



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 03:03 am BST

PDB ID : 3N2O  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

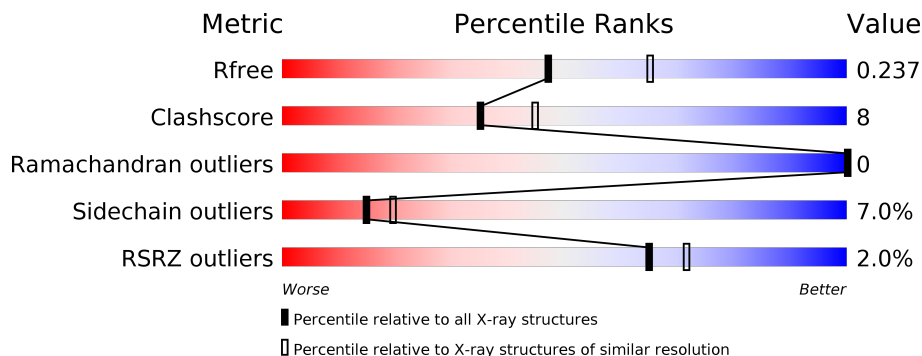
# 1 Overall quality at a glance

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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AG2	A	1002	-	X	-	X
3	AG2	B	1002	-	X	-	-
3	AG2	C	1002	-	-	-	X
3	AG2	D	1002	-	X	-	-

## 2 Entry composition i

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
			Total	C	N	O	S			
1	A	630	5022	3165	871	968	18	0	0	0
1	B	629	5013	3159	869	967	18	0	0	0
1	C	628	5005	3153	868	966	18	0	0	0
1	D	629	5013	3159	869	967	18	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

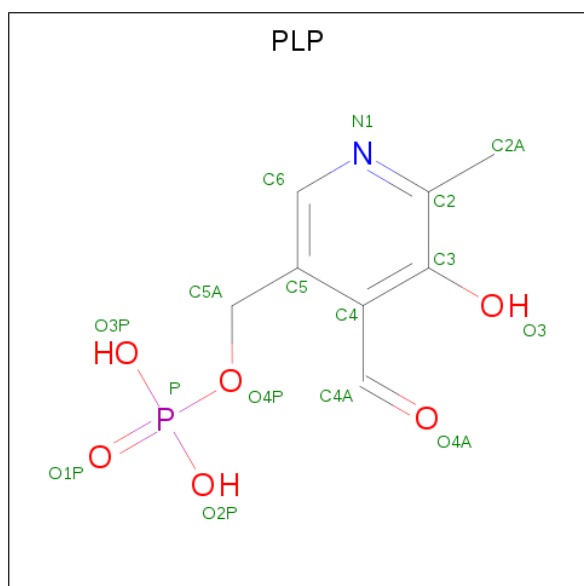
Chain	Residue	Modelled	Actual	Comment	Reference
A	641	LEU	-	EXPRESSION TAG	UNP Q7MK24
A	642	GLU	-	EXPRESSION TAG	UNP Q7MK24
A	643	HIS	-	EXPRESSION TAG	UNP Q7MK24
A	644	HIS	-	EXPRESSION TAG	UNP Q7MK24
A	645	HIS	-	EXPRESSION TAG	UNP Q7MK24
A	646	HIS	-	EXPRESSION TAG	UNP Q7MK24
A	647	HIS	-	EXPRESSION TAG	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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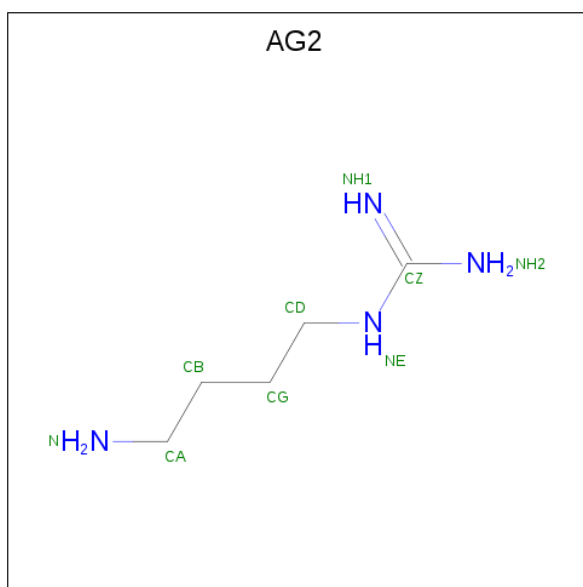
Chain	Residue	Modelled	Actual	Comment	Reference
C	646	HIS	-	EXPRESSION TAG	UNP Q7MK24
C	647	HIS	-	EXPRESSION TAG	UNP Q7MK24
C	648	HIS	-	EXPRESSION TAG	UNP Q7MK24
D	641	LEU	-	EXPRESSION TAG	UNP Q7MK24
D	642	GLU	-	EXPRESSION TAG	UNP Q7MK24
D	643	HIS	-	EXPRESSION TAG	UNP Q7MK24
D	644	HIS	-	EXPRESSION TAG	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 (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



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

- Molecule 3 is AGMATINE (three-letter code: AG2) (formula: C<sub>5</sub>H<sub>14</sub>N<sub>4</sub>).



