



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:46 AM UTC

PDB ID : 4WYA / pdb_00004wya
Title : Crystal structure of 7,8-diaminopelargonic acid synthase (BioA) from Mycobacterium tuberculosis, complexed with a fragment hit
Authors : Finzel, B.C.; Dai, D.; Geders, T.W.
Deposited on : 2014-11-17
Resolution : 2.50 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

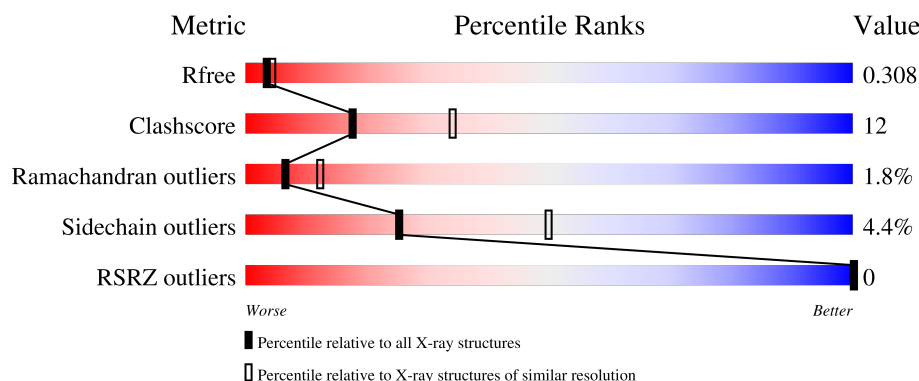
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	457	
1	B	457	
1	C	457	
1	D	457	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	3VQ	D	501	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12702 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 Adenosylmethionine-8-amino-7-oxononanoate aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	1	0	0
			3129	1989	554	567	19			
1	B	422	Total	C	N	O	S	0	1	0
			3147	2001	555	571	20			
1	C	419	Total	C	N	O	S	0	0	0
			3124	1987	551	566	20			
1	D	414	Total	C	N	O	S	0	1	0
			3100	1973	549	559	19			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P9WQ81
A	-18	GLY	-	expression tag	UNP P9WQ81
A	-17	SER	-	expression tag	UNP P9WQ81
A	-16	SER	-	expression tag	UNP P9WQ81
A	-15	HIS	-	expression tag	UNP P9WQ81
A	-14	HIS	-	expression tag	UNP P9WQ81
A	-13	HIS	-	expression tag	UNP P9WQ81
A	-12	HIS	-	expression tag	UNP P9WQ81
A	-11	HIS	-	expression tag	UNP P9WQ81
A	-10	HIS	-	expression tag	UNP P9WQ81
A	-9	SER	-	expression tag	UNP P9WQ81
A	-8	SER	-	expression tag	UNP P9WQ81
A	-7	GLY	-	expression tag	UNP P9WQ81
A	-6	LEU	-	expression tag	UNP P9WQ81
A	-5	VAL	-	expression tag	UNP P9WQ81
A	-4	PRO	-	expression tag	UNP P9WQ81
A	-3	ARG	-	expression tag	UNP P9WQ81
A	-2	GLY	-	expression tag	UNP P9WQ81
A	-1	SER	-	expression tag	UNP P9WQ81
A	0	HIS	-	expression tag	UNP P9WQ81

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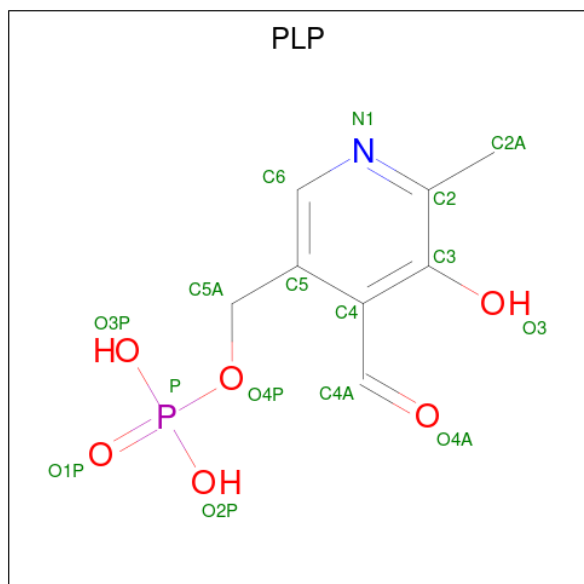
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP P9WQ81
B	-18	GLY	-	expression tag	UNP P9WQ81
B	-17	SER	-	expression tag	UNP P9WQ81
B	-16	SER	-	expression tag	UNP P9WQ81
B	-15	HIS	-	expression tag	UNP P9WQ81
B	-14	HIS	-	expression tag	UNP P9WQ81
B	-13	HIS	-	expression tag	UNP P9WQ81
B	-12	HIS	-	expression tag	UNP P9WQ81
B	-11	HIS	-	expression tag	UNP P9WQ81
B	-10	HIS	-	expression tag	UNP P9WQ81
B	-9	SER	-	expression tag	UNP P9WQ81
B	-8	SER	-	expression tag	UNP P9WQ81
B	-7	GLY	-	expression tag	UNP P9WQ81
B	-6	LEU	-	expression tag	UNP P9WQ81
B	-5	VAL	-	expression tag	UNP P9WQ81
B	-4	PRO	-	expression tag	UNP P9WQ81
B	-3	ARG	-	expression tag	UNP P9WQ81
B	-2	GLY	-	expression tag	UNP P9WQ81
B	-1	SER	-	expression tag	UNP P9WQ81
B	0	HIS	-	expression tag	UNP P9WQ81
C	-19	MET	-	initiating methionine	UNP P9WQ81
C	-18	GLY	-	expression tag	UNP P9WQ81
C	-17	SER	-	expression tag	UNP P9WQ81
C	-16	SER	-	expression tag	UNP P9WQ81
C	-15	HIS	-	expression tag	UNP P9WQ81
C	-14	HIS	-	expression tag	UNP P9WQ81
C	-13	HIS	-	expression tag	UNP P9WQ81
C	-12	HIS	-	expression tag	UNP P9WQ81
C	-11	HIS	-	expression tag	UNP P9WQ81
C	-10	HIS	-	expression tag	UNP P9WQ81
C	-9	SER	-	expression tag	UNP P9WQ81
C	-8	SER	-	expression tag	UNP P9WQ81
C	-7	GLY	-	expression tag	UNP P9WQ81
C	-6	LEU	-	expression tag	UNP P9WQ81
C	-5	VAL	-	expression tag	UNP P9WQ81
C	-4	PRO	-	expression tag	UNP P9WQ81
C	-3	ARG	-	expression tag	UNP P9WQ81
C	-2	GLY	-	expression tag	UNP P9WQ81
C	-1	SER	-	expression tag	UNP P9WQ81
C	0	HIS	-	expression tag	UNP P9WQ81
D	-19	MET	-	initiating methionine	UNP P9WQ81
D	-18	GLY	-	expression tag	UNP P9WQ81

