



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:49 PM UTC

PDB ID : 3N2O / pdb_00003n2o
Title : X-ray crystal structure of arginine decarboxylase complexed with Arginine from *Vibrio vulnificus*
Authors : Deng, X.; Lee, J.; Michael, A.J.; Tomchick, D.R.; Goldsmith, E.J.; Phillips, M.A.
Deposited on : 2010-05-18
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

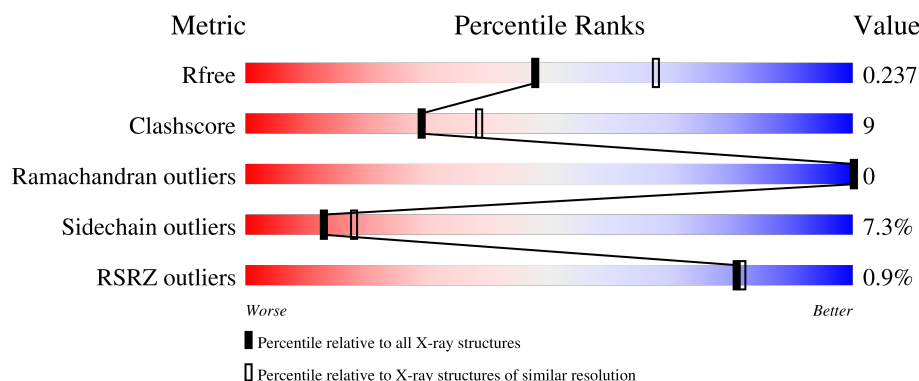
1 Overall quality at a glance

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	648	
1	B	648	
1	C	648	
1	D	648	

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	AG2	A	1002	-	X	-	-
3	AG2	B	1002	-	X	-	-
3	AG2	D	1002	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20592 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 Biosynthetic arginine decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	630	Total	C	N	O	S	0	0	0
			5022	3165	871	968	18			
1	B	629	Total	C	N	O	S	0	0	0
			5013	3159	869	967	18			
1	C	628	Total	C	N	O	S	0	0	0
			5005	3153	868	966	18			
1	D	629	Total	C	N	O	S	0	0	0
			5013	3159	869	967	18			

There are 32 discrepancies between the modelled and reference sequences:

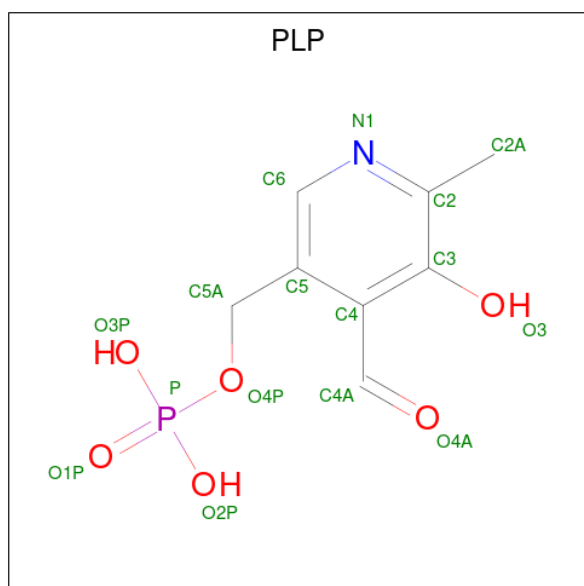
Chain	Residue	Modelled	Actual	Comment	Reference
A	641	LEU	-	expression tag	UNP Q7MK24
A	642	GLU	-	expression tag	UNP Q7MK24
A	643	HIS	-	expression tag	UNP Q7MK24
A	644	HIS	-	expression tag	UNP Q7MK24
A	645	HIS	-	expression tag	UNP Q7MK24
A	646	HIS	-	expression tag	UNP Q7MK24
A	647	HIS	-	expression tag	UNP Q7MK24
A	648	HIS	-	expression tag	UNP Q7MK24
B	641	LEU	-	expression tag	UNP Q7MK24
B	642	GLU	-	expression tag	UNP Q7MK24
B	643	HIS	-	expression tag	UNP Q7MK24
B	644	HIS	-	expression tag	UNP Q7MK24
B	645	HIS	-	expression tag	UNP Q7MK24
B	646	HIS	-	expression tag	UNP Q7MK24
B	647	HIS	-	expression tag	UNP Q7MK24
B	648	HIS	-	expression tag	UNP Q7MK24
C	641	LEU	-	expression tag	UNP Q7MK24
C	642	GLU	-	expression tag	UNP Q7MK24
C	643	HIS	-	expression tag	UNP Q7MK24
C	644	HIS	-	expression tag	UNP Q7MK24
C	645	HIS	-	expression tag	UNP Q7MK24

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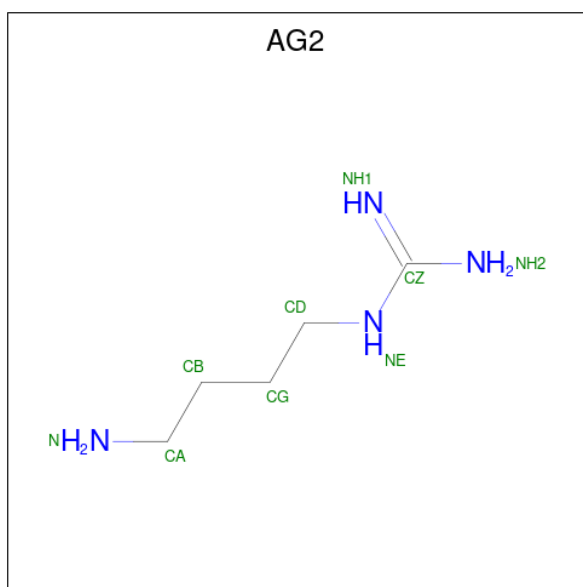
Chain	Residue	Modelled	Actual	Comment	Reference
C	646	HIS	-	expression tag	UNP Q7MK24
C	647	HIS	-	expression tag	UNP Q7MK24
C	648	HIS	-	expression tag	UNP Q7MK24
D	641	LEU	-	expression tag	UNP Q7MK24
D	642	GLU	-	expression tag	UNP Q7MK24
D	643	HIS	-	expression tag	UNP Q7MK24
D	644	HIS	-	expression tag	UNP Q7MK24
D	645	HIS	-	expression tag	UNP Q7MK24
D	646	HIS	-	expression tag	UNP Q7MK24
D	647	HIS	-	expression tag	UNP Q7MK24
D	648	HIS	-	expression tag	UNP Q7MK24

- 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		
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 AGMATINE (CCD ID: AG2) (formula: $C_5H_{14}N_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			9	5	4		
3	B	1	Total	C	N	0	0
			9	5	4		
3	C	1	Total	C	N	0	0
			9	5	4		
3	D	1	Total	C	N	0	0
			9	5	4		

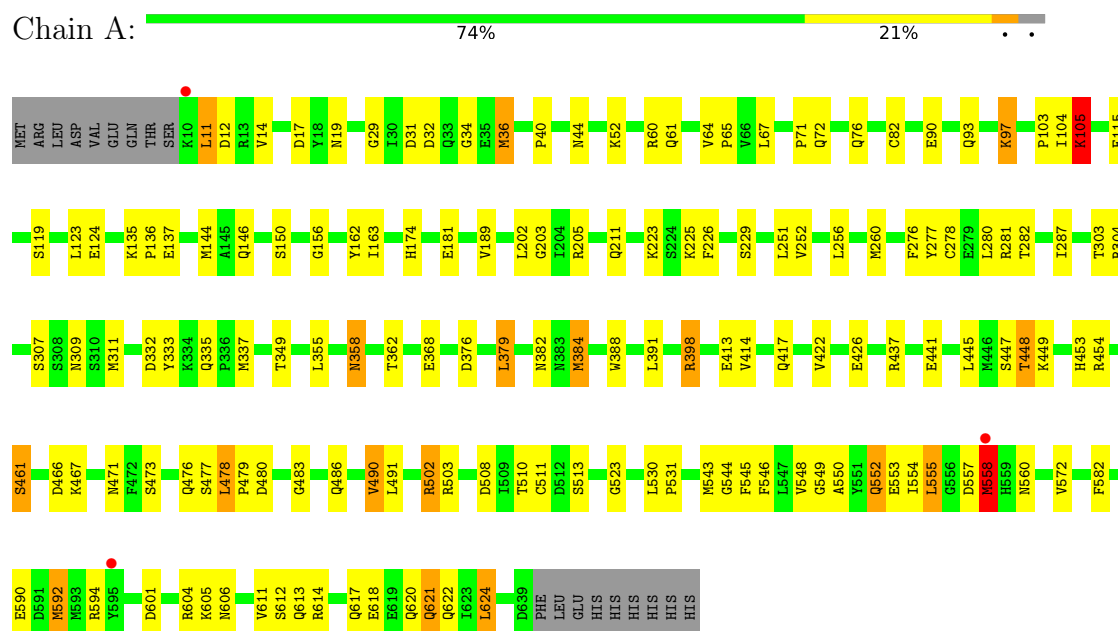
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	101	Total	O	0	0
			101	101		
4	B	140	Total	O	0	0
			140	140		
4	C	103	Total	O	0	0
			103	103		
4	D	99	Total	O	0	0
			99	99		

