



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 11:27 PM UTC

PDB ID : 4ADC / pdb_00004adc
Title : Structural and functional study of succinyl-ornithine transaminase from E. coli
Authors : Newman, J.; Peat, T.S.
Deposited on : 2011-12-23
Resolution : 2.30 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

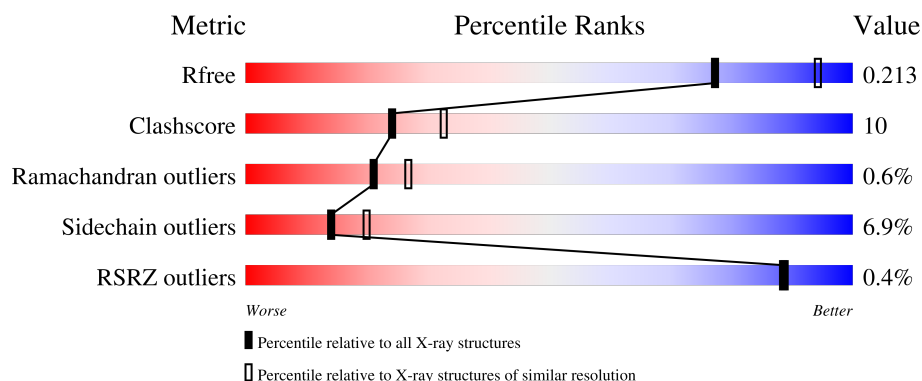
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	
1	B	406	
1	C	406	
1	D	406	

2 Entry composition [i](#)

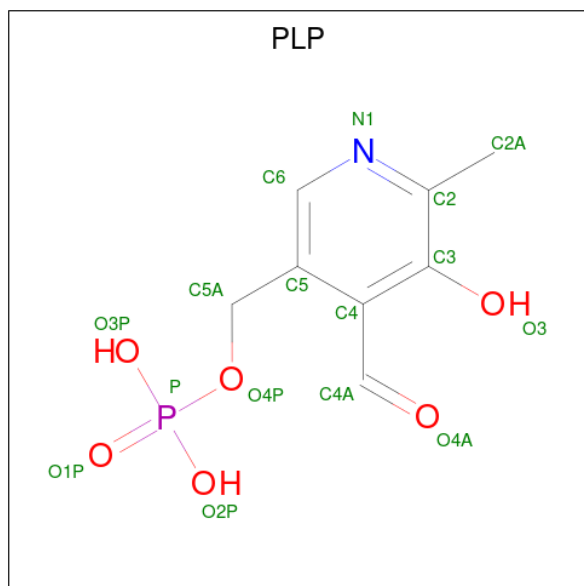
There are 5 unique types of molecules in this entry. The entry contains 12925 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	8	0
			3103	1961	551	580	11			
1	B	400	Total	C	N	O	S	0	7	0
			3092	1955	547	579	11			
1	C	400	Total	C	N	O	S	0	7	0
			3084	1950	545	578	11			
1	D	400	Total	C	N	O	S	0	4	0
			3061	1939	541	570	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
			16	8	1	6	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	D	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

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

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

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

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

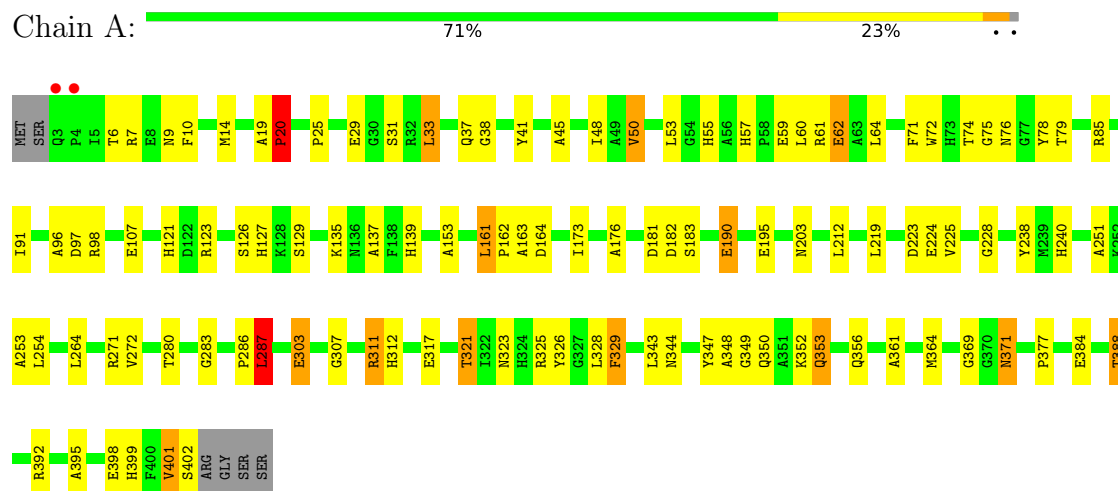
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	177	Total	O	0	0
			177	177		
5	B	146	Total	O	0	0
			146	146		
5	C	127	Total	O	0	0
			127	127		
5	D	68	Total	O	0	0
			68	68		

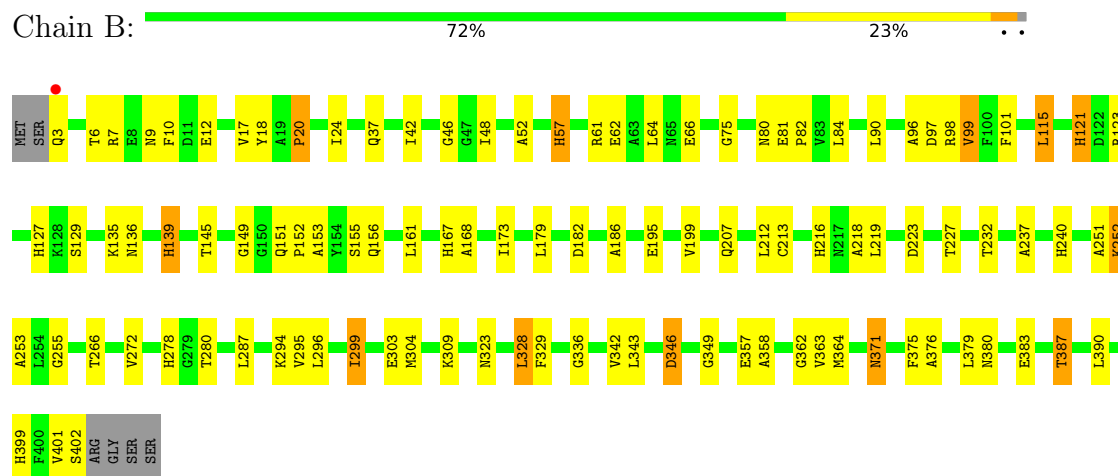
3 Residue-property plots [i](#)

