



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:31 AM UTC

PDB ID : 7AT1 / pdb_00007at1
Title : CRYSTAL STRUCTURES OF ASPARTATE CARBAMOYLTRANSFERASE LIGATED WITH PHOSPHONOACETAMIDE, MALONATE, AND CTP OR ATP AT 2.8-ANGSTROMS RESOLUTION AND NEUTRAL P*H
Authors : Gouaux, J.E.; Stevens, R.C.; Lipscomb, W.N.
Deposited on : 1989-09-22
Resolution : 2.80 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

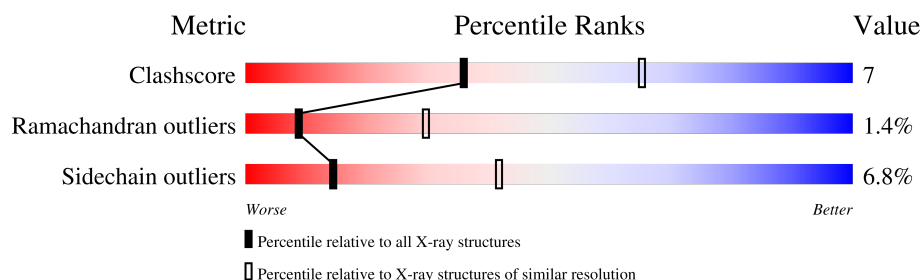
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	
3	E	2	
3	F	2	

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	GLC	E	2	X	X	-	-
3	GLC	F	2	X	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7169 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:

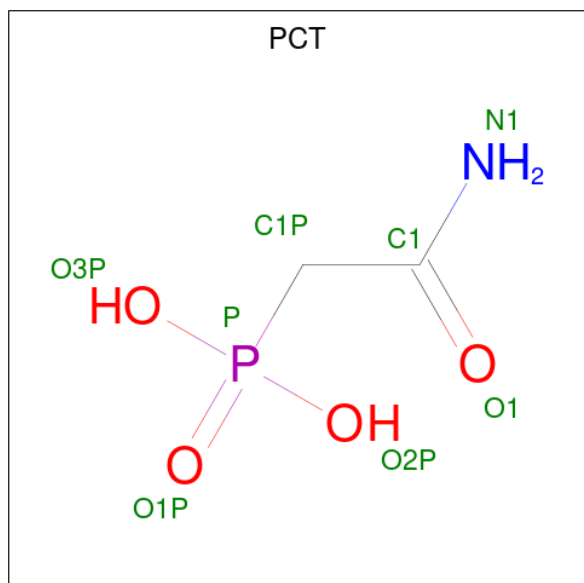
Chain	Residue	Modelled	Actual	Comment	Reference
B	8	GLY	GLN	conflict	UNP P0A7F3
D	8	GLY	GLN	conflict	UNP P0A7F3

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	E	2	Total	C	O	0	0	1
			7	4	3			
3	F	2	Total	C	O	0	0	1
			7	4	3			

- Molecule 4 is PHOSPHONOACETAMIDE (CCD ID: PCT) (formula: C₂H₆NO₄P).

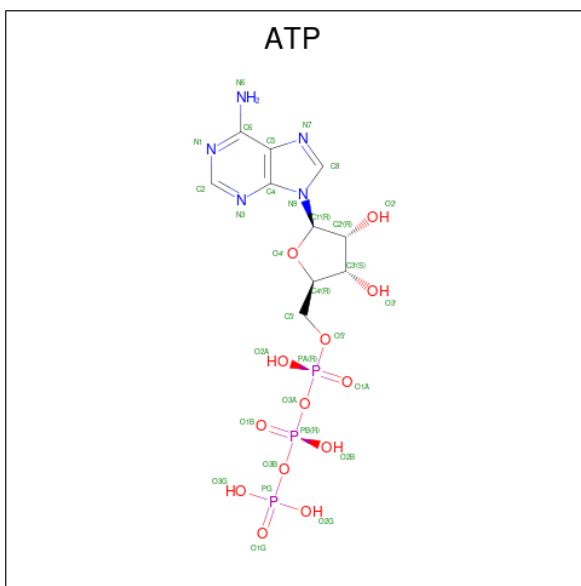


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			8	2	1	4	1		
4	C	1	Total	C	N	O	P	0	0
			8	2	1	4	1		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).



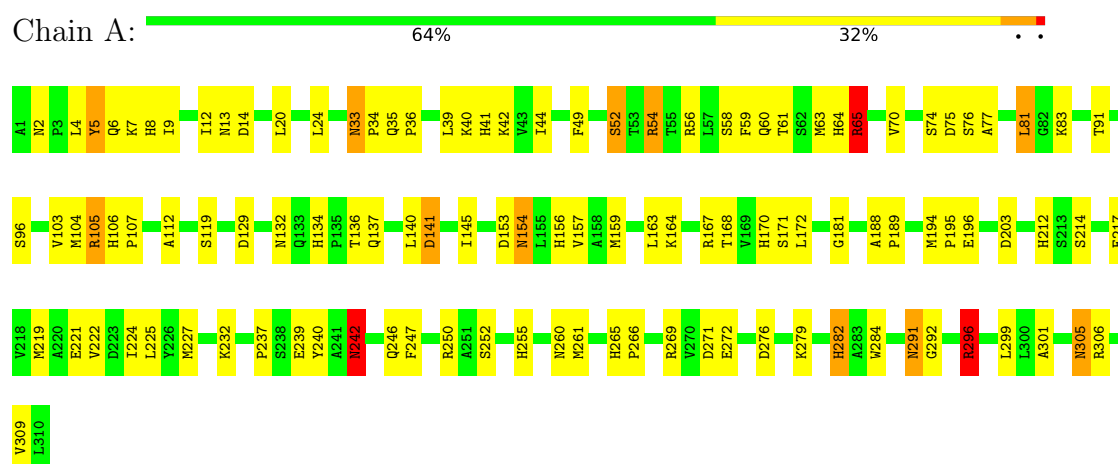
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