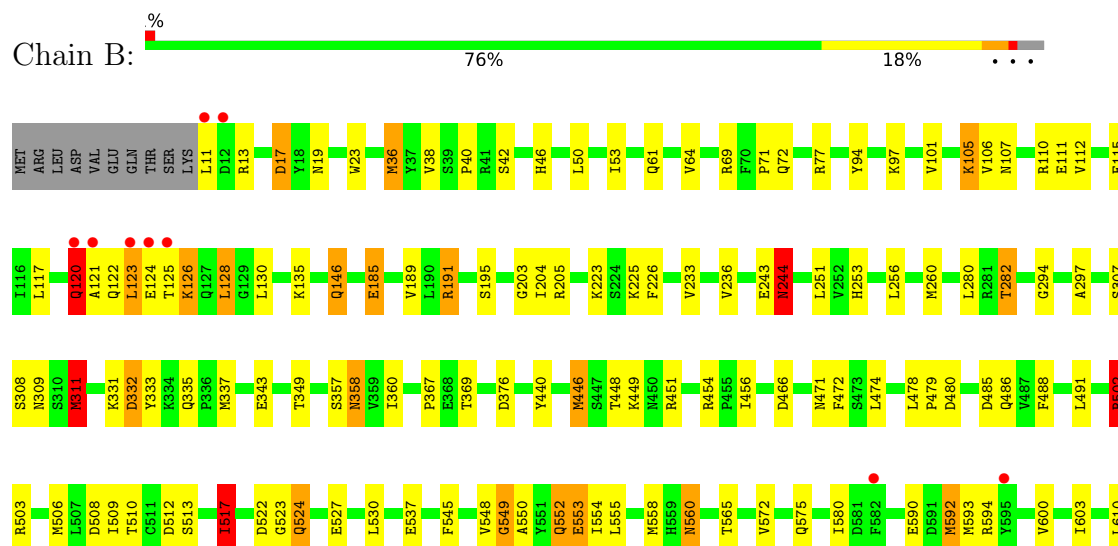
3 Residue-property plots [i](#)

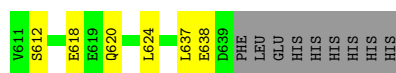
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

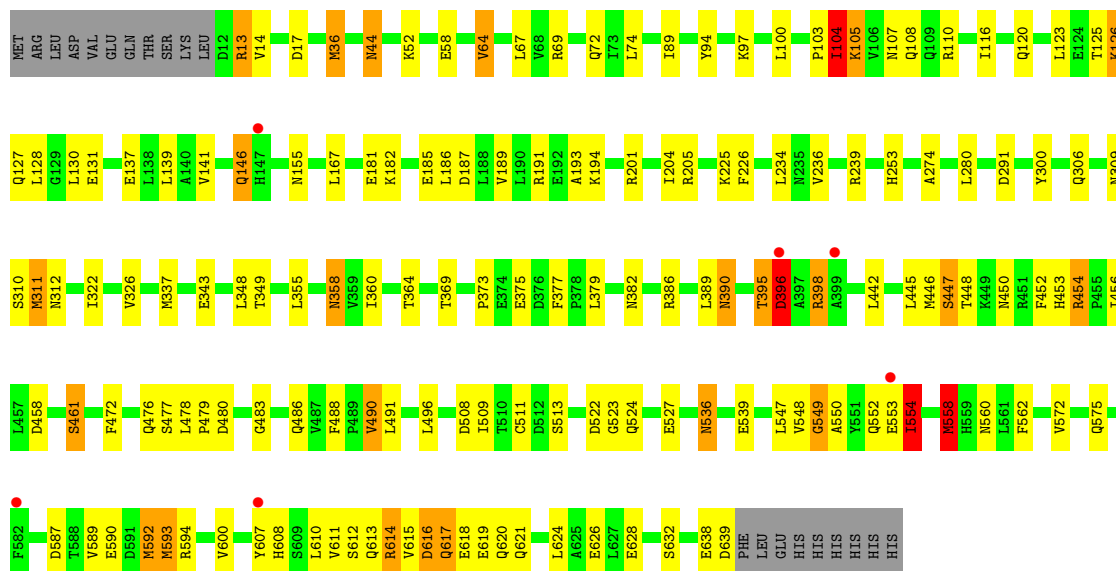


• Molecule 1: Biosynthetic arginine decarboxylase

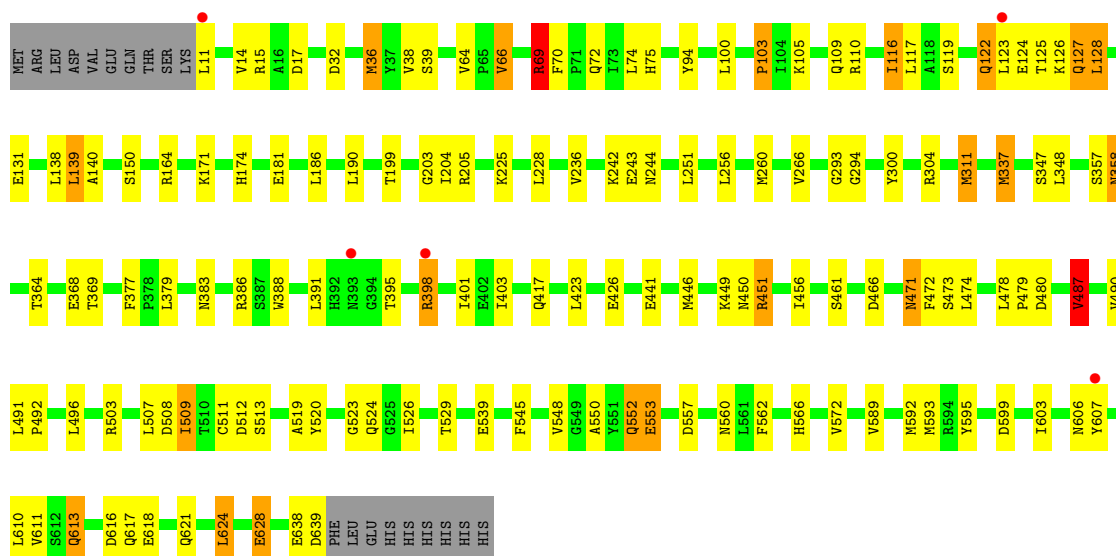
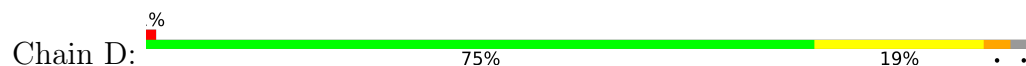




• Molecule 1: Biosynthetic arginine decarboxylase



• Molecule 1: Biosynthetic arginine decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.65Å 119.36Å 121.84Å 90.00° 96.30° 90.00°	Depositor
Resolution (Å)	121.10 – 2.30 121.10 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (121.10-2.30) 98.7 (121.10-2.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.179 , 0.239 0.179 , 0.237	Depositor DCC
R_{free} test set	6366 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20592	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: AG2, PLP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.19	12/5119 (0.2%)	1.17	16/6939 (0.2%)
1	B	1.31	18/5110 (0.4%)	1.22	22/6928 (0.3%)
1	C	1.31	14/5102 (0.3%)	1.18	16/6917 (0.2%)
1	D	1.23	19/5110 (0.4%)	1.18	21/6928 (0.3%)
All	All	1.26	63/20441 (0.3%)	1.19	75/27712 (0.3%)

