



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:02 PM UTC

PDB ID : 4ADB / pdb_00004adb
Title : Structural and functional study of succinyl-ornithine transaminase from E. coli
Authors : Newman, J.; Peat, T.S.
Deposited on : 2011-12-23
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

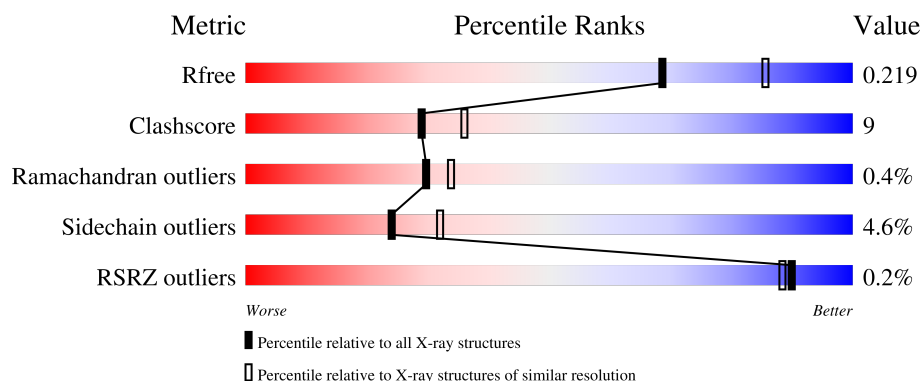
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	406	 78% 17% ..
1	B	406	 77% 19% ..
1	C	406	 75% 21% ..
1	D	406	 75% 20% ..

2 Entry composition [i](#)

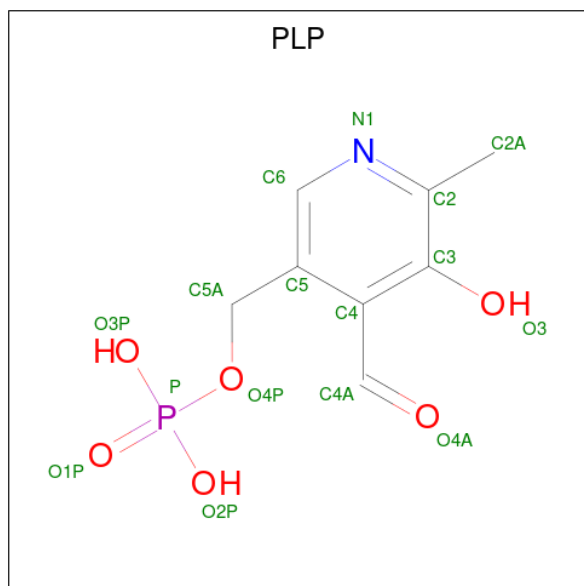
There are 5 unique types of molecules in this entry. The entry contains 13095 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SUCCINYLORNITHINE TRANSAMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	10	0
			3111	1968	552	580	11			
1	B	401	Total	C	N	O	S	0	7	0
			3095	1958	549	577	11			
1	C	399	Total	C	N	O	S	0	8	0
			3080	1951	540	577	12			
1	D	400	Total	C	N	O	S	0	9	0
			3099	1963	547	578	11			

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



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

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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		

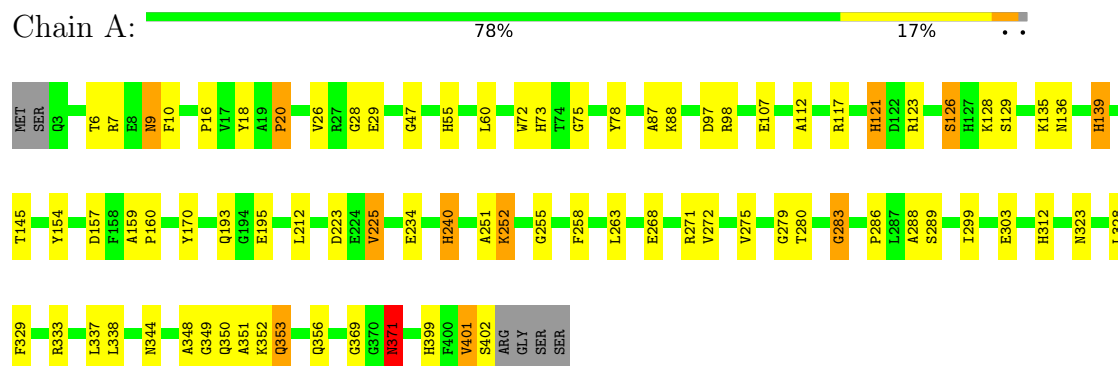
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	223	Total	O	0	0
			223	223		
5	B	181	Total	O	0	0
			181	181		
5	C	155	Total	O	0	0
			155	155		
5	D	85	Total	O	0	0
			85	85		