3 Residue-property plots

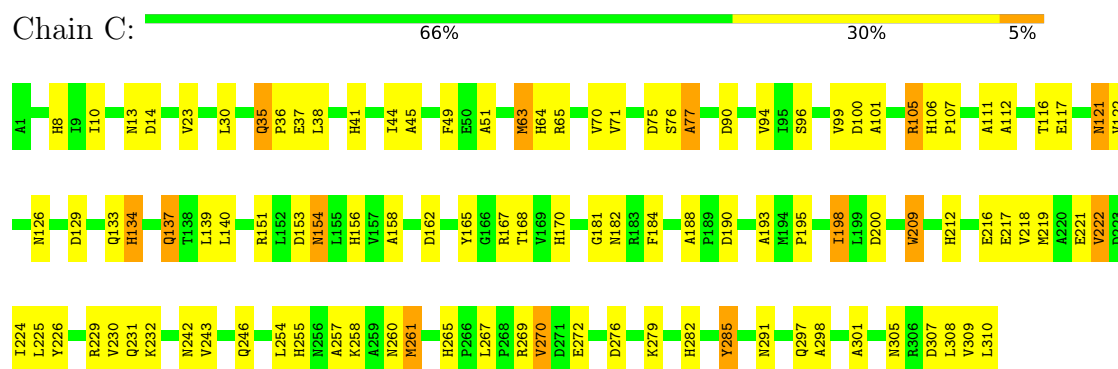
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

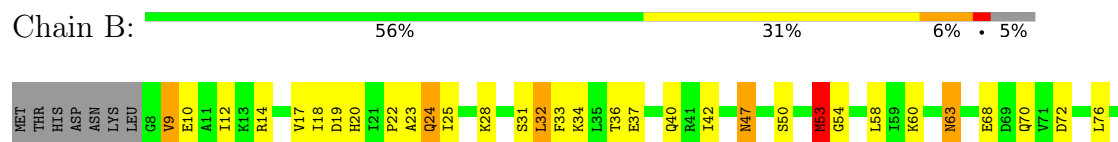
• Molecule 1: ASPARTATE CARBAMOYLTRANSFERASE (R STATE), CATALYTIC CHAIN



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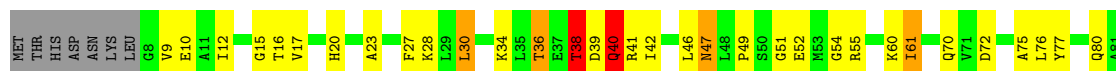


• Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN





- Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



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	122.50Å 122.50Å 156.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.183 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7169	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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: ATP, PCT, ZN, GLC

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	1.08	18/2461 (0.7%)	1.90	65/3339 (1.9%)
1	C	1.07	18/2461 (0.7%)	1.92	81/3339 (2.4%)
2	B	0.93	6/1155 (0.5%)	1.78	21/1561 (1.3%)
2	D	0.95	6/1155 (0.5%)	1.79	19/1561 (1.2%)
All	All	1.04	48/7232 (0.7%)	1.87	186/9800 (1.9%)

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	2
1	C	0	2
2	B	0	1
2	D	0	3
All	All	0	8

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	64	HIS	CD2-NE2	-7.67	1.29	1.37
1	C	156	HIS	CD2-NE2	-7.29	1.29	1.37
2	B	147	HIS	CD2-NE2	-7.03	1.30	1.37
1	A	265	HIS	CD2-NE2	-7.01	1.30	1.37
1	A	282	HIS	CD2-NE2	-7.00	1.30	1.37
1	A	106	HIS	CD2-NE2	-6.83	1.30	1.37
2	D	20	HIS	CD2-NE2	-6.78	1.30	1.37
2	B	117	HIS	CD2-NE2	-6.70	1.30	1.37
1	A	265	HIS	CG-ND1	-6.70	1.30	1.38
1	C	282	HIS	CD2-NE2	-6.62	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	HIS	CD2-NE2	-6.56	1.30	1.37
2	D	117	HIS	CD2-NE2	-6.49	1.30	1.37
1	C	255	HIS	CD2-NE2	-6.49	1.30	1.37
1	C	265	HIS	CD2-NE2	-6.48	1.30	1.37
1	C	212	HIS	CG-ND1	-6.43	1.31	1.38
1	C	212	HIS	CD2-NE2	-6.41	1.30	1.37
1	C	170	HIS	CD2-NE2	-6.23	1.30	1.37
1	C	8	HIS	CD2-NE2	-6.23	1.30	1.37
1	A	41	HIS	CD2-NE2	-6.18	1.31	1.37
1	A	212	HIS	CD2-NE2	-6.16	1.31	1.37
1	A	134	HIS	CD2-NE2	-6.14	1.31	1.37
1	A	282	HIS	CG-ND1	-6.08	1.31	1.38
1	A	8	HIS	CD2-NE2	-6.07	1.31	1.37
2	D	147	HIS	CD2-NE2	-6.06	1.31	1.37
1	C	106	HIS	CD2-NE2	-6.04	1.31	1.37
1	C	134	HIS	CD2-NE2	-6.04	1.31	1.37
2	B	20	HIS	CD2-NE2	-6.02	1.31	1.37
1	C	64	HIS	CG-ND1	-5.93	1.31	1.38
2	B	86	ILE	CA-CB	5.85	1.62	1.54
1	A	170	HIS	CD2-NE2	-5.85	1.31	1.37
1	A	212	HIS	CG-ND1	-5.82	1.31	1.38
1	C	106	HIS	CG-ND1	-5.79	1.31	1.38
1	A	106	HIS	CG-ND1	-5.77	1.31	1.38
1	A	156	HIS	CD2-NE2	-5.75	1.31	1.37
1	A	44	ILE	CA-CB	5.75	1.61	1.54
2	D	117	HIS	CG-ND1	-5.71	1.31	1.38
1	A	64	HIS	CG-ND1	-5.70	1.31	1.38
2	D	115	ILE	CA-CB	5.63	1.61	1.54
1	A	41	HIS	CG-ND1	-5.62	1.32	1.38
1	A	255	HIS	CD2-NE2	-5.55	1.31	1.37
1	C	282	HIS	CG-ND1	-5.52	1.32	1.38
2	D	20	HIS	CG-ND1	-5.46	1.32	1.38
1	C	41	HIS	CD2-NE2	-5.43	1.31	1.37
2	B	106	VAL	CA-CB	5.39	1.61	1.54
1	C	255	HIS	CG-ND1	-5.35	1.32	1.38
1	C	156	HIS	CG-ND1	-5.31	1.32	1.38
1	C	265	HIS	CG-ND1	-5.20	1.32	1.38
2	B	20	HIS	CG-ND1	-5.08	1.32	1.38