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	SER	-	expression tag	UNP P9WQ81
D	-16	SER	-	expression tag	UNP P9WQ81
D	-15	HIS	-	expression tag	UNP P9WQ81
D	-14	HIS	-	expression tag	UNP P9WQ81
D	-13	HIS	-	expression tag	UNP P9WQ81
D	-12	HIS	-	expression tag	UNP P9WQ81
D	-11	HIS	-	expression tag	UNP P9WQ81
D	-10	HIS	-	expression tag	UNP P9WQ81
D	-9	SER	-	expression tag	UNP P9WQ81
D	-8	SER	-	expression tag	UNP P9WQ81
D	-7	GLY	-	expression tag	UNP P9WQ81
D	-6	LEU	-	expression tag	UNP P9WQ81
D	-5	VAL	-	expression tag	UNP P9WQ81
D	-4	PRO	-	expression tag	UNP P9WQ81
D	-3	ARG	-	expression tag	UNP P9WQ81
D	-2	GLY	-	expression tag	UNP P9WQ81
D	-1	SER	-	expression tag	UNP P9WQ81
D	0	HIS	-	expression tag	UNP P9WQ81

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



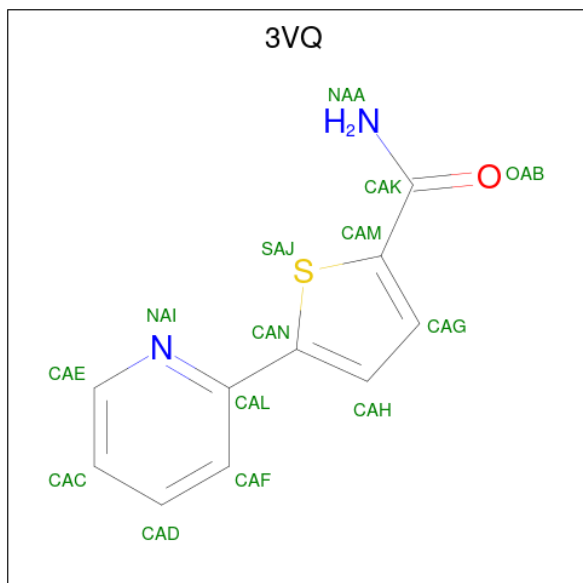
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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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 5-(pyridin-2-yl)thiophene-2-carboxamide (CCD ID: 3VQ) (formula: C₁₀H₈N₂OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			14	10	2	1	1		
3	D	1	Total	C	N	O	S	0	0
			14	10	2	1	1		

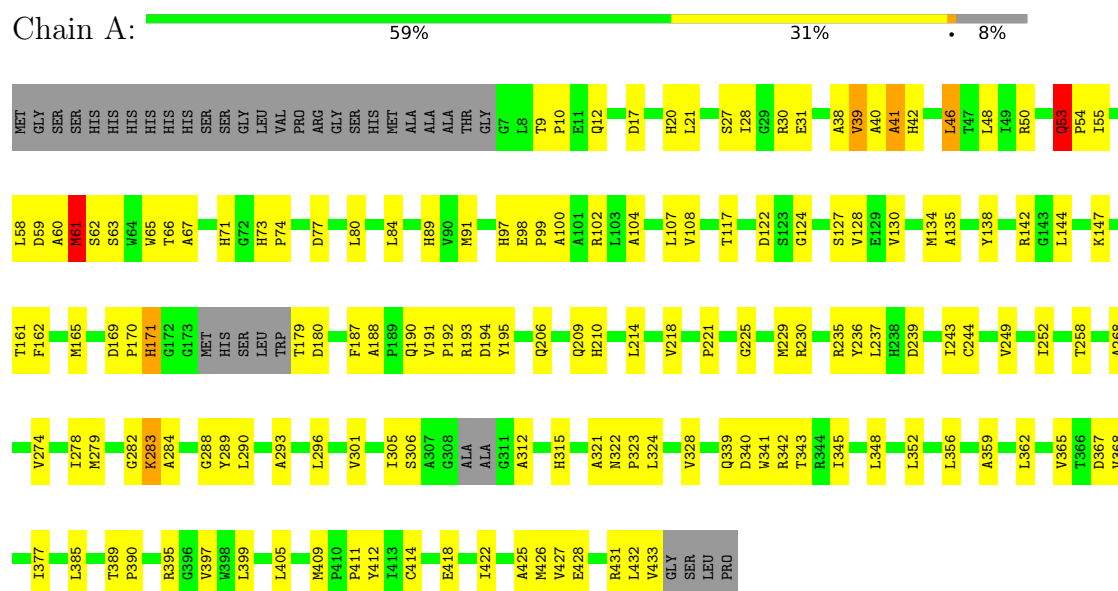
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	34	Total	O	0	0
			34	34		
4	B	25	Total	O	0	0
			25	25		
4	C	24	Total	O	0	0
			24	24		
4	D	31	Total	O	0	0
			31	31		

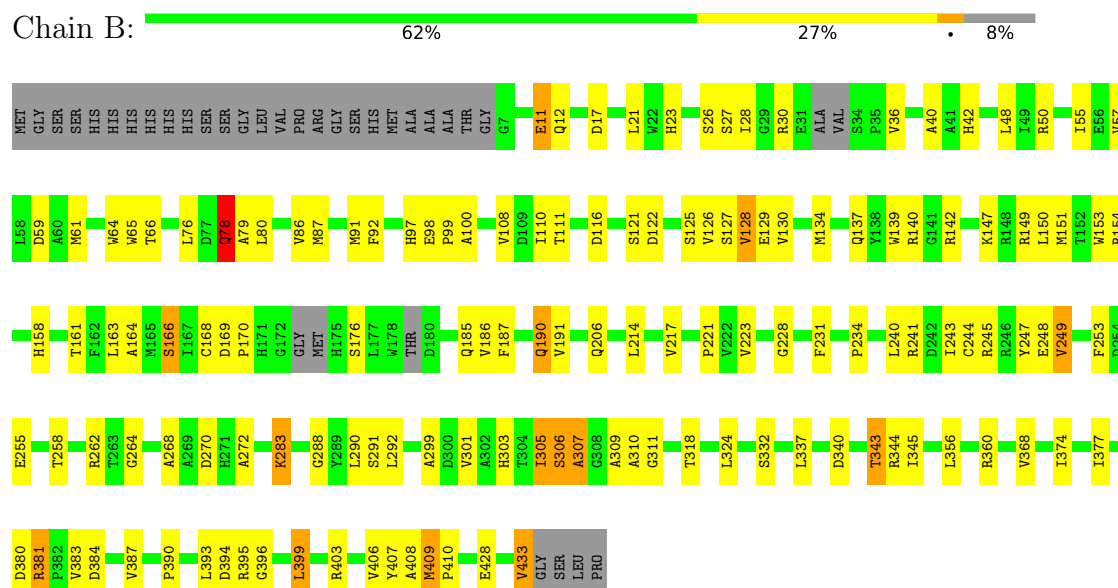
3 Residue-property plots

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: Adenosylmethionine-8-amino-7-oxononanoate aminotransferase