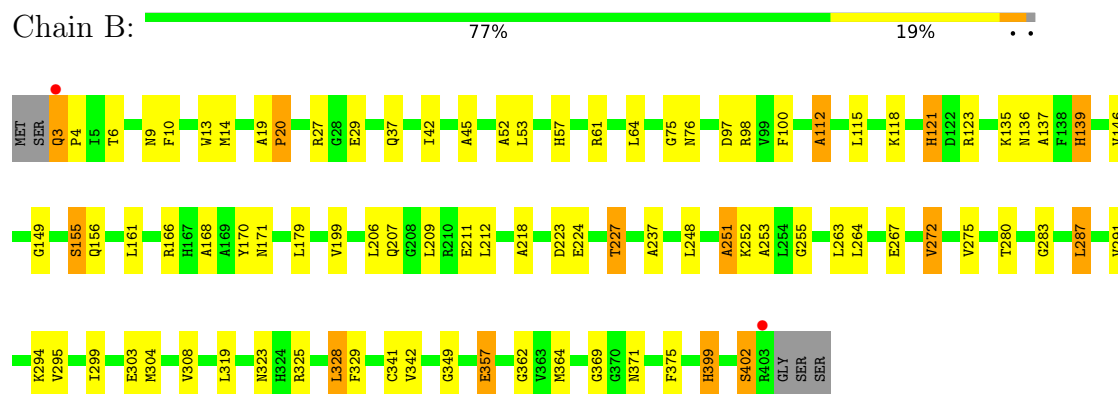
3 Residue-property plots

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

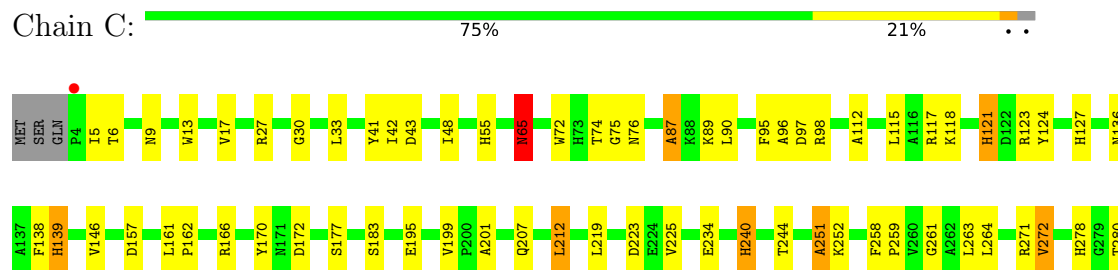
• Molecule 1: SUCCINYLORNITHINE TRANSAMINASE



• Molecule 1: SUCCINYLORNITHINE TRANSAMINASE



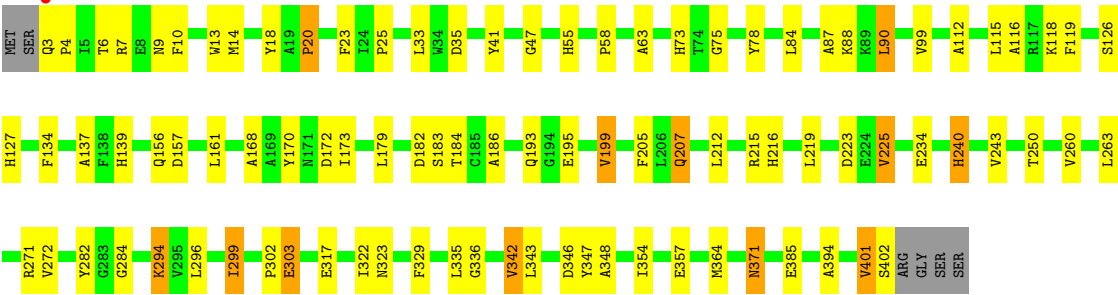
• Molecule 1: SUCCINYLORNITHINE TRANSAMINASE





● Molecule 1: SUCCINYLORNITHINE TRANSAMINASE

Chain D: 75% 20% . .



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.71Å 118.43Å 109.79Å 90.00° 96.69° 90.00°	Depositor
Resolution (Å)	109.05 – 2.20 109.04 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (109.05-2.20) 99.7 (109.04-2.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.171 , 0.219 0.171 , 0.219	Depositor DCC
R_{free} test set	5936 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13095	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, PLP, MG

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	1.54	25/3197 (0.8%)	1.29	10/4341 (0.2%)
1	B	1.54	20/3179 (0.6%)	1.32	16/4316 (0.4%)
1	C	1.44	20/3170 (0.6%)	1.27	10/4303 (0.2%)
1	D	1.35	9/3188 (0.3%)	1.25	11/4330 (0.3%)
All	All	1.47	74/12734 (0.6%)	1.29	47/17290 (0.3%)

