



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:46 PM UTC

PDB ID : 8ATC / pdb_00008atc
Title : COMPLEX OF N-PHOSPHONACETYL-L-ASPARTATE WITH ASPARTATE CARBAMOYLTRANSFERASE. X-RAY REFINEMENT, ANALYSIS OF CONFORMATIONAL CHANGES AND CATALYTIC AND ALLOSTERIC MECHANISMS
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Deposited on : 1989-08-25
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)
Xtrriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

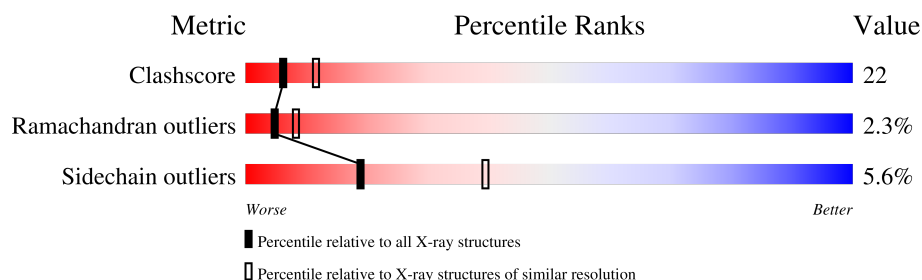
1 Overall quality at a glance

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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	310	
1	C	310	
2	B	153	
2	D	153	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8072 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 ASPARTATE CARBAMOYLTRANSFERASE (R STATE), CATALYTIC CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	C	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	GLN	GLU	conflict	UNP P0A786
A	147	GLN	GLU	conflict	UNP P0A786
A	149	GLU	GLN	conflict	UNP P0A786
A	196	GLU	GLN	conflict	UNP P0A786
C	60	GLN	GLU	conflict	UNP P0A786
C	147	GLN	GLU	conflict	UNP P0A786
C	149	GLU	GLN	conflict	UNP P0A786
C	196	GLU	GLN	conflict	UNP P0A786

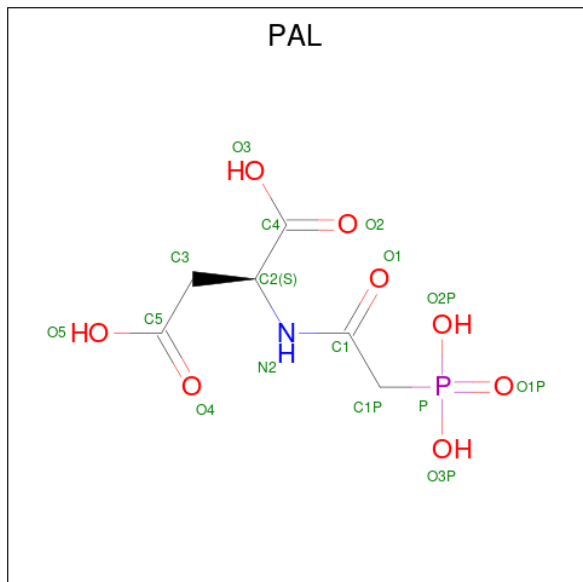
- Molecule 2 is a protein called ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1138	714	201	218	5			
2	D	146	Total	C	N	O	S	0	0	0
			1138	714	201	218	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	8	GLY	GLN	conflict	UNP P0A7F3
D	8	GLY	GLN	conflict	UNP P0A7F3

- Molecule 3 is N-(PHOSPHONACETYL)-L-ASPARTIC ACID (CCD ID: PAL) (formula: $C_6H_{10}NO_8P$).



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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		

- Molecule 5 is water.

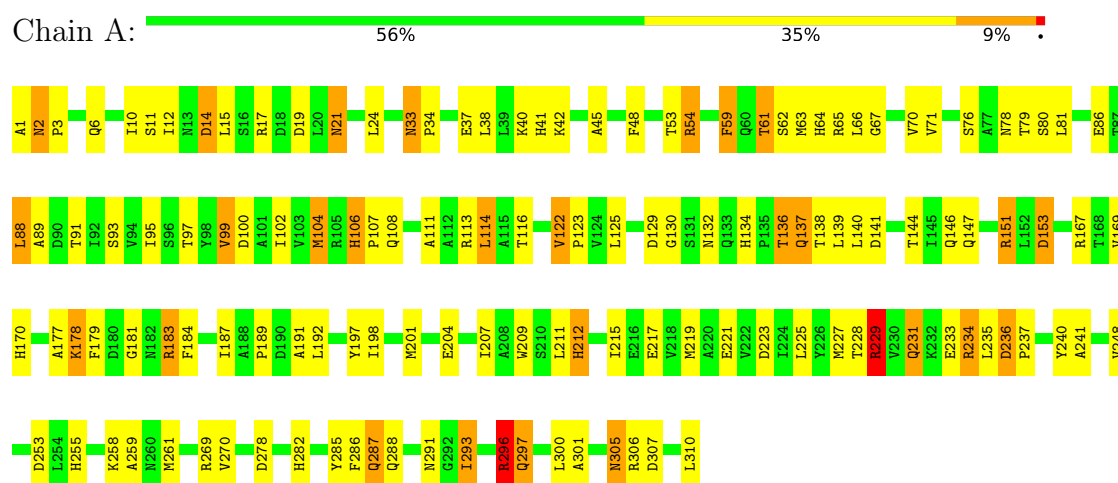
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	365	Total	O	0	0
			365	365		
5	B	128	Total	O	0	0
			128	128		
5	C	313	Total	O	0	0
			313	313		
5	D	126	Total	O	0	0
			126	126		

3 Residue-property plots

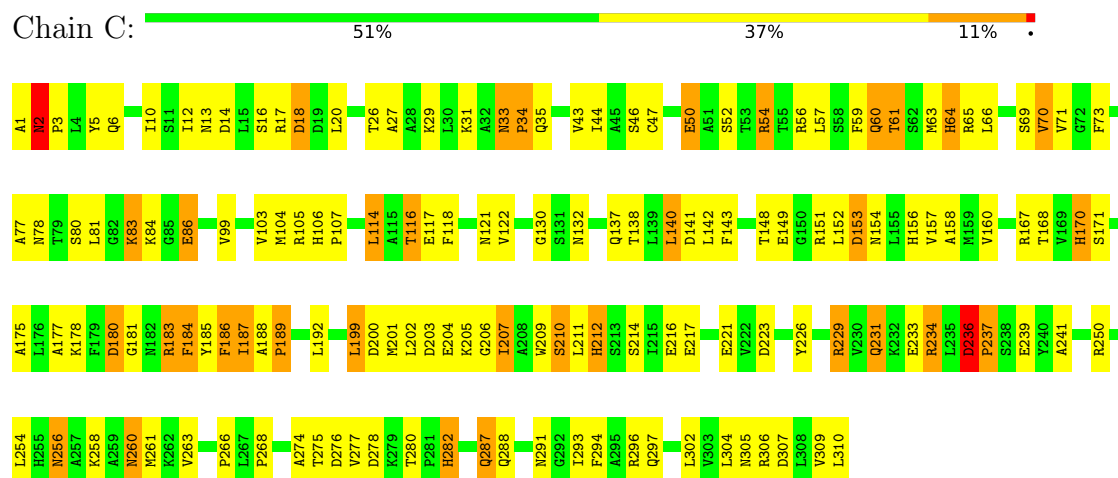
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: ASPARTATE CARBAMOYLTRANSFERASE (R STATE), CATALYTIC CHAIN

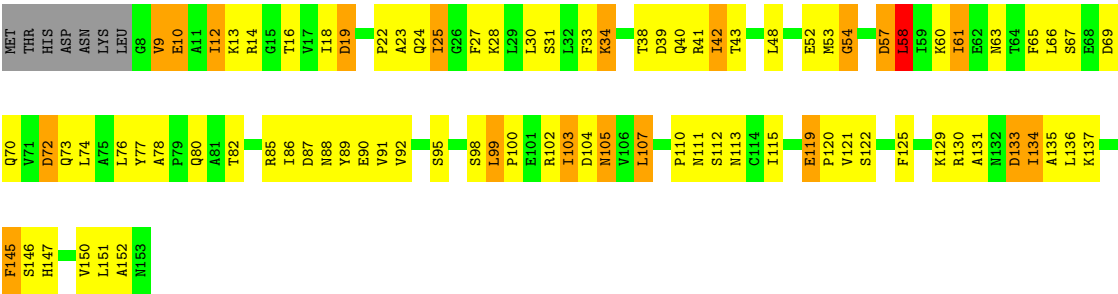


• Molecule 1: ASPARTATE CARBAMOYLTRANSFERASE (R STATE), CATALYTIC CHAIN

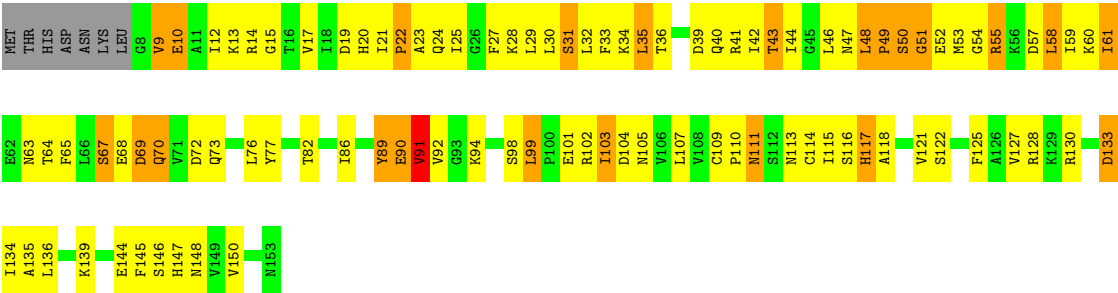
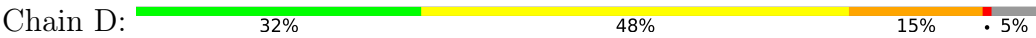


• Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN





● Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.11Å 122.11Å 156.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.165 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8072	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PAL, ZN

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	1.14	1/2461 (0.0%)	2.25	126/3339 (3.8%)
1	C	1.12	1/2461 (0.0%)	2.24	119/3339 (3.6%)
2	B	1.04	2/1155 (0.2%)	2.06	32/1561 (2.0%)
2	D	1.04	0/1155	2.13	43/1561 (2.8%)
All	All	1.10	4/7232 (0.1%)	2.20	320/9800 (3.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	229	ARG	CD-NE	-5.59	1.38	1.46
2	B	54	GLY	N-CA	-5.56	1.37	1.45
2	B	115	ILE	C-N	-5.37	1.26	1.33
1	C	229	ARG	NE-CZ	-5.13	1.27	1.33

All (320) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	229	ARG	CD-NE-CZ	18.88	150.83	124.40
1	A	229	ARG	CD-NE-CZ	17.67	149.14	124.40
1	C	14	ASP	CA-CB-CG	16.86	129.46	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	53	MET	CA-C-N	13.99	148.84	121.41
2	B	53	MET	C-N-CA	13.99	148.84	121.41
2	B	115	ILE	CA-C-N	13.99	139.55	120.38
2	B	115	ILE	C-N-CA	13.99	139.55	120.38
1	A	153	ASP	CA-CB-CG	12.52	125.11	112.60
1	A	183	ARG	CD-NE-CZ	-10.62	109.54	124.40
1	C	309	VAL	CA-C-N	10.29	140.23	121.70
1	C	309	VAL	C-N-CA	10.29	140.23	121.70
1	C	229	ARG	NE-CZ-NH1	9.70	131.20	121.50
1	A	146	GLN	OE1-CD-NE2	9.44	132.04	122.60
2	D	117	HIS	CA-C-N	9.38	132.64	120.44
2	D	117	HIS	C-N-CA	9.38	132.64	120.44
1	A	33	ASN	O-C-N	9.37	129.85	121.32
1	A	78	ASN	OD1-CG-ND2	9.37	131.97	122.60
1	A	10	ILE	N-CA-C	9.22	120.02	111.45
1	C	99	VAL	N-CA-CB	-9.06	100.91	112.60
1	C	234	ARG	CD-NE-CZ	-9.06	111.71	124.40
1	A	141	ASP	CA-CB-CG	9.06	121.66	112.60
1	C	180	ASP	CA-CB-CG	8.98	121.58	112.60
1	A	122	VAL	CB-CA-C	8.86	120.19	110.71
1	A	14	ASP	CA-CB-CG	8.77	121.37	112.60
1	C	83	LYS	N-CA-C	8.51	123.97	113.50
2	D	23	ALA	CA-C-N	8.50	134.99	122.74
2	D	23	ALA	C-N-CA	8.50	134.99	122.74
1	A	234	ARG	CD-NE-CZ	-8.47	112.53	124.40
2	D	90	GLU	CA-C-N	8.47	137.22	121.97
2	D	90	GLU	C-N-CA	8.47	137.22	121.97
1	C	2	ASN	CB-CA-C	8.45	121.02	108.86
2	D	115	ILE	CA-C-N	8.41	132.39	120.28
2	D	115	ILE	C-N-CA	8.41	132.39	120.28
1	A	229	ARG	NE-CZ-NH1	8.40	129.90	121.50
1	A	183	ARG	NE-CZ-NH1	-8.38	113.11	121.50
1	C	13	ASN	CA-CB-CG	-8.38	104.22	112.60
2	B	104	ASP	CA-C-N	8.30	137.40	121.54
2	B	104	ASP	C-N-CA	8.30	137.40	121.54
1	A	255	HIS	CA-CB-CG	8.18	121.98	113.80
1	C	170	HIS	CA-C-N	8.16	131.05	120.44
1	C	170	HIS	C-N-CA	8.16	131.05	120.44
1	A	212	HIS	CA-CB-CG	-8.00	105.80	113.80
2	D	65	PHE	CA-CB-CG	7.91	121.71	113.80
1	A	71	VAL	CA-C-O	-7.88	113.40	121.67
1	C	183	ARG	CD-NE-CZ	-7.85	113.42	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	229	ARG	NE-CZ-NH2	-7.80	112.18	119.20
2	D	133	ASP	CA-C-N	7.79	132.75	122.93
2	D	133	ASP	C-N-CA	7.79	132.75	122.93
2	D	68	GLU	N-CA-C	-7.79	105.74	114.62
1	A	139	LEU	CA-C-O	-7.63	112.81	120.82
2	B	48	LEU	N-CA-C	-7.59	100.51	110.07
1	C	6	GLN	OE1-CD-NE2	7.58	130.18	122.60
1	A	122	VAL	CA-C-O	7.58	123.62	119.15
1	C	43	VAL	O-C-N	7.57	129.79	122.97
1	A	54	ARG	CD-NE-CZ	7.48	134.88	124.40
2	D	31	SER	CA-C-N	7.43	130.45	120.65
2	D	31	SER	C-N-CA	7.43	130.45	120.65
1	C	70	VAL	N-CA-CB	-7.40	100.71	111.52
1	A	234	ARG	NE-CZ-NH1	-7.39	114.11	121.50
1	A	236	ASP	N-CA-C	-7.38	100.80	110.39
1	A	305	ASN	O-C-N	7.36	132.06	123.30
2	D	90	GLU	CA-C-O	7.36	128.65	120.70
1	C	70	VAL	CA-C-O	-7.35	112.57	120.36
1	A	48	PHE	CA-CB-CG	-7.34	106.46	113.80
1	A	6	GLN	OE1-CD-NE2	7.34	129.94	122.60
1	C	43	VAL	CA-C-O	-7.34	113.69	120.22
2	D	47	ASN	CA-CB-CG	7.33	119.93	112.60
1	C	86	GLU	CA-CB-CG	7.32	128.73	114.10
1	A	170	HIS	N-CA-C	-7.22	103.34	111.14
1	A	141	ASP	CA-C-N	7.18	129.90	120.28
1	A	141	ASP	C-N-CA	7.18	129.90	120.28
1	A	129	ASP	CA-CB-CG	7.17	119.77	112.60
2	D	53	MET	N-CA-CB	7.17	121.90	110.86
1	C	156	HIS	O-C-N	7.16	132.15	123.13
1	C	26	THR	CA-C-N	7.13	129.83	120.28
1	C	26	THR	C-N-CA	7.13	129.83	120.28
1	A	54	ARG	NE-CZ-NH1	7.11	128.61	121.50
2	D	68	GLU	O-C-N	7.11	130.91	121.67
2	B	54	GLY	N-CA-C	7.03	129.83	113.18
1	A	248	VAL	CA-C-O	-7.03	113.01	120.39
1	C	216	GLU	N-CA-C	7.02	121.43	113.01
1	A	305	ASN	CA-C-O	-7.00	112.81	120.36
1	A	147	GLN	OE1-CD-NE2	6.96	129.56	122.60
1	C	186	PHE	CA-CB-CG	6.94	120.74	113.80
1	C	188	ALA	N-CA-C	6.87	116.21	108.25
1	A	76	SER	CA-C-N	6.82	130.11	120.28
1	A	76	SER	C-N-CA	6.82	130.11	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	52	GLU	CA-C-N	6.82	130.88	121.33
2	D	52	GLU	C-N-CA	6.82	130.88	121.33
2	D	90	GLU	N-CA-C	6.82	120.52	109.40
1	A	106	HIS	O-C-N	6.80	126.71	121.88
1	A	282	HIS	CA-CB-CG	-6.76	107.04	113.80
1	C	118	PHE	CA-C-O	-6.76	111.51	119.48
1	C	121	ASN	CA-CB-CG	6.71	119.31	112.60
1	A	307	ASP	CA-CB-CG	6.70	119.30	112.60
1	A	146	GLN	CB-CG-CD	-6.69	101.23	112.60
1	C	199	LEU	CA-C-N	6.68	129.54	120.38
1	C	199	LEU	C-N-CA	6.68	129.54	120.38
1	A	179	PHE	CB-CA-C	6.68	122.00	110.45
2	B	72	ASP	CA-CB-CG	-6.67	105.93	112.60
1	A	236	ASP	CB-CA-C	6.65	118.78	108.61
1	A	113	ARG	CA-C-N	6.64	129.17	120.28
1	A	113	ARG	C-N-CA	6.64	129.17	120.28
1	A	17	ARG	NE-CZ-NH2	-6.58	113.28	119.20
1	C	274	ALA	CA-C-N	6.55	131.66	120.72
1	C	274	ALA	C-N-CA	6.55	131.66	120.72
1	C	277	VAL	CA-C-N	6.50	129.87	120.38
1	C	277	VAL	C-N-CA	6.50	129.87	120.38
2	B	119	GLU	N-CA-C	6.50	118.91	110.40
2	D	53	MET	CA-C-N	6.45	134.04	121.41
2	D	53	MET	C-N-CA	6.45	134.04	121.41
1	C	294	PHE	CA-CB-CG	-6.44	107.36	113.80
1	A	6	GLN	CA-CB-CG	-6.44	101.22	114.10
1	A	24	LEU	CA-C-O	-6.43	113.61	120.42
1	C	157	VAL	N-CA-C	6.42	117.12	107.75
1	A	93	SER	CA-C-O	-6.40	114.10	120.82
1	A	288	GLN	OE1-CD-NE2	6.39	128.99	122.60
1	C	61	THR	CA-CB-OG1	-6.36	100.06	109.60
1	C	59	PHE	CA-CB-CG	6.34	120.14	113.80
1	C	116	THR	N-CA-CB	6.32	120.07	110.28
1	A	33	ASN	CA-C-N	6.29	126.26	119.78
1	A	33	ASN	C-N-CA	6.29	126.26	119.78
1	A	80	SER	N-CA-C	-6.29	105.57	113.18
1	A	296	ARG	NE-CZ-NH2	6.28	124.85	119.20
1	C	282	HIS	CA-CB-CG	-6.27	107.53	113.80
1	C	18	ASP	CB-CA-C	6.26	120.61	110.96
1	C	52	SER	CA-C-N	6.26	129.78	121.90
1	C	52	SER	C-N-CA	6.26	129.78	121.90
1	A	181	GLY	N-CA-C	6.25	123.92	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	59	PHE	N-CA-CB	6.24	119.06	110.01
1	C	71	VAL	CA-C-O	-6.24	114.39	121.75
1	C	143	PHE	O-C-N	-6.23	115.51	122.12
1	C	260	ASN	CA-C-N	6.22	129.95	121.05
1	C	260	ASN	C-N-CA	6.22	129.95	121.05
1	C	34	PRO	CA-C-O	-6.22	114.25	121.34
2	B	133	ASP	O-C-N	6.21	129.64	122.99
1	A	223	ASP	CA-CB-CG	-6.21	106.39	112.60
1	A	78	ASN	CA-CB-CG	-6.21	106.39	112.60
1	C	305	ASN	CA-C-N	6.21	130.13	120.82
1	C	305	ASN	C-N-CA	6.21	130.13	120.82
1	A	6	GLN	N-CA-C	6.20	120.18	112.24
1	A	54	ARG	NE-CZ-NH2	-6.20	113.62	119.20
1	C	258	LYS	CA-C-O	-6.20	115.02	122.03
1	A	104	MET	N-CA-CB	-6.18	100.06	111.13
1	A	2	ASN	CA-CB-CG	6.15	118.75	112.60
1	A	269	ARG	CB-CG-CD	6.13	125.39	111.30
1	C	156	HIS	CA-C-O	-6.13	113.90	120.46
1	C	81	LEU	N-CA-C	-6.12	104.53	111.14
1	A	42	LYS	O-C-N	6.12	130.98	123.21
1	A	62	SER	CA-C-N	6.11	128.47	120.28
