



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:59 PM UTC

PDB ID : 2AT1 / pdb_00002at1
Title : CRYSTAL STRUCTURES OF PHOSPHONOACETAMIDE LIGATED T AND PHOSPHONOACETAMIDE AND MALONATE LIGATED R STATES OF ASPARTATE CARBAMOYLTRANSFERASE AT 2.8-ANGSTROMS RESOLUTION AND NEUTRAL PH
Authors : Gouaux, J.E.; 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)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
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

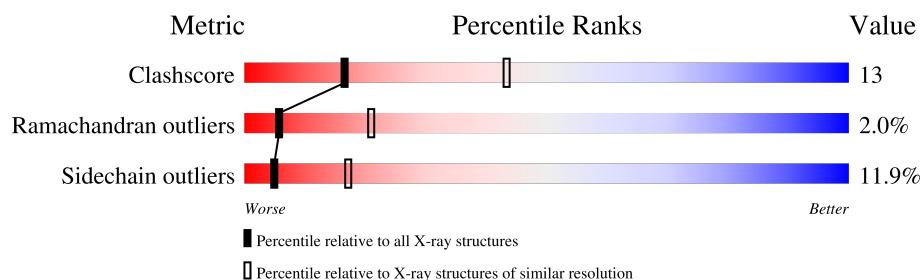
1 Overall quality at a glance

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	52% 37% 10% •
1	C	310	55% 37% 6% •
2	B	153	31% 46% 17% • 5%
2	D	153	45% 37% 11% • 5%
3	E	2	50% 50%
3	F	2	50% 50%

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	-	-
4	PCT	A	311	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7138 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:

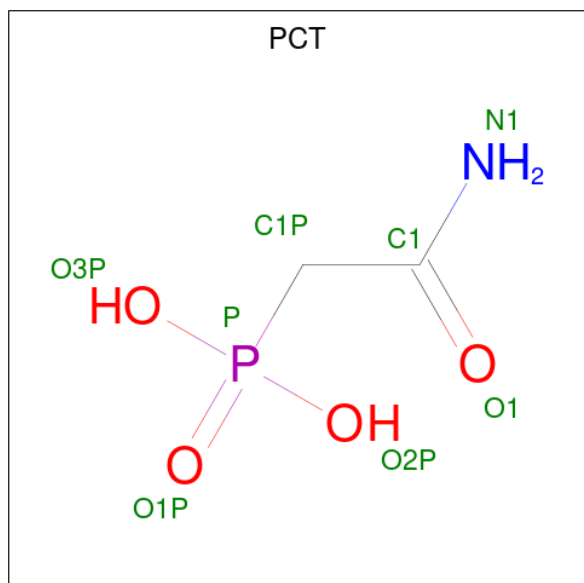
Chain	Residue	Modelled	Actual	Comment	Reference
B	8	GLY	GLN	conflict	UNP P0A7F3
D	8	GLY	GLN	conflict	UNP P0A7F3

- 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).

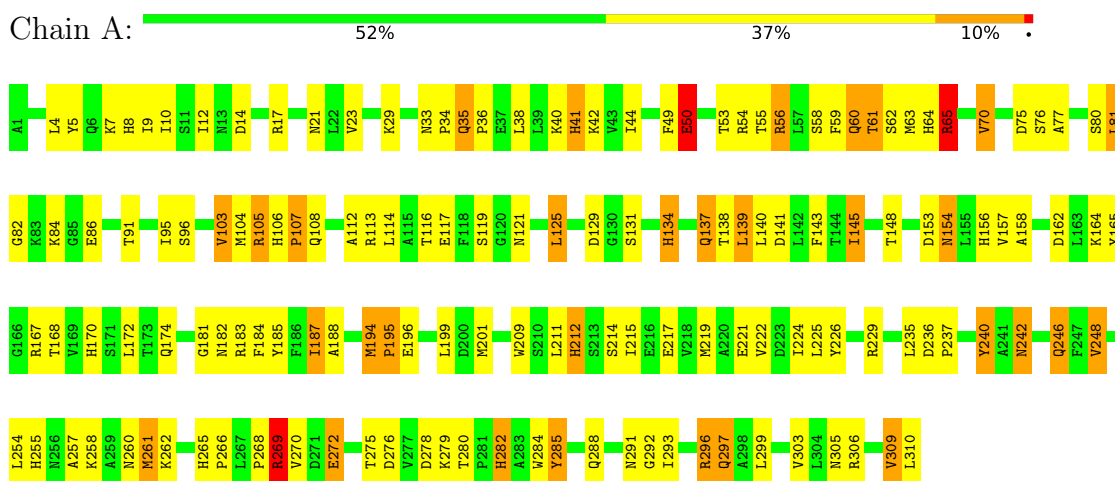
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		
5	D	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