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	139	HIS	ND1-CE1	7.39	1.40	1.32
1	A	121	HIS	CG-CD2	7.32	1.44	1.35
1	B	19	ALA	C-O	-7.27	1.15	1.24
1	B	139	HIS	CE1-NE2	7.26	1.39	1.32
1	B	137	ALA	C-O	7.14	1.32	1.23
1	C	312	HIS	CG-CD2	6.45	1.43	1.35
1	C	30	GLY	N-CA	6.35	1.54	1.45
1	A	26	VAL	N-CA	6.34	1.51	1.46
1	A	279	GLY	N-CA	6.28	1.52	1.45
1	B	75	GLY	C-O	6.26	1.31	1.23
1	A	28	GLY	N-CA	6.24	1.51	1.45
1	C	278	HIS	CG-CD2	6.23	1.42	1.35
1	C	261	GLY	N-CA	6.03	1.50	1.45
1	B	364	MET	C-O	6.02	1.31	1.24
1	D	385	GLU	C-O	-6.00	1.17	1.24
1	A	121	HIS	ND1-CE1	5.97	1.38	1.32
1	A	350	GLN	N-CA	5.96	1.53	1.46
1	C	399	HIS	CG-CD2	5.93	1.42	1.35
1	A	283	GLY	N-CA	5.92	1.51	1.45
1	D	260	VAL	CA-CB	5.91	1.61	1.55
1	A	399	HIS	CG-CD2	5.91	1.42	1.35
1	B	211	GLU	C-O	-5.86	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	275	VAL	C-O	-5.85	1.18	1.24
1	A	55	HIS	ND1-CE1	5.85	1.38	1.32
1	B	399	HIS	CG-CD2	5.80	1.42	1.35
1	B	209	LEU	N-CA	5.77	1.53	1.46
1	C	139	HIS	CE1-NE2	5.74	1.38	1.32
1	A	145	THR	C-O	5.74	1.31	1.24
1	D	73	HIS	CG-ND1	-5.70	1.31	1.38
1	B	139	HIS	CG-CD2	5.67	1.42	1.35
1	D	23	PHE	CA-C	5.64	1.59	1.52
1	B	255	GLY	C-O	-5.62	1.17	1.23
1	D	199	VAL	CA-CB	5.59	1.61	1.54
1	D	55	HIS	CG-CD2	5.54	1.42	1.35
1	C	87	ALA	N-CA	5.50	1.52	1.46
1	A	9	ASN	N-CA	5.48	1.53	1.46
1	C	258	PHE	CA-C	5.45	1.59	1.52
1	C	240	HIS	CG-CD2	5.45	1.41	1.35
1	A	240	HIS	CG-CD2	5.44	1.41	1.35
1	C	121	HIS	CG-CD2	5.44	1.41	1.35
1	A	344	ASN	C-O	5.43	1.30	1.23
1	A	351	ALA	C-O	-5.41	1.17	1.24
1	A	268	GLU	N-CA	5.37	1.52	1.46
1	B	100	PHE	N-CA	5.35	1.52	1.46
1	C	312	HIS	CE1-NE2	5.34	1.37	1.32
1	B	121	HIS	CG-CD2	5.33	1.41	1.35
1	B	402	SER	N-CA	5.32	1.52	1.46
1	C	312	HIS	ND1-CE1	5.31	1.37	1.32
1	A	289	SER	N-CA	-5.31	1.39	1.46
1	A	275	VAL	C-O	-5.29	1.18	1.24
1	A	73	HIS	CE1-NE2	5.26	1.37	1.32
1	A	128	LYS	CA-C	5.26	1.59	1.53
1	C	321	THR	C-O	5.25	1.30	1.24
1	C	342	VAL	C-O	-5.24	1.18	1.24
1	D	240	HIS	CE1-NE2	5.24	1.37	1.32
1	A	255	GLY	C-O	-5.20	1.20	1.24
1	B	291	VAL	C-O	5.20	1.29	1.24
1	B	362	GLY	N-CA	5.20	1.52	1.45
1	C	136	ASN	N-CA	5.19	1.53	1.46
1	A	139	HIS	CE1-NE2	5.18	1.37	1.32
1	B	42	ILE	C-O	5.16	1.30	1.24
1	C	166	ARG	C-O	5.15	1.30	1.23
1	A	78	TYR	N-CA	5.14	1.52	1.46
1	D	58	PRO	N-CA	5.13	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	115	LEU	N-CA	-5.13	1.40	1.46
1	C	55	HIS	CG-ND1	-5.11	1.32	1.38
1	B	53	LEU	N-CA	5.10	1.51	1.46
1	C	42	ILE	CA-C	5.05	1.58	1.52
1	A	312	HIS	CG-CD2	5.04	1.41	1.35
1	A	47	GLY	CA-C	5.04	1.57	1.51
1	A	338	LEU	C-O	5.02	1.29	1.24
1	D	78	TYR	N-CA	5.01	1.52	1.46
1	C	138	PHE	C-O	5.00	1.29	1.24
1	C	219	LEU	C-O	5.00	1.29	1.23

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	369	GLY	N-CA-C	-8.50	101.97	112.68
1	A	299	ILE	N-CA-C	-8.49	104.51	111.81
1	C	65	ASN	N-CA-C	8.41	120.07	111.07
1	B	199	VAL	CA-C-N	-8.14	111.51	120.14
1	B	199	VAL	C-N-CA	-8.14	111.51	120.14
1	C	199	VAL	N-CA-C	7.92	115.39	107.55
1	D	342	VAL	CB-CA-C	7.82	120.23	111.08
1	D	161	LEU	CA-C-N	-7.04	112.51	119.76
1	D	161	LEU	C-N-CA	-7.04	112.51	119.76
1	D	371	ASN	N-CA-C	7.01	121.86	113.16
1	C	240	HIS	N-CA-C	-6.99	103.09	111.69
1	B	115	LEU	N-CA-C	-6.47	104.31	111.36
1	B	369	GLY	N-CA-C	-6.37	104.37	112.65
1	C	244	THR	CA-C-N	6.33	126.79	120.52
1	C	244	THR	C-N-CA	6.33	126.79	120.52
1	D	84	LEU	N-CA-C	-6.18	104.44	112.23
1	A	117	ARG	N-CA-C	6.17	117.67	111.07
1	C	127	HIS	N-CA-C	-6.09	105.68	113.23
1	A	60	LEU	N-CA-C	-6.07	104.67	111.28
1	D	357	GLU	N-CA-C	-6.06	104.76	111.36
1	C	5	ILE	N-CA-C	5.88	116.77	108.36
1	A	75	GLY	N-CA-C	-5.84	104.16	112.81
1	D	63	ALA	N-CA-C	-5.76	105.13	111.82
1	A	107	GLU	N-CA-C	-5.72	105.19	111.82
1	B	45	ALA	N-CA-C	-5.71	105.41	112.90
1	B	357	GLU	N-CA-C	-5.68	105.09	111.28
1	D	299	ILE	CB-CA-C	-5.65	105.05	111.55
1	A	29	GLU	CB-CA-C	-5.63	100.38	109.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	GLY	N-CA-C	-5.58	105.40	112.54
1	B	75	GLY	N-CA-C	-5.55	104.59	112.81
1	A	371	ASN	N-CA-C	5.51	120.69	113.30
1	C	75	GLY	N-CA-C	-5.47	105.71	112.33
1	C	291	VAL	N-CA-C	5.46	115.66	110.42
1	B	27	ARG	NE-CZ-NH2	-5.42	114.32	119.20
1	C	331	GLU	N-CA-CB	-5.39	103.37	111.56
1	D	75	GLY	N-CA-C	-5.38	104.84	112.81
1	D	284	GLY	N-CA-C	-5.37	107.38	115.32
1	B	206	LEU	N-CA-C	5.33	117.09	111.28
1	A	333	ARG	NE-CZ-NH1	-5.31	116.19	121.50
1	A	333	ARG	NE-CZ-NH2	5.25	123.93	119.20
1	B	218	ALA	N-CA-C	-5.15	101.48	109.72
1	D	173	ILE	N-CA-C	5.14	116.48	110.62
1	B	375	PHE	CA-C-N	-5.11	117.16	122.89
1	B	375	PHE	C-N-CA	-5.11	117.16	122.89
1	B	112	ALA	N-CA-C	-5.09	105.43	111.69
1	B	155	SER	N-CA-C	5.09	120.14	113.88
1	B	251	ALA	N-CA-C	-5.01	100.13	110.80