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

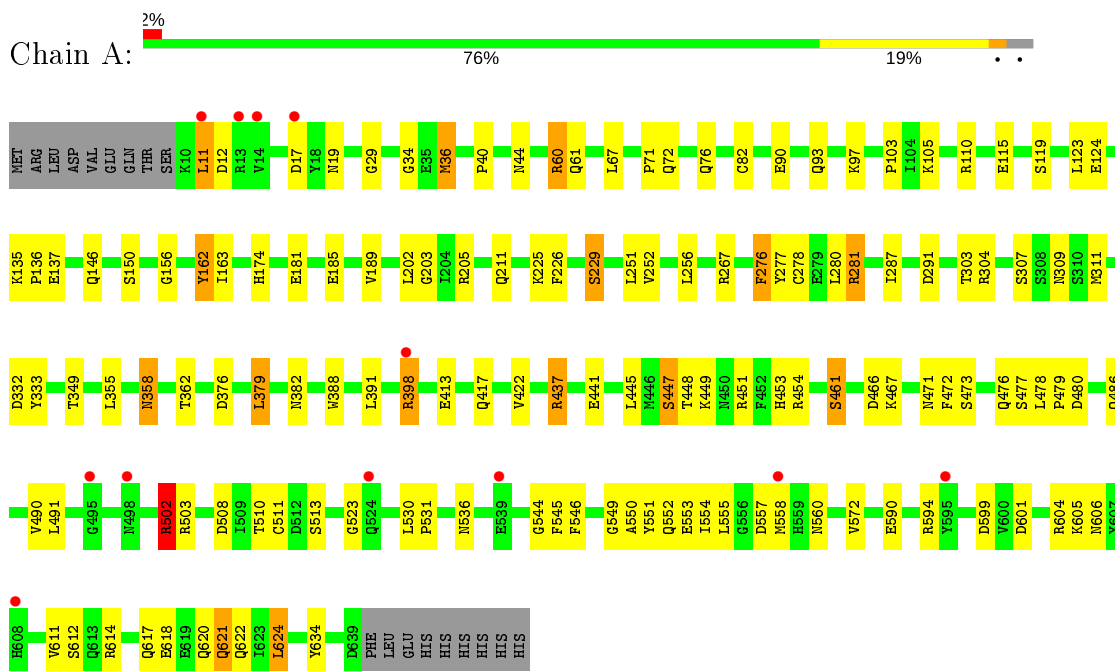
- Molecule 4 is water.

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

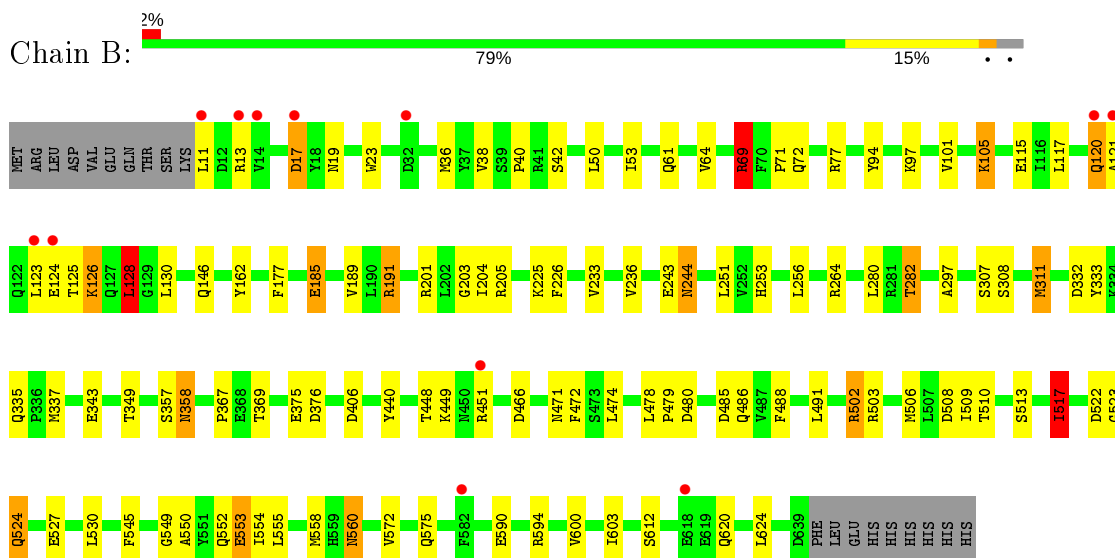
### 3 Residue-property plots [i](#)