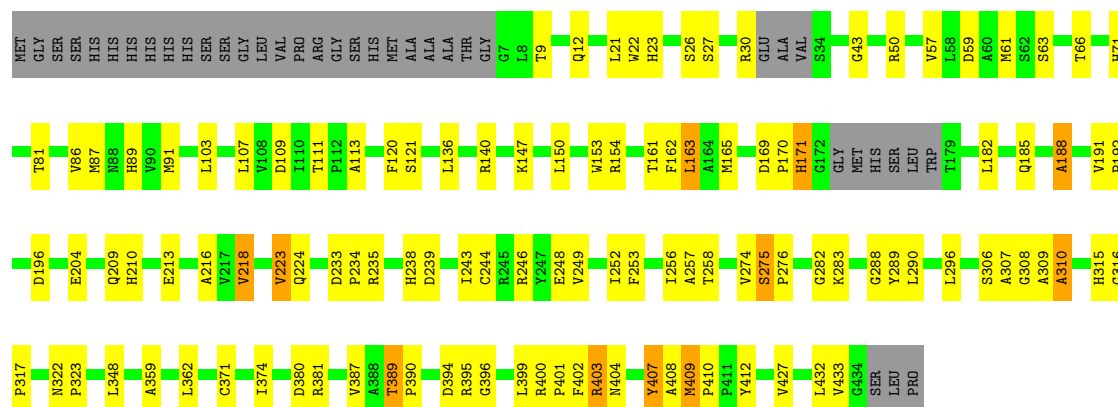


- Molecule 1: Adenosylmethionine-8-amino-7-oxononanoate aminotransferase



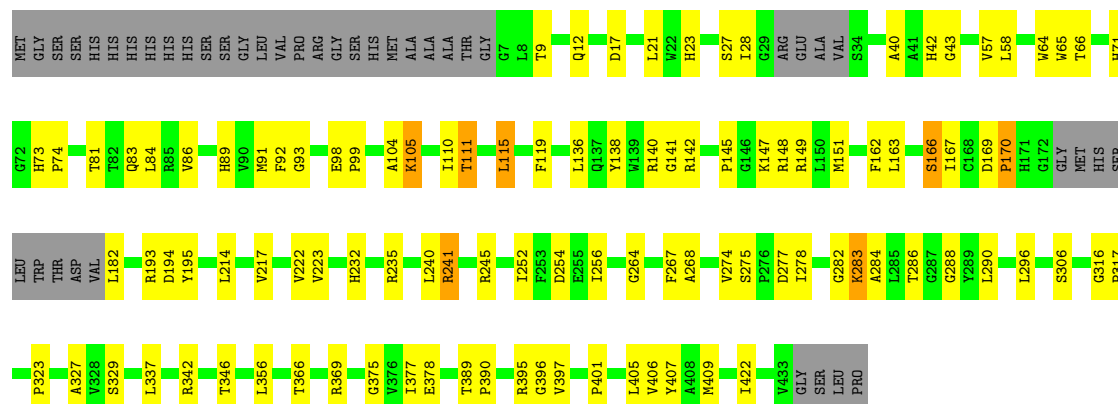
• Molecule 1: Adenosylmethionine-8-amino-7-oxononanoate aminotransferase

Chain C:  66% 23% 8%



• Molecule 1: Adenosylmethionine-8-amino-7-oxononanoate aminotransferase

Chain D:  67% 22% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.65Å 65.67Å 201.34Å 90.00° 90.29° 90.00°	Depositor
Resolution (Å)	29.87 – 2.50 29.87 – 2.50	Depositor EDS
% Data completeness (in resolution range)	87.6 (29.87-2.50) 86.1 (29.87-2.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.51Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.224 , 0.306 0.226 , 0.308	Depositor DCC
R_{free} test set	2568 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å ²)	40.1	Xtriage
Anisotropy	0.659	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 34.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.025 for -k,-h,-l 0.024 for k,h,-l 0.347 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12702	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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: PLP, 3VQ

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	0.56	0/3204	0.99	10/4378 (0.2%)
1	B	0.60	0/3220	0.99	11/4398 (0.3%)
1	C	0.58	0/3198	1.00	14/4369 (0.3%)
1	D	0.59	0/3175	0.98	8/4338 (0.2%)
All	All	0.58	0/12797	0.99	43/17483 (0.2%)

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	275	SER	CA-C-N	-7.84	112.76	120.52
1	C	275	SER	C-N-CA	-7.84	112.76	120.52
1	D	28	ILE	N-CA-C	-7.02	106.38	113.47
1	A	144	LEU	CA-C-N	6.69	126.83	119.87
1	A	144	LEU	C-N-CA	6.69	126.83	119.87
1	A	53	GLN	CA-C-N	6.46	127.91	119.84
1	A	53	GLN	C-N-CA	6.46	127.91	119.84
1	D	23	HIS	CA-C-N	-6.43	113.33	119.76
1	D	23	HIS	C-N-CA	-6.43	113.33	119.76
1	A	188	ALA	CA-C-N	-6.40	114.04	120.31
1	A	188	ALA	C-N-CA	-6.40	114.04	120.31
1	C	196	ASP	CA-C-N	6.39	127.82	119.84
1	C	196	ASP	C-N-CA	6.39	127.82	119.84
1	B	191	VAL	CA-C-N	6.27	127.68	119.84
1	B	191	VAL	C-N-CA	6.27	127.68	119.84
1	B	79	ALA	N-CA-C	-6.12	104.72	111.82
1	D	316	GLY	CA-C-N	6.12	126.33	119.90
1	D	316	GLY	C-N-CA	6.12	126.33	119.90
1	C	362	LEU	CA-C-N	5.88	125.58	119.82
1	C	362	LEU	C-N-CA	5.88	125.58	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	223	VAL	N-CA-C	5.84	116.28	107.75
1	D	169	ASP	CA-C-N	5.84	127.14	119.84
1	D	169	ASP	C-N-CA	5.84	127.14	119.84
1	C	410	PRO	CA-C-N	5.80	125.81	119.89
1	C	410	PRO	C-N-CA	5.80	125.81	119.89
1	B	23	HIS	CA-C-N	-5.77	113.76	119.99
1	B	23	HIS	C-N-CA	-5.77	113.76	119.99
1	A	142	ARG	N-CA-C	-5.68	105.93	112.92
1	C	188	ALA	CA-C-N	-5.52	112.94	119.84
1	C	188	ALA	C-N-CA	-5.52	112.94	119.84
1	B	128	VAL	N-CA-C	5.50	115.70	110.53
1	C	407	TYR	N-CA-C	5.44	117.11	108.79
1	B	78	GLN	N-CA-C	5.33	122.16	110.80
1	B	410	PRO	O-C-N	5.16	123.69	121.31
1	C	23	HIS	CA-C-N	-5.13	114.51	119.90
1	C	23	HIS	C-N-CA	-5.13	114.51	119.90
1	A	322	ASN	CA-C-N	5.10	126.22	119.84
1	A	322	ASN	C-N-CA	5.10	126.22	119.84
1	A	180	ASP	N-CA-C	5.09	117.85	108.58
1	D	223	VAL	N-CA-C	5.07	115.33	107.78
1	B	403	ARG	CB-CA-C	-5.06	110.72	116.54
1	B	30	ARG	N-CA-C	5.05	115.72	108.74
1	B	190	GLN	CA-CB-CG	5.03	124.15	114.10

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	3129	0	3091	101	0
1	B	3147	0	3105	93	0
1	C	3124	0	3100	74	1
1	D	3100	0	3075	71	1
2	A	15	0	6	0	0
2	B	15	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	15	0	6	1	0
2	D	15	0	6	1	0
3	B	14	0	8	0	0
3	D	14	0	8	8	0
4	A	34	0	0	2	0
4	B	25	0	0	1	0
4	C	24	0	0	1	1
4	D	31	0	0	0	1
All	All	12702	0	12411	309	2

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 12.