1	A	62	SER	C-N-CA	6.11	128.47	120.28
1	C	170	HIS	CA-CB-CG	-6.09	107.71	113.80
1	C	296	ARG	NE-CZ-NH1	6.09	127.59	121.50
2	D	69	ASP	N-CA-C	-6.08	104.57	111.14
2	B	152	ALA	N-CA-C	6.08	120.17	109.96
2	B	19	ASP	CA-C-O	-6.06	114.55	121.58
1	A	108	GLN	OE1-CD-NE2	6.04	128.64	122.60
1	C	236	ASP	N-CA-C	-6.04	101.33	110.50
1	C	103	VAL	CA-C-N	-6.01	111.36	121.94
1	C	103	VAL	C-N-CA	-6.01	111.36	121.94
1	A	134	HIS	CA-CB-CG	5.97	119.77	113.80
1	A	191	ALA	O-C-N	5.96	129.20	122.22
2	D	92	VAL	CA-C-N	5.95	125.69	121.65
2	D	92	VAL	C-N-CA	5.95	125.69	121.65
1	C	189	PRO	CA-C-O	-5.94	114.67	121.56
2	B	111	ASN	CA-C-N	5.93	128.82	120.28
2	B	111	ASN	C-N-CA	5.93	128.82	120.28
1	A	61	THR	O-C-N	5.92	128.49	122.09
1	C	31	LYS	CA-C-O	5.92	126.79	120.10
1	A	111	ALA	CA-C-N	5.91	128.68	120.29
1	A	111	ALA	C-N-CA	5.91	128.68	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	33	ASN	O-C-N	5.90	126.69	121.32
1	C	276	ASP	CA-CB-CG	5.89	118.49	112.60
1	C	137	GLN	OE1-CD-NE2	-5.89	116.71	122.60
2	D	104	ASP	CA-C-O	5.88	126.79	120.38
1	A	42	LYS	CA-C-O	-5.88	114.47	120.71
1	A	116	THR	N-CA-CB	5.88	119.27	110.22
2	D	91	VAL	CA-C-N	5.86	128.06	120.56
2	D	91	VAL	C-N-CA	5.86	128.06	120.56
1	A	241	ALA	CA-C-N	5.82	132.91	122.38
1	A	241	ALA	C-N-CA	5.82	132.91	122.38
1	C	27	ALA	CA-C-O	5.80	126.70	120.55
1	C	274	ALA	CA-C-O	-5.80	115.24	121.56
1	C	278	ASP	CA-CB-CG	5.80	118.40	112.60
2	B	57	ASP	N-CA-C	-5.78	100.47	109.72
1	A	93	SER	O-C-N	5.77	128.01	122.07
1	C	153	ASP	CA-CB-CG	5.75	118.35	112.60
1	A	297	GLN	N-CA-CB	5.72	118.31	110.01
1	C	148	THR	N-CA-C	5.72	120.32	113.23
2	D	39	ASP	CA-CB-CG	5.72	118.32	112.60
1	C	205	LYS	CA-C-N	5.72	130.72	120.77
1	C	205	LYS	C-N-CA	5.72	130.72	120.77
2	D	51	GLY	CA-C-N	5.72	128.21	120.38
2	D	51	GLY	C-N-CA	5.72	128.21	120.38
1	C	256	ASN	OD1-CG-ND2	-5.71	116.89	122.60
1	C	275	THR	N-CA-C	5.70	119.49	112.54
2	B	58	LEU	CB-CA-C	5.70	119.62	109.65
1	A	278	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	178	LYS	N-CA-C	-5.68	106.35	113.28
2	D	24	GLN	CA-CB-CG	-5.68	102.75	114.10
1	A	192	LEU	N-CA-CB	-5.67	101.87	111.17
1	C	212	HIS	CA-CB-CG	-5.66	108.14	113.80
1	C	234	ARG	NE-CZ-NH1	-5.66	115.84	121.50
1	C	307	ASP	CA-C-N	5.65	128.86	120.90
1	C	307	ASP	C-N-CA	5.65	128.86	120.90
1	C	236	ASP	CB-CA-C	5.63	117.53	108.91
1	C	214	SER	O-C-N	5.63	129.79	123.48
1	A	102	ILE	CA-C-O	-5.63	114.58	120.27
1	A	259	ALA	CA-C-N	5.63	130.99	121.14
1	A	259	ALA	C-N-CA	5.63	130.99	121.14
1	A	100	ASP	CA-C-N	5.61	131.46	121.75
1	A	100	ASP	C-N-CA	5.61	131.46	121.75
1	C	122	VAL	N-CA-C	5.61	112.67	107.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	ILE	CA-C-N	5.61	128.25	120.29
1	A	293	ILE	C-N-CA	5.61	128.25	120.29
2	B	135	ALA	CA-C-N	-5.61	115.27	123.00
2	B	135	ALA	C-N-CA	-5.61	115.27	123.00
1	C	29	LYS	CA-C-O	-5.60	114.94	120.82
1	A	19	ASP	O-C-N	5.59	127.83	122.07
2	D	70	GLN	OE1-CD-NE2	5.59	128.19	122.60
1	C	256	ASN	CA-CB-CG	5.59	118.19	112.60
1	C	60	GLN	CA-C-O	-5.58	114.64	120.55
1	A	114	LEU	CA-CB-CG	5.57	135.78	116.30
1	A	11	SER	CA-C-O	-5.55	114.28	120.66
1	C	50	GLU	CA-C-O	-5.54	115.35	121.33
1	C	184	PHE	N-CA-C	5.53	118.25	109.24
1	C	263	VAL	CA-C-O	-5.53	114.56	120.59
1	A	215	ILE	CA-C-N	5.53	128.45	120.38
1	A	215	ILE	C-N-CA	5.53	128.45	120.38
1	C	137	GLN	N-CA-C	-5.52	104.12	111.24
1	A	89	ALA	O-C-N	-5.52	116.35	122.09
1	A	223	ASP	N-CA-C	-5.50	106.25	113.12
1	C	137	GLN	N-CA-CB	5.49	118.14	110.07
1	C	47	CYS	N-CA-C	5.47	118.19	107.57
1	C	250	ARG	CA-C-O	-5.47	115.06	121.46
1	A	97	THR	N-CA-CB	5.47	119.05	110.46
1	C	221	GLU	CA-CB-CG	5.45	124.99	114.10
2	D	99	LEU	O-C-N	5.45	127.58	121.32
1	A	300	LEU	CA-C-N	5.43	127.55	120.28
1	A	300	LEU	C-N-CA	5.43	127.55	120.28
2	B	113	ASN	OD1-CG-ND2	5.43	128.03	122.60
2	B	82	THR	O-C-N	5.42	129.56	123.27
1	A	137	GLN	N-CA-C	-5.41	105.30	111.14
1	A	53	THR	N-CA-CB	5.40	121.75	111.00
1	A	99	VAL	N-CA-C	5.40	116.95	109.29
1	A	108	GLN	CA-CB-CG	-5.39	103.32	114.10
1	C	187	ILE	N-CA-C	5.39	114.50	106.85
1	C	268	PRO	O-C-N	5.38	131.33	121.10
1	C	35	GLN	CA-C-N	5.38	126.57	119.84
1	C	35	GLN	C-N-CA	5.38	126.57	119.84
2	B	74	LEU	O-C-N	5.38	127.61	122.07
2	B	99	LEU	O-C-N	5.37	125.98	121.31
1	A	122	VAL	N-CA-C	5.36	113.17	107.76
1	A	189	PRO	N-CA-C	-5.35	102.70	111.21
2	B	152	ALA	CA-C-N	5.35	131.32	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	152	ALA	C-N-CA	5.35	131.32	121.70
1	A	130	GLY	CA-C-O	-5.34	114.95	121.68
1	A	138	THR	CA-C-O	-5.34	115.21	120.82
1	A	235	LEU	CA-C-O	5.34	127.21	121.44
1	A	88	LEU	CB-CA-C	5.33	119.92	110.85
2	D	52	GLU	CB-CG-CD	5.33	121.67	112.60
1	C	43	VAL	N-CA-CB	5.32	119.26	112.34
1	C	275	THR	CA-C-N	5.31	129.59	120.72
1	C	275	THR	C-N-CA	5.31	129.59	120.72
2	B	19	ASP	N-CA-CB	-5.31	102.99	111.43
2	D	111	ASN	CA-CB-CG	-5.31	107.29	112.60
2	B	58	LEU	N-CA-CB	-5.30	101.90	110.81
1	A	71	VAL	N-CA-C	-5.28	100.24	108.95
1	A	79	THR	N-CA-C	-5.28	103.72	110.53
1	A	167	ARG	N-CA-C	-5.28	105.64	111.71
1	C	6	GLN	CA-CB-CG	-5.28	103.55	114.10
2	B	12	ILE	N-CA-C	-5.27	101.47	108.96
1	A	221	GLU	CB-CG-CD	-5.26	103.65	112.60
1	A	54	ARG	N-CA-C	5.24	116.80	111.14
1	A	286	PHE	CA-C-O	-5.24	113.61	119.79
1	A	183	ARG	NH1-CZ-NH2	5.24	126.11	119.30
2	B	145	PHE	CA-CB-CG	5.24	119.04	113.80
1	A	53	THR	N-CA-C	-5.23	103.07	111.02
1	C	64	HIS	CA-C-N	5.22	128.95	120.60
1	C	64	HIS	C-N-CA	5.22	128.95	120.60
2	D	49	PRO	CA-C-N	5.22	131.51	121.54
2	D	49	PRO	C-N-CA	5.22	131.51	121.54
2	D	133	ASP	CA-CB-CG	-5.21	107.39	112.60
1	A	67	GLY	N-CA-C	5.19	122.78	115.30
1	C	73	PHE	CA-CB-CG	5.18	118.98	113.80
1	C	70	VAL	N-CA-C	5.18	115.58	108.12
1	A	197	TYR	CA-C-N	5.17	128.14	120.74
1	A	197	TYR	C-N-CA	5.17	128.14	120.74
1	A	125	LEU	CB-CA-C	5.17	118.66	109.72
1	A	258	LYS	CA-C-O	-5.16	115.88	121.87
2	B	107	LEU	CB-CA-C	5.16	118.85	109.83
1	A	37	GLU	N-CA-C	5.15	118.61	111.71
1	A	217	GLU	CA-CB-CG	5.15	124.39	114.10
1	C	184	PHE	CA-CB-CG	-5.14	108.66	113.80
1	C	304	LEU	N-CA-CB	-5.14	102.85	110.61
1	C	78	ASN	CB-CA-C	5.13	119.24	110.56
2	D	113	ASN	CA-CB-CG	5.13	117.73	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	LYS	N-CA-C	-5.11	103.79	110.53
2	D	118	ALA	N-CA-C	5.10	116.53	111.07
1	C	231	GLN	O-C-N	5.10	129.37	122.59
1	A	204	GLU	CB-CA-C	-5.10	102.65	110.81
1	A	19	ASP	N-CA-C	-5.08	105.63	111.07
1	C	50	GLU	CG-CD-OE2	-5.07	106.75	118.40
2	B	134	ILE	O-C-N	5.07	128.30	122.93
1	C	241	ALA	CA-C-N	5.06	131.26	122.56
1	C	241	ALA	C-N-CA	5.06	131.26	122.56
1	C	2	ASN	CA-CB-CG	5.06	117.66	112.60
1	C	239	GLU	CA-C-O	-5.05	113.65	119.56
1	C	69	SER	CA-C-N	-5.05	115.97	122.99
1	C	69	SER	C-N-CA	-5.05	115.97	122.99
1	A	296	ARG	CD-NE-CZ	-5.04	117.34	124.40
2	D	39	ASP	N-CA-C	-5.04	106.88	112.57
1	C	168	THR	CA-C-O	-5.03	115.54	120.82
1	C	199	LEU	CB-CA-C	5.03	119.40	110.85
1	A	229	ARG	NE-CZ-NH2	-5.02	114.68	119.20
1	A	144	THR	CA-C-N	5.02	126.97	120.70
1	A	144	THR	C-N-CA	5.02	126.97	120.70
1	C	29	LYS	O-C-N	5.02	127.24	122.07
2	B	12	ILE	O-C-N	5.01	128.23	122.97
1	C	237	PRO	N-CD-CG	-5.01	95.69	103.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	296	ARG	Sidechain
1	C	54	ARG	Sidechain

