA	C2-N1-C6	2.16	122.56	118.77
3	A	600	PLP	O3P-P-O2P	2.19	116.47	107.61
2	B	500	SCA	O11-P1-O12	2.25	123.93	112.28
2	D	500	SCA	C2'-C3'-C4'	2.41	107.55	103.23
2	A	500	SCA	C2'-C3'-C4'	2.74	108.13	103.23
3	A	600	PLP	O3-C3-C2	2.81	123.66	117.78
2	D	500	SCA	CS2-CS3-CS4	3.46	118.57	112.66
3	A	600	PLP	C4A-C4-C5	3.49	124.38	120.86
2	B	500	SCA	CS3-CS2-CS1	3.96	118.36	112.41
2	A	500	SCA	O5'-C5'-C4'	4.08	123.46	109.00
3	A	600	PLP	C6-C5-C4	6.15	123.32	118.18
2	A	500	SCA	CS2-CS1-S	6.30	119.63	113.28
2	D	500	SCA	CS2-CS1-S	6.31	119.63	113.28
2	E	500	SCA	CS2-CS1-S	6.53	119.85	113.28
2	B	500	SCA	CS2-CS1-S	6.60	119.93	113.28
2	E	500	SCA	CS3-CS2-CS1	6.86	122.73	112.41
2	B	500	SCA	CS2-CS3-CS4	9.29	128.53	112.66
2	A	500	SCA	CS3-CS2-CS1	10.44	128.10	112.41
2	E	500	SCA	CS2-CS3-CS4	11.67	132.60	112.66
2	A	500	SCA	CS2-CS3-CS4	19.90	146.66	112.66

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	500	SCA	CS2-CS1-S-CP1
2	E	500	SCA	OS1-CS1-S-CP1

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Mol	Chain	Res	Type	Atoms
2	B	500	SCA	CS2-CS1-S-CP1
2	B	500	SCA	OS1-CS1-S-CP1
2	D	500	SCA	OS1-CS1-S-CP1
2	D	500	SCA	CS2-CS1-S-CP1

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	SCA	1	0
3	B	600	PLP	3	0
2	D	500	SCA	1	0
3	D	600	PLP	3	0
3	E	600	PLP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	398/401 (99%)	-0.49	2 (0%) 90 88	13, 24, 45, 77	0
1	B	399/401 (99%)	-0.39	0 100 100	13, 24, 46, 85	0
1	D	397/401 (99%)	-0.54	1 (0%) 93 92	13, 24, 46, 77	0
1	E	399/401 (99%)	-0.45	6 (1%) 74 67	13, 24, 45, 91	0
All	All	1593/1604 (99%)	-0.47	9 (0%) 89 86	13, 24, 46, 91	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1	MET	2.7
1	A	397	TRP	2.7
1	E	398	ALA	2.7
1	E	153	ALA	2.6
1	E	397	TRP	2.5
1	E	399	ARG	2.4
1	A	152	ASN	2.2
1	E	45	LYS	2.1
1	D	322	GLY	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SCA	D	500	55/55	0.91	0.18	1.16	29,62,100,101	55
2	SCA	B	500	55/55	0.90	0.19	1.10	28,71,113,114	55
2	SCA	E	500	55/55	0.89	0.20	1.06	33,79,130,131	55
2	SCA	A	500	55/55	0.89	0.20	0.96	18,80,121,122	55
3	PLP	E	600	16/16	0.96	0.16	0.88	29,46,60,67	0
3	PLP	D	600	16/16	0.97	0.12	-0.77	33,39,59,71	0
3	PLP	B	600	16/16	0.98	0.16	-0.79	38,47,67,73	0
3	PLP	A	600	15/16	0.98	0.11	-0.94	32,34,38,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.