All (309) 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:278:ILE:O	4:A:601:HOH:O	1.78	1.01
1:C:147:LYS:NZ	1:C:248:GLU:O	2.02	0.93
1:D:92:PHE:H	3:D:501:3VQ:H3	1.37	0.87
1:B:61:MET:HE3	1:B:399:LEU:HA	1.57	0.86
1:D:264:GLY:O	1:D:342:ARG:NH1	2.11	0.84
1:A:42:HIS:HA	1:A:71:HIS:HB2	1.63	0.80
1:B:147:LYS:NZ	1:B:248:GLU:O	2.17	0.77
1:A:195:TYR:CE1	1:A:235:ARG:HG2	2.21	0.76
1:A:315:HIS:O	4:A:602:HOH:O	2.03	0.74
1:D:241[A]:ARG:HE	1:D:274:VAL:HG13	1.51	0.74
1:D:147:LYS:NZ	1:D:214:LEU:O	2.19	0.74
1:D:91:MET:HB2	3:D:501:3VQ:H4	1.71	0.71
1:B:142:ARG:HH11	1:B:142:ARG:HG2	1.57	0.69
1:D:317:PRO:O	3:D:501:3VQ:H2	1.92	0.69
1:D:140:ARG:HH22	1:D:148:ARG:HB3	1.57	0.69
1:B:163:LEU:O	1:B:166:SER:HB3	1.94	0.68
1:C:307:ALA:C	1:C:309:ALA:HB3	2.19	0.67
1:C:91:MET:HE3	1:D:64:TRP:HB2	1.76	0.67
1:D:241[A]:ARG:HH21	1:D:275:SER:H	1.42	0.66
1:D:65:TRP:HB2	1:D:283:LYS:HD3	1.77	0.65
1:A:283:LYS:HG3	1:B:318:THR:HG21	1.77	0.65
1:A:61:MET:HE1	1:A:399:LEU:HA	1.77	0.65
1:A:190:GLN:NE2	1:A:191:VAL:O	2.24	0.65
1:A:98:GLU:HG2	1:A:102:ARG:HH21	1.61	0.65
1:B:27:SER:O	1:B:27:SER:OG	2.16	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:ALA:HB1	1:B:303:HIS:CE1	2.32	0.64
1:B:65:TRP:CZ2	1:B:409:MET:HE2	2.32	0.64
1:B:78:GLN:HE22	1:D:395:ARG:HA	1.63	0.64
1:D:93:GLY:H	3:D:501:3VQ:H4	1.63	0.64
1:C:256:ILE:HG22	1:C:283:LYS:HG3	1.80	0.63
1:A:63:SER:HB3	1:B:91:MET:H	1.63	0.63
1:C:9:THR:HG23	1:C:12:GLN:H	1.61	0.63
1:A:397:VAL:HG21	1:A:422:ILE:HA	1.81	0.62
1:A:282:GLY:O	1:A:284:ALA:N	2.32	0.62
1:A:301:VAL:O	1:A:305:ILE:HG12	1.99	0.62
1:C:61:MET:HE2	1:C:400:ARG:HB3	1.81	0.61
1:A:359:ALA:HA	1:A:362:LEU:HD23	1.82	0.61
1:C:89:HIS:HA	1:C:323:PRO:HG2	1.81	0.61
1:B:168:CYS:SG	1:B:169:ASP:N	2.74	0.61
1:A:359:ALA:HB2	1:A:427:VAL:HG22	1.83	0.60
1:C:309:ALA:HA	1:C:310:ALA:C	2.26	0.60
1:A:356:LEU:HD22	1:A:377:ILE:HD11	1.82	0.60
1:C:165:MET:HE3	1:C:182:LEU:HD21	1.84	0.60
1:B:76:LEU:HD21	1:B:332:SER:HB2	1.84	0.59
1:D:163:LEU:O	1:D:166:SER:HB3	2.02	0.59
1:A:61:MET:N	1:A:61:MET:HE2	2.18	0.59
1:A:89:HIS:HA	1:A:323:PRO:HG2	1.85	0.59
1:A:60:ALA:N	1:A:61:MET:O	2.35	0.59
1:D:375:GLY:O	1:D:407:TYR:HB2	2.02	0.59
1:C:26:SER:OG	1:C:27:SER:N	2.33	0.59
1:B:65:TRP:HB2	1:B:283:LYS:HD3	1.84	0.58
1:D:241[A]:ARG:HH11	1:D:245:ARG:HH22	1.52	0.58
1:B:66:THR:HB	1:B:288:GLY:HA2	1.86	0.58
1:C:204:GLU:OE2	1:C:246:ARG:NH1	2.21	0.58
1:B:142:ARG:HG2	1:B:142:ARG:NH1	2.18	0.58
1:C:57:VAL:HG12	1:C:396:GLY:HA2	1.86	0.57
1:B:150:LEU:O	1:B:185:GLN:HB3	2.04	0.57
1:A:59:ASP:HA	1:A:60:ALA:O	2.04	0.57
1:C:308:GLY:C	1:C:310:ALA:HB3	2.30	0.57
1:D:283:LYS:NZ	2:D:502:PLP:O3	2.38	0.57
1:C:87:MET:HE2	4:C:614:HOH:O	2.04	0.56
1:C:387:VAL:HG11	1:C:432:LEU:HD22	1.85	0.56
1:A:46:LEU:HG	1:A:59:ASP:HB2	1.86	0.56
1:A:65:TRP:CE2	1:A:409:MET:HE3	2.39	0.56
1:A:91:MET:HE3	1:B:64:TRP:HB2	1.87	0.56
1:D:57:VAL:HG12	1:D:396:GLY:HA2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:ASP:OD2	1:C:63:SER:OG	2.23	0.56
1:C:307:ALA:O	1:C:309:ALA:HB3	2.05	0.56
1:A:362:LEU:HD11	1:A:431:ARG:HE	1.71	0.55
1:B:270:ASP:OD2	4:B:601:HOH:O	2.18	0.55
1:B:356:LEU:HD22	1:B:377:ILE:HD11	1.89	0.55
1:B:407:TYR:CE2	1:B:409:MET:HE3	2.41	0.55
1:B:170:PRO:HD3	1:B:187:PHE:CE2	2.41	0.55
1:B:17:ASP:HA	1:B:21:LEU:HD12	1.89	0.54
1:B:153:TRP:HD1	1:B:154:ARG:O	1.91	0.54
1:A:385:LEU:HD12	1:A:385:LEU:H	1.71	0.54
1:D:91:MET:HB2	3:D:501:3VQ:CAE	2.37	0.54
1:D:98:GLU:HB3	1:D:99:PRO:HD3	1.88	0.54
1:B:11[A]:GLU:HG2	1:B:12:GLN:N	2.23	0.53
1:B:264:GLY:HA2	1:B:345:ILE:HG21	1.89	0.53
1:B:283:LYS:NZ	2:B:502:PLP:O3	2.42	0.53
1:C:163:LEU:HD22	1:D:162:PHE:CD2	2.43	0.53
1:C:308:GLY:HA2	1:C:309:ALA:C	2.33	0.53
1:D:241[B]:ARG:NH1	1:D:277:ASP:OD1	2.38	0.53
1:A:40:ALA:HB1	1:B:86:VAL:O	2.09	0.53
1:D:66:THR:HB	1:D:288:GLY:HA3	1.91	0.53
1:D:140:ARG:NH2	1:D:148:ARG:HB3	2.24	0.53
1:A:389:THR:HB	1:A:390:PRO:HD3	1.91	0.53
1:B:360:ARG:HE	1:B:368:VAL:HB	1.74	0.53
1:A:41:ALA:HA	1:A:46:LEU:HA	1.91	0.52
1:A:244:CYS:HB3	1:A:249:VAL:O	2.09	0.52
1:C:87:MET:HB2	1:D:40:ALA:HA	1.90	0.52
1:D:241[A]:ARG:NH2	1:D:275:SER:H	2.07	0.52
1:C:27:SER:HB2	1:D:306:SER:HB3	1.91	0.52
1:B:139:TRP:CD2	1:B:147:LYS:HD3	2.44	0.52
1:C:30:ARG:HA	1:C:30:ARG:NE	2.25	0.52
1:C:162:PHE:HA	1:C:165:MET:HE2	1.92	0.52
1:C:380:ASP:OD1	1:C:381:ARG:HG2	2.09	0.52
1:C:150:LEU:HD23	1:C:216:ALA:HB3	1.92	0.52
1:C:81:THR:HG22	1:D:81:THR:HG22	1.91	0.51
1:D:111:THR:HG21	1:D:296:LEU:HD22	1.92	0.51
1:A:39:VAL:HG13	1:A:39:VAL:O	2.11	0.51