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

• Molecule 1: SUCCINYLORNITHINE TRANSAMINASE

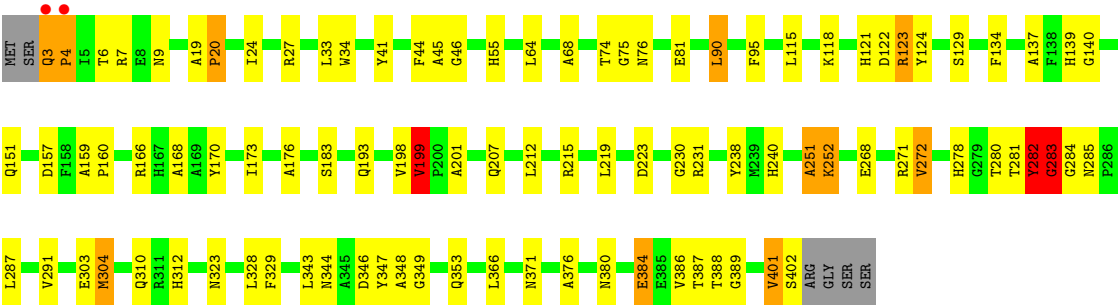


• Molecule 1: SUCCINYLORNITHINE TRANSAMINASE

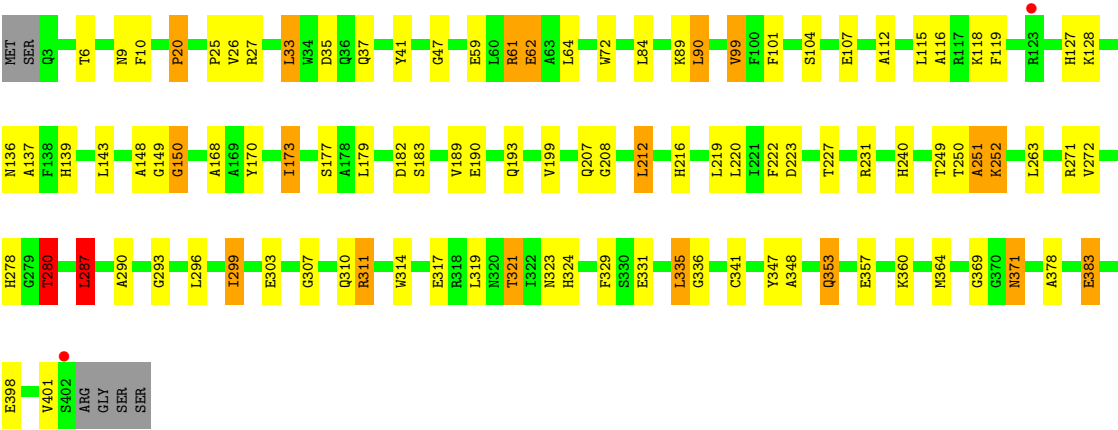


• Molecule 1: SUCCINYLORNITHINE TRANSAMINASE





● Molecule 1: SUCCINYLORNITHINE TRANSAMINASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.37Å 118.28Å 109.46Å 90.00° 96.80° 90.00°	Depositor
Resolution (Å)	108.69 – 2.30 108.69 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (108.69-2.30) 97.8 (108.69-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.170 , 0.213 0.171 , 0.213	Depositor DCC
R_{free} test set	5072 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12925	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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: 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	1.52	26/3180 (0.8%)	1.36	16/4319 (0.4%)
1	B	1.54	20/3170 (0.6%)	1.40	19/4305 (0.4%)
1	C	1.43	13/3165 (0.4%)	1.34	23/4298 (0.5%)
1	D	1.37	8/3143 (0.3%)	1.31	14/4269 (0.3%)
All	All	1.47	67/12658 (0.5%)	1.35	72/17191 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	3
1	D	0	1
All	All	0	4

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	377	PRO	N-CA	8.46	1.56	1.47
1	B	167	HIS	CE1-NE2	7.43	1.40	1.32
1	B	139	HIS	ND1-CE1	7.40	1.40	1.32
1	A	107	GLU	C-O	7.07	1.32	1.24
1	C	278	HIS	CG-CD2	7.02	1.43	1.35
1	B	42	ILE	C-O	6.66	1.31	1.24
1	A	127	HIS	CG-CD2	6.59	1.43	1.35
1	C	285	ASN	N-CA	6.55	1.55	1.46
1	C	281	THR	N-CA	6.48	1.54	1.46
1	A	79	THR	CA-C	6.30	1.62	1.53
1	B	57	HIS	CG-CD2	6.29	1.42	1.35
1	B	186	ALA	N-CA	6.16	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	278	HIS	CE1-NE2	6.12	1.38	1.32
1	B	127	HIS	CG-CD2	6.02	1.42	1.35
1	B	66	GLU	CA-C	5.98	1.60	1.52
1	D	311	ARG	CA-C	5.96	1.60	1.52
1	B	121	HIS	CG-CD2	5.93	1.42	1.35
1	A	224	GLU	C-O	5.90	1.31	1.24
1	D	249	THR	CA-C	-5.89	1.45	1.52
1	D	72	TRP	CA-C	-5.87	1.44	1.52
1	B	399	HIS	CG-CD2	5.85	1.42	1.35
1	D	278	HIS	CG-CD2	5.85	1.42	1.35
1	A	240	HIS	CG-CD2	5.81	1.42	1.35
1	C	386	VAL	C-O	5.79	1.30	1.24
1	A	329	PHE	CA-C	-5.78	1.45	1.52
1	B	240	HIS	CG-CD2	5.76	1.42	1.35
1	A	75	GLY	N-CA	5.76	1.51	1.45
1	A	20	PRO	C-O	5.76	1.30	1.23
1	A	45	ALA	C-O	5.75	1.30	1.24
1	C	387	THR	N-CA	5.74	1.53	1.46
1	B	255	GLY	C-O	-5.74	1.18	1.24
1	C	219	LEU	C-O	5.71	1.30	1.23
1	A	287	LEU	N-CA	5.67	1.53	1.46
1	A	344	ASN	C-O	5.67	1.31	1.23
1	B	278	HIS	CG-CD2	5.67	1.42	1.35
1	B	167	HIS	CG-CD2	5.56	1.42	1.35
1	A	228	GLY	C-O	5.55	1.29	1.23
1	A	55	HIS	CG-CD2	5.50	1.41	1.35
1	A	25	PRO	N-CA	5.47	1.53	1.47
1	C	312	HIS	CG-CD2	5.44	1.41	1.35
1	A	399	HIS	CG-CD2	5.36	1.41	1.35
1	D	324	HIS	CG-CD2	5.34	1.41	1.35
1	A	225	VAL	N-CA	-5.32	1.40	1.46
1	B	121	HIS	CE1-NE2	5.31	1.37	1.32
1	A	71	PHE	C-O	5.31	1.30	1.23
1	B	153	ALA	C-O	-5.31	1.17	1.24
1	A	311	ARG	C-O	-5.28	1.17	1.24
1	D	378	ALA	N-CA	5.28	1.53	1.46
1	C	240	HIS	CG-CD2	5.27	1.41	1.35
1	C	384	GLU	C-O	5.26	1.30	1.24
1	C	55	HIS	CD2-NE2	-5.26	1.32	1.37
1	A	57	HIS	CE1-NE2	5.21	1.37	1.32
1	A	343	LEU	C-O	5.19	1.30	1.23
1	B	362	GLY	N-CA	5.18	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	287	LEU	N-CA	5.14	1.52	1.46
1	B	62	GLU	CA-C	5.14	1.59	1.52
1	A	19	ALA	CA-C	5.12	1.59	1.52
1	B	309	LYS	N-CA	5.12	1.52	1.46
1	C	34	TRP	NE1-CE2	-5.11	1.31	1.37
1	A	312	HIS	CG-CD2	5.10	1.41	1.35
1	D	199	VAL	CA-CB	5.08	1.58	1.54
1	C	140	GLY	N-CA	5.07	1.50	1.45
1	C	312	HIS	ND1-CE1	5.07	1.37	1.32
1	A	190	GLU	CA-C	5.06	1.58	1.52
1	A	176	ALA	CA-C	-5.03	1.46	1.52
1	A	135	LYS	CA-C	-5.02	1.46	1.52
1	B	123	ARG	CA-C	5.01	1.59	1.52