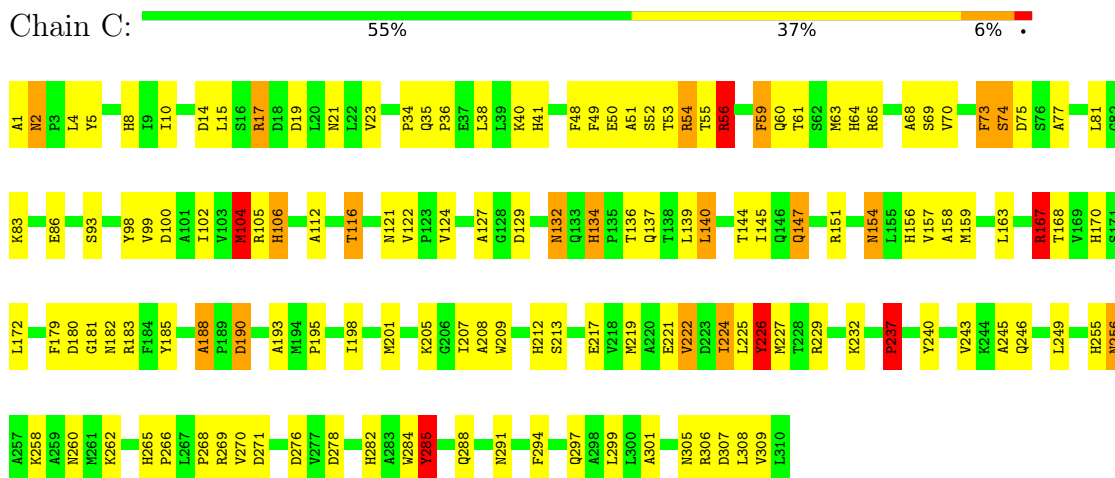
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

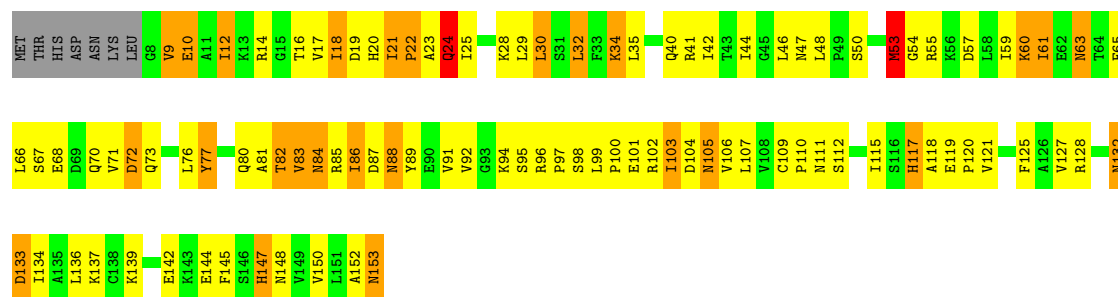


• Molecule 1: ASPARTATE CARBAMOYLTRANSFERASE (R STATE), CATALYTIC CHAIN



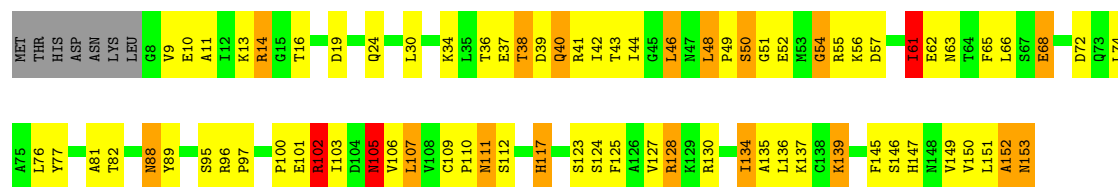
• Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN





• Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN

Chain D: 45% 37% 11% 5%



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

Chain E: 50% 50%



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

Chain F: 50% 50%



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	122.20Å 122.20Å 156.60Å 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}	0.170 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7138	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: 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	1.28	23/2461 (0.9%)	2.10	97/3339 (2.9%)
1	C	1.33	18/2461 (0.7%)	2.05	78/3339 (2.3%)
2	B	1.19	6/1155 (0.5%)	2.02	32/1561 (2.0%)
2	D	1.07	4/1155 (0.3%)	1.96	33/1561 (2.1%)
All	All	1.25	51/7232 (0.7%)	2.05	240/9800 (2.4%)

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	3
1	C	0	6
2	B	0	2
2	D	0	1
All	All	0	12