1:B:151:MET:HB3	1:B:217:VAL:HG22	1.91	0.51
1:B:78:GLN:NE2	1:D:395:ARG:HA	2.25	0.51
1:D:110:ILE:HG21	1:D:337:LEU:HD11	1.92	0.51
1:D:356:LEU:HD22	1:D:377:ILE:HD11	1.93	0.51
1:A:63:SER:HB3	1:B:91:MET:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:CYS:HB3	1:B:249:VAL:O	2.11	0.51
1:B:309:ALA:C	1:B:311:GLY:H	2.18	0.51
1:A:97:HIS:CE1	1:A:100:ALA:HB2	2.46	0.50
1:C:238:HIS:HA	1:C:274:VAL:HG11	1.92	0.50
1:B:234:PRO:O	1:B:272:ALA:HB2	2.11	0.50
1:C:9:THR:HG22	1:C:12:GLN:OE1	2.12	0.50
1:C:408:ALA:C	1:C:409:MET:HG3	2.36	0.50
1:D:140:ARG:NH2	1:D:145:PRO:O	2.45	0.50
1:B:122:ASP:O	1:B:291:SER:OG	2.24	0.50
1:B:97:HIS:HD2	1:B:100:ALA:H	1.59	0.49
1:C:50:ARG:NH2	1:C:394:ASP:OD1	2.35	0.49
1:A:283:LYS:HE2	1:B:318:THR:OG1	2.13	0.49
1:B:395:ARG:NE	1:B:428:GLU:HG3	2.27	0.49
1:A:55:ILE:HG13	1:A:55:ILE:O	2.13	0.49
1:A:192:PRO:HG2	1:A:236:TYR:OH	2.12	0.49
1:B:125:SER:HB3	1:B:161:THR:HG23	1.94	0.49
1:A:218:VAL:HG22	1:A:252:ILE:HB	1.94	0.49
1:A:348:LEU:O	1:A:352:LEU:HB2	2.13	0.49
1:A:428:GLU:OE2	1:A:431:ARG:NH2	2.45	0.49
1:B:98:GLU:HB3	1:B:99:PRO:HD3	1.95	0.49
1:B:153:TRP:C	1:B:153:TRP:CD1	2.90	0.49
1:C:111:THR:HG21	1:C:296:LEU:HD22	1.94	0.49
1:C:136:LEU:O	1:C:140:ARG:HG3	2.12	0.49
1:B:153:TRP:HZ3	1:B:240:LEU:HD11	1.77	0.49
1:C:43:GLY:O	1:C:71:HIS:N	2.43	0.49
1:C:244:CYS:HB3	1:C:249:VAL:O	2.11	0.49
1:C:359:ALA:HB2	1:C:427:VAL:HG22	1.94	0.49
1:B:158:HIS:O	1:B:164:ALA:HB1	2.12	0.49
1:B:50:ARG:NH1	1:B:394:ASP:OD1	2.46	0.49
1:A:60:ALA:C	1:A:61:MET:HE2	2.37	0.48
1:A:27:SER:HB2	1:B:306:SER:HB3	1.95	0.48
1:B:149:ARG:HB2	1:B:214:LEU:HD23	1.95	0.48
1:C:253:PHE:HB2	1:C:276:PRO:HG3	1.94	0.48
1:B:380:ASP:OD1	1:B:381:ARG:HG3	2.12	0.48
1:D:92:PHE:N	3:D:501:3VQ:H3	2.18	0.48
1:A:239:ASP:O	1:A:243:ILE:HG13	2.14	0.48
1:A:348:LEU:HD11	1:A:412:TYR:HA	1.94	0.48
1:B:262:ARG:HG3	1:B:374:ILE:HD11	1.95	0.48
1:C:306:SER:HB3	1:D:27:SER:HB2	1.94	0.48
1:A:38:ALA:O	1:A:39:VAL:HB	2.12	0.48
1:C:239:ASP:O	1:C:243:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:ARG:HB2	1:D:214:LEU:HD23	1.95	0.48
1:A:58:LEU:O	1:A:60:ALA:HB3	2.13	0.48
1:A:221:PRO:HA	1:A:237:LEU:HD21	1.95	0.48
1:A:362:LEU:HD11	1:A:431:ARG:NE	2.29	0.48
1:A:20:HIS:ND1	1:B:116:ASP:O	2.37	0.48
1:A:341:TRP:O	1:A:345:ILE:HG12	2.13	0.48
1:A:258:THR:HB	1:A:268:ALA:HB2	1.96	0.47
1:C:113:ALA:O	1:C:275:SER:OG	2.32	0.47
1:A:84:LEU:HD22	1:B:80:LEU:HD23	1.97	0.47
1:D:43:GLY:N	1:D:71:HIS:O	2.46	0.47
1:C:163:LEU:HD22	1:D:162:PHE:CE2	2.49	0.47
1:C:289:TYR:HE2	1:D:84:LEU:HD11	1.79	0.47
1:C:257:ALA:HB2	2:C:501:PLP:O3	2.14	0.47
1:B:384:ASP:HB3	1:B:387:VAL:HG22	1.94	0.47
1:C:153:TRP:CZ3	1:C:224:GLN:HG2	2.49	0.47
1:A:17:ASP:HA	1:A:21:LEU:HD12	1.97	0.47
1:A:279:MET:N	1:A:296:LEU:O	2.45	0.47
1:C:103:LEU:HD23	1:C:120:PHE:CE2	2.50	0.47
1:A:130:VAL:O	1:A:134:MET:HG3	2.15	0.47
1:B:395:ARG:HE	1:B:428:GLU:HG3	1.79	0.47
1:A:66:THR:HB	1:A:288:GLY:HA2	1.96	0.47
1:D:369:ARG:HH12	1:D:378:GLU:HB2	1.79	0.47
1:D:389:THR:HB	1:D:390:PRO:HD3	1.96	0.47
1:C:371:CYS:O	1:C:374:ILE:HB	2.14	0.46
1:A:418:GLU:O	1:A:422:ILE:HG13	2.15	0.46
1:B:65:TRP:CE2	1:B:409:MET:HE2	2.50	0.46
1:B:255:GLU:OE1	1:B:258:THR:OG1	2.31	0.46
1:C:66:THR:HB	1:C:288:GLY:HA2	1.98	0.46
1:B:57:VAL:HG12	1:B:396:GLY:HA2	1.97	0.46
1:B:40:ALA:HB1	1:B:42:HIS:NE2	2.30	0.46
1:A:60:ALA:HB2	1:A:422:ILE:HD13	1.96	0.46
1:B:147:LYS:HE2	1:B:214:LEU:O	2.15	0.46
1:C:223:VAL:HB	1:C:258:THR:HG22	1.97	0.46
1:B:130:VAL:O	1:B:134:MET:HG3	2.15	0.46
1:B:221:PRO:HB2	1:B:268:ALA:HB3	1.97	0.46
1:A:138:TYR:CD1	1:A:301:VAL:HA	2.51	0.46
1:B:381:ARG:CZ	1:B:433:VAL:HG13	2.46	0.46
1:D:286:THR:HG22	1:D:329:SER:HB2	1.97	0.46
1:C:395:ARG:HG2	1:C:395:ARG:HH21	1.80	0.45
1:A:65:TRP:HB2	1:A:283:LYS:CD	2.47	0.45
1:A:162:PHE:HD2	1:B:129:GLU:OE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:LEU:O	1:C:111:THR:OG1	2.12	0.45
1:D:17:ASP:HA	1:D:21:LEU:HD12	1.97	0.45
1:A:210:HIS:O	1:A:214:LEU:HG	2.17	0.45
1:B:383:VAL:HG21	1:B:406:VAL:HG23	1.98	0.45
1:A:27:SER:HB2	1:B:306:SER:CB	2.47	0.45
1:D:193:ARG:HA	1:D:232:HIS:HA	1.98	0.45
1:B:151:MET:HA	1:B:186:VAL:O	2.17	0.45
1:D:40:ALA:HB1	1:D:42:HIS:CE1	2.52	0.45
1:D:111:THR:HB	1:D:115:LEU:HD12	1.98	0.45
1:A:46:LEU:CG	1:A:59:ASP:HB2	2.46	0.45
1:C:154:ARG:HG3	1:C:188:ALA:O	2.17	0.45
1:C:290:LEU:HD22	1:D:290:LEU:HD22	1.99	0.45
1:A:135:ALA:O	1:A:138:TYR:HB3	2.17	0.45
1:B:187:PHE:O	1:B:206:GLN:NE2	2.48	0.45
1:B:340:ASP:OD2	1:B:343:THR:HB	2.17	0.44
1:D:92:PHE:H	3:D:501:3VQ:CAC	2.17	0.44