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	3111	0	3032	52	0
1	B	3095	0	3027	51	0
1	C	3080	0	3013	62	0
1	D	3099	0	3027	69	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0
2	C	15	0	6	2	0
2	D	15	0	6	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	223	0	0	7	1
5	B	181	0	0	8	0
5	C	155	0	0	6	1
5	D	85	0	0	1	0
All	All	13095	0	12123	214	1

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 9.

All (214) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353[A]:GLN:NE2	5:A:2199:HOH:O	1.56	1.32
1:A:7:ARG:NH2	1:A:20[A]:PRO:HD2	1.56	1.16
1:D:271[B]:ARG:CG	1:D:271[B]:ARG:HH11	1.64	1.08
1:A:87:ALA:CB	1:B:14:MET:HE1	1.85	1.06
1:D:7:ARG:NH2	1:D:20[A]:PRO:HD2	1.70	1.04
1:C:65:ASN:OD1	5:C:2042:HOH:O	1.76	1.03
1:D:271[B]:ARG:HH11	1:D:271[B]:ARG:HG2	1.25	1.00
1:C:207:GLN:OE1	5:C:2114:HOH:O	1.77	0.99
1:C:87:ALA:HB2	1:D:14:MET:HE1	1.50	0.92
1:A:349:GLY:H	1:A:371:ASN:ND2	1.68	0.91
1:B:227[A]:THR:HG21	1:B:237:ALA:HB2	1.53	0.90
1:B:227[A]:THR:CG2	1:B:237:ALA:HB2	2.01	0.89
1:C:87:ALA:CB	1:D:14:MET:HE1	2.02	0.87
1:A:10:PHE:CE1	1:A:20[A]:PRO:HD3	2.11	0.85
1:A:87:ALA:HB1	1:B:14:MET:HE1	1.58	0.85
1:C:252:LYS:HZ3	2:C:1404:PLP:C4A	1.55	0.84
1:D:7:ARG:HH21	1:D:20[A]:PRO:HD2	1.43	0.83
1:B:227[A]:THR:HG21	1:B:237:ALA:CB	2.09	0.82
1:D:271[B]:ARG:CG	1:D:271[B]:ARG:NH1	2.38	0.81
1:B:13:TRP:C	1:B:14:MET:HE2	2.09	0.78
1:D:18:TYR:HB3	1:D:20[B]:PRO:HD3	1.65	0.78
1:D:41:TYR:HB2	1:D:364:MET:HE2	1.67	0.77
1:A:10:PHE:CE1	1:A:20[B]:PRO:HD2	2.21	0.75
1:D:127:HIS:HD2	1:D:183:SER:HB3	1.51	0.75
1:C:41:TYR:HB2	1:C:364[A]:MET:HE2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166[B]:ARG:HG3	5:B:2089:HOH:O	1.86	0.74
1:D:271[B]:ARG:HH11	1:D:271[B]:ARG:HG3	1.51	0.73
1:D:323:ASN:HD21	1:D:329:PHE:H	1.36	0.73
1:D:41:TYR:CB	1:D:364:MET:HE2	2.20	0.71
1:A:87:ALA:HB2	1:B:14:MET:HE1	1.71	0.71
1:A:271[A]:ARG:HD3	1:C:271[A]:ARG:HD3	1.72	0.71
1:C:87:ALA:CB	1:D:14:MET:CE	2.68	0.71
1:A:223:ASP:OD1	1:A:225:VAL:HG13	1.91	0.71
1:C:352:LYS:O	1:C:356:GLN:HG3	1.91	0.70
1:D:303[A]:GLU:H	1:D:303[A]:GLU:CD	1.99	0.70
1:C:323:ASN:HD21	1:C:329:PHE:H	1.38	0.70
1:A:154:TYR:CD2	5:A:2129:HOH:O	2.43	0.70
1:D:33:LEU:HB3	1:D:364:MET:HE1	1.73	0.70
1:B:139:HIS:HD2	1:B:223:ASP:OD2	1.77	0.68
1:A:10:PHE:CZ	1:A:20[B]:PRO:HD2	2.29	0.68
1:A:139:HIS:HD2	1:A:223:ASP:OD2	1.77	0.67
1:D:41:TYR:HB2	1:D:364:MET:CE	2.25	0.66
1:A:323:ASN:HD21	1:A:329:PHE:H	1.43	0.66
1:A:7:ARG:HH21	1:A:20[A]:PRO:HD2	1.52	0.66
1:D:271[B]:ARG:HG2	1:D:271[B]:ARG:NH1	2.04	0.66
1:D:182:ASP:OD1	1:D:216:HIS:HD2	1.79	0.65
1:B:135:LYS:O	1:B:136:ASN:HB2	1.96	0.65
1:B:349:GLY:H	1:B:371:ASN:ND2	1.96	0.64
1:A:349:GLY:N	1:A:371:ASN:ND2	2.44	0.63
1:D:401:VAL:O	1:D:402:SER:CB	2.47	0.63
1:A:349:GLY:H	1:A:371:ASN:HD22	1.47	0.62
1:C:177:SER:HB3	1:C:212:LEU:HD21	1.81	0.62
1:D:18:TYR:C	1:D:20[B]:PRO:HD3	2.25	0.62
1:C:6:THR:H	1:C:9:ASN:ND2	1.98	0.61
1:B:10:PHE:CZ	1:B:20:PRO:HD3	2.36	0.61
1:B:123[A]:ARG:NH1	5:B:2077:HOH:O	1.72	0.61
1:B:227[A]:THR:CG2	1:B:227[A]:THR:O	2.47	0.61
1:A:18:TYR:C	1:A:20[B]:PRO:HD3	2.26	0.61
1:B:3:GLN:NE2	1:B:4:PRO:HD2	2.15	0.60
1:C:43:ASP:HA	1:C:364[A]:MET:HE3	1.83	0.60
1:C:139:HIS:HD2	1:C:223:ASP:OD2	1.84	0.59
1:D:127:HIS:CD2	1:D:183:SER:HB3	2.35	0.59
1:A:352:LYS:O	1:A:356:GLN:HG3	2.03	0.58
1:B:64:LEU:HD12	1:B:287:LEU:HD22	1.85	0.58