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	64	HIS	CD2-NE2	-8.23	1.28	1.37
2	B	12	ILE	CA-CB	8.22	1.65	1.54
1	C	156	HIS	CD2-NE2	-8.17	1.28	1.37
1	A	70	VAL	CA-CB	-8.15	1.44	1.54
1	A	64	HIS	CD2-NE2	-7.75	1.29	1.37
1	A	106	HIS	CD2-NE2	-7.48	1.29	1.37
2	B	106	VAL	CA-CB	7.46	1.64	1.54
1	A	282	HIS	CD2-NE2	-7.31	1.29	1.37
1	C	212	HIS	CD2-NE2	-7.25	1.29	1.37
1	A	134	HIS	CD2-NE2	-7.04	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	134	HIS	CD2-NE2	-6.93	1.30	1.37
1	A	212	HIS	CD2-NE2	-6.62	1.30	1.37
1	C	106	HIS	CD2-NE2	-6.61	1.30	1.37
1	C	170	HIS	CD2-NE2	-6.59	1.30	1.37
1	C	265	HIS	CD2-NE2	-6.56	1.30	1.37
1	A	170	HIS	CD2-NE2	-6.45	1.30	1.37
1	A	50	GLU	CD-OE2	-6.36	1.13	1.25
1	A	265	HIS	CG-ND1	-6.32	1.31	1.38
1	A	41	HIS	CD2-NE2	-6.30	1.30	1.37
1	C	8	HIS	CD2-NE2	-6.29	1.30	1.37
1	C	156	HIS	CG-ND1	-6.18	1.31	1.38
1	A	170	HIS	CG-ND1	-6.12	1.31	1.38
1	C	255	HIS	CD2-NE2	-6.05	1.31	1.37
1	C	41	HIS	CD2-NE2	-6.04	1.31	1.37
1	A	8	HIS	CD2-NE2	-6.03	1.31	1.37
1	C	226	TYR	CA-CB	-6.01	1.45	1.52
1	A	106	HIS	CA-CB	-6.01	1.45	1.54
2	D	117	HIS	CD2-NE2	-5.95	1.31	1.37
1	A	265	HIS	CD2-NE2	-5.89	1.31	1.37
2	B	147	HIS	CD2-NE2	-5.88	1.31	1.37
2	D	147	HIS	CD2-NE2	-5.88	1.31	1.37
2	B	20	HIS	CD2-NE2	-5.81	1.31	1.37
1	C	134	HIS	CB-CG	5.81	1.58	1.50
1	C	265	HIS	CG-ND1	-5.79	1.31	1.38
1	A	224	ILE	CA-CB	5.74	1.61	1.54
2	B	117	HIS	CD2-NE2	-5.67	1.31	1.37
1	C	282	HIS	CD2-NE2	-5.66	1.31	1.37
1	A	282	HIS	CG-ND1	-5.66	1.32	1.38
1	C	212	HIS	CG-ND1	-5.61	1.32	1.38
1	A	156	HIS	CD2-NE2	-5.57	1.31	1.37
1	C	285	TYR	CA-CB	5.46	1.62	1.53
1	A	34	PRO	CA-CB	-5.45	1.46	1.53
1	A	255	HIS	CD2-NE2	-5.33	1.31	1.37
1	A	106	HIS	CG-ND1	-5.24	1.32	1.38
2	D	117	HIS	CG-ND1	-5.24	1.32	1.38
1	A	56	ARG	CA-CB	-5.19	1.45	1.53
1	A	64	HIS	CG-ND1	-5.18	1.32	1.38
1	A	134	HIS	CG-ND1	-5.12	1.32	1.38
2	B	115	ILE	CA-CB	5.11	1.61	1.54
1	C	134	HIS	CA-CB	5.10	1.59	1.53
2	D	9	VAL	CA-CB	5.08	1.61	1.54