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

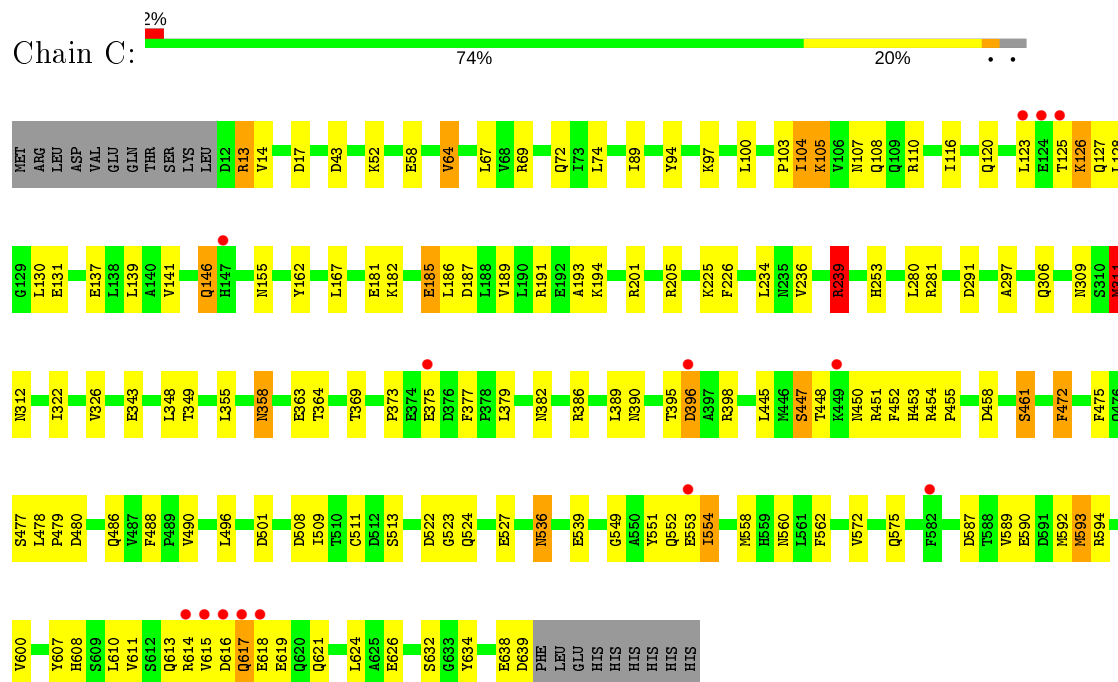
- Molecule 1: Biosynthetic arginine decarboxylase



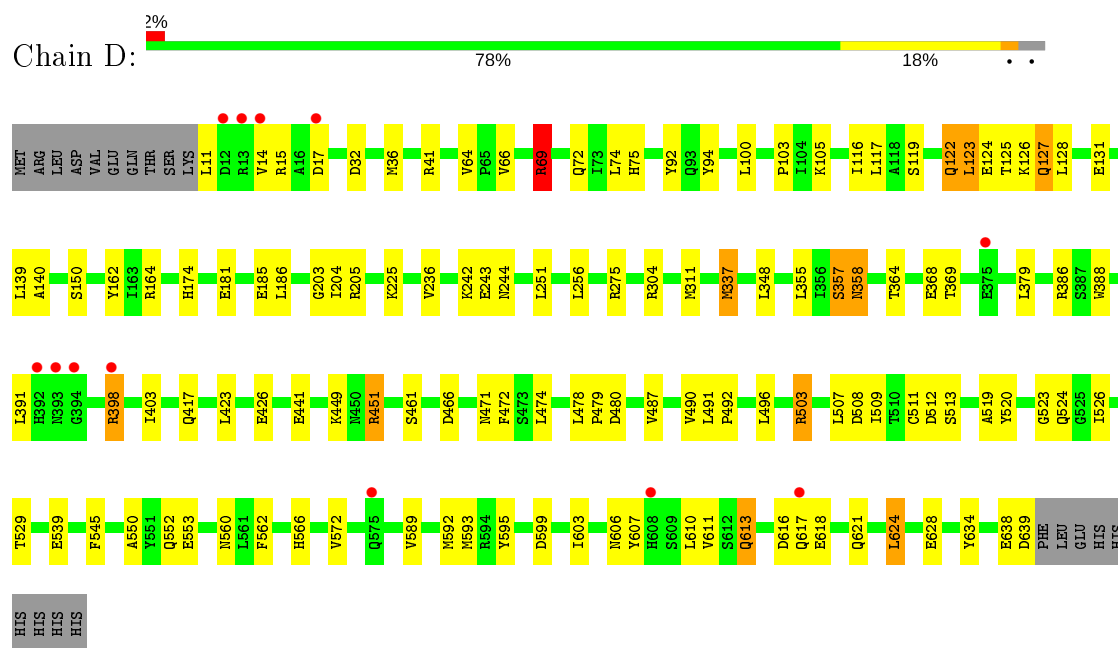
- Molecule 1: Biosynthetic arginine decarboxylase