All (186) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	VAL	O-C-N	10.10	133.26	122.45
1	A	41	HIS	ND1-CG-CD2	9.61	115.71	106.10
1	A	106	HIS	ND1-CG-CD2	9.39	115.49	106.10
1	C	14	ASP	CA-CB-CG	9.22	121.82	112.60
1	A	141	ASP	CA-CB-CG	8.83	121.43	112.60
2	D	153	ASN	CA-CB-CG	8.65	121.25	112.60
1	A	188	ALA	O-C-N	-8.34	116.37	121.71
1	C	75	ASP	CA-CB-CG	8.27	120.87	112.60
1	C	282	HIS	ND1-CG-CD2	8.25	114.35	106.10
1	A	105	ARG	NE-CZ-NH2	8.23	126.60	119.20
1	A	282	HIS	ND1-CG-CD2	8.08	114.18	106.10
2	D	105	ASN	N-CA-C	8.04	127.93	110.80
1	A	305	ASN	CA-CB-CG	-7.92	104.68	112.60
2	D	153	ASN	OD1-CG-ND2	-7.81	114.79	122.60
1	A	81	LEU	N-CA-C	-7.71	102.81	111.14
1	A	222	VAL	N-CA-C	7.71	119.53	109.58
1	C	260	ASN	OD1-CG-ND2	-7.66	114.94	122.60
1	A	272	GLU	N-CA-C	7.62	121.67	112.38
1	C	154	ASN	OD1-CG-ND2	-7.60	115.00	122.60
1	A	276	ASP	CA-CB-CG	7.50	120.10	112.60
1	C	243	VAL	N-CA-C	7.45	118.22	110.62
1	C	8	HIS	ND1-CG-CD2	7.45	113.55	106.10
1	C	265	HIS	CA-C-N	7.44	127.81	119.32
1	C	265	HIS	C-N-CA	7.44	127.81	119.32
1	C	229	ARG	O-C-N	-7.43	114.74	123.06
1	A	106	HIS	CG-CD2-NE2	-7.30	99.90	107.20
1	A	41	HIS	CG-CD2-NE2	-7.17	100.03	107.20
1	C	105	ARG	NE-CZ-NH2	7.13	125.62	119.20
1	C	309	VAL	N-CA-C	-7.13	94.85	107.18
1	A	269	ARG	CB-CG-CD	-7.12	94.92	111.30
2	D	40	GLN	OE1-CD-NE2	-6.96	115.64	122.60
2	D	147	HIS	ND1-CG-CD2	6.96	113.06	106.10
1	C	242	ASN	OD1-CG-ND2	-6.95	115.65	122.60
1	A	103	VAL	N-CA-C	-6.95	98.42	108.36
2	B	12	ILE	O-C-N	6.92	130.30	123.03
1	C	188	ALA	O-C-N	-6.91	117.01	121.85
1	C	200	ASP	CA-CB-CG	6.85	119.45	112.60
1	C	121	ASN	N-CA-C	-6.83	104.84	113.72
2	B	47	ASN	OD1-CG-ND2	-6.83	115.77	122.60
1	C	107	PRO	N-CA-C	6.79	122.81	113.65
1	C	265	HIS	ND1-CG-CD2	6.76	112.86	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	106	VAL	CB-CA-C	-6.75	104.03	110.65
1	A	33	ASN	CA-C-N	6.71	126.67	119.76
1	A	33	ASN	C-N-CA	6.71	126.67	119.76
1	A	54	ARG	NE-CZ-NH2	6.63	125.17	119.20
1	A	56	ARG	NE-CZ-NH1	-6.63	114.86	121.50
1	C	246	GLN	N-CA-C	6.63	118.51	111.28
1	C	122	VAL	N-CA-CB	-6.62	103.14	110.23
1	A	75	ASP	CA-CB-CG	6.56	119.16	112.60
1	A	242	ASN	CA-CB-CG	6.54	119.14	112.60
1	C	121	ASN	CA-CB-CG	6.54	119.14	112.60
2	B	84	ASN	OD1-CG-ND2	-6.52	116.08	122.60
2	B	106	VAL	N-CA-C	6.49	119.20	111.09
1	A	134	HIS	ND1-CG-CD2	6.47	112.57	106.10
1	C	122	VAL	CB-CA-C	6.47	116.95	110.94
2	B	105	ASN	CB-CG-ND2	6.43	126.05	116.40
2	B	37	GLU	CA-CB-CG	-6.42	101.27	114.10
2	B	53	MET	N-CA-C	-6.38	99.43	109.50
1	C	35	GLN	CA-C-N	6.35	126.03	119.56
1	C	35	GLN	C-N-CA	6.35	126.03	119.56
1	C	134	HIS	ND1-CG-CD2	6.33	112.43	106.10
1	C	99	VAL	N-CA-C	6.31	118.26	109.29
1	C	162	ASP	CA-CB-CG	6.31	118.91	112.60
1	C	126	ASN	OD1-CG-ND2	-6.31	116.29	122.60
1	C	154	ASN	CB-CG-ND2	6.29	125.83	116.40
1	C	269	ARG	N-CA-C	-6.25	99.52	109.59
2	D	38	THR	N-CA-CB	-6.25	100.88	111.31
1	A	153	ASP	CA-CB-CG	6.25	118.85	112.60
1	A	13	ASN	OD1-CG-ND2	-6.24	116.36	122.60
1	C	51	ALA	N-CA-C	6.21	119.37	110.24
1	C	282	HIS	CG-CD2-NE2	-6.21	100.99	107.20
2	B	70	GLN	OE1-CD-NE2	-6.20	116.40	122.60
1	A	56	ARG	NE-CZ-NH2	6.17	124.75	119.20
1	A	35	GLN	CA-C-N	6.15	125.84	119.56
1	A	35	GLN	C-N-CA	6.15	125.84	119.56
2	B	105	ASN	OD1-CG-ND2	-6.12	116.48	122.60
1	C	269	ARG	CB-CG-CD	-6.08	97.33	111.30
1	C	309	VAL	O-C-N	6.03	128.39	122.97
1	A	33	ASN	OD1-CG-ND2	-6.02	116.58	122.60
2	B	18	ILE	N-CA-C	-6.02	98.34	107.73
1	C	36	PRO	N-CA-C	6.00	121.64	113.84
2	D	85	ARG	NE-CZ-NH2	5.99	124.59	119.20
1	A	8	HIS	ND1-CG-CD2	5.98	112.08	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	151	ARG	NE-CZ-NH2	5.97	124.58	119.20
1	A	242	ASN	CB-CG-ND2	5.97	125.36	116.40
1	C	106	HIS	ND1-CG-CD2	5.97	112.07	106.10
1	C	190	ASP	CA-CB-CG	5.97	118.57	112.60
1	C	291	ASN	OD1-CG-ND2	-5.96	116.64	122.60
1	C	222	VAL	N-CA-C	5.96	117.59	108.71
1	C	260	ASN	CB-CG-ND2	5.92	125.27	116.40
1	C	198	ILE	N-CA-C	-5.88	104.59	111.00
2	D	28	LYS	N-CA-C	-5.87	104.88	111.28
1	A	232	LYS	N-CA-CB	-5.84	101.24	109.94
1	A	129	ASP	CA-CB-CG	5.78	118.38	112.60