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	284	GLY	N-CA-C	-12.01	99.60	115.21
1	B	149	GLY	N-CA-C	-9.69	99.45	112.82
1	C	81	GLU	CA-C-N	-9.01	109.64	119.19
1	C	81	GLU	C-N-CA	-9.01	109.64	119.19
1	C	238	TYR	N-CA-C	-8.95	101.44	111.82
1	B	75	GLY	N-CA-C	-8.41	100.36	112.81
1	B	115	LEU	N-CA-C	-7.83	102.82	111.36
1	D	357	GLU	N-CA-C	-7.57	102.38	111.69
1	D	280	THR	CB-CA-C	-7.44	96.54	110.16
1	D	299	ILE	N-CA-C	-7.33	105.51	111.81
1	B	299	ILE	N-CA-C	6.87	118.48	111.00
1	C	282	TYR	N-CA-C	6.79	121.27	112.72
1	D	324	HIS	N-CA-C	-6.43	104.27	111.28
1	A	62	GLU	N-CA-C	-6.40	103.81	111.69
1	C	75	GLY	N-CA-C	-6.33	105.58	112.04
1	B	199	VAL	CA-C-N	-6.31	113.45	119.76
1	B	199	VAL	C-N-CA	-6.31	113.45	119.76
1	B	24	ILE	N-CA-C	6.14	114.73	107.73
1	B	266	THR	N-CA-C	-6.08	102.34	110.55
1	B	375	PHE	CA-C-N	-6.05	115.87	122.59
1	B	375	PHE	C-N-CA	-6.05	115.87	122.59
1	B	357	GLU	N-CA-C	-6.05	104.77	111.36
1	A	59	GLU	N-CA-C	6.03	117.85	111.28
1	C	176	ALA	N-CA-C	-6.01	104.65	111.14
1	D	290	ALA	N-CA-C	-5.97	104.34	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	379	LEU	CA-C-N	-5.92	113.18	122.65
1	B	379	LEU	C-N-CA	-5.92	113.18	122.65
1	A	369	GLY	N-CA-C	-5.88	105.01	112.65
1	C	291	VAL	N-CA-C	5.86	116.05	110.42
1	B	96	ALA	N-CA-C	5.82	118.27	110.35
1	D	310	GLN	N-CA-C	-5.81	104.86	111.14
1	D	398	GLU	CA-C-O	-5.80	114.69	121.07
1	C	122	ASP	N-CA-C	5.80	118.55	111.82
1	A	85	ARG	CG-CD-NE	-5.71	99.45	112.00
1	B	336	GLY	CA-C-N	-5.68	114.17	122.86
1	B	336	GLY	C-N-CA	-5.68	114.17	122.86
1	C	183	SER	N-CA-C	5.66	119.81	113.02
1	C	24	ILE	CA-C-N	-5.64	113.89	119.92
1	C	24	ILE	C-N-CA	-5.64	113.89	119.92
1	C	283[A]	GLY	CA-C-N	-5.58	113.32	122.20
1	C	283[A]	GLY	C-N-CA	-5.58	113.32	122.20
1	C	283[B]	GLY	CA-C-N	-5.58	113.32	122.20
1	C	283[B]	GLY	C-N-CA	-5.58	113.32	122.20
1	A	153	ALA	N-CA-C	5.55	119.15	112.38
1	A	161	LEU	CA-C-N	-5.51	114.28	119.90
1	A	161	LEU	C-N-CA	-5.51	114.28	119.90
1	C	199	VAL	CA-C-N	-5.49	114.93	120.31
1	C	199	VAL	C-N-CA	-5.49	114.93	120.31
1	A	74	THR	CB-CA-C	-5.47	100.59	109.13
1	C	90	LEU	N-CA-C	-5.43	105.79	112.90
1	D	189	VAL	N-CA-C	5.41	115.50	108.35
1	C	304	MET	CG-SD-CE	-5.40	89.02	100.90
1	A	74	THR	N-CA-C	-5.39	107.71	114.56
1	D	62	GLU	N-CA-C	-5.37	105.09	111.69
1	B	127	HIS	N-CA-C	-5.35	106.60	113.23
1	A	38	GLY	N-CA-C	-5.30	108.00	115.32
1	D	369	GLY	N-CA-C	-5.30	106.00	112.68
1	A	57	HIS	CA-C-N	5.27	124.90	119.05
1	A	57	HIS	C-N-CA	5.27	124.90	119.05
1	D	148	ALA	CA-C-N	5.26	126.71	120.14
1	D	148	ALA	C-N-CA	5.26	126.71	120.14
1	A	50	VAL	CB-CA-C	-5.22	106.48	111.44
1	B	232	THR	CB-CA-C	-5.22	100.61	110.01
1	A	61	ARG	CA-CB-CG	-5.21	103.67	114.10
1	C	75	GLY	CA-C-O	-5.18	118.72	122.45
1	A	31	SER	N-CA-C	5.17	118.72	112.93
1	B	145	THR	N-CA-C	-5.14	105.75	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	19	ALA	CA-C-N	5.13	126.39	120.85
1	C	19	ALA	C-N-CA	5.13	126.39	120.85
1	D	150	GLY	N-CA-C	5.07	121.76	114.10
1	D	84	LEU	N-CA-C	-5.05	105.47	111.69
1	A	76	ASN	N-CA-C	5.04	119.06	113.02