- 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, $\alpha$ , $\beta$ , $\gamma$	101.65Å 119.36Å 121.84Å 90.00° 96.30° 90.00°	Depositor
Resolution (Å)	121.10 – 2.30 49.69 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (121.10-2.30) 98.8 (49.69-2.30)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.66 (at 2.29Å)	Xtrriage
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 (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.6	Xtrriage
Anisotropy	0.175	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 50.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	20592	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.99	3/5119 (0.1%)	0.90	7/6939 (0.1%)
1	B	1.05	3/5110 (0.1%)	0.96	9/6928 (0.1%)
1	C	1.05	6/5102 (0.1%)	0.93	7/6917 (0.1%)
1	D	1.01	2/5110 (0.0%)	0.91	8/6928 (0.1%)
All	All	1.03	14/20441 (0.1%)	0.93	31/27712 (0.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	185	GLU	CG-CD	6.70	1.61	1.51
1	B	185	GLU	CG-CD	6.58	1.61	1.51
1	C	311	MET	CG-SD	-6.52	1.64	1.81
1	A	185	GLU	CG-CD	6.20	1.61	1.51
1	C	551	TYR	CD1-CE1	-5.77	1.30	1.39
1	A	229	SER	CB-OG	-5.75	1.34	1.42
1	C	551	TYR	CD2-CE2	-5.72	1.30	1.39
1	C	363	GLU	CB-CG	5.51	1.62	1.52
1	A	551	TYR	CD1-CE1	-5.39	1.31	1.39
1	B	177	PHE	CE2-CZ	5.28	1.47	1.37
1	C	185	GLU	CG-CD	5.21	1.59	1.51
1	B	375	GLU	CB-CG	5.16	1.61	1.52
1	D	92	TYR	CE2-CZ	-5.05	1.31	1.38
1	C	475	PHE	CE2-CZ	5.04	1.47	1.37

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	69	ARG	NE-CZ-NH2	-9.01	115.80	120.30
1	B	517	ILE	CG1-CB-CG2	-8.84	91.94	111.40
1	B	201	ARG	NE-CZ-NH2	-8.17	116.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	123	LEU	CA-CB-CG	7.72	133.05	115.30
1	A	502	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	B	69	ARG	NE-CZ-NH2	-7.43	116.59	120.30
1	D	355	LEU	CA-CB-CG	-6.98	99.25	115.30
1	D	503	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	A	267	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	B	128	LEU	CA-CB-CG	6.21	129.58	115.30
1	A	502	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	D	550	ALA	C-N-CA	6.07	136.88	121.70
1	D	41	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	C	43	ASP	CB-CG-OD1	5.86	123.57	118.30
1	C	490	VAL	CB-CA-C	-5.82	100.33	111.40
1	B	406	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	550	ALA	C-N-CA	5.67	135.86	121.70
1	B	264	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	C	239	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	C	239	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	B	550	ALA	C-N-CA	5.38	135.15	121.70
1	A	599	ASP	CB-CG-OD1	5.36	123.12	118.30
1	D	275	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	C	478	LEU	CA-CB-CG	5.29	127.46	115.30
1	A	110	ARG	NE-CZ-NH1	-5.17	117.71	120.30
1	B	185	GLU	CB-CA-C	5.15	120.69	110.40
1	C	501	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	C	64	VAL	CG1-CB-CG2	5.11	119.07	110.90
1	A	291	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	B	264	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	D	474	LEU	CA-CB-CG	5.02	126.84	115.30

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	5022	0	4918	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5013	0	4905	83	0
1	C	5005	0	4893	102	0
1	D	5013	0	4905	82	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	1	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	326	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 8.