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	2415	0	2422	66	0
1	C	2415	0	2422	83	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1138	0	1154	71	0
2	D	1138	0	1154	113	1
3	A	16	0	5	0	0
3	C	16	0	6	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	365	0	0	5	1
5	B	128	0	0	1	0
5	C	313	0	0	1	1
5	D	126	0	0	3	0
All	All	8072	0	7163	321	4

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 22.

All (321) 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)
2:D:30:LEU:HD13	2:D:59:ILE:HD13	1.20	1.11
2:D:22:PRO:HB2	2:D:25:ILE:HD12	1.35	1.09
2:B:9:VAL:O	2:B:10:GLU:HG2	1.54	1.04
2:D:10:GLU:HB2	2:D:43:THR:HG21	1.44	1.00
1:A:287:GLN:HE21	1:A:287:GLN:N	1.63	0.96
2:D:22:PRO:HB2	2:D:25:ILE:CD1	1.96	0.95
2:D:82:THR:CG2	2:D:94:LYS:HE3	1.96	0.95
1:A:287:GLN:H	1:A:287:GLN:NE2	1.67	0.93
1:C:114:LEU:HD22	2:D:121:VAL:HG11	1.50	0.92
2:D:82:THR:HG21	2:D:94:LYS:HE3	1.51	0.92
1:C:234:ARG:HG3	1:C:234:ARG:HH11	1.35	0.91
2:D:40:GLN:OE1	2:D:63:ASN:HB2	1.72	0.90
2:D:134:ILE:H	2:D:147:HIS:HD2	1.20	0.89
2:D:46:LEU:HA	2:D:57:ASP:OD2	1.73	0.88
2:D:9:VAL:O	2:D:10:GLU:HG2	1.75	0.85
2:B:58:LEU:HD21	2:B:60:LYS:HE3	1.59	0.85
2:D:30:LEU:HD13	2:D:59:ILE:CD1	2.04	0.84
2:B:105:ASN:HB3	2:B:122:SER:HB3	1.58	0.83
1:A:287:GLN:HE21	1:A:287:GLN:H	0.84	0.82
2:B:42:ILE:HD13	2:B:61:ILE:HG23	1.62	0.82
2:D:30:LEU:CD1	2:D:59:ILE:HD13	2.08	0.82
1:C:287:GLN:H	1:C:287:GLN:HE21	1.25	0.82
2:D:134:ILE:H	2:D:147:HIS:CD2	1.98	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:ILE:H	2:B:147:HIS:CD2	1.98	0.81
2:D:30:LEU:HD21	2:D:44:ILE:CD1	2.11	0.81
2:D:30:LEU:HD21	2:D:44:ILE:HD13	1.63	0.81
2:B:134:ILE:H	2:B:147:HIS:HD2	1.28	0.80
1:C:234:ARG:HG3	1:C:234:ARG:NH1	1.97	0.78
1:A:234:ARG:HG3	1:A:234:ARG:HH11	1.48	0.78
2:D:42:ILE:HG12	2:D:61:ILE:HG23	1.66	0.77
2:B:72:ASP:HB3	2:B:100:PRO:HG3	1.65	0.77
2:D:36:THR:HG22	2:D:36:THR:O	1.81	0.77
2:D:133:ASP:HB2	2:D:147:HIS:CD2	2.20	0.77
2:D:9:VAL:HG11	2:D:58:LEU:HD13	1.69	0.75
2:D:58:LEU:HD21	2:D:60:LYS:CE	2.17	0.75
1:C:200:ASP:O	1:C:204:GLU:HG3	1.86	0.74
2:B:13:LYS:HG3	2:B:89:TYR:CE1	2.21	0.74
2:D:32:LEU:CD1	2:D:77:TYR:CZ	2.69	0.74
1:A:114:LEU:CD2	2:B:121:VAL:HG11	2.18	0.74
2:B:103:ILE:HD12	2:B:107:LEU:HD12	1.70	0.74
1:A:219:MET:HE3	1:A:253:ASP:O	1.88	0.74
2:B:10:GLU:HG3	2:B:43:THR:HG21	1.71	0.73
2:B:134:ILE:HB	2:B:147:HIS:CD2	2.23	0.73
2:D:32:LEU:HD11	2:D:77:TYR:OH	1.89	0.73
1:C:184:PHE:O	1:C:209:TRP:HA	1.88	0.73
1:C:66:LEU:HD21	1:C:297:GLN:HE21	1.53	0.72
2:D:58:LEU:C	2:D:58:LEU:HD23	2.15	0.72
2:D:9:VAL:HG11	2:D:58:LEU:CD1	2.19	0.72
1:A:64:HIS:HD2	5:A:325:HOH:O	1.72	0.72
2:D:10:GLU:CB	2:D:43:THR:HG21	2.19	0.72
2:B:76:LEU:HD11	2:B:103:ILE:HD13	1.71	0.72
1:C:287:GLN:H	1:C:287:GLN:NE2	1.87	0.71
1:A:106:HIS:ND1	1:A:107:PRO:HD2	2.05	0.70
2:D:99:LEU:HD21	2:D:134:ILE:HD13	1.73	0.70
2:B:67:SER:HB2	2:B:70:GLN:HG3	1.74	0.70
1:C:106:HIS:CG	1:C:107:PRO:HD2	2.26	0.70
2:B:38:THR:CG2	2:B:42:ILE:HD11	2.22	0.70
1:C:114:LEU:CD2	2:D:121:VAL:HG11	2.19	0.70
2:D:76:LEU:HD11	2:D:103:ILE:CD1	2.21	0.69
2:D:76:LEU:HD11	2:D:103:ILE:HD11	1.75	0.69
2:B:86:ILE:HA	2:B:90:GLU:O	1.93	0.69
1:A:65:ARG:HB2	1:A:297:GLN:HE21	1.57	0.69
1:A:137:GLN:NE2	5:A:378:HOH:O	2.26	0.68
1:A:234:ARG:HG3	1:A:234:ARG:NH1	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:82:THR:HG23	2:D:94:LYS:HE3	1.76	0.67
2:D:29:LEU:HD21	2:D:77:TYR:CB	2.25	0.67
1:C:106:HIS:ND1	1:C:107:PRO:HD2	2.10	0.67
2:D:48:LEU:O	2:D:55:ARG:HA	1.95	0.66
1:C:114:LEU:HD22	2:D:121:VAL:CG1	2.26	0.66
2:D:58:LEU:HD21	2:D:60:LYS:HE3	1.77	0.65
1:A:237:PRO:HA	1:A:240:TYR:CD1	2.31	0.65
2:B:38:THR:HG21	2:B:42:ILE:HD11	1.79	0.65
1:C:234:ARG:NH1	1:C:234:ARG:CG	2.54	0.65
1:A:236:ASP:OD2	1:A:237:PRO:HD2	1.96	0.65
2:D:58:LEU:HD21	2:D:60:LYS:HG3	1.79	0.65
2:D:21:ILE:O	2:D:22:PRO:C	2.40	0.64
2:D:67:SER:OG	2:D:70:GLN:HG3	1.98	0.64
1:C:141:ASP:OD1	1:C:288:GLN:NE2	2.29	0.64
2:D:14:ARG:HA	2:D:86:ILE:HG22	1.80	0.64
1:A:88:LEU:HD11	1:A:104:MET:HE3	1.81	0.62
2:B:40:GLN:OE1	2:B:63:ASN:HB2	1.98	0.62
1:C:261:MET:O	1:C:282:HIS:ND1	2.31	0.62
1:A:187:ILE:HG12	1:A:212:HIS:HB2	1.82	0.62
1:A:106:HIS:CG	1:A:107:PRO:HD2	2.35	0.62
2:B:10:GLU:HB2	2:B:60:LYS:HD2	1.82	0.61
2:B:99:LEU:HD12	2:B:129:LYS:HB3	1.81	0.61
2:B:134:ILE:N	2:B:147:HIS:HD2	1.98	0.61
2:B:69:ASP:O	2:B:72:ASP:N	2.34	0.61
2:B:9:VAL:O	2:B:10:GLU:CG	2.40	0.61
2:D:40:GLN:OE1	2:D:63:ASN:CB	2.45	0.61
2:D:25:ILE:O	2:D:29:LEU:HG	2.00	0.60
2:D:32:LEU:HD11	2:D:77:TYR:CZ	2.35	0.60
1:C:310:LEU:N	1:C:310:LEU:HD12	2.16	0.60
1:A:114:LEU:HD23	2:B:121:VAL:HG11	1.84	0.59
1:C:138:THR:OG1	1:C:171:SER:HB3	2.01	0.59
2:D:32:LEU:CD1	2:D:77:TYR:OH	2.48	0.59
2:D:145:PHE:HB2	2:D:150:VAL:HG23	1.84	0.59
1:A:225:LEU:HB3	1:A:261:MET:CE	2.33	0.58
2:B:76:LEU:HD11	2:B:103:ILE:CD1	2.33	0.58
2:D:13:LYS:HG3	2:D:89:TYR:CE1	2.39	0.58
2:B:99:LEU:CD1	2:B:129:LYS:HB3	2.33	0.58