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	266	VAL	CA-CB	7.04	1.62	1.54
1	C	311	MET	CG-SD	-6.62	1.64	1.80
1	D	103	PRO	C-O	-6.51	1.18	1.24
1	A	105	LYS	C-O	-6.43	1.16	1.24
1	B	360	ILE	C-O	-6.43	1.17	1.24
1	C	490	VAL	C-O	-6.37	1.17	1.24
1	D	70	PHE	C-O	-6.19	1.18	1.24
1	C	390	ASN	C-O	-6.09	1.17	1.24
1	D	548	VAL	C-O	-5.99	1.17	1.24
1	A	548	VAL	C-O	-5.92	1.17	1.24
1	D	550	ALA	C-O	-5.92	1.16	1.24
1	A	592	MET	SD-CE	-5.92	1.64	1.79
1	D	260	MET	C-O	-5.90	1.17	1.24
1	A	384	MET	SD-CE	-5.87	1.64	1.79
1	B	550	ALA	C-O	-5.85	1.17	1.24
1	B	260	MET	C-O	-5.85	1.17	1.24
1	D	472	PHE	C-O	-5.83	1.17	1.23
1	B	111	GLU	C-O	-5.82	1.17	1.24
1	C	549	GLY	C-O	-5.62	1.16	1.23
1	A	550	ALA	CA-CB	-5.61	1.45	1.53
1	B	311	MET	SD-CE	-5.58	1.65	1.79
1	D	471	ASN	C-O	-5.57	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	311	MET	C-O	-5.56	1.17	1.23
1	B	446	MET	SD-CE	-5.55	1.65	1.79
1	D	66	VAL	CA-CB	5.49	1.62	1.54
1	D	473	SER	C-O	-5.47	1.17	1.24
1	C	36	MET	C-O	-5.47	1.17	1.24
1	A	14	VAL	CA-CB	5.46	1.61	1.54
1	C	337	MET	C-O	-5.46	1.16	1.23
1	A	144	MET	C-O	-5.45	1.16	1.24
1	A	550	ALA	C-O	-5.43	1.17	1.24
1	A	260	MET	SD-CE	-5.42	1.66	1.79
1	D	550	ALA	CA-CB	-5.41	1.46	1.53
1	B	110	ARG	C-O	-5.38	1.17	1.24
1	C	274	ALA	CA-CB	-5.34	1.45	1.53
1	B	46	HIS	C-O	-5.33	1.17	1.24
1	B	592	MET	SD-CE	-5.32	1.66	1.79
1	B	106	VAL	C-O	-5.32	1.18	1.24
1	A	311	MET	SD-CE	-5.29	1.66	1.79
1	B	360	ILE	CA-CB	-5.29	1.48	1.54
1	B	36	MET	C-O	-5.29	1.17	1.24
1	C	548	VAL	C-O	-5.29	1.18	1.24
1	D	474	LEU	C-O	-5.27	1.17	1.24
1	C	592	MET	SD-CE	-5.26	1.66	1.79
1	B	107	ASN	C-O	-5.26	1.17	1.23
1	A	104	ILE	C-O	-5.24	1.16	1.24
1	C	550	ALA	C-O	-5.23	1.17	1.24
1	D	116	ILE	CA-CB	5.23	1.60	1.54
1	C	310	SER	C-O	-5.20	1.17	1.23
1	C	442	LEU	C-O	-5.19	1.18	1.24
1	D	347	SER	CA-C	5.19	1.59	1.52
1	B	593	MET	SD-CE	-5.17	1.66	1.79
1	D	595	TYR	CA-C	5.16	1.59	1.52
1	C	360	ILE	CA-CB	-5.12	1.48	1.54
1	D	553	GLU	C-O	-5.12	1.18	1.24
1	D	487	VAL	CA-CB	-5.11	1.48	1.54
1	A	543	MET	SD-CE	-5.10	1.66	1.79
1	B	120	GLN	N-CA	5.10	1.52	1.46
1	B	549	GLY	C-O	-5.09	1.17	1.23
1	D	69	ARG	N-CA	5.08	1.52	1.46
1	B	112	VAL	C-O	-5.06	1.18	1.24
1	B	111	GLU	N-CA	-5.05	1.40	1.46
1	C	547	LEU	C-O	-5.01	1.16	1.23

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	554	ILE	N-CA-C	9.67	120.48	110.72
1	A	552	GLN	N-CA-C	9.24	121.11	111.14
1	D	548	VAL	CA-C-N	8.56	129.48	119.98
1	D	548	VAL	C-N-CA	8.56	129.48	119.98
1	B	552	GLN	N-CA-C	8.22	120.02	111.14
1	A	337	MET	CA-C-N	7.97	127.86	120.21
1	A	337	MET	C-N-CA	7.97	127.86	120.21
1	B	548	VAL	CA-C-N	7.18	127.95	119.98
1	B	548	VAL	C-N-CA	7.18	127.95	119.98
1	C	616	ASP	N-CA-C	-6.95	100.16	110.23
1	B	244	ASN	CB-CA-C	-6.66	102.27	111.73
1	D	557	ASP	N-CA-C	6.60	118.16	108.86
1	D	300	TYR	N-CA-C	6.56	119.25	111.71
1	D	552	GLN	N-CA-C	6.37	118.30	111.36
1	B	294	GLY	CA-C-N	-6.35	116.57	123.30
1	B	294	GLY	C-N-CA	-6.35	116.57	123.30
1	C	490	VAL	CB-CA-C	-6.29	100.33	110.28
1	C	64	VAL	N-CA-CB	-6.26	102.44	111.21
1	B	517	ILE	CG1-CB-CG2	-6.25	91.94	110.70
1	B	309	ASN	N-CA-C	6.10	120.34	113.02
1	D	553	GLU	N-CA-C	6.10	117.93	111.28
1	B	122	GLN	N-CA-C	6.04	119.84	112.23
1	C	614	ARG	N-CA-C	6.04	120.65	113.28
1	D	199	THR	CA-C-N	-6.04	113.74	120.14
1	D	199	THR	C-N-CA	-6.04	113.74	120.14
1	C	483	GLY	N-CA-C	6.03	119.78	112.49
1	D	39	SER	CA-C-N	-5.96	114.09	120.47
1	D	39	SER	C-N-CA	-5.96	114.09	120.47
1	A	558	MET	N-CA-C	5.94	120.36	111.81
1	B	565	THR	N-CA-C	-5.89	102.05	110.59
1	D	550	ALA	CA-C-N	5.89	136.88	126.45
1	D	550	ALA	C-N-CA	5.89	136.88	126.45
1	C	300	TYR	N-CA-C	5.84	117.64	111.28
1	A	555	LEU	N-CA-C	5.80	120.20	113.18
1	A	426	GLU	N-CA-C	5.75	117.55	111.28
1	B	223	LYS	N-CA-C	5.65	119.80	113.02
1	C	548	VAL	CA-C-N	5.64	127.19	120.14
1	C	548	VAL	C-N-CA	5.64	127.19	120.14
1	B	331	LYS	N-CA-C	-5.61	105.31	111.82
1	B	195	SER	N-CA-C	5.57	118.06	111.33
1	B	502	ARG	N-CA-C	5.54	116.67	108.86
1	C	104	ILE	CA-CB-CG2	5.53	119.91	110.50
1	A	335	GLN	CA-C-N	-5.51	114.91	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	GLN	C-N-CA	-5.51	114.91	120.31
1	A	613	GLN	N-CA-C	5.49	116.95	110.97
1	B	332	ASP	N-CA-C	5.49	118.19	111.82
1	A	223	LYS	N-CA-C	5.47	119.59	113.02
1	C	558	MET	N-CA-C	5.47	120.16	112.72
1	D	377	PHE	CA-C-N	-5.45	114.98	120.21
1	D	377	PHE	C-N-CA	-5.45	114.98	120.21
1	A	582	PHE	N-CA-C	-5.44	101.02	109.24
1	D	383	ASN	N-CA-C	5.42	117.18	111.28
1	B	146	GLN	N-CA-C	5.40	117.59	111.11
1	C	396	ASP	N-CA-C	5.39	118.41	109.46
1	B	454	ARG	CA-C-N	-5.32	113.55	119.19
1	B	454	ARG	C-N-CA	-5.32	113.55	119.19
1	A	550	ALA	CA-C-N	5.32	135.86	126.45
1	A	550	ALA	C-N-CA	5.32	135.86	126.45
1	C	628	GLU	N-CA-C	5.29	116.86	111.14
1	D	293	GLY	N-CA-C	5.26	121.37	111.80
1	B	637	LEU	N-CA-C	5.21	118.15	110.59
1	A	483	GLY	N-CA-C	5.20	120.33	113.37
1	A	490	VAL	CB-CA-C	-5.19	102.08	110.28
1	D	190	LEU	CA-C-N	5.17	127.17	120.44
1	D	190	LEU	C-N-CA	5.17	127.17	120.44
1	C	44	ASN	N-CA-C	5.14	118.84	112.47
1	A	32	ASP	N-CA-C	5.12	118.79	112.54
1	B	185	GLU	CB-CA-C	5.12	120.69	109.99
1	B	135	LYS	CA-C-N	-5.08	113.81	119.19
1	B	135	LYS	C-N-CA	-5.08	113.81	119.19
1	C	454	ARG	CA-C-N	-5.06	114.45	119.56
1	C	454	ARG	C-N-CA	-5.06	114.45	119.56
1	D	294	GLY	CA-C-N	-5.03	117.97	123.30
1	D	294	GLY	C-N-CA	-5.03	117.97	123.30
1	D	138	LEU	N-CA-C	-5.03	105.71	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

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	5022	0	4918	98	0
1	B	5013	0	4905	88	0
1	C	5005	0	4893	107	0
1	D	5013	0	4905	88	0
2	A	15	0	6	1	0
2	B	15	0	7	0	0
2	C	15	0	6	1	0
2	D	15	0	6	0	0
3	A	9	0	14	3	0
3	B	9	0	14	2	0
3	C	9	0	14	0	0
3	D	9	0	14	0	0
4	A	101	0	0	0	0
4	B	140	0	0	1	0
4	C	103	0	0	1	0
4	D	99	0	0	0	0
All	All	20592	0	19702	347	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 9.