All (326) 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:HH11	1:B:191:ARG:HG3	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:HD22	1:C:358:ASN:H	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: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:CG2	1:C:395:THR:O	2.29	0.80
1:C:447:SER:H	1:C:453:HIS:HD2	1.30	0.80
1:C:205:ARG:HD2	1:C:253:HIS:HD2	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:B:358:ASN:HD22	1.33	0.77
1:D:511:CYS:H	1:D:560:ASN:HD21	1.33	0.77
1:D:358:ASN:H	1:D:358:ASN:HD22	1.33	0.76
1:C:395:THR:O	1:C:395:THR:HG22	1.86	0.73
1:B:191:ARG:CG	1:B:191:ARG:HH11	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:HG3	1:A:61:GLN:O	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: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:HD22	1:A:358:ASN:H	1.42	0.68
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
1:D:480:ASP:H	1:D:552:GLN:HE22	1.45	0.64
1:B:69:ARG:HH22	1:B:553:GLU:CD	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ARG:NH1	1:B:191:ARG:HG3	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: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:557:ASP:OD1	1:B:555:LEU:HA	2.03	0.57
1:A:72:GLN:NE2	1:A:572:VAL:H	1.99	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: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: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:C:139:LEU:HB3	1:D:593:MET:HE1	1.86	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
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:D:503:ARG:HH11	1:D:529:THR:HG23	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:LYS:HE3	1:D:512:ASP:O	2.07	0.54
1:C:74:LEU:HD22	1:C:116:ILE:HD11	1.89	0.54
1:C:13:ARG:NH1	1:C:13:ARG:HG2	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: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: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:D:181:GLU:HG2	1:D:205:ARG:HD3	1.91	0.52
1:B:524:GLN:HE22	1:B:527:GLU:CD	2.13	0.52
1:B:233:VAL:CG1	1:B:280:LEU:HD21	2.40	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:38:VAL:HG22	1:B:40:PRO:HD3	1.92	0.51
1:C:139:LEU:HB3	1:D:593:MET:CE	2.40	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:A:510:THR:HB	1:A:560:ASN:HD22	1.76	0.51
1:B:123:LEU:O	1:B:126:LYS:N	2.32	0.51
1:C:69:ARG:HH22	1:C:553:GLU:CD	2.13	0.51
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:135:LYS:HB3	1:A:136:PRO:HD3	1.93	0.50
1:A:11:LEU:HD21	1:A:34:GLY:CA	2.41	0.50
1:A:413:GLU:O	1:A:417:GLN:HG3	2.11	0.50
1:C:536:ASN:N	1:C:536:ASN:OD1	2.45	0.50
1:C:107:ASN:ND2	1:C:553:GLU:OE2	2.42	0.50
1:C:618:GLU:OE2	1:C:618:GLU:O	2.30	0.50
1:D:599:ASP:O	1:D:603:ILE:HG12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:508:ASP:C	1:B:508:ASP:OD1	2.50	0.50
1:C:358:ASN:ND2	1:C:358:ASN:H	2.02	0.50
1:C:390:ASN:HB2	1:C:396:ASP:OD2	2.12	0.50
1:C:349:THR:O	1:C:549:GLY:HA3	2.12	0.50
1:C:589:VAL:HG11	1:D:139:LEU:HD13	1.94	0.49
1:D:519:ALA:HB1	1:D:526:ILE:HG23	1.94	0.49
1:D:479:PRO:HD2	1:D:552:GLN:HE21	1.76	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:297:ALA:HB3	1:C:311:MET:HE3	1.94	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:C:587:ASP:HB3	1:C:592:MET:HE3	1.95	0.49
1:A:358:ASN:HD21	1:A:471:ASN:HD22	1.60	0.48
1:C:593:MET:HE1	1:D:140:ALA:HA	1.95	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
1:A:590:GLU:CD	1:A:594:ARG:HH21	2.17	0.48
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:C:187:ASP:CG	1:C:191:ARG:HE	2.16	0.48
1:B:19:ASN:HB2	1:B:523:GLY:HA2	1.95	0.48
1:A:398:ARG:HG3	1:D:304:ARG:HH12	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:97:LYS:HE2	1:A:97:LYS:HB2	1.46	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:B:128:LEU:C	1:B:128:LEU:HD23	2.34	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:N	1:D:358:ASN:HD22	2.07	0.46
1:B:36:MET:HE3	1:B:491:LEU:CB	2.46	0.46
1:C:105:LYS:HD3	2:C:1001:PLP:C4	2.33	0.46
1:A:29:GLY:O	1:A:36:MET:HE3	2.16	0.46
1:B:23:TRP:HZ2	1:B:491:LEU:HD11	1.80	0.46
1:C:615:VAL:O	1:C:616:ASP:C	2.47	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:D:69:ARG:HH22	1:D:553:GLU:CD	2.19	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:64:VAL:HB	1:B:357:SER:HA	1.99	0.45
1:A:303:THR:HA	1:D:451:ARG:HH12	1.82	0.45
1:C:508:ASP:OD1	1:D:225:LYS:NZ	2.50	0.45
1:C:89:ILE:HG23	1:C:94:TYR:HB3	1.99	0.45
1:D:391:LEU:HD13	1:D:403:ILE:HD13	1.98	0.45
1:C:97:LYS:HB2	1:C:97:LYS:HE3	1.79	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:A:621:GLN:HG3	1:A:622:GLN:N	2.32	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:ND2	1:B:358:ASN:H	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:A:391:LEU:CD1	1:A:445:LEU:HD12	2.48	0.43
1:B:517:ILE:HD12	1:B:517:ILE:HG21	1.37	0.43
1:B:50:LEU:HA	1:B:53:ILE:HD12	1.99	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:HB2	1:B:524:GLN:HE21	1.43	0.43
1:D:613:GLN:HB3	1:D:613:GLN:HE21	1.71	0.43
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: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:C:593:MET:CE	1:D:140:ALA:HA	2.49	0.43
1:A:203:GLY:HA2	1:A:251:LEU:O	2.19	0.43
1:D:119:SER:O	1:D:122:GLN:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:105:LYS:HB3	1:A:105:LYS:HE3	1.81	0.42
1:C:104:ILE:HD13	1:C:141:VAL:HG22	2.00	0.42
1:C:280:LEU:HA	1:C:280:LEU:HD23	1.78	0.42
1:D:364:THR:HG22	1:D:466:ASP:CG	2.40	0.42
1:A:618:GLU:H	1:A:618:GLU:CD	2.20	0.42
1:B:203:GLY:HA2	1:B:251:LEU:O	2.19	0.42
1:C:496:LEU:HA	1:C:496:LEU:HD23	1.89	0.42
1:C:617:GLN:HE21	1:C:617:GLN:HB2	1.49	0.42
1:C:587:ASP:CB	1:C:592:MET:HE3	2.50	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: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: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:D:592:MET:HE2	1:D:595:TYR:CD2	2.55	0.41
1:B:204:ILE:HD13	1:B:204:ILE:HG21	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
1:C:445:LEU:HA	1:C:445:LEU:HD23	1.93	0.41
1:D:204:ILE:HD13	1:D:204:ILE:HG21	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:C:509:ILE:CD1	1:C:562:PHE:CZ	3.04	0.41
1:D:256:LEU:HD23	1:D:256:LEU:HA	1.72	0.41
1:A:437:ARG:HA	1:A:437:ARG:HD2	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:554:ILE:HG22	1:A:555:LEU:HD13	1.99	0.41
1:C:103:PRO:HA	1:C:131:GLU:HB3	2.02	0.41
1:C:14:VAL:O	1:C:17:ASP:HB2	2.21	0.41
3:B:1002:AG2:HG1	3:B:1002:AG2:HN1	1.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:LEU:HD23	1:C:389:LEU:HA	1.86	0.41
1:A:358:ASN:N	1:A:358:ASN:HD22	2.14	0.41
1:A:388:TRP:HZ3	1:A:441:GLU:HG3	1.86	0.41
1:B:560:ASN:HD22	1:B:560:ASN:HA	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:624:LEU:O	1:D:628:GLU:HG3	2.21	0.41
1:A:40:PRO:O	1:A:76:GLN:NE2	2.54	0.41
1:D:487:VAL:CG2	1:D:519:ALA:HB3	2.50	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:B:117:LEU:HA	1:B:117:LEU:HD23	1.95	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:189:VAL:HG11	1:A:202:LEU:HD21	2.03	0.40
1:A:478:LEU:N	1:A:479:PRO:CD	2.85	0.40
1:A:225:LYS:NZ	1:B:508:ASP:OD1	2.52	0.40
1:A:146:GLN:HE22	1:B:603:ILE:HG23	1.86	0.40
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	516 (94%)	33 (6%)	19	26
1	B	548/567 (97%)	509 (93%)	39 (7%)	14	19
1	C	547/567 (96%)	502 (92%)	45 (8%)	11	14
1	D	548/567 (97%)	511 (93%)	37 (7%)	16	21
All	All	2192/2268 (97%)	2038 (93%)	154 (7%)	15	19