1:A:280:THR:HG21	1:A:283:GLY:HA3	1.85	0.58
1:C:96:ALA:HB2	1:C:264:LEU:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:LYS:NZ	2:C:1404:PLP:C4	2.60	0.58
1:A:234:GLU:HG3	1:A:240:HIS:HB2	1.86	0.58
1:C:280:THR:HG21	1:C:283:GLY:HA3	1.86	0.58
1:A:157:ASP:OD2	1:B:118:LYS:HE2	2.04	0.58
1:C:43:ASP:CA	1:C:364[A]:MET:HE3	2.34	0.57
1:A:72:TRP:O	1:A:286:PRO:HD2	2.04	0.57
1:D:401:VAL:O	1:D:402:SER:HB3	2.05	0.57
1:C:121:HIS:HB3	5:C:2082:HOH:O	2.05	0.57
1:D:14:MET:HA	1:D:14:MET:HE2	1.86	0.56
1:B:227[A]:THR:O	1:B:227[A]:THR:HG22	2.04	0.55
1:D:10:PHE:CZ	1:D:20[B]:PRO:HD2	2.42	0.55
1:A:121:HIS:HE1	1:A:129:SER:OG	1.90	0.55
1:A:139:HIS:HE1	5:A:2123:HOH:O	1.89	0.55
1:D:223:ASP:OD1	1:D:225:VAL:HG13	2.07	0.55
1:C:115:LEU:C	1:C:115:LEU:HD23	2.32	0.54
1:D:18:TYR:CB	1:D:20[B]:PRO:HD3	2.37	0.54
1:D:90:LEU:HD13	1:D:296:LEU:HD11	1.90	0.53
1:A:6:THR:H	1:A:9:ASN:ND2	2.07	0.53
1:A:271[B]:ARG:HG2	1:A:271[B]:ARG:NH1	2.22	0.53
1:C:323:ASN:ND2	1:C:328:LEU:H	2.07	0.53
1:B:323:ASN:ND2	1:B:328:LEU:H	2.07	0.53
1:C:76:ASN:O	1:D:20[B]:PRO:HG3	2.08	0.53
1:A:271[B]:ARG:HG2	1:A:271[B]:ARG:HH11	1.74	0.53
1:D:6:THR:H	1:D:9:ASN:ND2	2.06	0.53
1:A:126:SER:HB3	5:A:2119:HOH:O	2.08	0.52
1:D:13:TRP:O	1:D:14:MET:HE2	2.09	0.52
1:B:224:GLU:OE1	1:B:227[A]:THR:HG22	2.10	0.52
1:B:323:ASN:HD21	1:B:329:PHE:H	1.57	0.52
1:A:10:PHE:CZ	1:A:20[B]:PRO:CD	2.94	0.51
1:B:156:GLN:HE22	1:D:156:GLN:HE22	1.58	0.51
1:D:116:ALA:HA	1:D:219:LEU:HD12	1.92	0.51
1:B:272:VAL:HG22	5:B:2076:HOH:O	2.10	0.51
1:C:353:GLN:HE21	1:C:353:GLN:H	1.59	0.50
1:B:248:LEU:HD22	1:B:264:LEU:HD22	1.94	0.50
1:C:157:ASP:OD2	1:D:118:LYS:HE2	2.11	0.50
1:C:123:ARG:HD3	1:C:124:TYR:CE2	2.46	0.50
1:A:7:ARG:NH2	1:A:20[A]:PRO:CD	2.50	0.50
1:D:335:LEU:O	1:D:336:GLY:C	2.53	0.50
1:B:139:HIS:HE1	5:B:2090:HOH:O	1.93	0.50
1:C:74:THR:O	1:D:47:GLY:HA2	2.12	0.50
1:A:348:ALA:HA	1:A:371:ASN:HD21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:ALA:HB2	1:D:179:LEU:HD12	1.93	0.49
1:B:280:THR:HG21	1:B:283:GLY:HA3	1.95	0.49
1:B:399:HIS:CD2	5:B:2180:HOH:O	2.64	0.49
1:C:87:ALA:HB1	1:D:14:MET:CE	2.43	0.49
1:B:121:HIS:HB3	5:B:2074:HOH:O	2.12	0.48
1:A:195[B]:GLU:HG3	5:A:2153:HOH:O	2.13	0.48
1:B:295:VAL:CG1	1:B:299:ILE:HD12	2.44	0.48
1:C:170:TYR:OH	1:C:201:ALA:HB2	2.13	0.48
1:D:139:HIS:HD2	1:D:223:ASP:OD2	1.95	0.48
1:C:303[A]:GLU:H	1:C:303[A]:GLU:CD	2.21	0.48
1:D:170:TYR:CE2	1:D:193:GLN:HG3	2.47	0.48
1:C:161:LEU:O	1:C:162:PRO:C	2.53	0.48
1:C:112:ALA:HB2	1:C:263:LEU:HD13	1.96	0.48
1:A:121:HIS:CE1	1:A:129:SER:OG	2.65	0.48
1:C:89:LYS:NZ	1:C:297[A]:GLU:HG3	2.29	0.48
1:D:271[B]:ARG:NH1	1:D:271[B]:ARG:HG3	2.15	0.48
1:B:319:LEU:HD13	1:B:341:CYS:SG	2.53	0.48
1:C:295:VAL:HG13	1:C:299:ILE:HD12	1.95	0.47
1:A:16:PRO:HB2	5:A:2013:HOH:O	2.14	0.47
1:A:258:PHE:CE1	1:A:288:ALA:HB2	2.49	0.47
1:A:328:LEU:HD21	1:A:401:VAL:HG23	1.96	0.47
1:B:6:THR:H	1:B:9:ASN:ND2	2.12	0.47
1:B:329:PHE:HA	1:B:342:VAL:O	2.15	0.47
1:C:43:ASP:CB	1:C:364[A]:MET:HE3	2.44	0.47
1:C:87:ALA:HB1	1:D:14:MET:HE1	1.91	0.47
1:B:112:ALA:HB2	1:B:263:LEU:HD13	1.97	0.47
1:B:227[A]:THR:CG2	1:B:237:ALA:CB	2.78	0.47
5:B:2163:HOH:O	1:C:183:SER:HB3	2.14	0.46
1:D:115:LEU:C	1:D:115:LEU:HD23	2.41	0.46
1:D:87:ALA:HA	1:D:99[A]:VAL:HG11	1.98	0.46
1:A:223:ASP:OD1	1:A:223:ASP:C	2.58	0.46
1:C:41:TYR:CB	1:C:364[A]:MET:HE2	2.41	0.46