All (347) 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:554:ILE:HG23	1:A:555:LEU:CD1	1.79	1.12
1:A:554:ILE:HG23	1:A:555:LEU:HD12	1.31	1.08
1:B:590:GLU:HG3	1:B:600:VAL:HG11	1.35	1.06
1:C:396:ASP:OD1	1:C:398:ARG:HD3	1.61	1.00
1:B:191:ARG:HG3	1:B:191:ARG:HH11	1.27	0.98
1:C:13:ARG:HG2	1:C:13:ARG:HH11	1.32	0.95
1:D:503:ARG:HD2	1:D:529:THR:HG23	1.51	0.92
1:C:358:ASN:H	1:C:358:ASN:HD22	1.22	0.87
1:A:71:PRO:HB3	1:A:115:GLU:HG3	1.58	0.85
1:D:503:ARG:HD2	1:D:529:THR:CG2	2.06	0.85
1:C:67:LEU:HD21	1:C:553:GLU:OE1	1.78	0.83
1:A:554:ILE:CG2	1:A:555:LEU:CD1	2.58	0.82
1:C:139:LEU:HB3	1:D:593:MET:HE1	1.60	0.82
1:A:447:SER:H	1:A:453:HIS:HD2	1.28	0.81
1:B:297:ALA:HB3	1:B:311:MET:HG3	1.62	0.81
1:D:150:SER:H	1:D:174:HIS:HD2	1.27	0.81
1:C:395:THR:O	1:C:395:THR:CG2	2.29	0.80
1:C:447:SER:H	1:C:453:HIS:HD2	1.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:ARG:HD2	1:C:253:HIS:HD2	1.48	0.79
1:C:593:MET:HE1	1:D:140:ALA:HA	1.62	0.78
1:B:120:GLN:HG3	1:B:121:ALA:N	1.97	0.78
1:B:71:PRO:HB3	1:B:115:GLU:HG3	1.63	0.78
1:A:72:GLN:HE22	1:A:572:VAL:H	1.31	0.78
1:B:297:ALA:HB3	1:B:311:MET:CG	2.13	0.78
1:B:358:ASN:HD22	1:B:358:ASN:H	1.33	0.77
1:D:511:CYS:H	1:D:560:ASN:HD21	1.33	0.77
1:D:358:ASN:HD22	1:D:358:ASN:H	1.33	0.76
1:C:593:MET:HE1	1:D:140:ALA:CA	2.16	0.75
1:C:395:THR:O	1:C:395:THR:HG22	1.86	0.73
1:B:191:ARG:HH11	1:B:191:ARG:CG	2.02	0.72
1:C:72:GLN:HE22	1:C:572:VAL:H	1.38	0.72
1:C:226:PHE:HE2	1:D:511:CYS:HA	1.54	0.72
1:C:146:GLN:HE22	1:D:606:ASN:HD22	1.37	0.72
1:C:390:ASN:HB3	1:C:396:ASP:OD2	1.90	0.71
1:B:297:ALA:CB	1:B:311:MET:HG3	2.20	0.71
1:B:69:ARG:NH2	1:B:553:GLU:OE1	2.22	0.71
1:A:61:GLN:O	1:A:61:GLN:HG3	1.91	0.71
1:C:390:ASN:CB	1:C:396:ASP:OD2	2.39	0.70
1:A:466:ASP:OD2	1:A:502:ARG:HD3	1.92	0.70
1:A:480:ASP:H	1:A:552:GLN:HE22	1.40	0.70
1:A:67:LEU:HD21	1:A:553:GLU:OE2	1.92	0.70
1:C:205:ARG:HD2	1:C:253:HIS:CD2	2.27	0.70
1:D:72:GLN:HE22	1:D:572:VAL:H	1.38	0.69
1:A:554:ILE:HG23	1:A:555:LEU:HD13	1.74	0.69
1:A:554:ILE:CG2	1:A:555:LEU:HD13	2.22	0.69
1:B:69:ARG:HH22	1:B:553:GLU:CD	2.00	0.69
1:A:612:SER:HA	1:A:620:GLN:NE2	2.08	0.69
1:B:522:ASP:OD2	1:B:527:GLU:HG3	1.92	0.68
1:A:358:ASN:H	1:A:358:ASN:HD22	1.42	0.68
1:B:592:MET:HA	1:B:592:MET:HE2	1.77	0.66
1:A:67:LEU:CD2	1:A:553:GLU:OE2	2.43	0.66
1:A:511:CYS:H	1:A:560:ASN:ND2	1.93	0.66
1:A:447:SER:H	1:A:453:HIS:CD2	2.14	0.66
1:A:590:GLU:OE2	1:A:604:ARG:NH2	2.28	0.65
1:C:146:GLN:NE2	1:D:606:ASN:HD22	1.94	0.65
1:B:480:ASP:H	1:B:552:GLN:HE22	1.45	0.64
1:D:511:CYS:H	1:D:560:ASN:ND2	1.94	0.64
1:A:398:ARG:HG2	1:D:304:ARG:HH22	1.61	0.64
1:C:447:SER:H	1:C:453:HIS:CD2	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:480:ASP:H	1:D:552:GLN:HE22	1.45	0.64
1:C:13:ARG:HH11	1:C:13:ARG:CG	2.09	0.64
1:B:554:ILE:O	1:B:554:ILE:HG13	1.97	0.64
1:A:11:LEU:HD21	1:A:34:GLY:HA2	1.80	0.63
1:B:36:MET:HE1	1:B:491:LEU:HD13	1.81	0.62
1:B:191:ARG:HG3	1:B:191:ARG:NH1	2.05	0.62
1:A:511:CYS:H	1:A:560:ASN:HD21	1.46	0.62
1:C:594:ARG:NH1	1:C:600:VAL:HB	2.15	0.62
1:A:181:GLU:HG2	1:A:205:ARG:HD3	1.82	0.61
1:B:204:ILE:HD11	1:B:236:VAL:HG11	1.80	0.61
1:C:105:LYS:HE3	1:D:511:CYS:SG	2.40	0.61
1:D:100:LEU:HD21	1:D:348:LEU:HD21	1.82	0.61
1:D:503:ARG:CD	1:D:529:THR:HG23	2.29	0.60
1:D:15:ARG:NH2	1:D:32:ASP:OD1	2.34	0.60
1:A:211:GLN:OE1	1:A:256:LEU:HD22	2.02	0.60
1:A:60:ARG:O	1:A:61:GLN:HG2	2.02	0.59
1:A:19:ASN:HB2	1:A:523:GLY:HA2	1.83	0.59
1:D:490:VAL:O	1:D:491:LEU:HD23	2.03	0.59
1:A:309:ASN:ND2	1:A:486:GLN:OE1	2.36	0.59
1:B:282:THR:HG21	4:B:705:HOH:O	2.03	0.58
1:C:446:MET:HE1	1:C:456:ILE:HG21	1.85	0.58
1:D:127:GLN:HE21	1:D:127:GLN:HA	1.68	0.58
1:A:156:GLY:N	1:A:181:GLU:OE1	2.36	0.58
1:D:74:LEU:HD22	1:D:116:ILE:HD11	1.86	0.57
1:A:72:GLN:NE2	1:A:572:VAL:H	1.99	0.57
1:A:557:ASP:OD1	1:B:555:LEU:HA	2.03	0.57
1:B:71:PRO:HB3	1:B:115:GLU:CG	2.35	0.57
1:C:480:ASP:H	1:C:552:GLN:HE22	1.51	0.57
1:B:524:GLN:HE22	1:B:527:GLU:CD	2.13	0.57
1:C:615:VAL:HG12	1:C:616:ASP:O	2.04	0.56
1:B:506:MET:HB2	1:B:517:ILE:HG13	1.87	0.56
1:B:590:GLU:CG	1:B:600:VAL:HG11	2.24	0.56
1:A:29:GLY:O	1:A:36:MET:HE3	2.05	0.56
1:A:163:ILE:HD12	1:A:189:VAL:HG22	1.87	0.56
1:D:75:HIS:HA	1:D:119:SER:OG	2.06	0.56
1:D:203:GLY:HA2	1:D:251:LEU:O	2.06	0.56
1:A:384:MET:HE1	1:A:414:VAL:HG21	1.87	0.56
1:B:120:GLN:HB3	1:B:128:LEU:HD22	1.87	0.56
1:B:297:ALA:HB3	1:B:311:MET:HG2	1.87	0.56
1:C:187:ASP:HB2	1:C:239:ARG:HH22	1.71	0.56
1:B:486:GLN:HG2	1:B:488:PHE:CZ	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:ARG:HH22	1:C:553:GLU:CD	2.13	0.55
1:B:590:GLU:OE1	1:B:594:ARG:NH2	2.39	0.55
1:C:522:ASP:OD2	1:C:527:GLU:HG3	2.07	0.55
1:B:117:LEU:O	1:B:120:GLN:HG2	2.07	0.55
1:D:204:ILE:HD11	1:D:236:VAL:HG11	1.89	0.55
1:B:358:ASN:HD21	1:B:471:ASN:HD22	1.54	0.55
1:B:479:PRO:HD2	1:B:552:GLN:HE21	1.71	0.55
1:D:492:PRO:HB2	1:D:496:LEU:HD21	1.89	0.55
1:C:225:LYS:HE3	1:D:512:ASP:O	2.07	0.54
1:D:503:ARG:HH11	1:D:529:THR:HG23	1.72	0.54
1:B:508:ASP:C	1:B:508:ASP:OD1	2.50	0.54
1:C:74:LEU:HD22	1:C:116:ILE:HD11	1.89	0.54
1:C:13:ARG:HG2	1:C:13:ARG:NH1	2.11	0.54
1:D:186:LEU:HD22	1:D:236:VAL:HG22	1.89	0.54
1:B:72:GLN:HE22	1:B:572:VAL:H	1.54	0.54
1:A:417:GLN:HB3	1:A:422:VAL:HB	1.91	0.53
1:D:479:PRO:HD2	1:D:552:GLN:NE2	2.23	0.53
1:D:509:ILE:HD12	1:D:562:PHE:CZ	2.44	0.53
1:A:590:GLU:CD	1:A:594:ARG:HH21	2.17	0.53
1:C:104:ILE:HG23	1:C:108:GLN:HG3	1.91	0.53
1:D:117:LEU:HD22	1:D:128:LEU:HG	1.89	0.53
1:C:187:ASP:CG	1:C:191:ARG:HE	2.16	0.53
1:C:610:LEU:HG	1:C:614:ARG:HD2	1.91	0.53
1:B:349:THR:O	1:B:549:GLY:HA3	2.09	0.52
1:C:373:PRO:HB3	1:C:377:PHE:CD1	2.45	0.52
1:C:589:VAL:O	1:C:593:MET:HG2	2.09	0.52
1:A:558:MET:HB3	1:A:592:MET:HE1	1.90	0.52
1:D:181:GLU:HG2	1:D:205:ARG:HD3	1.91	0.52
1:B:233:VAL:CG1	1:B:280:LEU:HD21	2.40	0.52
1:A:384:MET:HE1	1:A:414:VAL:CG2	2.39	0.52
1:C:186:LEU:HD22	1:C:236:VAL:HG22	1.92	0.52
1:A:71:PRO:HB3	1:A:115:GLU:CG	2.35	0.52
1:D:478:LEU:HA	1:D:552:GLN:HE21	1.75	0.52
1:B:185:GLU:O	1:B:189:VAL:HG23	2.10	0.51
1:D:503:ARG:HD2	1:D:529:THR:HG21	1.90	0.51
1:B:128:LEU:C	1:B:128:LEU:HD23	2.34	0.51
1:B:38:VAL:HG22	1:B:40:PRO:HD3	1.92	0.51
1:C:100:LEU:HD21	1:C:348:LEU:HD21	1.91	0.51
1:D:487:VAL:HG22	1:D:519:ALA:HB3	1.92	0.51
1:C:615:VAL:O	1:C:616:ASP:C	2.47	0.51
1:A:510:THR:HB	1:A:560:ASN:HD22	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:LEU:O	1:B:126:LYS:N	2.32	0.51
1:D:69:ARG:HH22	1:D:553:GLU:CD	2.19	0.50
1:C:72:GLN:NE2	1:C:572:VAL:H	2.07	0.50
1:A:276:PHE:O	1:A:280:LEU:HG	2.11	0.50
1:B:17:ASP:O	1:B:523:GLY:N	2.37	0.50
1:B:243:GLU:O	1:B:244:ASN:HB2	2.12	0.50
1:C:450:ASN:OD1	1:C:452:PHE:N	2.40	0.50
1:A:11:LEU:HD21	1:A:34:GLY:CA	2.41	0.50
1:A:135:LYS:HB3	1:A:136:PRO:HD3	1.93	0.50
1:A:413:GLU:O	1:A:417:GLN:HG3	2.11	0.50
1:C:107:ASN:ND2	1:C:553:GLU:OE2	2.42	0.50
1:C:536:ASN:OD1	1:C:536:ASN:N	2.45	0.50
1:C:618:GLU:O	1:C:618:GLU:OE2	2.30	0.50
1:D:599:ASP:O	1:D:603:ILE:HG12	2.12	0.50
1:B:472:PHE:HE1	1:B:478:LEU:HD13	1.74	0.50
1:C:123:LEU:HD13	1:C:125:THR:HG22	1.94	0.50
1:D:391:LEU:HD13	1:D:403:ILE:CD1	2.41	0.50
1:A:618:GLU:CD	1:A:618:GLU:H	2.20	0.50
1:D:388:TRP:HZ3	1:D:441:GLU:HG3	1.77	0.50
1:D:607:TYR:O	1:D:611:VAL:HG23	2.12	0.50
1:C:358:ASN:H	1:C:358:ASN:ND2	2.02	0.50
1:C:349:THR:O	1:C:549:GLY:HA3	2.12	0.50
1:C:390:ASN:HB2	1:C:396:ASP:OD2	2.12	0.50
1:C:589:VAL:HG11	1:D:139:LEU:HD13	1.94	0.49
1:D:479:PRO:HD2	1:D:552:GLN:HE21	1.76	0.49
1:D:519:ALA:HB1	1:D:526:ILE:HG23	1.94	0.49
1:A:379:LEU:HA	1:A:382:ASN:HD22	1.77	0.49
1:A:490:VAL:O	1:A:491:LEU:HD23	2.13	0.49
3:A:1002:AG2:HB2	1:B:105:LYS:HZ1	1.77	0.49
1:C:358:ASN:HD22	1:C:358:ASN:N	1.99	0.49
1:A:225:LYS:NZ	1:B:510:THR:O	2.44	0.49
1:C:291:ASP:OD2	1:C:343:GLU:OE2	2.31	0.49
1:C:607:TYR:O	1:C:611:VAL:HG23	2.11	0.49
1:B:367:PRO:HG3	1:B:440:TYR:CZ	2.48	0.49
1:D:358:ASN:HD21	1:D:471:ASN:HD22	1.59	0.49
1:C:17:ASP:O	1:C:523:GLY:N	2.38	0.49
1:C:182:LYS:O	1:C:185:GLU:HG2	2.12	0.49
1:A:358:ASN:HD21	1:A:471:ASN:HD22	1.60	0.48
1:C:587:ASP:HB3	1:C:592:MET:HE3	1.94	0.48