All (154) 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	60	ARG
1	A	119	SER
1	A	124	GLU
1	A	162	TYR
1	A	229	SER
1	A	276	PHE
1	A	281	ARG
1	A	307	SER
1	A	311	MET
1	A	332	ASP
1	A	358	ASN
1	A	376	ASP
1	A	379	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	398	ARG
1	A	437	ARG
1	A	447	SER
1	A	449	LYS
1	A	451	ARG
1	A	461	SER
1	A	472	PHE
1	A	502	ARG
1	A	513	SER
1	A	536	ASN
1	A	558	MET
1	A	614	ARG
1	A	617	GLN
1	A	621	GLN
1	A	624	LEU
1	A	634	TYR
1	B	11	LEU
1	B	13	ARG
1	B	17	ASP
1	B	42	SER
1	B	61	GLN
1	B	69	ARG
1	B	97	LYS
1	B	105	LYS
1	B	120	GLN
1	B	124	GLU
1	B	125	THR
1	B	126	LYS
1	B	128	LEU
1	B	162	TYR
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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	553	GLU
1	B	560	ASN
1	B	575	GLN
1	B	624	LEU
1	C	13	ARG
1	C	52	LYS
1	C	58	GLU
1	C	64	VAL
1	C	104	ILE
1	C	105	LYS
1	C	110	ARG
1	C	126	LYS
1	C	127	GLN
1	C	146	GLN
1	C	162	TYR
1	C	194	LYS
1	C	201	ARG
1	C	239	ARG
1	C	281	ARG
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	396	ASP
1	C	447	SER
1	C	451	ARG
1	C	455	PRO
1	C	461	SER
1	C	472	PHE
1	C	511	CYS
1	C	513	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	634	TYR
1	C	638	GLU
1	C	639	ASP
1	D	11	LEU
1	D	36	MET
1	D	69	ARG
1	D	105	LYS
1	D	122	GLN
1	D	123	LEU
1	D	126	LYS
1	D	127	GLN
1	D	162	TYR
1	D	242	LYS
1	D	244	ASN
1	D	311	MET
1	D	337	MET
1	D	357	SER
1	D	358	ASN
1	D	368	GLU
1	D	369	THR
1	D	379	LEU
1	D	386	ARG
1	D	398	ARG
1	D	449	LYS
1	D	451	ARG
1	D	461	SER
1	D	472	PHE
1	D	513	SER
1	D	524	GLN

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Mol	Chain	Res	Type
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	634	TYR
1	D	638	GLU
1	D	639	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) 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	321	ASN
1	A	358	ASN
1	A	382	ASN
1	A	453	HIS
1	A	552	GLN
1	A	560	ASN
1	A	571	ASN
1	A	602	GLN
1	A	606	ASN
1	B	19	ASN
1	B	72	GLN
1	B	120	GLN
1	B	146	GLN
1	B	147	HIS
1	B	271	ASN
1	B	358	ASN
1	B	393	ASN
1	B	486	GLN
1	B	498	ASN
1	B	524	GLN
1	B	536	ASN
1	B	552	GLN
1	B	571	ASN