1:A:2:ASN:HB2	1:A:3:PRO:HD2	1.86	0.58
1:A:65:ARG:HB2	1:A:297:GLN:NE2	2.19	0.58
2:D:9:VAL:HG13	2:D:60:LYS:HE3	1.85	0.58
2:D:13:LYS:O	2:D:13:LYS:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ASP:OD2	5:A:474:HOH:O	2.17	0.57
2:B:87:ASP:HB3	2:B:92:VAL:HG21	1.86	0.57
2:B:91:VAL:HG12	2:B:91:VAL:O	2.03	0.57
1:A:88:LEU:HD21	1:A:104:MET:HE1	1.87	0.57
1:A:231:GLN:HE21	1:A:234:ARG:HH12	1.53	0.57
2:B:16:THR:OG1	2:B:65:PHE:HA	2.05	0.56
2:D:107:LEU:HD13	2:D:150:VAL:HG11	1.87	0.56
2:B:119:GLU:OE2	2:B:120:PRO:HD2	2.05	0.56
2:D:12:ILE:HD11	2:D:17:VAL:CG2	2.35	0.56
2:D:20:HIS:HE1	5:D:916:HOH:O	1.89	0.56
1:A:61:THR:HB	1:A:293:ILE:HD11	1.88	0.56
1:A:234:ARG:NH1	1:A:234:ARG:CG	2.60	0.56
1:C:236:ASP:HB2	1:C:237:PRO:HD2	1.87	0.56
1:A:106:HIS:CE1	1:A:107:PRO:HD2	2.41	0.55
1:A:229:ARG:NH2	1:A:233:GLU:OE1	2.32	0.55
1:A:12:ILE:O	1:A:12:ILE:CG2	2.54	0.55
1:A:88:LEU:HD11	1:A:104:MET:CE	2.36	0.55
1:C:114:LEU:CD2	2:D:121:VAL:CG1	2.82	0.55
1:C:130:GLY:O	1:C:167:ARG:HD3	2.06	0.55
1:C:201:MET:HG2	1:C:201:MET:O	1.97	0.55
2:B:10:GLU:CB	2:B:60:LYS:HD2	2.37	0.55
1:C:189:PRO:HG2	1:C:192:LEU:HB2	1.87	0.55
1:A:169:VAL:CG1	1:A:228:THR:HG21	2.37	0.54
2:B:27:PHE:CE2	2:D:27:PHE:CE2	2.96	0.54
1:C:204:GLU:C	1:C:206:GLY:H	2.15	0.54
2:D:10:GLU:OE1	2:D:41:ARG:NH2	2.41	0.54
2:B:133:ASP:OD2	2:B:146:SER:OG	2.24	0.54
2:B:10:GLU:HB2	2:B:60:LYS:HZ2	1.73	0.54
2:B:130:ARG:HB2	2:B:133:ASP:O	2.07	0.54
1:C:10:ILE:HD11	1:C:116:THR:CG2	2.38	0.54
1:C:154:ASN:HA	1:C:181:GLY:O	2.08	0.54
2:B:102:ARG:HA	2:B:125:PHE:O	2.08	0.54
1:A:225:LEU:CB	1:A:261:MET:CE	2.87	0.53
2:B:40:GLN:O	2:B:42:ILE:HG12	2.09	0.53
2:D:29:LEU:HD22	2:D:33:PHE:HE1	1.73	0.53
2:D:17:VAL:HG23	2:D:86:ILE:HD12	1.90	0.53
2:B:85:ARG:C	2:B:86:ILE:HG13	2.34	0.52
2:B:22:PRO:O	2:B:25:ILE:HB	2.10	0.52
2:B:136:LEU:HD12	2:B:150:VAL:HG21	1.91	0.52
1:A:65:ARG:CB	1:A:297:GLN:NE2	2.73	0.52
2:B:39:ASP:OD1	2:D:55:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:ILE:HD12	2:B:107:LEU:CD1	2.39	0.52
1:C:138:THR:HG21	1:C:175:ALA:HB2	1.91	0.52
1:A:287:GLN:N	1:A:287:GLN:NE2	2.40	0.52
1:C:140:LEU:HD12	1:C:140:LEU:C	2.35	0.52
1:C:310:LEU:N	1:C:310:LEU:CD1	2.73	0.52
1:A:81:LEU:HA	1:A:86:GLU:HB3	1.92	0.51
2:B:102:ARG:HB2	2:B:125:PHE:O	2.09	0.51
2:D:29:LEU:HD21	2:D:77:TYR:CG	2.45	0.51
1:A:225:LEU:HB3	1:A:261:MET:HE2	1.91	0.51
1:C:310:LEU:CD1	1:C:310:LEU:H	2.23	0.51
1:A:1:ALA:HA	1:A:306:ARG:CG	2.41	0.51
1:A:38:LEU:HD12	1:A:66:LEU:HD22	1.91	0.51
2:D:107:LEU:HD13	2:D:150:VAL:CG1	2.39	0.51
1:A:1:ALA:HA	1:A:306:ARG:HG2	1.91	0.51
2:D:90:GLU:CG	2:D:91:VAL:N	2.73	0.51
1:C:61:THR:O	1:C:65:ARG:HG2	2.11	0.51
2:D:58:LEU:CD2	2:D:60:LYS:HG3	2.40	0.51
2:B:78:ALA:C	2:B:80:GLN:H	2.19	0.50
2:D:9:VAL:CG1	2:D:60:LYS:HE3	2.42	0.50
1:C:229:ARG:NH2	1:C:233:GLU:OE1	2.42	0.50
2:D:58:LEU:C	2:D:58:LEU:CD2	2.85	0.50
2:D:49:PRO:O	2:D:50:SER:HB2	2.11	0.50
2:B:73:GLN:O	2:B:77:TYR:HD2	1.94	0.49
1:C:202:LEU:O	1:C:207:ILE:N	2.40	0.49
2:D:15:GLY:HA2	2:D:64:THR:O	2.11	0.49
1:A:45:ALA:HB2	1:A:99:VAL:HG11	1.94	0.49
2:B:23:ALA:O	2:B:24:GLN:HB2	2.11	0.49
2:D:130:ARG:HD2	2:D:135:ALA:HB2	1.95	0.49
1:C:151:ARG:O	1:C:152:LEU:HD23	2.13	0.49
1:A:114:LEU:CD2	2:B:121:VAL:CG1	2.89	0.49
1:C:80:SER:OG	1:C:84:LYS:HD2	2.13	0.49
2:D:10:GLU:O	2:D:60:LYS:NZ	2.45	0.49
2:B:134:ILE:CB	2:B:147:HIS:CD2	2.95	0.48
1:A:140:LEU:HD12	1:A:140:LEU:C	2.37	0.48
2:D:76:LEU:HD23	2:D:134:ILE:HD12	1.94	0.48
1:C:77:ALA:O	1:C:83:LYS:HE3	2.13	0.48
1:C:5:TYR:CD2	1:C:306:ARG:HA	2.47	0.48
2:D:69:ASP:O	2:D:73:GLN:HG3	2.14	0.48
2:D:30:LEU:HD21	2:D:44:ILE:HD11	1.93	0.48
1:A:177:ALA:HB1	1:A:207:ILE:HD12	1.95	0.48
1:C:64:HIS:HE1	5:C:345:HOH:O	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:ASP:O	2:B:88:ASN:HB3	2.14	0.48
1:C:2:ASN:HA	1:C:3:PRO:HD3	1.79	0.48
1:C:63:MET:SD	1:C:70:VAL:HG22	2.53	0.48
2:D:36:THR:O	2:D:36:THR:CG2	2.50	0.48
1:C:20:LEU:HD13	1:C:142:LEU:CD1	2.44	0.47
2:B:41:ARG:NH1	5:B:224:HOH:O	2.48	0.47
2:B:85:ARG:C	2:B:86:ILE:CG1	2.87	0.47
1:C:203:ASP:O	1:C:206:GLY:HA2	2.14	0.47
1:A:106:HIS:CG	1:A:107:PRO:CD	2.97	0.47
2:B:125:PHE:HA	2:B:137:LYS:O	2.15	0.47
1:C:16:SER:C	1:C:18:ASP:N	2.72	0.47
1:C:160:VAL:HG22	1:C:187:ILE:HB	1.97	0.47
1:A:122:VAL:HA	1:A:123:PRO:HD3	1.78	0.47
1:C:12:ILE:HD13	1:C:12:ILE:HA	1.75	0.47
1:C:151:ARG:NH1	1:C:154:ASN:O	2.47	0.47
2:D:28:LYS:HE3	5:D:835:HOH:O	2.14	0.47
2:D:102:ARG:HA	2:D:127:VAL:HG23	1.96	0.47
2:D:134:ILE:N	2:D:147:HIS:HD2	1.99	0.47
2:D:133:ASP:OD1	2:D:133:ASP:N	2.34	0.47
2:B:33:PHE:HD2	2:B:33:PHE:HA	1.57	0.47
1:C:287:GLN:NE2	1:C:287:GLN:N	2.61	0.47
1:C:151:ARG:HD2	1:C:153:ASP:O	2.15	0.46
2:D:42:ILE:CG1	2:D:61:ILE:HG23	2.40	0.46
1:A:225:LEU:CB	1:A:261:MET:HE2	2.44	0.46
1:C:231:GLN:HE21	1:C:234:ARG:HH12	1.63	0.46
2:D:32:LEU:HD13	2:D:77:TYR:CZ	2.49	0.46
1:C:114:LEU:HD13	1:C:114:LEU:O	2.15	0.46