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	282	TYR	Peptide
1	C	283[B]	GLY	Mainchain,Peptide
1	D	150	GLY	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3103	0	3012	71	0
1	B	3092	0	3019	58	0
1	C	3084	0	3009	53	0
1	D	3061	0	2991	71	0
2	A	16	0	7	0	0
2	B	16	0	7	0	0
2	C	16	0	7	0	0
2	D	16	0	7	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	B	1	0	0	0	0
5	A	177	0	0	5	0
5	B	146	0	0	5	0
5	C	127	0	0	4	0
5	D	68	0	0	1	0
All	All	12925	0	12059	245	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 10.

All (245) 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:271[B]:ARG:HG2	1:A:271[B]:ARG:HH11	1.06	1.14
1:A:271[A]:ARG:HD3	1:C:271[A]:ARG:CD	1.78	1.11
1:A:271[A]:ARG:CD	1:C:271[A]:ARG:HD3	1.82	1.09
1:A:14:MET:HE3	5:A:2012:HOH:O	1.53	1.08
1:B:387[A]:THR:CG2	5:B:2125:HOH:O	2.04	1.04
1:A:271[A]:ARG:HD3	1:C:271[A]:ARG:HD3	1.02	1.01
1:D:271[B]:ARG:HH11	1:D:271[B]:ARG:CG	1.75	0.97
1:A:271[B]:ARG:HG2	1:A:271[B]:ARG:NH1	1.83	0.91
1:A:271[B]:ARG:HH11	1:A:271[B]:ARG:CG	1.83	0.91
1:D:271[B]:ARG:HH11	1:D:271[B]:ARG:HG2	1.36	0.88
1:D:90:LEU:HD13	1:D:296:LEU:HD11	1.56	0.84
1:C:304:MET:HE1	1:C:380:ASN:HB3	1.61	0.82
1:C:349:GLY:H	1:C:371:ASN:HD22	1.28	0.81
1:B:387[A]:THR:HG23	5:B:2125:HOH:O	1.69	0.81
1:A:349:GLY:H	1:A:371:ASN:HD22	1.29	0.79
1:B:227[A]:THR:CG2	1:B:237:ALA:HB2	2.13	0.79
1:A:348:ALA:HA	1:A:371:ASN:HD21	1.47	0.79
1:A:33:LEU:HD12	1:A:364:MET:HE1	1.65	0.79
1:B:387[A]:THR:HG22	5:B:2125:HOH:O	1.72	0.77
1:A:353[A]:GLN:HE21	1:A:353[A]:GLN:H	1.33	0.76
1:B:7:ARG:NH2	1:B:20:PRO:HD2	2.00	0.76
1:B:195:GLU:OE1	5:B:2098:HOH:O	2.04	0.75
1:D:323:ASN:HD21	1:D:329:PHE:H	1.32	0.75
1:C:323:ASN:HD21	1:C:329:PHE:H	1.36	0.73
1:D:271[B]:ARG:CG	1:D:271[B]:ARG:NH1	2.47	0.73
1:D:41:TYR:HB2	1:D:364:MET:HE2	1.69	0.72
1:A:349:GLY:H	1:A:371:ASN:ND2	1.87	0.72
1:B:227[A]:THR:HG21	1:B:237:ALA:HB2	1.72	0.72
1:A:325:ARG:HD3	1:A:326:TYR:CZ	2.26	0.71
1:A:323:ASN:HD21	1:A:329:PHE:H	1.39	0.71
1:D:182:ASP:OD1	1:D:216:HIS:HD2	1.74	0.71
1:A:328:LEU:HD21	1:A:401:VAL:HG23	1.72	0.70
1:A:139:HIS:HD2	1:A:223:ASP:OD2	1.73	0.70
1:B:182:ASP:OD1	1:B:216:HIS:HD2	1.75	0.69
5:C:2127:HOH:O	1:D:280:THR:HG23	1.92	0.69
1:D:89:LYS:HE2	1:D:293:GLY:O	1.92	0.69
1:D:90:LEU:CD1	1:D:296:LEU:HD11	2.22	0.68
1:A:395:ALA:O	1:A:398:GLU:HB3	1.95	0.67
1:D:41:TYR:HB2	1:D:364:MET:CE	2.23	0.67
1:D:41:TYR:CB	1:D:364:MET:HE2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:HIS:HE1	1:C:129:SER:OG	1.78	0.66
1:C:198:VAL:HG12	1:C:198:VAL:O	1.96	0.66
1:A:384:GLU:OE2	1:A:388:THR:HG21	1.96	0.65
1:B:139:HIS:HD2	1:B:223:ASP:OD2	1.78	0.65
1:D:271[B]:ARG:HH11	1:D:271[B]:ARG:HG3	1.62	0.65
1:A:384:GLU:O	1:A:388:THR:HG23	1.98	0.64
1:D:182:ASP:OD1	1:D:216:HIS:CD2	2.50	0.64
1:A:348:ALA:CA	1:A:371:ASN:HD21	2.10	0.64
1:B:349:GLY:H	1:B:371:ASN:ND2	1.95	0.64
1:D:6:THR:H	1:D:9:ASN:ND2	1.96	0.64
1:B:64:LEU:HD12	1:B:287:LEU:HD22	1.80	0.63
1:A:91:ILE:O	5:A:2075:HOH:O	2.15	0.63
1:C:193:GLN:HB2	1:C:199:VAL:HG13	1.80	0.63
1:B:227[A]:THR:HG22	1:B:237:ALA:HB2	1.80	0.63
1:D:33:LEU:HD12	1:D:364:MET:HE1	1.80	0.63
1:C:74:THR:O	1:D:47:GLY:HA2	1.99	0.63
1:D:90:LEU:HD13	1:D:296:LEU:CD1	2.27	0.62
1:A:10:PHE:CZ	1:A:20:PRO:HD3	2.35	0.62
1:D:353:GLN:H	1:D:353:GLN:HE21	1.47	0.62
1:A:41:TYR:HB2	1:A:364:MET:CE	2.30	0.62
5:A:2148:HOH:O	1:B:252:LYS:NZ	2.30	0.62
1:C:3:GLN:HG2	1:C:4:PRO:HD2	1.80	0.62
1:C:349:GLY:H	1:C:371:ASN:ND2	1.94	0.62
1:B:99:VAL:HG21	1:B:101:PHE:CZ	2.34	0.61
1:C:348:ALA:HA	1:C:371:ASN:HD21	1.66	0.61
1:A:139:HIS:HE1	5:A:2098:HOH:O	1.83	0.61
1:A:41:TYR:HB2	1:A:364:MET:HE2	1.81	0.61
1:C:121:HIS:CE1	1:C:129:SER:OG	2.54	0.61
1:A:384:GLU:OE2	1:A:388:THR:CG2	2.50	0.60
1:D:64:LEU:HD12	1:D:287:LEU:HD22	1.82	0.60
1:D:104:SER:OG	1:D:107:GLU:HG3	2.01	0.60
1:C:115:LEU:C	1:C:115:LEU:HD23	2.27	0.60
1:D:137:ALA:O	1:D:149:GLY:O	2.21	0.59
1:A:10:PHE:CE1	1:A:20:PRO:HD3	2.37	0.59