2	D	80	GLN	OE1-CD-NE2	-5.78	116.82	122.60
1	C	272	GLU	N-CA-C	5.77	120.05	112.89
1	A	106	HIS	CB-CG-CD2	-5.77	123.70	131.20
1	C	122	VAL	CA-C-N	5.77	125.70	119.76
1	C	122	VAL	C-N-CA	5.77	125.70	119.76
2	B	47	ASN	CA-CB-CG	5.74	118.34	112.60
1	C	117	GLU	CA-CB-CG	-5.74	102.63	114.10
1	C	231	GLN	OE1-CD-NE2	-5.73	116.87	122.60
2	D	9	VAL	N-CA-CB	-5.72	106.51	112.06
1	A	282	HIS	CG-CD2-NE2	-5.70	101.50	107.20
2	D	127	VAL	N-CA-C	5.70	115.54	106.88
1	C	276	ASP	CA-CB-CG	5.68	118.28	112.60
2	D	102	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	A	107	PRO	N-CA-C	5.67	120.95	113.86
2	B	95	SER	N-CA-CB	-5.65	101.81	110.85
1	A	291	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	C	122	VAL	N-CA-C	5.65	113.49	108.63
2	B	84	ASN	CB-CG-ND2	5.64	124.86	116.40
1	C	265	HIS	CG-CD2-NE2	-5.64	101.56	107.20
1	C	216	GLU	N-CA-C	-5.60	105.25	111.36
1	C	231	GLN	CG-CD-NE2	5.58	124.77	116.40
1	A	269	ARG	N-CA-C	-5.57	100.61	109.59
1	A	14	ASP	CA-CB-CG	5.55	118.15	112.60
1	C	94	VAL	CA-C-O	-5.55	114.89	121.05
2	D	61	ILE	CA-CB-CG2	-5.54	101.07	110.50
2	B	19	ASP	CA-CB-CG	5.53	118.13	112.60
1	C	291	ASN	CB-CG-ND2	5.53	124.70	116.40
1	A	91	THR	CA-CB-OG1	-5.49	101.36	109.60
1	A	132	ASN	OD1-CG-ND2	-5.49	117.11	122.60
1	C	270	VAL	O-C-N	-5.49	115.71	122.57
1	A	105	ARG	NE-CZ-NH1	-5.47	116.03	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	63	MET	CA-C-O	-5.47	115.08	120.82
1	C	182	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	C	209	TRP	CB-CG-CD1	-5.46	118.71	126.90
1	A	104	MET	CG-SD-CE	-5.46	88.90	100.90
2	D	117	HIS	N-CA-C	5.45	117.22	111.28
1	A	52	SER	N-CA-C	5.45	116.81	108.42
2	D	153	ASN	CB-CG-ND2	5.43	124.54	116.40
1	C	193	ALA	N-CA-C	5.40	117.49	110.53
1	C	133	GLN	O-C-N	5.38	130.15	123.15
1	A	164	LYS	N-CA-C	5.37	117.21	111.36
2	D	70	GLN	OE1-CD-NE2	-5.36	117.24	122.60
1	C	265	HIS	CB-CG-CD2	-5.34	124.26	131.20
1	A	196	GLU	N-CA-C	5.31	117.76	111.33
1	C	285	TYR	N-CA-C	5.31	119.01	112.54
1	A	36	PRO	N-CA-C	5.30	120.73	113.84
2	B	100	PRO	CB-CA-C	5.29	118.31	110.85
1	A	282	HIS	CB-CG-CD2	-5.29	124.33	131.20
1	A	65	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	A	260	ASN	CB-CG-ND2	5.26	124.28	116.40
2	B	18	ILE	N-CA-CB	5.25	117.76	111.31
1	C	129	ASP	CA-CB-CG	5.25	117.85	112.60
1	C	30	LEU	N-CA-C	-5.24	105.57	111.28
1	C	267	LEU	O-C-N	-5.23	115.31	121.32
2	D	9	VAL	N-CA-C	-5.23	98.97	106.55
2	B	63	ASN	OD1-CG-ND2	-5.22	117.38	122.60
1	A	203	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	260	ASN	OD1-CG-ND2	-5.21	117.39	122.60
1	C	77	ALA	N-CA-C	5.21	121.89	110.80
1	C	225	LEU	N-CA-C	-5.21	99.93	108.41
1	A	271	ASP	CA-CB-CG	5.19	117.79	112.60
2	D	134	ILE	N-CA-CB	-5.19	105.08	111.00
1	A	250	ARG	NE-CZ-NH2	5.18	123.86	119.20
2	B	33	PHE	N-CA-C	-5.17	101.28	109.76
2	B	121	VAL	O-C-N	-5.17	117.44	122.97
1	C	35	GLN	N-CA-C	5.17	118.37	108.97
1	A	154	ASN	OD1-CG-ND2	-5.16	117.44	122.60
1	C	305	ASN	OD1-CG-ND2	-5.16	117.44	122.60
1	A	239	GLU	CA-CB-CG	-5.16	103.79	114.10
1	C	90	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	58	SER	N-CA-C	-5.13	105.69	111.28
1	C	106	HIS	CA-C-N	5.11	124.90	119.28
1	C	106	HIS	C-N-CA	5.11	124.90	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	TRP	CE2-CD2-CG	-5.09	101.09	107.20
1	C	261	MET	CG-SD-CE	-5.08	89.72	100.90
1	C	298	ALA	CB-CA-C	-5.08	102.90	110.88
1	C	100	ASP	CA-C-O	5.08	125.22	119.27
1	A	296	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	C	297	GLN	OE1-CD-NE2	-5.07	117.53	122.60
2	B	152	ALA	O-C-N	5.06	129.32	122.59
1	C	111	ALA	N-CA-C	5.05	117.45	111.33
1	C	137	GLN	CA-C-N	5.05	127.01	120.44
1	C	137	GLN	C-N-CA	5.05	127.01	120.44
1	C	153	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	224	ILE	N-CA-C	-5.03	101.06	108.11
1	A	60	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	C	13	ASN	OD1-CG-ND2	-5.03	117.57	122.60
1	A	76	SER	N-CA-C	5.03	117.65	111.82
1	A	112	ALA	O-C-N	-5.02	116.43	122.15
1	A	157	VAL	N-CA-C	5.01	115.24	107.28
1	A	252	SER	N-CA-C	5.01	117.39	111.33
2	B	105	ASN	N-CA-C	5.00	121.46	110.80