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Mol	Chain	Res	Type
1	C	44	ASN
1	C	72	GLN
1	C	146	GLN
1	C	253	HIS
1	C	309	ASN
1	C	358	ASN
1	C	453	HIS
1	C	552	GLN
1	C	613	GLN
1	C	617	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	253	HIS
1	D	306	GLN
1	D	309	ASN
1	D	358	ASN
1	D	498	ASN
1	D	524	GLN
1	D	552	GLN
1	D	560	ASN
1	D	571	ASN
1	D	613	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry i

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PLP	D	1001	1	15,15,16	2.19	6 (40%)	20,22,23	1.51	6 (30%)
2	PLP	B	1001	1	15,15,16	1.79	3 (20%)	20,22,23	1.58	3 (15%)
3	AG2	A	1002	-	8,8,8	2.85	3 (37%)	7,8,8	3.20	3 (42%)
3	AG2	C	1002	-	8,8,8	2.98	3 (37%)	7,8,8	2.93	3 (42%)
3	AG2	D	1002	-	8,8,8	3.04	3 (37%)	7,8,8	2.89	3 (42%)
2	PLP	C	1001	1	15,15,16	2.29	5 (33%)	20,22,23	1.93	6 (30%)
2	PLP	A	1001	1	15,15,16	2.07	4 (26%)	20,22,23	1.41	4 (20%)
3	AG2	B	1002	-	8,8,8	3.00	3 (37%)	7,8,8	2.60	3 (42%)

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

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	AG2	CZ-NE	7.09	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1002	AG2	CZ-NE	7.06	1.47	1.33
3	D	1002	AG2	CZ-NE	6.86	1.46	1.33
3	A	1002	AG2	CZ-NE	6.76	1.46	1.33
2	C	1001	PLP	C3-C2	-4.19	1.36	1.40
3	D	1002	AG2	CZ-NH1	4.19	1.49	1.32
2	B	1001	PLP	C4A-C4	4.18	1.60	1.51
2	D	1001	PLP	C4A-C4	-4.07	1.43	1.51
2	A	1001	PLP	P-O2P	-4.07	1.39	1.54
2	C	1001	PLP	P-O2P	-3.98	1.39	1.54
2	A	1001	PLP	P-O3P	-3.96	1.39	1.54
2	D	1001	PLP	P-O2P	-3.81	1.40	1.54
3	C	1002	AG2	CZ-NH1	3.63	1.46	1.32
3	B	1002	AG2	CZ-NH1	3.56	1.46	1.32
2	C	1001	PLP	C4A-C4	-3.53	1.44	1.51
3	A	1002	AG2	CZ-NH1	3.53	1.46	1.32
2	C	1001	PLP	P-O3P	-3.51	1.41	1.54
2	A	1001	PLP	C3-C2	-3.33	1.37	1.40
2	D	1001	PLP	C3-C2	-3.20	1.37	1.40
2	D	1001	PLP	P-O3P	-3.18	1.42	1.54
2	A	1001	PLP	P-O1P	-3.06	1.40	1.50
2	C	1001	PLP	P-O1P	-3.06	1.40	1.50
3	D	1002	AG2	CZ-NH2	2.90	1.46	1.34
3	B	1002	AG2	CZ-NH2	2.82	1.46	1.34
2	B	1001	PLP	C2-N1	2.67	1.38	1.33
3	C	1002	AG2	CZ-NH2	2.60	1.45	1.34
3	A	1002	AG2	CZ-NH2	2.45	1.44	1.34
2	B	1001	PLP	C5-C4	2.44	1.43	1.40
2	D	1001	PLP	P-O1P	-2.28	1.43	1.50
2	D	1001	PLP	O4P-C5A	-2.04	1.37	1.45