1:D:94:TYR:CE1	1:D:337:MET:HG2	2.47	0.48
1:A:349:THR:O	1:A:549:GLY:HA3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLN:NE2	1:B:603:ILE:HG23	2.28	0.48
1:A:508:ASP:O	1:B:225:LYS:HE2	2.13	0.48
1:A:398:ARG:HG3	1:D:304:ARG:HH12	1.79	0.48
1:B:19:ASN:HB2	1:B:523:GLY:HA2	1.95	0.48
1:C:509:ILE:HD13	1:C:562:PHE:CZ	2.49	0.48
1:D:243:GLU:OE1	1:D:243:GLU:HA	2.13	0.48
1:C:139:LEU:HD13	1:D:589:VAL:HG11	1.96	0.48
1:A:17:ASP:O	1:A:523:GLY:N	2.47	0.47
1:C:309:ASN:HD21	1:C:486:GLN:HA	1.79	0.47
1:C:486:GLN:HG2	1:C:488:PHE:CZ	2.49	0.47
1:D:72:GLN:NE2	1:D:572:VAL:H	2.07	0.47
1:A:103:PRO:HG3	2:A:1001:PLP:H5A2	1.96	0.47
1:C:594:ARG:HH12	1:C:600:VAL:HB	1.76	0.47
1:A:137:GLU:OE2	1:B:560:ASN:HA	2.14	0.47
1:B:77:ARG:HD2	1:B:77:ARG:HA	1.62	0.47
1:D:545:PHE:N	1:D:545:PHE:CD1	2.82	0.47
1:A:97:LYS:HB2	1:A:97:LYS:HE2	1.46	0.47
1:A:362:THR:HA	1:A:467:LYS:O	2.15	0.47
1:A:606:ASN:HD22	1:B:146:GLN:NE2	2.12	0.47
1:A:355:LEU:HD22	1:A:477:SER:HB3	1.97	0.47
1:A:448:THR:O	1:A:454:ARG:HD3	2.15	0.47
1:D:520:TYR:O	1:D:526:ILE:HA	2.15	0.47
1:B:466:ASP:OD2	1:B:502:ARG:HD3	2.14	0.46
1:C:590:GLU:HA	1:C:593:MET:HG3	1.98	0.46
1:D:64:VAL:HB	1:D:357:SER:HA	1.97	0.46
1:A:473:SER:HB3	1:A:476:GLN:HB3	1.98	0.46
1:D:358:ASN:HD22	1:D:358:ASN:N	2.07	0.46
1:D:364:THR:HG22	1:D:466:ASP:CG	2.40	0.46
1:C:105:LYS:HD3	2:C:1001:PLP:C4	2.33	0.46
1:B:23:TRP:HZ2	1:B:491:LEU:HD11	1.80	0.46
1:D:589:VAL:HG12	1:D:593:MET:HE3	1.98	0.46
1:A:461:SER:OG	1:A:503:ARG:HD2	2.16	0.46
1:B:333:TYR:HB3	1:B:335:GLN:HG3	1.98	0.46
1:A:150:SER:H	1:A:174:HIS:HD2	1.64	0.46
1:C:187:ASP:OD1	1:C:239:ARG:NH2	2.49	0.46
1:D:17:ASP:O	1:D:523:GLY:N	2.38	0.46
1:A:554:ILE:HD11	1:B:558:MET:CE	2.45	0.46
1:C:234:LEU:HD11	1:D:426:GLU:HA	1.98	0.46
1:C:306:GLN:HG2	1:C:312:ASN:ND2	2.30	0.46
1:C:395:THR:O	1:C:395:THR:HG23	2.14	0.46
1:A:162:TYR:HD2	1:A:162:TYR:O	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:MET:HE2	1:D:36:MET:HB3	1.82	0.45
3:A:1002:AG2:CB	1:B:105:LYS:NZ	2.80	0.45
1:C:185:GLU:O	1:C:189:VAL:HG23	2.16	0.45
1:D:509:ILE:CD1	1:D:562:PHE:CZ	2.99	0.45
1:A:82:CYS:SG	1:A:123:LEU:HD11	2.56	0.45
1:A:252:VAL:HG23	1:A:287:ILE:HG21	1.98	0.45
1:B:101:VAL:O	1:B:343:GLU:HA	2.16	0.45
1:D:417:GLN:HB2	1:D:423:LEU:HD12	1.99	0.45
1:A:391:LEU:HD11	1:A:445:LEU:HD12	1.98	0.45
1:C:448:THR:O	1:C:454:ARG:HD3	2.17	0.45
1:A:490:VAL:HA	1:A:544:GLY:O	2.17	0.45
1:B:517:ILE:HD13	1:B:517:ILE:HG23	1.07	0.45
1:C:225:LYS:HG2	1:D:507:LEU:HD22	1.98	0.45
1:C:139:LEU:HB3	1:D:593:MET:CE	2.40	0.45
1:A:303:THR:HA	1:D:451:ARG:HH12	1.82	0.45
1:B:64:VAL:HB	1:B:357:SER:HA	1.99	0.45
1:C:89:ILE:HG23	1:C:94:TYR:HB3	1.99	0.45
1:C:508:ASP:OD1	1:D:225:LYS:NZ	2.50	0.45
1:D:391:LEU:HD13	1:D:403:ILE:HD13	1.98	0.45
1:C:97:LYS:HE3	1:C:97:LYS:HB2	1.79	0.44
1:D:592:MET:HA	1:D:592:MET:HE2	1.99	0.44
1:C:322:ILE:O	1:C:326:VAL:HG23	2.18	0.44
1:C:472:PHE:O	1:C:508:ASP:HB2	2.17	0.44
1:B:121:ALA:O	1:B:126:LYS:HE2	2.18	0.44
1:B:503:ARG:HA	1:B:530:LEU:O	2.18	0.44
1:C:155:ASN:OD1	1:C:181:GLU:OE2	2.34	0.44
1:C:479:PRO:HD2	1:C:552:GLN:HE21	1.83	0.44
1:D:124:GLU:HG2	1:D:125:THR:H	1.82	0.44
1:B:243:GLU:O	1:B:244:ASN:CB	2.65	0.44
1:B:358:ASN:H	1:B:358:ASN:ND2	2.10	0.44
1:A:601:ASP:O	1:A:605:LYS:HG3	2.18	0.44
1:B:94:TYR:CZ	1:B:337:MET:HB3	2.52	0.44
1:C:490:VAL:C	1:C:491:LEU:HG	2.42	0.44
1:C:587:ASP:CB	1:C:592:MET:HE3	2.48	0.44
1:A:391:LEU:CD1	1:A:445:LEU:HD12	2.48	0.43
1:B:50:LEU:HA	1:B:53:ILE:HD12	1.99	0.43
1:B:517:ILE:HG21	1:B:517:ILE:HD12	1.37	0.43
1:C:479:PRO:HD2	1:C:552:GLN:NE2	2.33	0.43
1:B:358:ASN:HD22	1:B:358:ASN:N	2.05	0.43
1:B:524:GLN:HE21	1:B:524:GLN:HB2	1.43	0.43
1:D:613:GLN:HE21	1:D:613:GLN:HB3	1.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:LEU:HD12	1:A:531:PRO:HD2	2.00	0.43
1:B:517:ILE:H	1:B:517:ILE:HG12	1.37	0.43
1:C:104:ILE:CD1	1:C:130:LEU:HD22	2.48	0.43
1:B:612:SER:HA	1:B:620:GLN:NE2	2.33	0.43
1:B:479:PRO:HD2	1:B:552:GLN:NE2	2.33	0.43
1:B:545:PHE:CD1	1:B:545:PHE:N	2.87	0.43
1:D:446:MET:HE1	1:D:456:ILE:HG21	2.01	0.43
1:A:181:GLU:HB3	1:A:226:PHE:HB3	2.01	0.43
1:A:277:TYR:CZ	1:A:281:ARG:HD3	2.54	0.43
1:A:203:GLY:HA2	1:A:251:LEU:O	2.19	0.43
1:A:621:GLN:HG3	1:A:622:GLN:N	2.32	0.43
1:D:119:SER:O	1:D:122:GLN:N	2.47	0.43
3:A:1002:AG2:HB1	1:B:105:LYS:HZ2	1.84	0.42
1:C:123:LEU:O	1:C:126:LYS:N	2.44	0.42
1:C:612:SER:HA	1:C:620:GLN:CD	2.44	0.42
1:A:105:LYS:HE3	1:A:105:LYS:HB3	1.81	0.42
1:C:104:ILE:HD13	1:C:141:VAL:HG22	2.00	0.42
1:C:450:ASN:OD1	1:C:450:ASN:C	2.62	0.42
1:C:280:LEU:HD23	1:C:280:LEU:HA	1.78	0.42
1:B:203:GLY:HA2	1:B:251:LEU:O	2.19	0.42
1:C:496:LEU:HD23	1:C:496:LEU:HA	1.89	0.42
1:C:617:GLN:HE21	1:C:617:GLN:HB2	1.49	0.42
1:C:626:GLU:OE1	1:D:164:ARG:NH2	2.37	0.42
1:A:304:ARG:NH1	1:D:398:ARG:HD2	2.35	0.42
1:A:511:CYS:HA	1:B:226:PHE:HE2	1.85	0.42
1:A:554:ILE:HD11	1:B:558:MET:HE3	2.01	0.42
1:C:476:GLN:OE1	1:C:558:MET:HE3	2.19	0.42
1:B:69:ARG:NH1	1:B:553:GLU:OE1	2.52	0.42
1:A:611:VAL:HG21	1:A:624:LEU:HD22	2.02	0.42
1:C:225:LYS:NZ	1:D:508:ASP:OD1	2.53	0.42
1:D:14:VAL:HG11	1:D:496:LEU:O	2.20	0.42
1:A:64:VAL:HA	1:A:65:PRO:C	2.45	0.42
1:B:117:LEU:HD11	1:B:130:LEU:HD11	2.02	0.42
1:C:137:GLU:OE2	1:D:560:ASN:HA	2.19	0.42
1:C:554:ILE:HG23	4:C:657:HOH:O	2.19	0.42
1:D:66:VAL:HG23	1:D:566:HIS:HB2	2.02	0.42
1:B:506:MET:HB2	1:B:517:ILE:CG1	2.49	0.41
1:C:355:LEU:HD22	1:C:477:SER:HB3	2.01	0.41
1:B:204:ILE:HG21	1:B:204:ILE:HD13	1.82	0.41
1:C:120:GLN:OE1	1:C:128:LEU:HA	2.20	0.41
1:C:167:LEU:HD13	1:C:193:ALA:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445:LEU:HD23	1:C:445:LEU:HA	1.93	0.41
1:D:204:ILE:HG21	1:D:204:ILE:HD13	1.76	0.41
1:D:358:ASN:H	1:D:358:ASN:ND2	2.10	0.41
1:A:90:GLU:O	1:A:93:GLN:NE2	2.53	0.41
1:B:512:ASP:CG	3:B:1002:AG2:HG2	2.45	0.41
1:C:509:ILE:CD1	1:C:562:PHE:CZ	3.04	0.41
1:C:626:GLU:CD	1:D:164:ARG:HH21	2.25	0.41
1:D:256:LEU:HA	1:D:256:LEU:HD23	1.72	0.41
1:D:450:ASN:OD1	1:D:450:ASN:C	2.63	0.41
1:A:437:ARG:HD2	1:A:437:ARG:HA	1.75	0.41
1:A:546:PHE:N	1:A:546:PHE:CD2	2.87	0.41
1:C:226:PHE:CE2	1:D:511:CYS:HA	2.45	0.41
1:A:508:ASP:OD1	1:A:508:ASP:C	2.63	0.41
1:A:554:ILE:HG22	1:A:555:LEU:HD13	1.99	0.41
1:C:14:VAL:O	1:C:17:ASP:HB2	2.21	0.41
1:C:103:PRO:HA	1:C:131:GLU:HB3	2.02	0.41
3:B:1002:AG2:HN1	3:B:1002:AG2:HG1	1.47	0.41
1:C:389:LEU:HD23	1:C:389:LEU:HA	1.86	0.41
1:A:40:PRO:O	1:A:76:GLN:NE2	2.54	0.41
1:A:358:ASN:HD22	1:A:358:ASN:N	2.14	0.41
1:A:388:TRP:HZ3	1:A:441:GLU:HG3	1.86	0.41
1:B:446:MET:HE1	1:B:456:ILE:HG21	2.02	0.41
1:B:560:ASN:HA	1:B:560:ASN:HD22	1.61	0.41
1:C:458:ASP:O	1:C:461:SER:HB2	2.21	0.41
1:C:608:HIS:CD2	1:C:624:LEU:HD22	2.55	0.41
1:D:487:VAL:CG2	1:D:519:ALA:HB3	2.50	0.41
1:D:624:LEU:O	1:D:628:GLU:HG3	2.21	0.41
1:A:355:LEU:HB3	1:A:545:PHE:HB2	2.03	0.41
1:B:205:ARG:HA	1:B:253:HIS:O	2.21	0.41
1:D:103:PRO:HA	1:D:131:GLU:HB3	2.03	0.41
1:D:589:VAL:CG1	1:D:593:MET:HE3	2.51	0.41
1:B:117:LEU:HD23	1:B:117:LEU:HA	1.95	0.40
1:A:557:ASP:CG	1:B:555:LEU:HA	2.47	0.40
1:C:306:GLN:CG	1:C:312:ASN:HD22	2.34	0.40
1:D:124:GLU:HG2	1:D:125:THR:N	2.36	0.40
1:A:278:CYS:HB3	1:A:333:TYR:CD1	2.56	0.40
1:A:31:ASP:OD1	1:A:31:ASP:C	2.65	0.40
1:A:189:VAL:HG11	1:A:202:LEU:HD21	2.03	0.40
1:A:146:GLN:HE22	1:B:603:ILE:HG23	1.86	0.40
1:A:225:LYS:NZ	1:B:508:ASP:OD1	2.52	0.40
1:A:478:LEU:N	1:A:479:PRO:CD	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:ASN:HB3	1:C:386:ARG:HH12	1.86	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	628/648 (97%)	606 (96%)	22 (4%)	0	100	100
1	B	627/648 (97%)	610 (97%)	17 (3%)	0	100	100
1	C	626/648 (97%)	605 (97%)	21 (3%)	0	100	100
1	D	627/648 (97%)	606 (97%)	21 (3%)	0	100	100
All	All	2508/2592 (97%)	2427 (97%)	81 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	549/567 (97%)	520 (95%)	29 (5%)	20	30
1	B	548/567 (97%)	505 (92%)	43 (8%)	11	16
1	C	547/567 (96%)	503 (92%)	44 (8%)	11	15
1	D	548/567 (97%)	503 (92%)	45 (8%)	10	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2192/2268 (97%)	2031 (93%)	161 (7%)	13	18