1:A:53:GLN:HA	1:A:54:PRO:HD3	1.72	0.44
1:A:229:MET:HB2	1:A:405:LEU:HD13	1.98	0.44
1:C:348:LEU:HD11	1:C:412:TYR:HA	1.99	0.44
1:D:151:MET:O	1:D:217:VAL:HA	2.18	0.44
1:D:397:VAL:HG21	1:D:422:ILE:HA	1.99	0.44
1:A:161:THR:O	1:A:165:MET:HG3	2.18	0.44
1:B:110:ILE:HG21	1:B:337:LEU:HD11	1.98	0.44
1:D:256:ILE:O	1:D:283:LYS:HB2	2.16	0.44
1:D:369:ARG:NH1	1:D:378:GLU:OE1	2.49	0.44
1:B:344:ARG:HB2	1:B:344:ARG:CZ	2.48	0.44
1:D:401:PRO:HG3	1:D:406:VAL:HG12	1.99	0.44
1:A:324:LEU:O	1:A:328:VAL:HG23	2.17	0.44
1:C:109:ASP:OD2	1:C:109:ASP:N	2.51	0.44
1:D:254:ASP:OD1	1:D:256:ILE:HD12	2.17	0.44
1:D:241[A]:ARG:HD2	1:D:245:ARG:HH22	1.83	0.44
1:B:48:LEU:O	1:B:55:ILE:HG12	2.16	0.44
1:A:21:LEU:HD22	1:B:92:PHE:HE2	1.83	0.44
1:B:108:VAL:HG22	1:B:116:ASP:HA	2.00	0.44
1:C:21:LEU:HD21	1:D:104:ALA:HB2	2.00	0.44
1:A:414:CYS:HA	1:A:418:GLU:OE1	2.18	0.43
1:A:290:LEU:HD22	1:B:290:LEU:HD22	1.99	0.43
1:A:97:HIS:NE2	1:A:321:ALA:O	2.51	0.43
1:A:340:ASP:OD2	1:A:343:THR:OG1	2.25	0.43
1:A:395:ARG:HD2	1:A:425:ALA:HA	2.00	0.43
1:C:150:LEU:HD22	1:C:218:VAL:CG2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ALA:HB1	1:B:26:SER:O	2.19	0.43
1:B:301:VAL:O	1:B:305:ILE:HG12	2.17	0.43
1:B:128:VAL:HG21	1:B:158:HIS:O	2.19	0.43
1:C:399:LEU:HD12	1:C:399:LEU:HA	1.83	0.43
1:B:243:ILE:O	1:B:247:TYR:HD1	2.02	0.43
1:A:104:ALA:HB2	1:B:21:LEU:HD21	2.00	0.43
1:C:308:GLY:O	1:C:310:ALA:HB3	2.19	0.43
1:C:402:PHE:HB3	1:C:407:TYR:CE1	2.53	0.43
1:C:403:ARG:HB3	1:C:404:ASN:H	1.67	0.43
1:B:408:ALA:C	1:B:409:MET:HG3	2.43	0.43
1:A:41:ALA:HB3	1:B:87:MET:HG3	2.00	0.42
1:D:105:LYS:HD3	1:D:105:LYS:HA	1.61	0.42
1:B:50:ARG:NH2	1:B:390:PRO:HB3	2.34	0.42
1:B:97:HIS:CD2	1:B:100:ALA:H	2.37	0.42
1:D:378:GLU:HA	1:D:405:LEU:HD23	2.00	0.42
1:A:27:SER:HB2	1:B:306:SER:OG	2.19	0.42
1:C:161:THR:O	1:C:165:MET:HG3	2.19	0.42
1:B:121:SER:O	1:B:292:LEU:HD12	2.20	0.42
1:A:147:LYS:NZ	1:A:214:LEU:O	2.39	0.42
1:B:262:ARG:HH12	1:B:409:MET:C	2.27	0.42
1:C:402:PHE:HB3	1:C:407:TYR:HE1	1.83	0.42
1:D:138:TYR:CE2	1:D:142:ARG:HD3	2.54	0.42
1:A:59:ASP:HA	1:A:60:ALA:C	2.45	0.42
1:A:62:SER:HB3	1:A:67:ALA:H	1.85	0.42
1:A:169:ASP:O	1:A:171:HIS:N	2.50	0.42
1:A:169:ASP:OD2	1:A:171:HIS:HB2	2.20	0.42
1:A:170:PRO:O	1:A:171:HIS:CG	2.73	0.42
1:B:126:VAL:O	1:B:130:VAL:HG23	2.20	0.42
1:B:154:ARG:O	1:B:190:GLN:OE1	2.38	0.42
1:C:309:ALA:CA	1:C:310:ALA:C	2.91	0.42
1:D:65:TRP:CE2	1:D:409:MET:SD	3.12	0.42
1:B:97:HIS:NE2	1:B:100:ALA:HB2	2.35	0.42
1:D:9:THR:OG1	1:D:12:GLN:HG3	2.19	0.42
1:A:73:HIS:HA	1:A:74:PRO:HD3	1.89	0.42
1:D:73:HIS:HA	1:D:74:PRO:HD3	1.96	0.42
1:C:22:TRP:CD1	1:D:119:PHE:HB2	2.55	0.42
1:C:150:LEU:HD12	1:C:185:GLN:NE2	2.34	0.42
1:C:233:ASP:HA	1:C:234:PRO:HD3	1.91	0.42
1:A:365:VAL:HG13	1:A:377:ILE:HG23	2.02	0.41
1:A:422:ILE:O	1:A:426:MET:HG3	2.19	0.41
1:D:66:THR:HB	1:D:288:GLY:CA	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:GLY:O	1:D:284:ALA:N	2.52	0.41
1:A:193:ARG:NE	1:A:194:ASP:OD1	2.53	0.41
1:C:103:LEU:HD23	1:C:120:PHE:CZ	2.55	0.41
1:A:117:THR:O	1:A:296:LEU:HA	2.19	0.41
1:D:89:HIS:HA	1:D:323:PRO:HG2	2.01	0.41
1:A:124:GLY:O	1:A:128:VAL:HG23	2.20	0.41
1:A:206:GLN:O	1:A:209:GLN:HG2	2.21	0.41
1:B:241:ARG:HG3	1:B:245:ARG:HH12	1.85	0.41
1:C:66:THR:HB	1:C:288:GLY:CA	2.51	0.41
1:D:195:TYR:CE1	1:D:235:ARG:HG2	2.55	0.41
1:A:61:MET:O	1:A:411:PRO:HD3	2.20	0.41
1:A:170:PRO:HD3	1:A:187:PHE:CE2	2.56	0.41
1:B:306:SER:O	1:B:307:ALA:CB	2.69	0.41
1:C:191:VAL:HA	1:C:192:PRO:HD3	1.93	0.41
1:D:83:GLN:HG2	1:D:327:ALA:CB	2.50	0.41
1:D:83:GLN:HG2	1:D:327:ALA:HB2	2.03	0.41
1:D:93:GLY:H	3:D:501:3VQ:CAE	2.33	0.41
1:A:9:THR:HG22	1:A:12:GLN:OE1	2.21	0.41
1:A:98:GLU:HB3	1:A:99:PRO:HD3	2.03	0.41
1:A:107:LEU:HD23	1:A:107:LEU:HA	1.78	0.41
1:A:283:LYS:HE3	1:A:283:LYS:HB2	1.91	0.41
1:A:339:GLN:O	1:A:341:TRP:N	2.53	0.41
1:B:324:LEU:HD23	1:B:324:LEU:HA	1.94	0.41
1:C:210:HIS:O	1:C:213:GLU:HG2	2.21	0.41
1:C:315:HIS:HD2	1:C:317:PRO:HD3	1.86	0.41
1:D:252:ILE:HG12	1:D:278:ILE:HB	2.03	0.41
1:A:77:ASP:OD2	1:A:289:TYR:OH	2.30	0.41
1:B:221:PRO:HG3	1:B:253:PHE:CG	2.56	0.41
1:C:169:ASP:C	1:C:171:HIS:H	2.29	0.41
1:C:389:THR:OG1	1:C:390:PRO:HD3	2.21	0.41
1:B:223:VAL:HG22	1:B:231:PHE:CD2	2.56	0.40
1:D:110:ILE:HG13	1:D:267:PHE:HE1	1.86	0.40
1:A:46:LEU:HB2	1:A:48:LEU:HD21	2.03	0.40
1:A:367:ASP:OD1	1:A:368:VAL:N	2.54	0.40
1:C:63:SER:O	1:C:66:THR:OG1	2.33	0.40
1:C:322:ASN:HA	1:C:323:PRO:HD3	1.97	0.40
1:A:65:TRP:NE1	1:A:409:MET:HE3	2.36	0.40
1:A:127:SER:HB3	1:A:293:ALA:HB1	2.03	0.40