1:A:348:ALA:CA	1:A:371:ASN:HD21	2.29	0.46
1:D:343:LEU:HD21	1:D:354:ILE:CD1	2.45	0.46
1:A:20[B]:PRO:HG3	1:B:76:ASN:O	2.16	0.46
1:B:168:ALA:HB2	1:B:179:LEU:HD12	1.98	0.46
1:C:13:TRP:CE2	1:D:88:LYS:HD3	2.51	0.46
1:C:41:TYR:N	1:C:41:TYR:CD1	2.84	0.46
1:C:118:LYS:HD3	1:C:272:VAL:HG13	1.97	0.46
1:B:155:SER:HB2	1:B:161:LEU:HD11	1.98	0.45
1:D:139:HIS:HE1	5:D:2048:HOH:O	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271[B]:ARG:HH11	1:A:271[B]:ARG:CG	2.29	0.45
1:D:119:PHE:C	1:D:119:PHE:CD1	2.95	0.45
1:D:6:THR:H	1:D:9:ASN:HD22	1.65	0.45
1:C:280:THR:CG2	1:C:283:GLY:HA3	2.47	0.44
1:D:215:ARG:HE	1:D:215:ARG:HB2	1.49	0.44
1:A:280:THR:CG2	1:A:283:GLY:HA3	2.47	0.44
1:C:294:LYS:HE2	1:C:294:LYS:HB2	1.56	0.44
1:A:170:TYR:CZ	1:A:193:GLN:HG3	2.53	0.44
1:D:10:PHE:CE1	1:D:20[A]:PRO:HD3	2.52	0.44
1:B:57:HIS:O	1:B:61:ARG:HG3	2.18	0.44
1:B:13:TRP:O	1:B:14:MET:HE2	2.16	0.44
1:C:223:ASP:C	1:C:223:ASP:OD1	2.61	0.44
1:B:295:VAL:HG13	1:B:299:ILE:HD12	2.00	0.43
1:C:384:GLU:OE2	1:C:388:THR:OG1	2.32	0.43
1:A:225:VAL:HG23	1:A:252:LYS:HG3	2.00	0.43
1:B:13:TRP:HB2	1:B:14:MET:HE3	2.00	0.43
1:D:347:TYR:O	1:D:348:ALA:C	2.59	0.43
1:B:97:ASP:C	1:B:98:ARG:HG2	2.42	0.43
1:C:89:LYS:CE	1:C:297[A]:GLU:HG3	2.48	0.43
1:D:294:LYS:HD3	1:D:294:LYS:HA	1.69	0.43
1:C:118:LYS:HG3	1:D:157:ASP:HB3	1.99	0.43
1:B:29:GLU:HG2	5:B:2020:HOH:O	2.17	0.43
1:D:170:TYR:C	1:D:172:ASP:H	2.27	0.43
1:B:52:ALA:HB2	1:B:253:ALA:HB1	1.99	0.43
1:C:115:LEU:HD23	1:C:115:LEU:O	2.19	0.43
1:C:225:VAL:HG13	1:C:251:ALA:HB3	2.01	0.42
1:A:112:ALA:HB2	1:A:263:LEU:HD13	2.00	0.42
1:C:27:ARG:O	1:C:33:LEU:HD12	2.19	0.42
1:C:95:PHE:CD2	1:C:95:PHE:C	2.98	0.42
1:C:195[A]:GLU:HG2	5:C:2111:HOH:O	2.18	0.42
1:B:170:TYR:O	1:B:171:ASN:HB2	2.19	0.42
1:C:87:ALA:HB2	1:D:14:MET:CE	2.32	0.42
1:C:335:LEU:O	1:C:336:GLY:C	2.63	0.42
1:A:88:LYS:HD3	1:B:13:TRP:CE2	2.55	0.41
5:A:2008:HOH:O	1:B:267:GLU:OE1	2.21	0.41
1:C:366:LEU:HB2	1:C:374:ARG:HB3	2.02	0.41
1:C:72:TRP:O	1:C:286:PRO:HD2	2.19	0.41
1:C:97:ASP:O	1:C:98:ARG:HG2	2.20	0.41
1:C:172:ASP:OD1	1:C:172:ASP:C	2.64	0.41
1:A:328:LEU:HA	1:A:328:LEU:HD23	1.80	0.41
1:B:135:LYS:O	1:B:136:ASN:CB	2.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:ARG:HH11	1:C:117:ARG:HD2	1.67	0.41
1:C:121:HIS:CB	5:C:2082:HOH:O	2.66	0.41
1:A:135:LYS:O	1:A:136:ASN:HB2	2.21	0.41
1:C:234:GLU:HG3	1:C:240:HIS:HB2	2.03	0.41
1:D:3:GLN:HB3	1:D:4:PRO:HD3	2.02	0.41
1:B:6:THR:H	1:B:9:ASN:HD22	1.69	0.41
1:B:14:MET:HE2	1:B:14:MET:N	2.36	0.41
1:D:234:GLU:HG3	1:D:240:HIS:HB2	2.03	0.41
1:D:322:ILE:HG12	1:D:394:ALA:HB2	2.03	0.41
1:A:337:LEU:HD23	1:A:337:LEU:HA	1.95	0.41
1:A:6:THR:H	1:A:9:ASN:HD22	1.69	0.40
1:A:159:ALA:HA	1:A:160:PRO:C	2.46	0.40
1:C:259:PRO:HA	1:D:282:TYR:CE2	2.55	0.40
1:D:25:PRO:HA	1:D:35:ASP:HA	2.04	0.40
1:D:207:GLN:HE21	1:D:243:VAL:HG22	1.86	0.40
1:D:225:VAL:HG22	2:D:1404:PLP:C3	2.50	0.40
1:D:112:ALA:HB2	1:D:263:LEU:HD13	2.03	0.40
1:D:137:ALA:HB1	1:D:139:HIS:CE1	2.56	0.40
1:D:184:THR:HG22	1:D:186:ALA:H	1.86	0.40
1:D:219:LEU:HA	1:D:219:LEU:HD23	1.78	0.40
1:B:304:MET:O	1:B:308:VAL:HG23	2.22	0.40
1:C:139:HIS:HE1	5:C:2091:HOH:O	2.05	0.40
1:A:97:ASP:O	1:A:98:ARG:HG2	2.21	0.40
1:D:134:PHE:CE2	1:D:205:PHE:HZ	2.40	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2037:HOH:O	5:C:2022:HOH:O[3_445]	2.09	0.11