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	TYR	Sidechain
1	A	5	TYR	Sidechain
2	B	89	TYR	Sidechain
1	C	165	TYR	Sidechain
1	C	226	TYR	Sidechain
2	D	27	PHE	Sidechain
2	D	77	TYR	Sidechain
2	D	89	TYR	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	33	0
1	C	2415	0	2422	27	0
2	B	1138	0	1154	24	0
2	D	1138	0	1154	23	0
3	E	7	0	0	1	0
3	F	7	0	0	1	0
4	A	8	0	4	1	0
4	C	8	0	4	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	B	31	0	12	1	0
All	All	7169	0	7172	105	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 7.

All (105) 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:C:10:ILE:HD11	1:C:116:THR:HG21	1.56	0.86
2:D:23:ALA:HB2	2:D:55:ARG:HG3	1.59	0.85
2:D:72:ASP:HB3	2:D:100:PRO:HG3	1.72	0.69
1:A:136:THR:HB	1:A:296:ARG:HH21	1.57	0.69
2:B:22:PRO:HB2	2:B:25:ILE:HD12	1.75	0.68
2:D:17:VAL:HG13	2:D:60:LYS:HG2	1.75	0.67
1:A:63:MET:SD	1:A:70:VAL:HG22	2.37	0.65
2:B:40:GLN:HE21	2:B:63:ASN:HB2	1.65	0.61
1:C:137:GLN:HG2	1:C:168:THR:HG22	1.82	0.60
2:B:14:ARG:HG3	2:B:87:ASP:HA	1.83	0.60
2:B:133:ASP:HB2	2:B:147:HIS:CE1	2.35	0.60
1:C:49:PHE:HD2	1:C:76:SER:HB3	1.67	0.59
1:A:301:ALA:O	1:A:305:ASN:HB2	2.03	0.59
2:B:40:GLN:NE2	2:B:63:ASN:HB2	2.17	0.59
2:B:84:ASN:HD21	2:B:91:VAL:HG13	1.68	0.58
1:A:214:SER:HB3	1:A:217:GLU:HG3	1.84	0.58
2:D:130:ARG:HD2	2:D:135:ALA:HB2	1.86	0.57
1:C:154:ASN:HA	1:C:181:GLY:O	2.05	0.56
1:A:137:GLN:HG2	1:A:168:THR:HG22	1.88	0.56
1:C:23:VAL:HG11	1:C:139:LEU:HD13	1.86	0.56
2:D:87:ASP:HB3	2:D:92:VAL:HG21	1.88	0.55
2:B:137:LYS:HG3	2:B:144:GLU:HG3	1.89	0.55
1:C:45:ALA:HA	1:C:71:VAL:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:GLY:O	1:A:296:ARG:HB2	2.07	0.54
2:B:50:SER:HB3	2:B:53:MET:O	2.07	0.54
1:C:254:LEU:CD2	1:C:261:MET:HE1	2.38	0.53
1:C:63:MET:SD	1:C:70:VAL:HG22	2.49	0.53
2:B:53:MET:SD	2:B:54:GLY:N	2.82	0.53
1:C:35:GLN:HB3	1:C:38:LEU:HB2	1.90	0.53
2:D:30:LEU:CD1	2:D:36:THR:HG23	2.39	0.52
1:C:301:ALA:HB1	1:C:308:LEU:HD11	1.92	0.52
2:B:23:ALA:O	2:B:24:GLN:HB2	2.08	0.52
1:C:10:ILE:HD11	1:C:116:THR:CG2	2.35	0.51
1:A:9:ILE:HG13	1:A:299:LEU:HD11	1.92	0.51
1:A:194:MET:SD	1:A:195:PRO:HD2	2.49	0.51
2:D:49:PRO:HA	2:D:54:GLY:O	2.11	0.51
2:B:58:LEU:HD21	2:B:60:LYS:HE3	1.93	0.51
2:D:30:LEU:HD11	2:D:36:THR:HG23	1.94	0.50
1:C:195:PRO:HG2	1:C:198:ILE:HD12	1.92	0.50
2:D:23:ALA:CB	2:D:55:ARG:HG3	2.36	0.50
1:C:137:GLN:O	1:C:140:LEU:HG	2.11	0.50
1:C:254:LEU:HD22	1:C:261:MET:HE1	1.94	0.50
1:C:279:LYS:N	1:C:279:LYS:HD2	2.27	0.50
6:B:155:ATP:H5'1	6:B:155:ATP:H8	1.77	0.49
1:C:134:HIS:HB2	1:C:167:ARG:HD3	1.93	0.49
1:A:12:ILE:HG13	1:A:171:SER:HB3	1.95	0.49
2:B:47:ASN:ND2	2:D:39:ASP:HA	2.27	0.49
2:B:36:THR:HG23	2:D:46:LEU:HD13	1.94	0.49
2:B:80:GLN:HA	2:B:96:ARG:HH22	1.78	0.49
1:A:189:PRO:HD3	1:A:247:PHE:HE1	1.78	0.49
1:A:61:THR:O	1:A:65:ARG:HG3	2.13	0.48
1:C:230:VAL:O	1:C:232:LYS:HD2	2.15	0.46
1:A:4:LEU:HA	1:A:7:LYS:HD2	1.96	0.46
1:A:5:TYR:CZ	1:A:306:ARG:HG2	2.50	0.46
1:A:77:ALA:O	1:A:83:LYS:HG2	2.16	0.46
1:C:158:ALA:HB2	1:C:222:VAL:HG11	1.98	0.46
1:A:52:SER:HB2	1:A:105:ARG:HH11	1.81	0.45
1:A:20:LEU:O	1:A:24:LEU:HG	2.15	0.45
2:D:146:SER:HB3	2:D:149:VAL:HG23	1.98	0.45
1:C:219:MET:SD	1:C:261:MET:HE2	2.57	0.45
1:A:167:ARG:HD2	3:E:2:GLC:C4	2.46	0.45
1:A:141:ASP:O	1:A:145:ILE:HG13	2.16	0.45
2:D:47:ASN:HD21	2:D:55:ARG:HE	1.64	0.45
1:C:49:PHE:CD2	1:C:76:SER:HB3	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:75:ALA:HB2	2:D:97:PRO:HB2	1.98	0.44
2:B:143:LYS:HB2	2:B:145:PHE:CZ	2.52	0.44
1:A:242:ASN:HB3	1:A:246:GLN:HE22	1.83	0.44
2:B:28:LYS:O	2:B:32:LEU:HB2	2.18	0.44
1:A:227:MET:O	1:A:266:PRO:HD2	2.17	0.44
2:B:84:ASN:ND2	2:B:91:VAL:HG13	2.31	0.43
1:C:167:ARG:HH21	1:C:167:ARG:HD2	1.71	0.43
1:A:154:ASN:HA	1:A:181:GLY:O	2.19	0.43
2:B:110:PRO:HG2	2:B:145:PHE:CD2	2.53	0.43
2:B:96:ARG:HA	2:B:97:PRO:HD3	1.83	0.43
2:B:111:ASN:HB3	2:B:114:CYS:HB2	1.99	0.43
2:D:127:VAL:HG22	2:D:136:LEU:HD23	2.01	0.43
1:A:33:ASN:HA	1:A:34:PRO:HD3	1.77	0.43
1:A:39:LEU:O	1:A:42:LYS:HB2	2.19	0.43
1:A:219:MET:HE1	1:A:225:LEU:HD22	2.01	0.43
2:D:133:ASP:HB2	2:D:147:HIS:CE1	2.53	0.42
2:D:99:LEU:HD23	2:D:99:LEU:HA	1.86	0.42
2:B:111:ASN:O	2:B:117:HIS:CE1	2.73	0.42
1:C:167:ARG:HD2	3:F:2:GLC:C4	2.50	0.42
1:A:261:MET:HE3	1:A:282:HIS:ND1	2.34	0.42
1:C:184:PHE:O	1:C:209:TRP:HA	2.19	0.42
1:A:2:ASN:ND2	1:A:305:ASN:O	2.53	0.41
1:C:112:ALA:O	1:C:116:THR:HG23	2.19	0.41
1:A:105:ARG:NH1	4:A:311:PCT:O3P	2.53	0.41
1:A:59:PHE:O	1:A:63:MET:HG3	2.21	0.41
1:A:163:LEU:O	1:A:195:PRO:HD3	2.20	0.41
2:D:38:THR:HG23	2:D:40:GLN:H	1.85	0.41
1:C:257:ALA:HB1	1:C:261:MET:HE3	2.01	0.41
2:D:102:ARG:HA	2:D:125:PHE:O	2.20	0.41
1:A:49:PHE:HE2	1:A:81:LEU:HD13	1.86	0.41
1:A:159:MET:HE2	1:A:172:LEU:HD23	2.03	0.41
1:C:217:GLU:HG3	1:C:218:VAL:HG13	2.03	0.41
2:D:16:THR:CG2	2:D:83:VAL:HG13	2.50	0.41
1:A:96:SER:OG	1:A:119:SER:HA	2.20	0.40
2:B:17:VAL:HG22	2:B:60:LYS:HG2	2.02	0.40
2:B:42:ILE:HB	2:D:46:LEU:HB2	2.03	0.40
2:B:17:VAL:HG13	2:B:60:LYS:HG2	2.02	0.40
1:C:44:ILE:HG23	1:C:101:ALA:HB3	2.02	0.40
2:D:12:ILE:HD12	2:D:15:GLY:HA3	2.03	0.40
2:D:42:ILE:HA	2:D:60:LYS:O	2.22	0.40
1:A:137:GLN:O	1:A:140:LEU:HG	2.22	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	308/310 (99%)	289 (94%)	17 (6%)	2 (1%)	21	51
1	C	308/310 (99%)	297 (96%)	9 (3%)	2 (1%)	21	51
2	B	144/153 (94%)	128 (89%)	12 (8%)	4 (3%)	4	14
2	D	144/153 (94%)	126 (88%)	13 (9%)	5 (4%)	3	10
All	All	904/926 (98%)	840 (93%)	51 (6%)	13 (1%)	9	30