All (2) 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)
4:C:620:HOH:O	4:D:622:HOH:O[1_565]	2.11	0.09
1:C:209:GLN:NE2	1:D:141:GLY:O[2_655]	2.19	0.01

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	414/457 (91%)	374 (90%)	32 (8%)	8 (2%)	6	11
1	B	415/457 (91%)	385 (93%)	21 (5%)	9 (2%)	5	9
1	C	413/457 (90%)	376 (91%)	31 (8%)	6 (2%)	8	16
1	D	409/457 (90%)	373 (91%)	30 (7%)	6 (2%)	8	16
All	All	1651/1828 (90%)	1508 (91%)	114 (7%)	29 (2%)	6	12

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	VAL
1	B	283	LYS
1	D	283	LYS
1	A	41	ALA
1	A	283	LYS
1	B	307	ALA
1	D	166	SER
1	D	268	ALA
1	A	61	MET
1	A	306	SER
1	D	170	PRO
1	A	31	GLU
1	B	59	ASP
1	C	171	HIS
1	D	115	LEU
1	A	225	GLY

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Mol	Chain	Res	Type
1	B	78	GLN
1	B	176	SER
1	B	228	GLY
1	B	305	ILE
1	C	310	ALA
1	C	316	GLY
1	D	222	VAL
1	A	171	HIS
1	B	28	ILE
1	B	310	ALA
1	C	282	GLY
1	C	401	PRO
1	C	170	PRO

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	315/346 (91%)	299 (95%)	16 (5%)	21	43
1	B	316/346 (91%)	299 (95%)	17 (5%)	20	41
1	C	316/346 (91%)	306 (97%)	10 (3%)	34	62
1	D	313/346 (90%)	299 (96%)	14 (4%)	24	49
All	All	1260/1384 (91%)	1203 (96%)	57 (4%)	25	49

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	PRO
1	A	28	ILE
1	A	30	ARG
1	A	46	LEU
1	A	50	ARG
1	A	53	GLN
1	A	61	MET
1	A	80	LEU

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Mol	Chain	Res	Type
1	A	108	VAL
1	A	122	ASP
1	A	179	THR
1	A	230	ARG
1	A	274	VAL
1	A	342	ARG
1	A	432	LEU
1	A	433	VAL
1	B	11[A]	GLU
1	B	11[B]	GLU
1	B	36	VAL
1	B	78	GLN
1	B	111	THR
1	B	127	SER
1	B	137	GLN
1	B	140	ARG
1	B	166	SER
1	B	249	VAL
1	B	306	SER
1	B	343	THR
1	B	381	ARG
1	B	393	LEU
1	B	399	LEU
1	B	409	MET
1	B	433	VAL
1	C	86	VAL
1	C	121	SER
1	C	163	LEU
1	C	218	VAL
1	C	235	ARG
1	C	252	ILE
1	C	389	THR
1	C	403	ARG
1	C	409	MET
1	C	433	VAL
1	D	58	LEU
1	D	86	VAL
1	D	105	LYS
1	D	111	THR
1	D	136	LEU
1	D	167	ILE
1	D	170	PRO