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	408/406 (100%)	390 (96%)	16 (4%)	2 (0%)	24	27
1	B	406/406 (100%)	387 (95%)	17 (4%)	2 (0%)	24	27
1	C	405/406 (100%)	387 (96%)	17 (4%)	1 (0%)	43	51
1	D	407/406 (100%)	384 (94%)	22 (5%)	1 (0%)	43	51
All	All	1626/1624 (100%)	1548 (95%)	72 (4%)	6 (0%)	30	34

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	252	LYS
1	A	251	ALA
1	B	251	ALA
1	A	252	LYS
1	C	251	ALA
1	D	401	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	316/312 (101%)	302 (96%)	14 (4%)	25	34
1	B	314/312 (101%)	297 (95%)	17 (5%)	20	25
1	C	314/312 (101%)	301 (96%)	13 (4%)	27	37
1	D	316/312 (101%)	295 (93%)	21 (7%)	15	18
All	All	1260/1248 (101%)	1195 (95%)	65 (5%)	24	26

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20[A]	PRO
1	A	20[B]	PRO
1	A	123	ARG

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Mol	Chain	Res	Type
1	A	126	SER
1	A	212	LEU
1	A	225	VAL
1	A	272	VAL
1	A	303[A]	GLU
1	A	303[B]	GLU
1	A	353[A]	GLN
1	A	353[B]	GLN
1	A	371	ASN
1	A	401	VAL
1	A	402	SER
1	B	3	GLN
1	B	20	PRO
1	B	37	GLN
1	B	146	VAL
1	B	207	GLN
1	B	212	LEU
1	B	227[A]	THR
1	B	227[B]	THR
1	B	272	VAL
1	B	287	LEU
1	B	294	LYS
1	B	303[A]	GLU
1	B	303[B]	GLU
1	B	325	ARG
1	B	328	LEU
1	B	357	GLU
1	B	402	SER
1	C	17	VAL
1	C	48	ILE
1	C	65	ASN
1	C	90	LEU
1	C	146	VAL
1	C	212	LEU
1	C	272	VAL
1	C	303[A]	GLU
1	C	303[B]	GLU
1	C	352	LYS
1	C	353	GLN
1	C	371	ASN
1	C	401	VAL
1	D	20[A]	PRO

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Mol	Chain	Res	Type
1	D	20[B]	PRO
1	D	90	LEU
1	D	126	SER
1	D	195[A]	GLU
1	D	195[B]	GLU
1	D	199	VAL
1	D	207	GLN
1	D	212	LEU
1	D	225	VAL
1	D	250	THR
1	D	272	VAL
1	D	294	LYS
1	D	299	ILE
1	D	302	PRO
1	D	303[A]	GLU
1	D	303[B]	GLU
1	D	317	GLU
1	D	342	VAL
1	D	346	ASP
1	D	371	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	121	HIS
1	A	139	HIS
1	A	207	GLN
1	A	216	HIS
1	A	323	ASN
1	A	350	GLN
1	A	356	GLN
1	A	371	ASN
1	A	399	HIS
1	B	3	GLN
1	B	9	ASN
1	B	139	HIS
1	B	156	GLN
1	B	214	ASN
1	B	310	GLN
1	B	323	ASN
1	B	371	ASN