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	12	ASP
1	A	36	MET
1	A	44	ASN
1	A	52	LYS
1	A	97	LYS
1	A	105	LYS
1	A	119	SER
1	A	124	GLU
1	A	229	SER
1	A	282	THR
1	A	307	SER
1	A	332	ASP
1	A	358	ASN
1	A	368	GLU
1	A	376	ASP
1	A	379	LEU
1	A	398	ARG
1	A	448	THR
1	A	449	LYS
1	A	461	SER
1	A	478	LEU
1	A	502	ARG
1	A	513	SER
1	A	558	MET
1	A	614	ARG
1	A	617	GLN
1	A	621	GLN
1	A	624	LEU
1	B	11	LEU
1	B	13	ARG
1	B	17	ASP
1	B	42	SER
1	B	61	GLN
1	B	97	LYS
1	B	105	LYS
1	B	120	GLN

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Mol	Chain	Res	Type
1	B	123	LEU
1	B	124	GLU
1	B	125	THR
1	B	126	LYS
1	B	128	LEU
1	B	191	ARG
1	B	244	ASN
1	B	256	LEU
1	B	282	THR
1	B	307	SER
1	B	308	SER
1	B	311	MET
1	B	332	ASP
1	B	358	ASN
1	B	369	THR
1	B	376	ASP
1	B	448	THR
1	B	449	LYS
1	B	451	ARG
1	B	474	LEU
1	B	485	ASP
1	B	502	ARG
1	B	509	ILE
1	B	513	SER
1	B	517	ILE
1	B	524	GLN
1	B	537	GLU
1	B	553	GLU
1	B	560	ASN
1	B	575	GLN
1	B	580	ILE
1	B	610	LEU
1	B	618	GLU
1	B	624	LEU
1	B	638	GLU
1	C	13	ARG
1	C	36	MET
1	C	44	ASN
1	C	52	LYS
1	C	58	GLU
1	C	64	VAL
1	C	104	ILE