1:C:159:ALA:HB1	1:C:160:PRO:HA	1.84	0.59
1:A:353[A]:GLN:HE21	1:A:353[A]:GLN:N	2.00	0.59
1:D:128:LYS:HG3	1:D:183:SER:HA	1.85	0.59
1:A:97:ASP:O	1:A:98:ARG:HG2	2.03	0.58
1:B:121:HIS:CE1	1:B:129:SER:OG	2.57	0.58
1:A:33:LEU:CD1	1:A:364:MET:HE1	2.34	0.58
1:A:14:MET:HE2	1:B:84:LEU:HD23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:LYS:O	1:B:136:ASN:HB2	2.03	0.58
1:B:10:PHE:CZ	1:B:20:PRO:HD3	2.39	0.58
1:C:118:LYS:HD3	1:C:272:VAL:HG13	1.86	0.58
1:A:328:LEU:CD2	1:A:401:VAL:HG23	2.34	0.57
1:A:6:THR:H	1:A:9:ASN:ND2	2.02	0.57
1:A:348:ALA:HA	1:A:371:ASN:ND2	2.18	0.57
1:B:323:ASN:ND2	1:B:328:LEU:H	2.03	0.57
1:A:64:LEU:HD12	1:A:287:LEU:HD22	1.87	0.57
1:B:6:THR:H	1:B:9:ASN:ND2	2.03	0.56
1:C:68:ALA:O	1:D:61:ARG:HD2	2.06	0.56
1:C:349:GLY:N	1:C:371:ASN:HD22	2.01	0.56
1:D:173:ILE:HD13	1:D:208:GLY:HA3	1.88	0.56
5:C:2126:HOH:O	1:D:280:THR:HG22	2.06	0.55
1:C:347:TYR:OH	1:C:401:VAL:HG13	2.06	0.55
1:B:121:HIS:HE1	1:B:129:SER:OG	1.88	0.55
1:C:115:LEU:HD23	1:C:115:LEU:O	2.07	0.54
1:A:10:PHE:CE1	1:A:20:PRO:CD	2.90	0.54
1:B:152:PRO:O	1:B:156:GLN:HG3	2.07	0.54
1:C:157:ASP:OD2	1:D:118:LYS:HE2	2.08	0.54
1:D:10:PHE:CZ	1:D:20:PRO:HD3	2.43	0.54
1:D:139:HIS:HD2	1:D:223:ASP:OD2	1.89	0.54
1:C:280:THR:HG21	1:C:283[B]:GLY:HA3	1.90	0.53
1:A:353[A]:GLN:H	1:A:353[A]:GLN:NE2	2.04	0.53
1:C:6:THR:H	1:C:9:ASN:ND2	2.06	0.53
1:D:348:ALA:HB1	1:D:371:ASN:HD21	1.73	0.53
1:A:349:GLY:N	1:A:371:ASN:HD22	2.03	0.53
1:B:323:ASN:HD21	1:B:329:PHE:H	1.55	0.53
1:A:280:THR:HG21	1:A:283:GLY:HA3	1.91	0.52
1:D:137:ALA:HB1	1:D:139:HIS:CE1	2.43	0.52
1:A:181:ASP:OD1	1:A:183:SER:HB2	2.09	0.52
1:A:7:ARG:NH2	1:A:20:PRO:HD2	2.24	0.52
1:A:33:LEU:HB3	1:A:364:MET:HE1	1.90	0.52
1:A:121[A]:HIS:HE1	1:A:129:SER:OG	1.93	0.51
1:D:271[B]:ARG:NH1	1:D:271[B]:ARG:HG3	2.23	0.51
1:C:323:ASN:ND2	1:C:329:PHE:H	2.06	0.51
1:A:253:ALA:O	1:A:254:LEU:C	2.53	0.51
1:B:10:PHE:CE1	1:B:20:PRO:HD3	2.45	0.51
1:D:323:ASN:HD21	1:D:329:PHE:N	2.05	0.51
1:B:358:ALA:HB1	1:B:363:VAL:HG13	1.93	0.51
1:D:116:ALA:HA	1:D:219:LEU:HD12	1.93	0.50
1:D:307:GLY:O	1:D:311:ARG:HD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:THR:H	1:A:9:ASN:HD22	1.57	0.50
1:A:195[A]:GLU:OE1	5:A:2128:HOH:O	2.19	0.50
1:B:182:ASP:OD1	1:B:216:HIS:CD2	2.62	0.50
5:C:2127:HOH:O	1:D:280:THR:CG2	2.57	0.50
1:C:7:ARG:NH2	1:C:20:PRO:HD2	2.27	0.50
1:B:346:ASP:OD1	1:B:346:ASP:N	2.44	0.49
1:D:26:VAL:HG23	1:D:27:ARG:HG2	1.93	0.49
1:C:401:VAL:O	1:C:402:SER:OG	2.28	0.49
1:A:41:TYR:CB	1:A:364:MET:HE2	2.41	0.49
1:C:268[B]:GLU:CD	1:C:268[B]:GLU:H	2.20	0.49
1:B:295:VAL:HG13	1:B:299:ILE:HD12	1.95	0.49
1:C:46:GLY:HA3	1:C:376:ALA:O	2.12	0.48
1:A:317:GLU:O	1:A:321:THR:HG23	2.13	0.48
1:A:347:TYR:O	1:A:350:GLN:HB2	2.12	0.48
1:C:76:ASN:HD21	1:C:283[A]:GLY:HA2	1.78	0.48
1:D:353:GLN:HE21	1:D:353:GLN:N	2.10	0.48
1:B:115:LEU:HD23	1:B:115:LEU:O	2.14	0.48
1:B:383:GLU:O	1:B:387[B]:THR:HG22	2.12	0.48
1:D:127:HIS:CD2	1:D:183:SER:HB3	2.49	0.48
1:D:317:GLU:O	1:D:321:THR:HG23	2.13	0.48
1:D:127:HIS:HD2	1:D:183:SER:HB3	1.77	0.48
1:D:314:TRP:CH2	1:D:383:GLU:HB2	2.49	0.47
1:D:136:ASN:HB2	1:D:193:GLN:HE22	1.79	0.47
1:B:52:ALA:HB2	1:B:253:ALA:HB1	1.97	0.47
1:B:227[A]:THR:HG21	1:B:237:ALA:CB	2.42	0.47
1:B:296:LEU:HD23	1:B:296:LEU:HA	1.65	0.47
1:C:123:ARG:HD3	1:C:124:TYR:CE2	2.50	0.47
1:C:344[A]:ASN:C	1:C:344[A]:ASN:OD1	2.58	0.47
1:D:33:LEU:HB3	1:D:364:MET:HE1	1.97	0.47
1:D:115:LEU:HD23	1:D:115:LEU:C	2.39	0.47
1:A:96:ALA:HB2	1:A:264:LEU:HB3	1.96	0.47
1:A:349:GLY:N	1:A:371:ASN:ND2	2.60	0.47
1:D:6:THR:H	1:D:9:ASN:HD22	1.62	0.47
1:C:41:TYR:CD1	1:C:41:TYR:N	2.82	0.47
1:B:155:SER:HB2	1:B:161:LEU:HD11	1.96	0.46
1:C:230:GLY:O	1:C:231:ARG:C	2.56	0.46
1:B:81:GLU:N	1:B:82:PRO:CD	2.79	0.46
1:C:170:TYR:OH	1:C:201:ALA:HB2	2.16	0.46
1:A:223:ASP:OD1	1:A:223:ASP:C	2.58	0.46
1:A:163:ALA:O	1:A:164:ASP:HB2	2.16	0.46