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	24	GLN
2	D	105	ASN
1	A	54	ARG
2	B	132	ASN
2	D	51	GLY
2	B	9	VAL
2	B	34	LYS
1	C	270	VAL
2	D	10	GLU
1	A	6	GLN
1	C	77	ALA
2	D	89	TYR
2	D	120	PRO

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	261/261 (100%)	252 (97%)	9 (3%)	32	68
1	C	261/261 (100%)	250 (96%)	11 (4%)	26	61
2	B	129/136 (95%)	113 (88%)	16 (12%)	4	16
2	D	129/136 (95%)	112 (87%)	17 (13%)	4	14
All	All	780/794 (98%)	727 (93%)	53 (7%)	14	42

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LYS
1	A	65	ARG
1	A	74	SER
1	A	221	GLU
1	A	237	PRO
1	A	242	ASN
1	A	279	LYS
1	A	291	ASN
1	A	296	ARG
2	B	9	VAL
2	B	10	GLU
2	B	31	SER
2	B	32	LEU
2	B	53	MET
2	B	68	GLU
2	B	72	ASP
2	B	76	LEU
2	B	84	ASN
2	B	86	ILE
2	B	88	ASN
2	B	103	ILE
2	B	105	ASN
2	B	132	ASN
2	B	147	HIS
2	B	153	ASN
1	C	37	GLU
1	C	65	ARG
1	C	96	SER
1	C	105	ARG
1	C	121	ASN

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Mol	Chain	Res	Type
1	C	221	GLU
1	C	224	ILE
1	C	258	LYS
1	C	285	TYR
1	C	307	ASP
1	C	310	LEU
2	D	30	LEU
2	D	34	LYS
2	D	36	THR
2	D	38	THR
2	D	40	GLN
2	D	41	ARG
2	D	47	ASN
2	D	52	GLU
2	D	61	ILE
2	D	76	LEU
2	D	82	THR
2	D	95	SER
2	D	98	SER
2	D	102	ARG
2	D	112	SER
2	D	122	SER
2	D	153	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	21	ASN
1	A	60	GLN
1	A	147	GLN
1	A	174	GLN
1	A	291	ASN
2	B	40	GLN
2	B	117	HIS
2	B	147	HIS
2	B	148	ASN
2	B	153	ASN
1	C	13	ASN
1	C	64	HIS
1	C	108	GLN
1	C	126	ASN

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Mol	Chain	Res	Type
2	D	24	GLN
2	D	47	ASN
2	D	63	ASN
2	D	88	ASN
2	D	113	ASN
2	D	117	HIS
2	D	148	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

Of 4 monosaccharides modelled in this entry, 2 were used 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	GLC	E	2	3	5,5,12	4.16	3 (60%)	5,5,17	1.98	3 (60%)
3	GLC	F	2	3	5,5,12	3.92	3 (60%)	5,5,17	1.93	2 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLC	E	2	3	2/2/1/5	2/3/3/22	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLC	F	2	3	2/2/1/5	1/3/3/22	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	GLC	C4-C3	-6.91	1.22	1.51
3	F	2	GLC	C4-C3	-6.50	1.24	1.51
3	E	2	GLC	O3-C3	-4.99	1.22	1.43
3	F	2	GLC	O3-C3	-4.52	1.24	1.43
3	F	2	GLC	O5-C1	-3.71	1.23	1.42
3	E	2	GLC	O5-C1	-3.59	1.23	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	GLC	O3-C3-C4	3.08	122.69	109.45
3	E	2	GLC	O3-C3-C4	2.82	121.58	109.45
3	E	2	GLC	O5-C1-C2	2.44	119.34	111.34
3	E	2	GLC	O3-C3-C2	2.21	119.30	109.56
3	F	2	GLC	O3-C3-C2	2.12	118.92	109.56