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Mol	Chain	Res	Type
1	C	9	ASN
1	C	37	GLN
1	C	139	HIS
1	C	207	GLN
1	C	310	GLN
1	C	323	ASN
1	C	350	GLN
1	C	353	GLN
1	C	371	ASN
1	D	9	ASN
1	D	121	HIS
1	D	127	HIS
1	D	139	HIS
1	D	151	GLN
1	D	207	GLN
1	D	216	HIS
1	D	310	GLN
1	D	323	ASN
1	D	324	HIS
1	D	350	GLN
1	D	371	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	C	1404	1	15,15,16	3.03	3 (20%)	21,22,23	1.67	5 (23%)
2	PLP	A	1404	1	15,15,16	2.53	5 (33%)	21,22,23	1.67	3 (14%)
2	PLP	D	1404	1	15,15,16	2.78	4 (26%)	21,22,23	1.51	4 (19%)
2	PLP	B	1404	1	15,15,16	2.50	5 (33%)	21,22,23	2.12	8 (38%)

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	C	1404	1	-	0/6/6/8	0/1/1/1
2	PLP	A	1404	1	-	0/6/6/8	0/1/1/1
2	PLP	D	1404	1	-	2/6/6/8	0/1/1/1
2	PLP	B	1404	1	-	3/6/6/8	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1404	PLP	C5-C4	7.51	1.49	1.40
2	C	1404	PLP	C3-C2	7.42	1.48	1.41
2	C	1404	PLP	C5-C4	7.35	1.48	1.40
2	D	1404	PLP	C5-C4	6.54	1.47	1.40
2	A	1404	PLP	C3-C2	6.07	1.47	1.41
2	D	1404	PLP	C3-C2	5.67	1.46	1.41
2	A	1404	PLP	C5-C4	5.37	1.46	1.40
2	D	1404	PLP	C3-C4	5.15	1.49	1.40
2	C	1404	PLP	C3-C4	4.68	1.49	1.40
2	B	1404	PLP	C3-C4	4.22	1.48	1.40
2	A	1404	PLP	C3-C4	3.05	1.45	1.40
2	A	1404	PLP	C4A-C4	-2.77	1.46	1.51
2	A	1404	PLP	C6-C5	2.35	1.42	1.37
2	D	1404	PLP	C2A-C2	-2.31	1.46	1.50
2	B	1404	PLP	C3-C2	2.27	1.43	1.41
2	B	1404	PLP	P-O3P	-2.21	1.46	1.54
2	B	1404	PLP	C4A-C4	-2.09	1.47	1.51

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1404	PLP	C6-N1-C2	4.76	127.82	119.20
2	A	1404	PLP	C6-N1-C2	4.02	126.48	119.20
2	A	1404	PLP	C3-C2-N1	-3.58	116.44	120.96
2	C	1404	PLP	C2A-C2-C3	3.37	124.74	120.80
2	B	1404	PLP	C6-C5-C4	-3.34	115.36	118.10
2	D	1404	PLP	C6-N1-C2	3.29	125.17	119.20
2	A	1404	PLP	C2A-C2-N1	3.27	123.80	117.64
2	C	1404	PLP	O2P-P-O4P	-3.22	98.26	106.67
2	B	1404	PLP	C3-C2-N1	-3.01	117.16	120.96
2	B	1404	PLP	O2P-P-O4P	-2.97	98.94	106.67
2	C	1404	PLP	C6-N1-C2	2.78	124.25	119.20
2	B	1404	PLP	C2A-C2-N1	2.71	122.75	117.64
2	B	1404	PLP	O3P-P-O2P	2.47	117.08	107.80
2	C	1404	PLP	O3P-P-O2P	2.46	117.04	107.80
2	C	1404	PLP	C3-C2-N1	-2.44	117.89	120.96
2	B	1404	PLP	O2P-P-O1P	2.32	119.88	110.83
2	D	1404	PLP	O2P-P-O4P	-2.32	100.62	106.67
2	D	1404	PLP	O3P-P-O2P	2.13	115.80	107.80
2	D	1404	PLP	O3-C3-C2	2.12	121.98	117.58
2	B	1404	PLP	O4P-P-O1P	-2.04	100.92	106.44

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1404	PLP	C5A-O4P-P-O1P
2	B	1404	PLP	C5A-O4P-P-O1P
2	B	1404	PLP	C5A-O4P-P-O2P
2	B	1404	PLP	C5A-O4P-P-O3P
2	D	1404	PLP	C5A-O4P-P-O2P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1404	PLP	2	0
2	D	1404	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	400/406 (98%)	-0.84	0 100 100	9, 21, 33, 72	25 (6%)
1	B	401/406 (98%)	-0.87	2 (0%) 87 85	8, 20, 32, 56	23 (5%)
1	C	399/406 (98%)	-0.73	1 (0%) 90 88	13, 25, 38, 61	26 (6%)
1	D	400/406 (98%)	-0.48	1 (0%) 90 88	15, 31, 47, 78	28 (7%)
All	All	1600/1624 (98%)	-0.73	4 (0%) 90 88	8, 24, 40, 78	102 (6%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	403	ARG	6.3
1	B	3	GLN	3.6
1	C	4	PRO	2.9
1	D	3	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	D	1405	1/1	0.93	0.07	36,36,36,36	0
3	NA	B	1405	1/1	0.94	0.07	21,21,21,21	0
4	MG	A	1999	1/1	0.95	0.07	27,27,27,27	1
4	MG	B	1999	1/1	0.96	0.04	38,38,38,38	1
3	NA	C	1405	1/1	0.98	0.03	27,27,27,27	0
2	PLP	D	1404	15/16	0.98	0.05	20,24,26,26	0
2	PLP	C	1404	15/16	0.99	0.04	23,27,31,32	0
2	PLP	A	1404	15/16	0.99	0.04	13,17,20,22	0
3	NA	A	1405	1/1	0.99	0.05	23,23,23,23	0
2	PLP	B	1404	15/16	0.99	0.04	13,15,19,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.