1:C:175:ALA:O	1:C:178:LYS:HB2	2.15	0.46
1:C:229:ARG:HH22	1:C:233:GLU:CD	2.22	0.46
1:A:209:TRP:HZ3	1:A:211:LEU:HD21	1.81	0.46
2:B:110:PRO:HG2	2:B:145:PHE:CG	2.50	0.46
1:C:61:THR:HB	1:C:293:ILE:HD11	1.98	0.46
2:D:99:LEU:HD21	2:D:134:ILE:CD1	2.44	0.46
2:D:146:SER:O	2:D:147:HIS:C	2.59	0.46
1:C:149:GLU:OE2	1:C:260:ASN:ND2	2.40	0.46
2:D:14:ARG:CA	2:D:86:ILE:HG22	2.45	0.46
2:D:58:LEU:HD21	2:D:60:LYS:HE2	1.97	0.46
2:D:130:ARG:CD	2:D:135:ALA:HB2	2.46	0.46
2:B:25:ILE:O	2:B:25:ILE:CG2	2.64	0.46
2:D:20:HIS:O	2:D:22:PRO:HD3	2.15	0.46
1:A:61:THR:HB	1:A:293:ILE:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:MET:O	1:C:201:MET:CG	2.59	0.46
2:D:12:ILE:HD11	2:D:17:VAL:HG23	1.97	0.46
1:C:223:ASP:O	1:C:261:MET:HA	2.16	0.45
2:D:9:VAL:HG11	2:D:58:LEU:HD11	1.96	0.45
2:D:46:LEU:CA	2:D:57:ASP:OD2	2.57	0.45
1:A:261:MET:HG3	5:A:639:HOH:O	2.16	0.45
2:B:130:ARG:HB3	2:B:131:ALA:H	1.45	0.45
1:C:199:LEU:HD13	1:C:209:TRP:CH2	2.52	0.45
1:A:151:ARG:HG3	1:A:153:ASP:O	2.17	0.45
1:A:237:PRO:HA	1:A:240:TYR:CE1	2.52	0.45
1:C:186:PHE:CE1	1:C:199:LEU:HD21	2.51	0.45
2:D:9:VAL:HG13	2:D:60:LYS:CE	2.46	0.45
1:A:12:ILE:O	1:A:12:ILE:HG22	2.15	0.45
2:D:19:ASP:O	2:D:20:HIS:HB2	2.16	0.45
1:C:170:HIS:N	1:C:170:HIS:CD2	2.82	0.45
1:C:204:GLU:OE1	2:D:128:ARG:NH2	2.50	0.45
1:C:226:TYR:CZ	1:C:266:PRO:HD3	2.52	0.45
1:A:59:PHE:HZ	1:A:136:THR:HG21	1.82	0.44
1:C:50:GLU:HB3	1:C:105:ARG:HG2	1.99	0.44
2:D:136:LEU:O	2:D:144:GLU:HA	2.18	0.44
2:B:30:LEU:HD23	2:D:27:PHE:HE2	1.83	0.44
2:B:99:LEU:HD21	2:B:134:ILE:HD13	1.98	0.44
1:C:212:HIS:N	1:C:212:HIS:CD2	2.86	0.44
2:D:98:SER:O	2:D:99:LEU:C	2.61	0.44
2:B:19:ASP:OD2	2:B:58:LEU:HD12	2.18	0.44
1:C:56:ARG:O	1:C:60:GLN:HG3	2.18	0.43
1:A:33:ASN:HA	1:A:34:PRO:HD2	1.84	0.43
2:B:119:GLU:HB3	2:B:120:PRO:HD2	2.00	0.43
1:C:177:ALA:HB1	1:C:207:ILE:HD12	2.00	0.43
1:A:291:ASN:HD22	1:A:291:ASN:HA	1.49	0.43
1:A:40:LYS:O	1:A:41:HIS:HB2	2.18	0.43
1:C:186:PHE:HE1	1:C:199:LEU:CD2	2.31	0.43
2:D:12:ILE:HD11	2:D:17:VAL:HG22	2.01	0.43
2:B:105:ASN:HB3	2:B:122:SER:CB	2.41	0.43
1:C:211:LEU:C	1:C:212:HIS:CD2	2.97	0.43
2:B:23:ALA:HA	2:B:57:ASP:OD1	2.19	0.43
1:A:184:PHE:O	1:A:209:TRP:HA	2.19	0.43
2:B:10:GLU:HB2	2:B:60:LYS:NZ	2.33	0.43
2:B:33:PHE:O	2:B:34:LYS:CB	2.66	0.43
1:C:210:SER:HB2	1:C:212:HIS:NE2	2.34	0.43
1:C:254:LEU:HD12	1:C:280:THR:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:35:LEU:O	2:D:42:ILE:HD11	2.19	0.43
2:B:28:LYS:O	2:B:31:SER:HB3	2.18	0.43
1:C:106:HIS:CE1	1:C:107:PRO:HD2	2.54	0.43
2:D:70:GLN:HA	2:D:73:GLN:OE1	2.19	0.43
2:D:76:LEU:HD11	2:D:103:ILE:HD13	1.99	0.43
2:B:103:ILE:CD1	2:B:107:LEU:CD1	2.97	0.42
1:C:261:MET:SD	1:C:261:MET:C	3.02	0.42
2:D:21:ILE:O	2:D:22:PRO:O	2.37	0.42
2:D:28:LYS:CE	5:D:835:HOH:O	2.67	0.42
2:D:91:VAL:O	2:D:91:VAL:HG12	2.19	0.42
1:C:186:PHE:CE1	1:C:199:LEU:CD2	3.02	0.42
1:A:64:HIS:HE1	5:A:388:HOH:O	2.02	0.42
2:D:110:PRO:HD2	2:D:145:PHE:CZ	2.54	0.42
1:A:227:MET:HE3	1:A:227:MET:HB3	1.87	0.42
1:C:33:ASN:HA	1:C:34:PRO:HD2	1.74	0.42
2:D:103:ILE:HG13	2:D:127:VAL:CG2	2.50	0.42
1:A:169:VAL:HG13	1:A:228:THR:HG21	2.00	0.42
1:C:158:ALA:HA	1:C:185:TYR:O	2.20	0.42
2:D:90:GLU:HG2	2:D:91:VAL:N	2.34	0.42
2:D:133:ASP:CB	2:D:147:HIS:CD2	2.99	0.42
2:B:76:LEU:HD13	2:B:151:LEU:HD21	2.01	0.42
2:B:73:GLN:O	2:B:77:TYR:CD2	2.73	0.42
2:D:82:THR:HG21	2:D:94:LYS:CE	2.36	0.42
2:D:102:ARG:HB2	2:D:125:PHE:O	2.20	0.42
2:D:109:CYS:O	2:D:117:HIS:HE1	2.03	0.42
2:B:14:ARG:HA	2:B:86:ILE:O	2.20	0.41
1:C:66:LEU:HD23	1:C:66:LEU:HA	1.82	0.41
1:C:66:LEU:CD2	1:C:297:GLN:HE21	2.28	0.41
2:D:114:CYS:HB3	2:D:116:SER:HB3	2.03	0.41
1:A:21:ASN:HD22	1:A:21:ASN:HA	1.73	0.41
2:D:111:ASN:O	2:D:117:HIS:NE2	2.47	0.41
1:C:61:THR:HB	1:C:293:ILE:CD1	2.50	0.41
1:C:117:GLU:OE1	2:D:139:LYS:NZ	2.33	0.41
1:A:15:LEU:O	1:A:178:LYS:HE3	2.21	0.41
1:C:16:SER:O	1:C:17:ARG:C	2.63	0.41
2:D:9:VAL:HG13	2:D:60:LYS:NZ	2.36	0.41
2:D:99:LEU:HD23	2:D:99:LEU:HA	1.87	0.41
1:A:137:GLN:O	1:A:140:LEU:HG	2.22	0.40
1:C:160:VAL:HG22	1:C:187:ILE:HD12	2.03	0.40
2:D:105:ASN:HD22	2:D:122:SER:HB3	1.85	0.40
1:A:91:THR:HG22	1:A:95:ILE:HD12	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ARG:HH11	1:A:296:ARG:HD2	1.56	0.40
2:B:134:ILE:HB	2:B:147:HIS:CG	2.56	0.40
1:A:301:ALA:O	1:A:305:ASN:HB2	2.21	0.40
1:C:2:ASN:HD21	1:C:302:LEU:HA	1.86	0.40
1:C:114:LEU:CD1	1:C:114:LEU:C	2.94	0.40
1:C:291:ASN:HD22	1:C:291:ASN:HA	1.60	0.40
1:A:63:MET:SD	1:A:70:VAL:HG22	2.62	0.40
2:D:72:ASP:OD2	2:D:98:SER:O	2.40	0.40
2:B:110:PRO:HG2	2:B:145:PHE:CD2	2.57	0.40
1:C:46:SER:OG	1:C:60:GLN:NE2	2.52	0.40
2:D:148:ASN:HD22	2:D:148:ASN:HA	1.65	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:602:HOH:O	5:C:602:HOH:O[2_655]	1.34	0.86
5:A:332:HOH:O	5:A:398:HOH:O[2_655]	1.98	0.22
1:C:54:ARG:NH2	1:C:86:GLU:OE2[2_655]	2.02	0.18
1:C:1:ALA:N	2:D:101:GLU:OE1[4_555]	2.03	0.17