1:A:325:ARG:HD3	1:A:326:TYR:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:ALA:HB2	1:D:263:LEU:HD13	1.97	0.46
1:C:123:ARG:HD3	1:C:124:TYR:CZ	2.51	0.46
1:C:323:ASN:ND2	1:C:328:LEU:H	2.14	0.46
1:C:134:PHE:HA	1:C:168:ALA:O	2.16	0.46
1:D:319:LEU:HD13	1:D:341:CYS:SG	2.56	0.46
1:A:50:VAL:O	1:A:253:ALA:HA	2.15	0.46
1:B:99:VAL:CG2	1:B:101:PHE:CE2	2.99	0.46
1:A:33:LEU:HD12	1:A:364:MET:CE	2.42	0.46
1:D:335:LEU:O	1:D:336:GLY:C	2.59	0.45
1:C:384:GLU:OE2	1:C:388:THR:OG1	2.32	0.45
1:A:161:LEU:O	1:A:162:PRO:C	2.54	0.45
1:D:223:ASP:C	1:D:223:ASP:OD1	2.60	0.45
1:C:45:ALA:HB1	1:C:366:LEU:HD21	1.99	0.45
1:C:139:HIS:HD2	1:C:223:ASP:OD2	1.99	0.45
1:D:25:PRO:HA	1:D:35:ASP:HA	1.99	0.45
1:B:115:LEU:HD23	1:B:115:LEU:C	2.42	0.45
1:B:323:ASN:HD21	1:B:328:LEU:H	1.65	0.45
1:D:33:LEU:CB	1:D:364:MET:HE1	2.47	0.45
1:D:347:TYR:O	1:D:348:ALA:C	2.59	0.45
1:B:48:ILE:O	1:B:252:LYS:CE	2.64	0.45
1:D:177:SER:HB3	1:D:212:LEU:HD11	1.98	0.45
1:A:53:LEU:HD12	1:A:60:LEU:HD11	1.99	0.44
1:B:151:GLN:HG3	5:B:2076:HOH:O	2.16	0.44
1:D:170:TYR:CE2	1:D:193:GLN:HG3	2.53	0.44
1:C:173:ILE:HG22	5:C:2090:HOH:O	2.17	0.44
1:D:227:THR:O	1:D:231:ARG:HB3	2.16	0.44
1:D:139:HIS:HE1	5:D:2038:HOH:O	1.99	0.44
1:B:48:ILE:O	1:B:252:LYS:HE2	2.17	0.44
1:C:348:ALA:HA	1:C:371:ASN:ND2	2.30	0.44
1:D:137:ALA:HA	1:D:190:GLU:OE2	2.17	0.44
1:A:401:VAL:O	1:A:401:VAL:HG13	2.18	0.44
1:D:41:TYR:CB	1:D:364:MET:CE	2.92	0.44
1:C:76:ASN:HD21	1:C:283[A]:GLY:CA	2.30	0.43
1:D:170:TYR:CZ	1:D:193:GLN:HG3	2.53	0.43
1:D:251:ALA:O	1:D:252:LYS:C	2.60	0.43
1:C:280:THR:CG2	1:C:283[B]:GLY:HA3	2.48	0.43
1:B:80:ASN:OD1	1:B:82:PRO:HD2	2.18	0.43
1:B:390:LEU:HD23	1:B:390:LEU:HA	1.83	0.43
1:B:213:CYS:HB3	1:B:218:ALA:O	2.18	0.43
1:C:344[A]:ASN:OD1	1:C:346:ASP:HB2	2.18	0.43
1:B:401:VAL:O	1:B:401:VAL:CG1	2.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:PHE:CZ	1:C:389:GLY:HA3	2.53	0.43
1:D:99:VAL:HG22	1:D:101:PHE:CE2	2.53	0.43
1:A:303[A]:GLU:CD	1:A:303[A]:GLU:H	2.26	0.43
1:C:329:PHE:CD1	1:C:343:LEU:HD23	2.53	0.43
1:A:323:ASN:ND2	1:A:329:PHE:H	2.11	0.43
1:A:137:ALA:HB1	1:A:139:HIS:CE1	2.53	0.43
1:B:6:THR:H	1:B:9:ASN:HD22	1.66	0.43
1:D:33:LEU:HD12	1:D:364:MET:CE	2.49	0.43
1:D:143:LEU:HD12	1:D:143:LEU:HA	1.84	0.43
1:A:121[A]:HIS:CE1	1:A:129:SER:OG	2.71	0.42
1:D:119:PHE:CD1	1:D:119:PHE:C	2.98	0.42
1:B:57:HIS:O	1:B:61:ARG:HG3	2.20	0.42
1:B:349:GLY:N	1:B:371:ASN:ND2	2.65	0.42
1:D:240:HIS:CD2	1:D:335:LEU:HD21	2.54	0.42
1:A:307:GLY:O	1:A:311:ARG:HD2	2.20	0.42
1:B:329:PHE:HA	1:B:342:VAL:O	2.20	0.42
1:D:33:LEU:CD1	1:D:364:MET:HE1	2.48	0.42
1:B:46:GLY:HA3	1:B:376:ALA:O	2.20	0.42
1:D:35:ASP:C	1:D:35:ASP:OD1	2.61	0.42
1:D:271[B]:ARG:HG2	1:D:271[B]:ARG:NH1	2.17	0.42
1:B:223:ASP:C	1:B:223:ASP:OD1	2.62	0.42
1:B:227[A]:THR:HG22	1:B:227[A]:THR:O	2.19	0.41
1:D:168:ALA:HB2	1:D:179:LEU:HD12	2.02	0.41
1:A:72:TRP:O	1:A:286:PRO:HD2	2.20	0.41
1:C:223:ASP:OD1	1:C:223:ASP:C	2.63	0.41
1:A:361:ALA:O	1:A:392:ARG:HB3	2.20	0.41
1:B:97:ASP:C	1:B:98:ARG:HG2	2.45	0.41
1:C:282:TYR:O	1:C:283[A]:GLY:C	2.61	0.41
1:C:137:ALA:HB1	1:C:139:HIS:CE1	2.56	0.41
1:A:271[B]:ARG:NH1	1:A:271[B]:ARG:CG	2.54	0.41
1:A:352:LYS:O	1:A:356:GLN:HG3	2.20	0.41
1:B:168:ALA:HB2	1:B:179:LEU:HD12	2.02	0.41
1:B:304:MET:HE1	1:B:380:ASN:HB3	2.03	0.41
1:C:251:ALA:O	1:C:252:LYS:C	2.64	0.41
1:A:78:TYR:CZ	1:B:364:MET:HE3	2.56	0.41
1:B:17:VAL:HG23	1:B:18:TYR:CD2	2.55	0.41
1:A:238:TYR:CD1	1:A:238:TYR:C	2.98	0.40
1:C:95:PHE:CD2	1:C:95:PHE:C	2.95	0.40
1:A:137:ALA:HA	1:A:190:GLU:OE2	2.22	0.40
1:D:220:LEU:HD11	1:D:222:PHE:HE1	1.87	0.40
1:B:343:LEU:HD23	1:B:343:LEU:HA	1.88	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	406/406 (100%)	383 (94%)	21 (5%)	2 (0%)	24	31
1	B	405/406 (100%)	387 (96%)	16 (4%)	2 (0%)	24	31
1	C	405/406 (100%)	378 (93%)	23 (6%)	4 (1%)	12	15
1	D	402/406 (99%)	382 (95%)	17 (4%)	3 (1%)	18	23
All	All	1618/1624 (100%)	1530 (95%)	77 (5%)	11 (1%)	21	23