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	2	GLC	C3
3	E	2	GLC	C1
3	F	2	GLC	C3
3	F	2	GLC	C1

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	2	GLC	C1-C2-C3-C4
3	E	2	GLC	C1-C2-C3-O3
3	E	2	GLC	C1-C2-C3-C4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

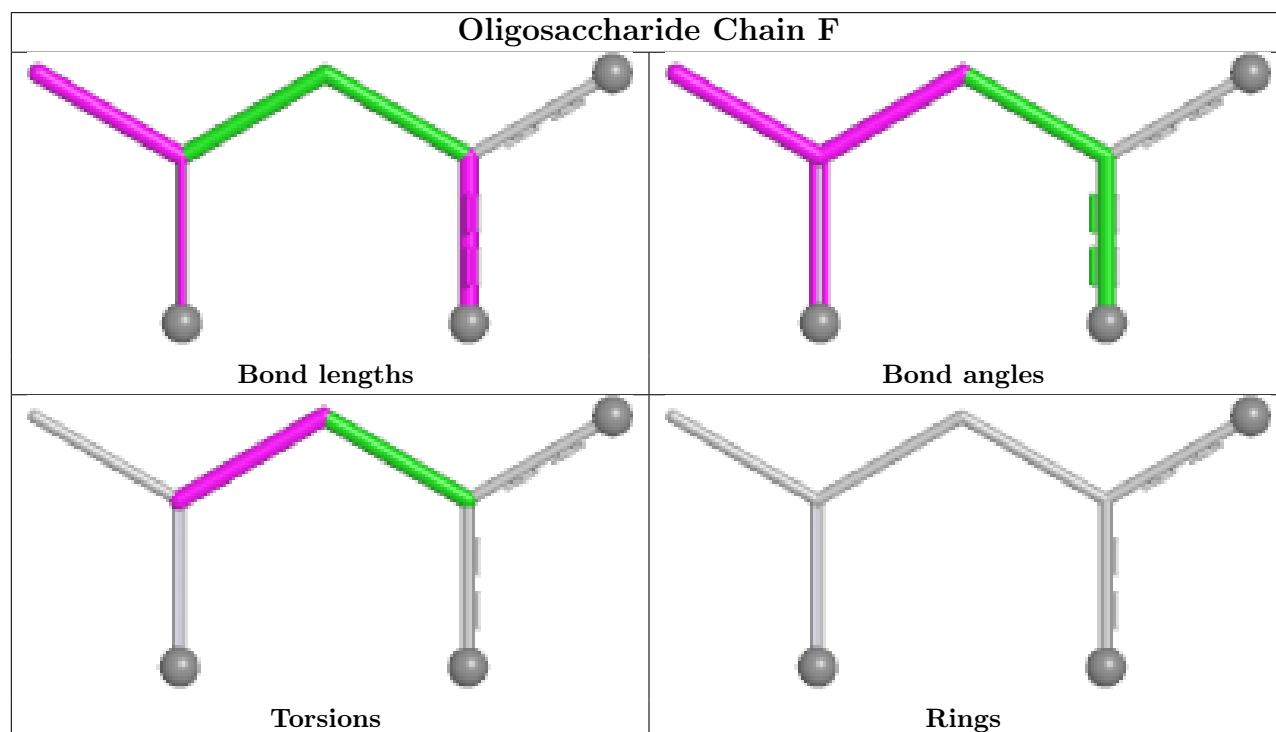
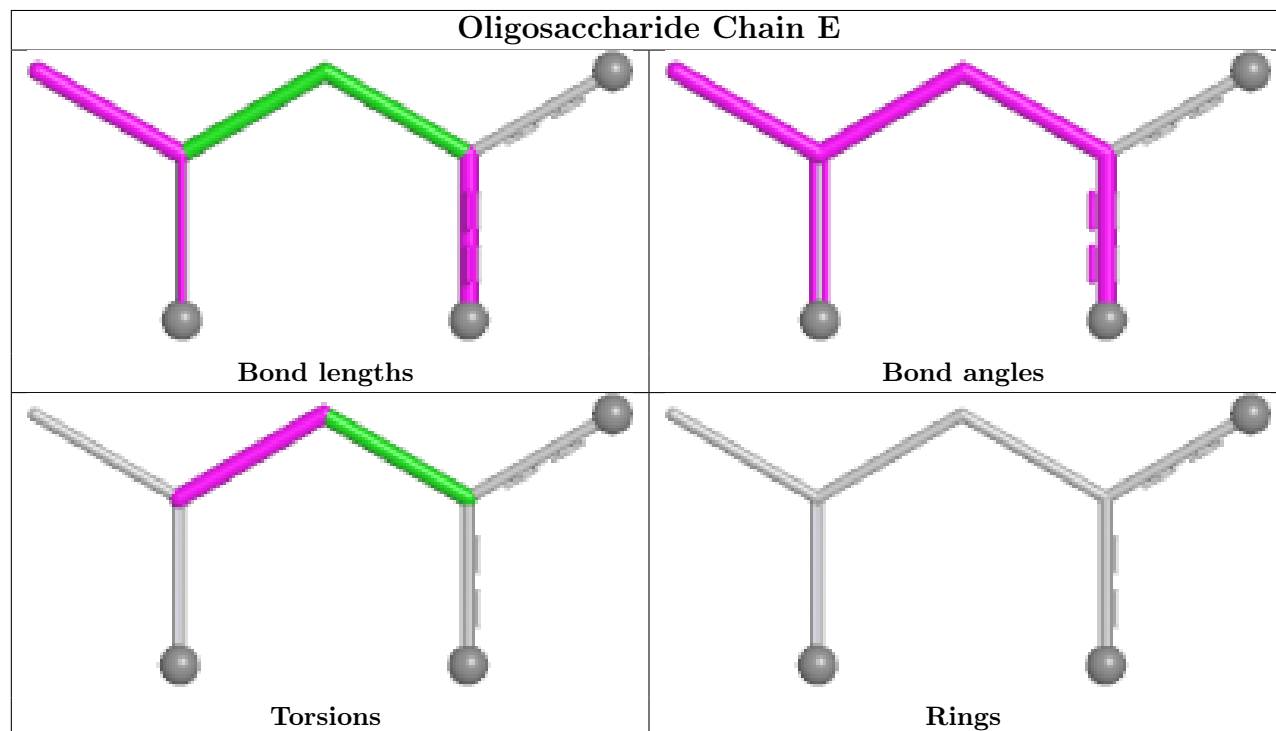
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2	GLC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	GLC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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
4	PCT	A	311	-	7,7,7	2.18	2 (28%)	9,10,10	1.93	2 (22%)
6	ATP	B	155	-	32,33,33	2.23	7 (21%)	48,52,52	1.38	7 (14%)
4	PCT	C	311	-	7,7,7	1.64	2 (28%)	9,10,10	1.44	1 (11%)