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Mol	Chain	Res	Type
1	D	182	LEU
1	D	194	ASP
1	D	240	LEU
1	D	241[A]	ARG
1	D	241[B]	ARG
1	D	346	THR
1	D	366	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	HIS
1	B	53	GLN
1	B	78	GLN
1	B	190	GLN
1	B	209	GLN
1	D	42	HIS
1	D	97	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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
3	3VQ	B	501	-	15,15,15	3.12	4 (26%)	20,20,20	1.82	5 (25%)
3	3VQ	D	501	-	15,15,15	3.59	4 (26%)	20,20,20	1.44	5 (25%)
2	PLP	B	502	1	15,15,16	3.05	3 (20%)	21,22,23	1.55	1 (4%)
2	PLP	D	502	1	15,15,16	2.93	3 (20%)	21,22,23	1.88	5 (23%)
2	PLP	C	501	1	15,15,16	2.66	3 (20%)	21,22,23	1.70	6 (28%)
2	PLP	A	501	1	15,15,16	3.20	3 (20%)	21,22,23	1.88	5 (23%)

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
3	3VQ	B	501	-	-	0/8/8/8	0/2/2/2
3	3VQ	D	501	-	-	0/8/8/8	0/2/2/2
2	PLP	B	502	1	-	0/6/6/8	0/1/1/1
2	PLP	D	502	1	-	3/6/6/8	0/1/1/1
2	PLP	C	501	1	-	0/6/6/8	0/1/1/1
2	PLP	A	501	1	-	5/6/6/8	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	3VQ	CAL-CAN	-10.81	1.31	1.46
3	B	501	3VQ	CAL-CAN	-8.83	1.34	1.46
2	A	501	PLP	C5-C4	8.74	1.50	1.40
2	D	502	PLP	C5-C4	8.02	1.49	1.40
2	B	502	PLP	C5-C4	7.62	1.49	1.40
3	D	501	3VQ	CAK-CAM	-7.51	1.35	1.49
2	B	502	PLP	C3-C2	7.46	1.48	1.41
2	A	501	PLP	C3-C2	7.30	1.48	1.41
3	B	501	3VQ	CAK-CAM	-7.18	1.36	1.49
2	C	501	PLP	C5-C4	6.93	1.48	1.40
2	D	502	PLP	C3-C2	6.45	1.47	1.41
2	C	501	PLP	C3-C2	6.06	1.47	1.41
2	A	501	PLP	C3-C4	4.43	1.48	1.40
2	B	502	PLP	C3-C4	4.24	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	PLP	C3-C4	3.80	1.47	1.40
2	D	502	PLP	C3-C4	3.69	1.47	1.40
3	D	501	3VQ	CAN-SAJ	-3.44	1.58	1.73
3	B	501	3VQ	CAE-NAI	2.61	1.40	1.34
3	B	501	3VQ	CAN-SAJ	-2.59	1.62	1.73
3	D	501	3VQ	CAE-NAI	2.01	1.38	1.34

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	502	PLP	C4A-C4-C5	5.43	126.54	120.94
2	A	501	PLP	C4A-C4-C5	4.70	125.78	120.94
2	B	502	PLP	C4A-C4-C5	4.34	125.41	120.94
3	B	501	3VQ	CAN-SAJ-CAM	3.58	95.05	92.37
2	C	501	PLP	C4A-C4-C5	3.49	124.54	120.94
3	B	501	3VQ	CAE-NAI-CAL	3.45	121.38	116.93
3	B	501	3VQ	CAC-CAE-NAI	-3.11	118.49	123.42
2	C	501	PLP	C2A-C2-N1	2.83	122.97	117.64
2	A	501	PLP	O4P-C5A-C5	2.82	114.64	109.36
2	D	502	PLP	O4P-C5A-C5	2.78	114.56	109.36
2	C	501	PLP	C2A-C2-C3	-2.77	117.56	120.80
3	B	501	3VQ	CAG-CAM-SAJ	-2.68	106.59	110.49
2	A	501	PLP	C5A-C5-C6	-2.60	115.11	119.36
3	D	501	3VQ	CAG-CAM-SAJ	-2.54	106.79	110.49
2	A	501	PLP	C6-N1-C2	2.54	123.81	119.20
2	D	502	PLP	C2A-C2-N1	2.53	122.41	117.64
2	C	501	PLP	C6-N1-C2	2.50	123.73	119.20
2	D	502	PLP	C2A-C2-C3	-2.49	117.89	120.80
2	C	501	PLP	O3P-P-O2P	2.44	116.94	107.80
3	D	501	3VQ	CAN-SAJ-CAM	2.40	94.17	92.37
3	D	501	3VQ	CAE-NAI-CAL	2.36	119.97	116.93
2	D	502	PLP	C4A-C4-C3	-2.25	116.77	120.52
2	A	501	PLP	O2P-P-O4P	-2.16	101.03	106.67
3	D	501	3VQ	CAK-CAM-SAJ	2.16	128.62	118.76
3	D	501	3VQ	CAC-CAE-NAI	-2.12	120.07	123.42
3	B	501	3VQ	CAL-CAN-SAJ	2.04	123.15	119.63
2	C	501	PLP	O3P-P-O4P	-2.03	101.37	106.67

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PLP	C4-C5-C5A-O4P
2	A	501	PLP	C6-C5-C5A-O4P
2	A	501	PLP	C5A-O4P-P-O1P
2	A	501	PLP	C5A-O4P-P-O2P
2	A	501	PLP	C5A-O4P-P-O3P
2	D	502	PLP	C4-C5-C5A-O4P
2	D	502	PLP	C6-C5-C5A-O4P
2	D	502	PLP	C5A-O4P-P-O2P

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	3VQ	8	0
2	B	502	PLP	1	0
2	D	502	PLP	1	0
2	C	501	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	420/457 (91%)	-1.25	0 100 100	30, 44, 60, 73	1 (0%)
1	B	422/457 (92%)	-1.24	0 100 100	23, 43, 54, 70	2 (0%)
1	C	419/457 (91%)	-1.27	0 100 100	29, 41, 59, 74	0
1	D	414/457 (90%)	-1.27	0 100 100	23, 40, 52, 67	1 (0%)
All	All	1675/1828 (91%)	-1.26	0 100 100	23, 42, 57, 74	4 (0%)

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	PLP	A	501	15/16	0.98	0.04	32,37,42,42	0
3	3VQ	B	501	14/14	0.98	0.04	36,44,52,52	0
2	PLP	C	501	15/16	0.99	0.02	28,31,38,40	0
2	PLP	D	502	15/16	0.99	0.04	28,31,38,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PLP	B	502	15/16	0.99	0.03	27,34,37,39	0
3	3VQ	D	501	14/14	0.99	0.04	38,45,52,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.