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	252	LYS
1	C	283[A]	GLY
1	C	283[B]	GLY
1	D	251	ALA
1	D	252	LYS
1	B	251	ALA
1	C	251	ALA
1	A	182	ASP
1	A	251	ALA
1	C	252	LYS
1	D	401	VAL

5.3.2 Protein sidechains [i](#)

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	314/312 (101%)	291 (93%)	23 (7%)	13	18
1	B	314/312 (101%)	293 (93%)	21 (7%)	15	21
1	C	313/312 (100%)	292 (93%)	21 (7%)	15	21
1	D	310/312 (99%)	285 (92%)	25 (8%)	11	14
All	All	1251/1248 (100%)	1161 (93%)	90 (7%)	14	18

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	PRO
1	A	29	GLU
1	A	33	LEU
1	A	37	GLN
1	A	48	ILE
1	A	62	GLU
1	A	123	ARG
1	A	126	SER
1	A	173	ILE
1	A	203	ASN
1	A	212	LEU
1	A	219	LEU
1	A	272	VAL
1	A	287	LEU
1	A	303[A]	GLU
1	A	303[B]	GLU
1	A	321	THR
1	A	353[A]	GLN
1	A	353[B]	GLN
1	A	371	ASN
1	A	388	THR
1	A	401	VAL
1	A	402	SER
1	B	3	GLN
1	B	12	GLU
1	B	20	PRO
1	B	37	GLN
1	B	90	LEU
1	B	99	VAL
1	B	173	ILE
1	B	207	GLN
1	B	212	LEU
1	B	219	LEU

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Mol	Chain	Res	Type
1	B	272	VAL
1	B	280	THR
1	B	294	LYS
1	B	303[A]	GLU
1	B	303[B]	GLU
1	B	328	LEU
1	B	346	ASP
1	B	371	ASN
1	B	387[A]	THR
1	B	387[B]	THR
1	B	402	SER
1	C	3	GLN
1	C	4	PRO
1	C	20	PRO
1	C	27	ARG
1	C	33	LEU
1	C	64	LEU
1	C	90	LEU
1	C	123	ARG
1	C	151	GLN
1	C	166	ARG
1	C	199	VAL
1	C	207	GLN
1	C	212	LEU
1	C	215	ARG
1	C	272	VAL
1	C	287	LEU
1	C	303[A]	GLU
1	C	303[B]	GLU
1	C	310	GLN
1	C	353	GLN
1	C	401	VAL
1	D	20	PRO
1	D	33	LEU
1	D	37	GLN
1	D	59	GLU
1	D	61	ARG
1	D	62	GLU
1	D	90	LEU
1	D	99	VAL
1	D	173	ILE
1	D	207	GLN

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Mol	Chain	Res	Type
1	D	212	LEU
1	D	250	THR
1	D	272	VAL
1	D	280	THR
1	D	287	LEU
1	D	299	ILE
1	D	303[A]	GLU
1	D	303[B]	GLU
1	D	321	THR
1	D	331	GLU
1	D	335	LEU
1	D	353	GLN
1	D	360	LYS
1	D	371	ASN
1	D	383	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	67	GLN
1	A	139	HIS
1	A	167	HIS
1	A	203	ASN
1	A	323	ASN
1	A	356	GLN
1	A	371	ASN
1	B	9	ASN
1	B	57	HIS
1	B	67	GLN
1	B	103	ASN
1	B	121	HIS
1	B	139	HIS
1	B	156	GLN
1	B	203	ASN
1	B	216	HIS
1	B	217	ASN
1	B	240	HIS
1	B	310	GLN
1	B	323	ASN
1	B	353	GLN
1	B	371	ASN