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	-5.35	106.84	119.19
3	B	1002	AG2	NE-CZ-NH1	-5.24	111.48	120.70
3	C	1002	AG2	NE-CZ-NH1	-5.09	111.74	120.70
3	A	1002	AG2	NE-CZ-NH1	-4.89	112.10	120.70
3	A	1002	AG2	NH2-CZ-NE	-4.86	107.98	119.19
3	D	1002	AG2	NE-CZ-NH1	-4.48	112.82	120.70
3	A	1002	AG2	NH2-CZ-NH1	-4.44	106.59	120.26
3	C	1002	AG2	NH2-CZ-NE	-4.41	109.02	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	PLP	C6-C5-C4	4.00	121.31	118.16
2	B	1001	PLP	C5-C6-N1	-3.87	117.37	123.82
3	C	1002	AG2	NH2-CZ-NH1	-3.49	109.51	120.26
3	B	1002	AG2	NH2-CZ-NH1	-3.05	110.87	120.26
2	A	1001	PLP	C4A-C4-C5	2.82	123.84	120.94
3	B	1002	AG2	NH2-CZ-NE	-2.77	112.80	119.19
2	A	1001	PLP	O4P-C5A-C5	2.63	114.36	109.35
2	D	1001	PLP	O4P-P-O1P	2.63	113.84	106.47
2	D	1001	PLP	C6-C5-C4	2.62	120.22	118.16
2	D	1001	PLP	C4A-C4-C5	2.54	123.55	120.94
2	C	1001	PLP	C4A-C4-C3	-2.52	116.23	120.50
2	C	1001	PLP	O4P-P-O1P	2.50	113.50	106.47
2	A	1001	PLP	O4P-P-O1P	2.44	113.31	106.47
2	C	1001	PLP	C5A-C5-C6	-2.37	115.47	119.37
3	D	1002	AG2	NH2-CZ-NH1	-2.35	113.02	120.26
2	C	1001	PLP	C6-C5-C4	2.24	119.92	118.16
2	D	1001	PLP	C5A-C5-C6	-2.23	115.70	119.37
2	B	1001	PLP	C6-N1-C2	2.20	123.24	119.17
2	D	1001	PLP	C2A-C2-C3	-2.11	118.28	120.89
2	A	1001	PLP	O2P-P-O4P	2.08	112.27	106.73
2	C	1001	PLP	O3P-P-O1P	-2.03	102.72	110.68
2	D	1001	PLP	C2A-C2-N1	2.03	121.63	117.67

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1001	PLP	C4-C5-C5A-O4P
3	A	1002	AG2	NH1-CZ-NE-CD
3	C	1002	AG2	NH1-CZ-NE-CD
2	C	1001	PLP	C4-C5-C5A-O4P
3	B	1002	AG2	NH1-CZ-NE-CD
3	D	1002	AG2	NE-CD-CG-CB
3	C	1002	AG2	NE-CD-CG-CB
3	D	1002	AG2	NH1-CZ-NE-CD
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	N-CA-CB-CG
3	B	1002	AG2	CA-CB-CG-CD
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 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	AG2	3	0
2	C	1001	PLP	1	0
2	A	1001	PLP	1	0
3	B	1002	AG2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	630/648 (97%)	-0.10	12 (1%) 66 73	16, 26, 46, 68	0
1	B	629/648 (97%)	0.02	12 (1%) 66 73	13, 25, 45, 69	0
1	C	628/648 (96%)	-0.04	14 (2%) 62 69	14, 26, 50, 68	0
1	D	629/648 (97%)	-0.03	12 (1%) 66 73	15, 26, 51, 68	0
All	All	2516/2592 (97%)	-0.04	50 (1%) 65 71	13, 26, 48, 69	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	11	LEU	6.9
1	D	393	ASN	5.6
1	D	398	ARG	4.7
1	B	124	GLU	4.7
1	D	617	GLN	4.1
1	C	125	THR	4.1
1	C	396	ASP	4.0
1	D	13	ARG	4.0
1	C	618	GLU	3.9
1	C	124	GLU	3.8
1	C	123	LEU	3.7
1	B	11	LEU	3.6
1	B	13	ARG	3.6
1	D	14	VAL	3.3
1	D	394	GLY	3.2
1	A	498	ASN	3.2
1	A	14	VAL	3.1
1	D	17	ASP	3.1
1	B	618	GLU	3.0
1	C	147	HIS	3.0
1	B	451	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	375	GLU	2.8
1	A	398	ARG	2.8
1	D	12	ASP	2.7
1	C	617	GLN	2.7
1	C	375	GLU	2.7
1	B	14	VAL	2.6
1	D	575	GLN	2.5
1	B	121	ALA	2.5
1	A	13	ARG	2.5
1	D	608	HIS	2.4
1	B	17	ASP	2.4
1	C	553	GLU	2.4
1	B	123	LEU	2.3
1	C	616	ASP	2.3
1	C	449	LYS	2.3
1	A	608	HIS	2.3
1	C	614	ARG	2.2
1	A	524	GLN	2.2
1	A	539	GLU	2.2
1	A	595	TYR	2.2
1	A	495	GLY	2.2
1	B	120	GLN	2.2
1	D	392	HIS	2.1
1	B	582	PHE	2.1
1	A	17	ASP	2.1
1	C	615	VAL	2.1
1	C	582	PHE	2.1
1	B	32	ASP	2.0
1	A	558	MET	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.



## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	AG2	C	1002	9/9	0.61	0.42	49,54,63,64	0
3	AG2	D	1002	9/9	0.67	0.31	41,46,52,52	0
3	AG2	B	1002	9/9	0.70	0.35	45,49,53,54	0
3	AG2	A	1002	9/9	0.79	0.53	49,52,58,58	0
2	PLP	D	1001	15/16	0.92	0.14	19,27,34,36	0
2	PLP	C	1001	15/16	0.95	0.14	20,30,36,40	0
2	PLP	A	1001	15/16	0.97	0.10	25,28,34,35	0
2	PLP	B	1001	15/16	0.97	0.16	21,29,32,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.