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
4	PCT	A	311	-	-	1/4/5/5	-
6	ATP	B	155	-	-	3/22/38/38	0/3/3/3
4	PCT	C	311	-	-	3/4/5/5	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	155	ATP	PB-O3B	6.40	1.66	1.59
6	B	155	ATP	PB-O3A	6.16	1.66	1.59
6	B	155	ATP	PA-O3A	4.87	1.64	1.59
4	A	311	PCT	P-C1P	3.85	1.85	1.79
6	B	155	ATP	C8-N9	-3.78	1.31	1.37
4	A	311	PCT	P-O1P	3.52	1.57	1.50
4	C	311	PCT	P-C1P	3.06	1.84	1.79
6	B	155	ATP	PG-O1G	3.05	1.60	1.50
6	B	155	ATP	C5-N7	-2.70	1.34	1.39
6	B	155	ATP	PA-O1A	2.50	1.59	1.50
4	C	311	PCT	P-O1P	2.16	1.54	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	311	PCT	O1-C1-C1P	4.88	125.00	119.86
6	B	155	ATP	O4'-C1'-N9	4.08	115.93	108.09
6	B	155	ATP	C6-C5-N7	2.84	137.56	132.09
6	B	155	ATP	C5-C4-N3	2.80	130.57	126.72
6	B	155	ATP	C6-C5-C4	-2.76	113.41	117.18
6	B	155	ATP	N3-C4-N9	-2.62	122.72	127.17
6	B	155	ATP	O2B-PB-O3B	2.34	113.58	107.27
4	A	311	PCT	O1P-P-C1P	-2.33	105.71	111.10
6	B	155	ATP	C3'-C2'-C1'	2.15	105.53	101.46
4	C	311	PCT	O1-C1-C1P	2.06	122.03	119.86

There are no chirality outliers.

All (7) torsion outliers are listed below:

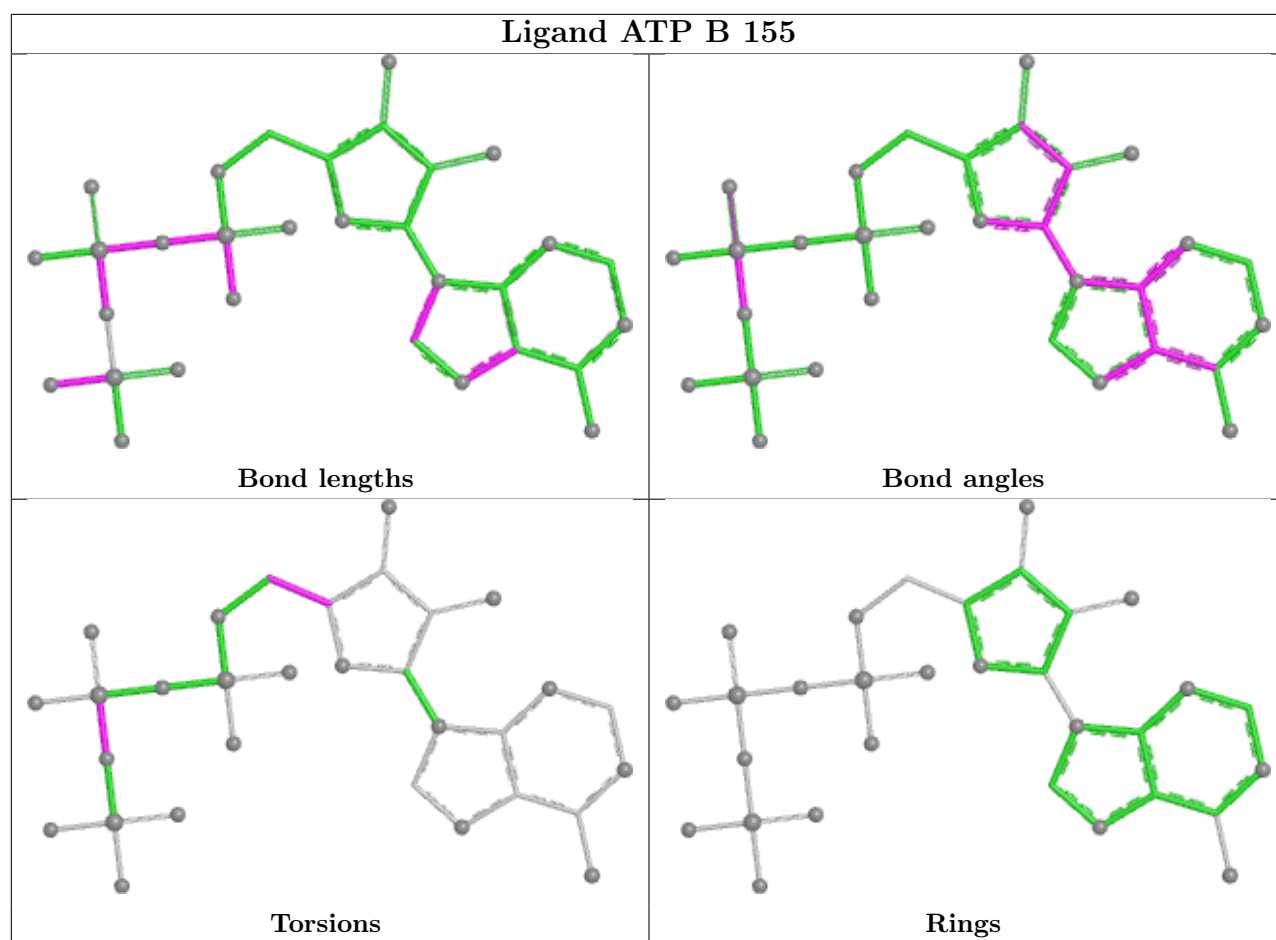
Mol	Chain	Res	Type	Atoms
4	C	311	PCT	C1-C1P-P-O1P
4	C	311	PCT	C1-C1P-P-O2P
4	C	311	PCT	C1-C1P-P-O3P
6	B	155	ATP	O4'-C4'-C5'-O5'
4	A	311	PCT	O1-C1-C1P-P
6	B	155	ATP	PG-O3B-PB-O2B
6	B	155	ATP	PG-O3B-PB-O1B

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	311	PCT	1	0
6	B	155	ATP	1	0

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.



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.