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Mol	Chain	Res	Type
1	C	105	LYS
1	C	110	ARG
1	C	126	LYS
1	C	127	GLN
1	C	146	GLN
1	C	194	LYS
1	C	201	ARG
1	C	204	ILE
1	C	311	MET
1	C	358	ASN
1	C	364	THR
1	C	369	THR
1	C	375	GLU
1	C	379	LEU
1	C	395	THR
1	C	396	ASP
1	C	398	ARG
1	C	447	SER
1	C	461	SER
1	C	478	LEU
1	C	511	CYS
1	C	513	SER
1	C	524	GLN
1	C	536	ASN
1	C	539	GLU
1	C	554	ILE
1	C	558	MET
1	C	560	ASN
1	C	575	GLN
1	C	593	MET
1	C	613	GLN
1	C	617	GLN
1	C	619	GLU
1	C	621	GLN
1	C	632	SER
1	C	638	GLU
1	C	639	ASP
1	D	11	LEU
1	D	36	MET
1	D	38	VAL
1	D	69	ARG
1	D	105	LYS

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Mol	Chain	Res	Type
1	D	109	GLN
1	D	110	ARG
1	D	122	GLN
1	D	123	LEU
1	D	126	LYS
1	D	127	GLN
1	D	128	LEU
1	D	139	LEU
1	D	171	LYS
1	D	228	LEU
1	D	242	LYS
1	D	244	ASN
1	D	311	MET
1	D	337	MET
1	D	358	ASN
1	D	368	GLU
1	D	369	THR
1	D	379	LEU
1	D	386	ARG
1	D	395	THR
1	D	398	ARG
1	D	401	ILE
1	D	449	LYS
1	D	451	ARG
1	D	461	SER
1	D	487	VAL
1	D	509	ILE
1	D	513	SER
1	D	524	GLN
1	D	539	GLU
1	D	610	LEU
1	D	613	GLN
1	D	616	ASP
1	D	617	GLN
1	D	618	GLU
1	D	621	GLN
1	D	624	LEU
1	D	628	GLU
1	D	638	GLU
1	D	639	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	72	GLN
1	A	93	GLN
1	A	271	ASN
1	A	306	GLN
1	A	358	ASN
1	A	382	ASN
1	A	453	HIS
1	A	552	GLN
1	A	560	ASN
1	A	602	GLN
1	A	606	ASN
1	A	620	GLN
1	B	19	ASN
1	B	33	GLN
1	B	44	ASN
1	B	72	GLN
1	B	120	GLN
1	B	147	HIS
1	B	271	ASN
1	B	358	ASN
1	B	393	ASN
1	B	408	GLN
1	B	443	ASN
1	B	486	GLN
1	B	498	ASN
1	B	524	GLN
1	B	536	ASN
1	B	552	GLN
1	B	613	GLN
1	B	622	GLN
1	C	44	ASN
1	C	72	GLN
1	C	146	GLN
1	C	211	GLN
1	C	245	GLN
1	C	253	HIS
1	C	306	GLN
1	C	309	ASN
1	C	358	ASN
1	C	417	GLN
1	C	443	ASN
1	C	453	HIS

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Mol	Chain	Res	Type
1	C	486	GLN
1	C	524	GLN
1	C	552	GLN
1	C	613	GLN
1	C	617	GLN
1	C	622	GLN
1	D	19	ASN
1	D	33	GLN
1	D	72	GLN
1	D	127	GLN
1	D	146	GLN
1	D	174	HIS
1	D	250	GLN
1	D	306	GLN
1	D	358	ASN
1	D	443	ASN
1	D	476	GLN
1	D	486	GLN
1	D	498	ASN
1	D	524	GLN
1	D	552	GLN
1	D	560	ASN
1	D	571	ASN
1	D	602	GLN
1	D	613	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLP	B	1001	1	15,15,16	1.86	4 (26%)	21,22,23	1.58	3 (14%)
3	AG2	D	1002	-	8,8,8	3.24	3 (37%)	7,8,8	2.96	3 (42%)
3	AG2	A	1002	-	8,8,8	3.02	3 (37%)	7,8,8	3.31	3 (42%)
2	PLP	A	1001	1	15,15,16	2.13	4 (26%)	21,22,23	1.41	4 (19%)
3	AG2	B	1002	-	8,8,8	3.18	3 (37%)	7,8,8	2.67	3 (42%)
2	PLP	C	1001	1	15,15,16	2.34	5 (33%)	21,22,23	1.91	6 (28%)
3	AG2	C	1002	-	8,8,8	3.15	3 (37%)	7,8,8	3.02	3 (42%)
2	PLP	D	1001	1	15,15,16	2.24	6 (40%)	21,22,23	1.49	6 (28%)