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Mol	Chain	Res	Type
1	C	9	ASN
1	C	36	GLN
1	C	37	GLN
1	C	76	ASN
1	C	121	HIS
1	C	139	HIS
1	C	174	ASN
1	C	203	ASN
1	C	323	ASN
1	C	371	ASN
1	D	9	ASN
1	D	37	GLN
1	D	127	HIS
1	D	139	HIS
1	D	193	GLN
1	D	207	GLN
1	D	216	HIS
1	D	323	ASN
1	D	353	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 7 ligands modelled in this entry, 3 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	B	1403	-	16,16,16	2.38	3 (18%)	20,23,23	2.24	7 (35%)
2	PLP	A	1403	-	16,16,16	2.17	4 (25%)	20,23,23	1.95	6 (30%)
2	PLP	D	1403	-	16,16,16	1.74	3 (18%)	20,23,23	1.90	7 (35%)
2	PLP	C	1403	-	16,16,16	2.16	3 (18%)	20,23,23	2.19	8 (40%)

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	B	1403	-	-	2/8/8/8	0/1/1/1
2	PLP	A	1403	-	-	3/8/8/8	0/1/1/1
2	PLP	D	1403	-	-	3/8/8/8	0/1/1/1
2	PLP	C	1403	-	-	2/8/8/8	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1403	PLP	C3-C2	5.82	1.47	1.41
2	B	1403	PLP	C4-C5	5.60	1.49	1.42
2	C	1403	PLP	C4-C3	5.43	1.50	1.41
2	A	1403	PLP	C3-C2	4.79	1.45	1.41
2	D	1403	PLP	C4-C3	4.45	1.48	1.41
2	C	1403	PLP	C4-C5	4.37	1.48	1.42
2	A	1403	PLP	C4-C5	4.30	1.48	1.42
2	C	1403	PLP	C3-C2	4.26	1.45	1.41
2	A	1403	PLP	C4-C3	4.05	1.47	1.41
2	B	1403	PLP	C4-C3	3.91	1.47	1.41
2	D	1403	PLP	C3-C2	3.34	1.44	1.41
2	D	1403	PLP	C4-C5	2.90	1.46	1.42
2	A	1403	PLP	P-O3P	-2.80	1.44	1.54

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1403	PLP	C4-C3-C2	-5.46	117.07	120.14
2	A	1403	PLP	O4A-C4A-C4	-4.98	113.00	124.80
2	C	1403	PLP	O4A-C4A-C4	-4.59	113.92	124.80
2	C	1403	PLP	C4-C3-C2	-4.30	117.72	120.14
2	B	1403	PLP	C6-N1-C2	4.27	126.94	119.20
2	B	1403	PLP	O2P-P-O4P	-3.76	96.87	106.67
2	D	1403	PLP	O4A-C4A-C4	-3.72	115.99	124.80
2	C	1403	PLP	C6-N1-C2	3.63	125.78	119.20
2	D	1403	PLP	O3P-P-O4P	-3.62	97.23	106.67
2	A	1403	PLP	C6-N1-C2	3.24	125.07	119.20
2	B	1403	PLP	C5-C6-N1	-3.02	118.92	123.83
2	A	1403	PLP	O4P-C5A-C5	-2.99	103.76	109.36
2	A	1403	PLP	O3P-P-O4P	2.98	114.43	106.67
2	D	1403	PLP	C3-C4-C5	-2.97	115.89	118.28
2	C	1403	PLP	O2P-P-O4P	-2.97	98.92	106.67
2	A	1403	PLP	C3-C2-N1	-2.95	117.24	120.96
2	B	1403	PLP	O4P-C5A-C5	-2.89	103.93	109.36
2	D	1403	PLP	O3P-P-O1P	2.69	121.33	110.83
2	C	1403	PLP	C2A-C2-C3	2.67	123.93	120.80
2	D	1403	PLP	C2A-C2-N1	2.46	122.27	117.64
2	D	1403	PLP	C6-N1-C2	2.38	123.52	119.20
2	D	1403	PLP	C2A-C2-C3	-2.33	118.07	120.80
2	C	1403	PLP	O3P-P-O2P	2.20	116.06	107.80
2	A	1403	PLP	C2A-C2-N1	2.18	121.75	117.64
2	B	1403	PLP	O3-C3-C2	2.13	122.01	117.58
2	C	1403	PLP	O3P-P-O4P	-2.08	101.24	106.67
2	B	1403	PLP	O4A-C4A-C4	-2.04	119.95	124.80
2	C	1403	PLP	O2P-P-O1P	2.01	118.69	110.83

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1403	PLP	C5A-O4P-P-O1P
2	D	1403	PLP	C5A-O4P-P-O2P
2	B	1403	PLP	C3-C4-C4A-O4A
2	C	1403	PLP	C3-C4-C4A-O4A
2	A	1403	PLP	C3-C4-C4A-O4A
2	A	1403	PLP	C5A-O4P-P-O1P
2	C	1403	PLP	C5-C4-C4A-O4A
2	D	1403	PLP	C3-C4-C4A-O4A
2	A	1403	PLP	C5-C4-C4A-O4A
2	B	1403	PLP	C5-C4-C4A-O4A

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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%)	-0.77	2 (0%) 87 87	8, 18, 31, 55	22 (5%)
1	B	400/406 (98%)	-0.81	1 (0%) 90 90	8, 17, 31, 65	21 (5%)
1	C	400/406 (98%)	-0.66	2 (0%) 87 87	8, 22, 36, 70	24 (6%)
1	D	400/406 (98%)	-0.48	2 (0%) 87 87	14, 28, 46, 77	20 (5%)
All	All	1600/1624 (98%)	-0.68	7 (0%) 88 89	8, 21, 38, 77	87 (5%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3	GLN	5.6
1	B	3	GLN	3.3
1	A	3	GLN	2.9
1	D	123	ARG	2.6
1	D	402	SER	2.4
1	C	4	PRO	2.2
1	A	4	PRO	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 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
4	MG	B	1999	1/1	0.94	0.04	36,36,36,36	1
3	NA	B	1404	1/1	0.96	0.04	21,21,21,21	0
3	NA	C	1404	1/1	0.98	0.02	25,25,25,25	0
2	PLP	D	1403	16/16	0.98	0.05	14,17,20,26	0
2	PLP	B	1403	16/16	0.99	0.03	8,10,12,18	0
2	PLP	C	1403	16/16	0.99	0.05	17,24,27,32	0
2	PLP	A	1403	16/16	0.99	0.05	14,15,19,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.