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	308/310 (99%)	292 (95%)	13 (4%)	3 (1%)	12	24
1	C	308/310 (99%)	290 (94%)	17 (6%)	1 (0%)	36	55
2	B	144/153 (94%)	121 (84%)	17 (12%)	6 (4%)	2	2
2	D	144/153 (94%)	111 (77%)	22 (15%)	11 (8%)	1	0
All	All	904/926 (98%)	814 (90%)	69 (8%)	21 (2%)	5	8

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	10	GLU
2	B	52	GLU
2	B	54	GLY
2	B	105	ASN
2	D	34	LYS
2	D	50	SER
2	D	51	GLY
2	D	54	GLY
2	D	89	TYR
2	D	91	VAL
2	B	9	VAL
2	D	9	VAL
2	D	10	GLU
1	C	132	ASN
2	D	22	PRO
2	B	34	LYS
2	D	35	LEU
1	A	132	ASN
1	A	231	GLN
2	D	67	SER
1	A	270	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	261/261 (100%)	249 (95%)	12 (5%)	24	48
1	C	261/261 (100%)	247 (95%)	14 (5%)	20	41
2	B	129/136 (95%)	118 (92%)	11 (8%)	10	22
2	D	129/136 (95%)	122 (95%)	7 (5%)	20	41
All	All	780/794 (98%)	736 (94%)	44 (6%)	19	39

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	54	ARG
1	A	59	PHE
1	A	136	THR
1	A	151	ARG
1	A	183	ARG
1	A	198	ILE
1	A	201	MET
1	A	229	ARG
1	A	285	TYR
1	A	287	GLN
1	A	310	LEU
2	B	12	ILE
2	B	18	ILE
2	B	25	ILE
2	B	42	ILE
2	B	58	LEU
2	B	61	ILE
2	B	66	LEU
2	B	95	SER
2	B	98	SER
2	B	103	ILE
2	B	112	SER
1	C	2	ASN
1	C	44	ILE
1	C	57	LEU
1	C	104	MET
1	C	114	LEU
1	C	140	LEU
1	C	180	ASP
1	C	183	ARG
1	C	207	ILE
1	C	210	SER
1	C	217	GLU
1	C	236	ASP
1	C	256	ASN
1	C	287	GLN
2	D	31	SER
2	D	43	THR
2	D	48	LEU
2	D	55	ARG
2	D	58	LEU
2	D	61	ILE