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	1001	1	-	1/6/6/8	0/1/1/1
3	AG2	D	1002	-	-	3/6/6/6	-
3	AG2	A	1002	-	-	4/6/6/6	-
2	PLP	A	1001	1	-	0/6/6/8	0/1/1/1
3	AG2	B	1002	-	-	5/6/6/6	-
2	PLP	C	1001	1	-	3/6/6/8	0/1/1/1
3	AG2	C	1002	-	-	2/6/6/6	-
2	PLP	D	1001	1	-	2/6/6/8	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	AG2	CZ-NE	7.27	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1002	AG2	CZ-NE	7.24	1.47	1.33
3	D	1002	AG2	CZ-NE	7.03	1.46	1.33
3	A	1002	AG2	CZ-NE	6.92	1.46	1.33
3	D	1002	AG2	CZ-NH1	4.70	1.49	1.32
2	B	1001	PLP	C4A-C4	4.37	1.60	1.51
2	D	1001	PLP	C4A-C4	-4.23	1.43	1.51
2	A	1001	PLP	P-O2P	-4.21	1.39	1.54
2	C	1001	PLP	P-O2P	-4.12	1.39	1.54
2	C	1001	PLP	C3-C2	-4.10	1.36	1.41
2	A	1001	PLP	P-O3P	-4.10	1.39	1.54
3	C	1002	AG2	CZ-NH1	4.08	1.46	1.32
3	B	1002	AG2	CZ-NH1	4.00	1.46	1.32
3	A	1002	AG2	CZ-NH1	3.96	1.46	1.32
2	D	1001	PLP	P-O2P	-3.94	1.40	1.54
2	C	1001	PLP	C4A-C4	-3.67	1.44	1.51
2	C	1001	PLP	P-O3P	-3.63	1.41	1.54
3	D	1002	AG2	CZ-NH2	3.38	1.46	1.34
2	D	1001	PLP	P-O3P	-3.29	1.42	1.54
3	B	1002	AG2	CZ-NH2	3.29	1.46	1.34
2	A	1001	PLP	C3-C2	-3.28	1.37	1.41
2	A	1001	PLP	P-O1P	-3.15	1.40	1.50
2	C	1001	PLP	P-O1P	-3.15	1.40	1.50
2	D	1001	PLP	C3-C2	-3.15	1.37	1.41
3	C	1002	AG2	CZ-NH2	3.04	1.45	1.34
3	A	1002	AG2	CZ-NH2	2.88	1.44	1.34
2	B	1001	PLP	C2-N1	2.83	1.38	1.33
2	B	1001	PLP	C5-C4	2.36	1.43	1.40
2	D	1001	PLP	P-O1P	-2.34	1.43	1.50
2	D	1001	PLP	O4P-C5A	-2.04	1.37	1.44
2	B	1001	PLP	C2A-C2	2.02	1.53	1.50

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1001	PLP	C4A-C4-C5	5.53	126.64	120.94
3	D	1002	AG2	NH2-CZ-NE	-5.47	106.84	119.27
3	B	1002	AG2	NE-CZ-NH1	-5.35	111.48	120.67
3	C	1002	AG2	NE-CZ-NH1	-5.20	111.74	120.67
3	A	1002	AG2	NE-CZ-NH1	-4.99	112.10	120.67
3	A	1002	AG2	NH2-CZ-NE	-4.97	107.98	119.27
3	A	1002	AG2	NH2-CZ-NH1	-4.74	106.59	120.07
3	D	1002	AG2	NE-CZ-NH1	-4.57	112.82	120.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1002	AG2	NH2-CZ-NE	-4.51	109.02	119.27
2	B	1001	PLP	C5-C6-N1	-3.97	117.37	123.83
2	B	1001	PLP	C6-C5-C4	3.92	121.31	118.10
3	C	1002	AG2	NH2-CZ-NH1	-3.71	109.51	120.07
3	B	1002	AG2	NH2-CZ-NH1	-3.23	110.87	120.07
3	B	1002	AG2	NH2-CZ-NE	-2.85	112.80	119.27
2	A	1001	PLP	C4A-C4-C5	2.81	123.84	120.94
2	D	1001	PLP	O4P-P-O1P	2.74	113.84	106.44
2	A	1001	PLP	O4P-C5A-C5	2.67	114.36	109.36
2	C	1001	PLP	O4P-P-O1P	2.61	113.50	106.44
2	D	1001	PLP	C6-C5-C4	2.59	120.22	118.10
2	C	1001	PLP	C4A-C4-C3	-2.57	116.23	120.52
2	A	1001	PLP	O4P-P-O1P	2.54	113.31	106.44
2	D	1001	PLP	C4A-C4-C5	2.54	123.55	120.94
3	D	1002	AG2	NH2-CZ-NH1	-2.48	113.02	120.07
2	C	1001	PLP	C5A-C5-C6	-2.39	115.47	119.36
2	D	1001	PLP	C5A-C5-C6	-2.24	115.70	119.36
2	B	1001	PLP	C6-N1-C2	2.23	123.24	119.20
2	C	1001	PLP	C6-C5-C4	2.23	119.92	118.10
2	A	1001	PLP	O2P-P-O4P	2.15	112.27	106.67
2	D	1001	PLP	C2A-C2-C3	-2.15	118.28	120.80
2	D	1001	PLP	C2A-C2-N1	2.12	121.63	117.64
2	C	1001	PLP	O3P-P-O1P	-2.08	102.72	110.83

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1001	PLP	C4-C5-C5A-O4P
2	D	1001	PLP	C4-C5-C5A-O4P
3	A	1002	AG2	NH1-CZ-NE-CD
3	B	1002	AG2	NH1-CZ-NE-CD
3	C	1002	AG2	NH1-CZ-NE-CD
3	D	1002	AG2	NE-CD-CG-CB
3	C	1002	AG2	NE-CD-CG-CB
3	A	1002	AG2	NE-CD-CG-CB
3	B	1002	AG2	NE-CD-CG-CB
3	A	1002	AG2	N-CA-CB-CG
3	B	1002	AG2	N-CA-CB-CG
2	C	1001	PLP	C6-C5-C5A-O4P
3	A	1002	AG2	NH2-CZ-NE-CD
2	C	1001	PLP	C5A-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
3	D	1002	AG2	NH1-CZ-NE-CD
3	B	1002	AG2	CA-CB-CG-CD
3	D	1002	AG2	N-CA-CB-CG
2	D	1001	PLP	C6-C5-C5A-O4P
3	B	1002	AG2	CG-CD-NE-CZ
2	B	1001	PLP	C4-C5-C5A-O4P

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	AG2	3	0
2	A	1001	PLP	1	0
3	B	1002	AG2	2	0
2	C	1001	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	630/648 (97%)	-0.32	3 (0%) 87 87	16, 26, 46, 68	0
1	B	629/648 (97%)	-0.39	9 (1%) 73 75	13, 25, 45, 69	0
1	C	628/648 (96%)	-0.29	6 (0%) 79 80	14, 26, 50, 68	0
1	D	629/648 (97%)	-0.24	5 (0%) 82 83	15, 26, 51, 68	0
All	All	2516/2592 (97%)	-0.31	23 (0%) 81 82	13, 26, 48, 69	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	11	LEU	5.0
1	B	121	ALA	4.1
1	B	11	LEU	4.1
1	B	123	LEU	3.5
1	B	124	GLU	3.3
1	C	553	GLU	3.3
1	B	120	GLN	3.2
1	A	10	LYS	3.0
1	C	582	PHE	2.8
1	A	558	MET	2.8
1	B	125	THR	2.7
1	D	123	LEU	2.6
1	D	398	ARG	2.5
1	C	147	HIS	2.5
1	C	396	ASP	2.4
1	D	393	ASN	2.4
1	B	582	PHE	2.3
1	D	607	TYR	2.3
1	B	595	TYR	2.3
1	A	595	TYR	2.2
1	C	607	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	12	ASP	2.1
1	C	399	ALA	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
3	AG2	C	1002	9/9	0.75	0.23	49,54,63,64	0
3	AG2	D	1002	9/9	0.75	0.22	41,46,52,52	0
3	AG2	B	1002	9/9	0.77	0.20	45,49,53,54	0
3	AG2	A	1002	9/9	0.81	0.19	49,52,58,58	0
2	PLP	D	1001	15/16	0.91	0.11	19,27,34,36	0
2	PLP	C	1001	15/16	0.95	0.09	20,30,36,40	0
2	PLP	A	1001	15/16	0.96	0.08	25,28,34,35	0
2	PLP	B	1001	15/16	0.96	0.07	21,29,32,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.