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Mol	Chain	Res	Type
2	D	103	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	78	ASN
1	A	132	ASN
1	A	137	GLN
1	A	147	GLN
1	A	231	GLN
1	A	242	ASN
1	A	246	GLN
1	A	256	ASN
1	A	287	GLN
1	A	291	ASN
1	A	297	GLN
2	B	20	HIS
2	B	63	ASN
2	B	132	ASN
2	B	147	HIS
1	C	21	ASN
1	C	132	ASN
1	C	137	GLN
1	C	231	GLN
1	C	287	GLN
1	C	291	ASN
1	C	297	GLN
2	D	84	ASN
2	D	105	ASN
2	D	147	HIS
2	D	148	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PAL	A	311	-	15,15,15	1.82	5 (33%)	20,21,21	1.93	6 (30%)
3	PAL	C	311	-	15,15,15	1.75	3 (20%)	20,21,21	2.31	12 (60%)

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	PAL	A	311	-	-	0/17/17/17	-
3	PAL	C	311	-	-	2/17/17/17	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	311	PAL	P-O2P	-3.84	1.46	1.55
3	C	311	PAL	O3-C4	-2.72	1.22	1.30
3	C	311	PAL	P-O2P	-2.62	1.49	1.55
3	C	311	PAL	O4-C5	2.39	1.29	1.22
3	A	311	PAL	C2-N2	-2.35	1.41	1.45
3	A	311	PAL	P-O3P	2.31	1.60	1.55
3	A	311	PAL	O1-C1	2.22	1.27	1.23
3	A	311	PAL	O3-C4	-2.19	1.23	1.30

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	311	PAL	C1P-C1-N2	5.36	120.29	115.19
3	A	311	PAL	C1P-C1-N2	4.39	119.38	115.19
3	A	311	PAL	C2-N2-C1	4.19	132.18	121.68
3	C	311	PAL	O4-C5-C3	-3.61	111.76	122.84
3	C	311	PAL	O1-C1-C1P	-2.89	114.74	121.45
3	C	311	PAL	O2P-P-O1P	2.68	119.32	112.39
3	A	311	PAL	O4-C5-C3	-2.63	114.76	122.84
3	A	311	PAL	C3-C2-C4	-2.54	105.72	110.79
3	A	311	PAL	C4-C2-N2	2.53	116.44	110.57
3	C	311	PAL	O3P-P-O1P	-2.46	106.03	112.39
3	C	311	PAL	C2-C3-C5	2.38	119.43	112.75
3	C	311	PAL	C3-C2-C4	-2.34	106.11	110.79
3	C	311	PAL	O5-C5-C3	2.27	121.06	114.00
3	C	311	PAL	C2-N2-C1	2.10	126.96	121.68
3	C	311	PAL	O1-C1-N2	-2.10	119.39	122.95
3	C	311	PAL	O2-C4-C2	-2.10	115.49	122.26
3	A	311	PAL	O2P-P-C1P	2.09	111.23	106.84
3	C	311	PAL	O3-C4-C2	2.05	120.45	113.51

There are no chirality outliers.

All (2) torsion outliers are listed below:

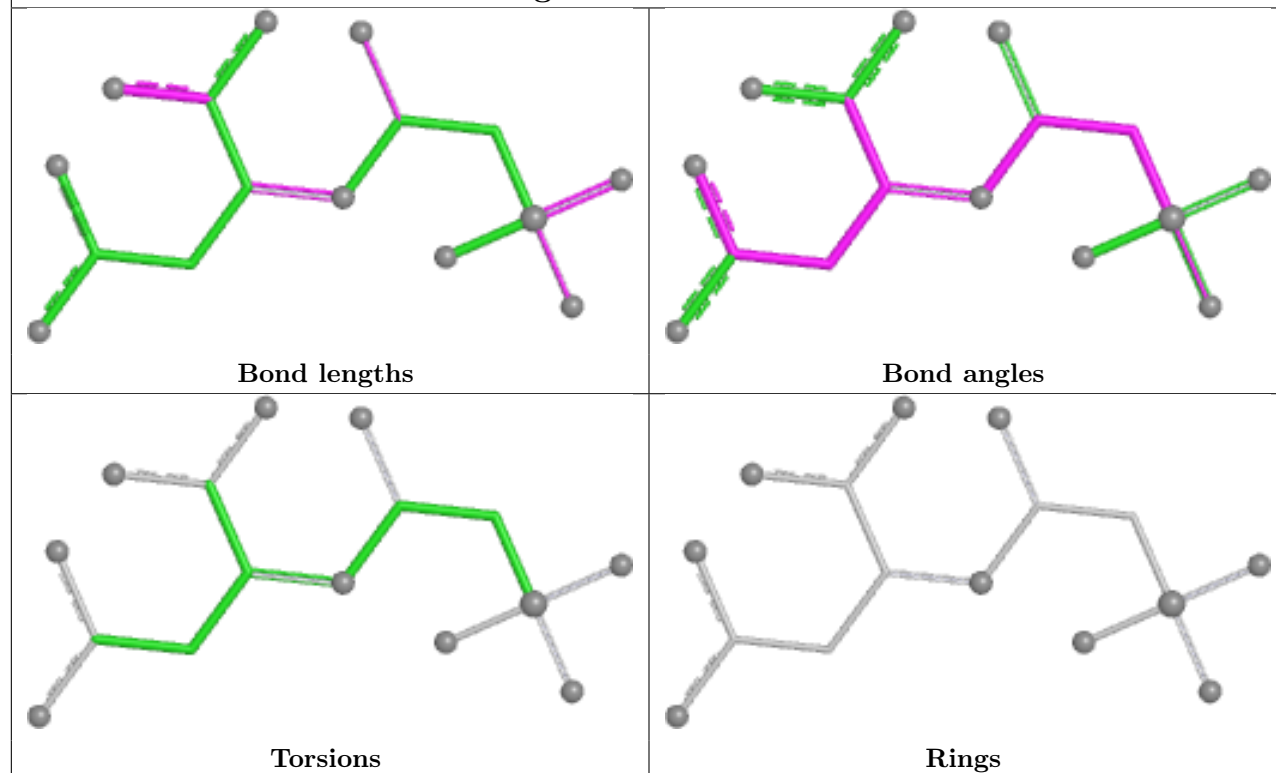
Mol	Chain	Res	Type	Atoms
3	C	311	PAL	O1-C1-N2-C2
3	C	311	PAL	C4-C2-C3-C5

There are no ring outliers.

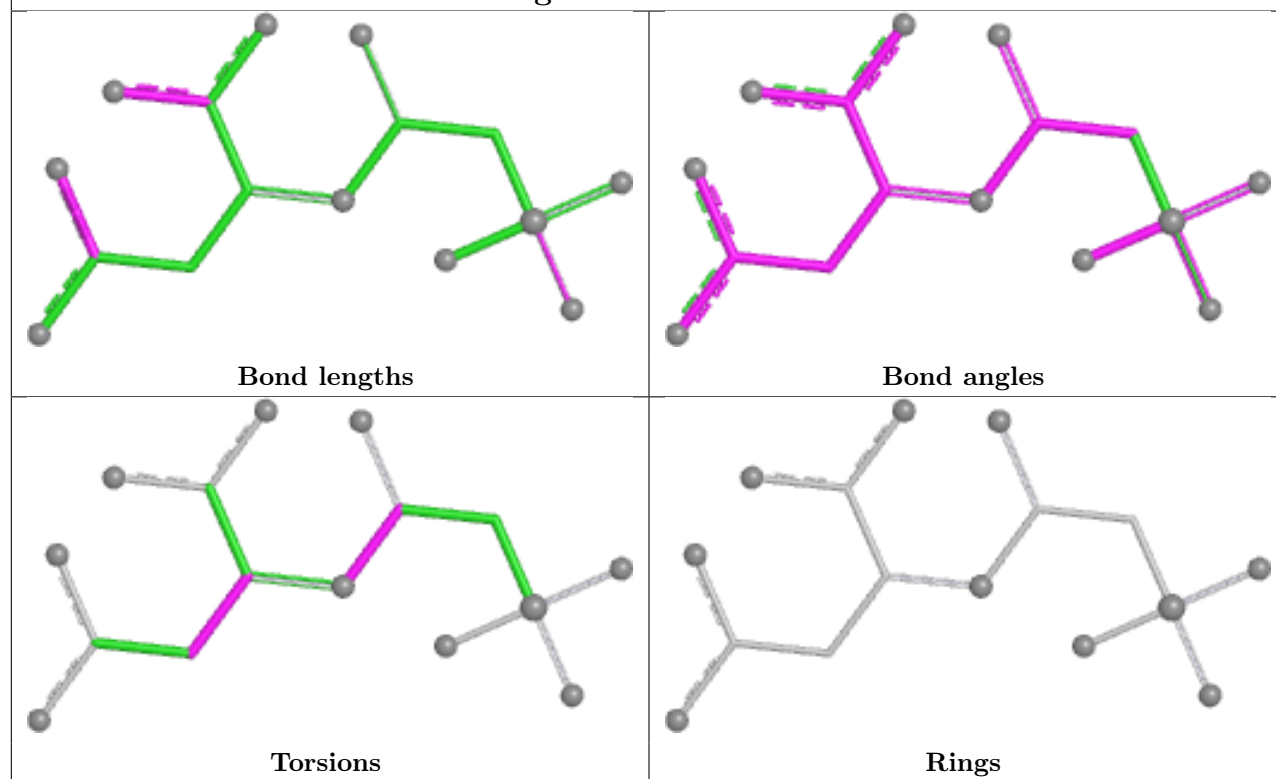
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PAL A 311



Ligand PAL C 311



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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.