All (240) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	84	ASN	CA-CB-CG	-12.65	99.95	112.60
1	A	56	ARG	NE-CZ-NH1	-11.02	110.48	121.50
1	A	309	VAL	O-C-N	10.26	135.40	122.57
1	C	75	ASP	CA-CB-CG	10.07	122.67	112.60
1	A	56	ARG	NE-CZ-NH2	9.59	127.83	119.20
1	C	53	THR	N-CA-C	-9.27	99.70	112.12
1	A	134	HIS	CA-CB-CG	9.17	122.97	113.80
2	B	21	ILE	N-CA-C	-9.08	100.82	108.63
1	C	73	PHE	CA-CB-CG	9.01	122.81	113.80
1	A	54	ARG	NE-CZ-NH2	8.95	127.25	119.20
1	C	51	ALA	N-CA-C	8.92	122.81	110.24
1	C	182	ASN	OD1-CG-ND2	-8.79	113.81	122.60
1	C	260	ASN	OD1-CG-ND2	-8.69	113.91	122.60
2	B	34	LYS	N-CA-C	8.14	128.14	110.80
1	A	269	ARG	NE-CZ-NH2	8.13	126.52	119.20
1	A	260	ASN	OD1-CG-ND2	-8.05	114.55	122.60
1	A	60	GLN	OE1-CD-NE2	-8.02	114.58	122.60
1	A	129	ASP	CA-CB-CG	8.01	120.61	112.60
1	C	297	GLN	OE1-CD-NE2	-7.96	114.64	122.60
1	A	42	LYS	O-C-N	-7.96	114.14	123.22
1	A	188	ALA	O-C-N	-7.83	114.66	121.32
1	A	153	ASP	CA-CB-CG	7.70	120.30	112.60
2	B	152	ALA	N-CA-C	7.70	127.19	110.80
1	C	154	ASN	CB-CG-ND2	7.67	127.90	116.40
2	B	53	MET	N-CA-C	-7.61	98.35	110.14
1	A	242	ASN	CA-CB-CG	7.55	120.15	112.60
2	B	47	ASN	OD1-CG-ND2	-7.55	115.05	122.60
1	A	143	PHE	N-CA-C	-7.44	103.11	111.07
1	C	151	ARG	NE-CZ-NH2	7.39	125.85	119.20
1	A	91	THR	CA-CB-OG1	-7.29	98.67	109.60
1	C	147	GLN	OE1-CD-NE2	-7.20	115.40	122.60
2	D	134	ILE	N-CA-CB	-7.20	102.42	111.41
2	D	147	HIS	CA-CB-CG	7.16	120.96	113.80
1	A	174	GLN	OE1-CD-NE2	-7.16	115.44	122.60
2	D	153	ASN	OD1-CG-ND2	-7.15	115.45	122.60
1	C	278	ASP	CA-CB-CG	7.08	119.68	112.60
1	C	309	VAL	N-CA-C	-7.08	97.29	107.77
2	B	18	ILE	N-CA-C	-7.05	97.45	108.23
1	A	33	ASN	CA-C-N	7.02	127.02	119.78
1	A	33	ASN	C-N-CA	7.02	127.02	119.78
1	A	106	HIS	ND1-CG-CD2	7.02	113.12	106.10
1	C	190	ASP	CA-CB-CG	7.01	119.61	112.60
1	A	260	ASN	CB-CG-ND2	7.00	126.91	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	256	ASN	OD1-CG-ND2	-6.95	115.65	122.60
1	A	75	ASP	CA-CB-CG	6.94	119.54	112.60
1	C	156	HIS	N-CA-C	-6.94	97.10	108.41
1	C	86	GLU	CA-CB-CG	6.92	127.93	114.10
1	A	103	VAL	O-C-N	-6.87	115.40	123.03
1	A	86	GLU	N-CA-C	6.87	120.68	110.52
2	D	102	ARG	NE-CZ-NH2	6.85	125.36	119.20
1	C	60	GLN	CA-CB-CG	-6.83	100.44	114.10
1	A	54	ARG	NE-CZ-NH1	-6.82	114.68	121.50
1	A	272	GLU	N-CA-C	6.77	120.64	112.38
2	D	111	ASN	CA-CB-CG	6.72	119.32	112.60
2	B	97	PRO	N-CA-C	6.71	121.03	110.50
1	A	257	ALA	O-C-N	6.70	131.44	123.33
2	B	119	GLU	N-CA-C	6.67	119.29	110.36
2	D	39	ASP	N-CA-C	-6.62	104.83	113.17
1	C	17	ARG	N-CA-C	-6.62	104.14	111.82
1	C	229	ARG	O-C-N	-6.58	115.49	123.19
1	A	106	HIS	CA-C-N	6.56	127.40	120.12
1	A	106	HIS	C-N-CA	6.56	127.40	120.12
1	A	35	GLN	CA-C-N	6.55	127.07	119.47
1	A	35	GLN	C-N-CA	6.55	127.07	119.47
2	D	109	CYS	CA-C-N	6.49	127.00	119.47
2	D	109	CYS	C-N-CA	6.49	127.00	119.47
1	A	64	HIS	CB-CA-C	-6.47	99.85	110.85
1	A	33	ASN	OD1-CG-ND2	-6.47	116.13	122.60
1	C	222	VAL	N-CA-C	6.43	118.94	108.97
1	C	54	ARG	N-CA-C	6.40	118.05	111.14
2	B	18	ILE	N-CA-CB	6.37	118.26	111.00
1	C	86	GLU	N-CA-C	6.36	119.14	110.55
2	B	118	ALA	O-C-N	-6.35	115.39	122.12
1	A	64	HIS	N-CA-CB	6.34	119.55	110.16
1	C	154	ASN	OD1-CG-ND2	-6.34	116.26	122.60
1	A	56	ARG	CG-CD-NE	-6.34	98.06	112.00
1	C	237	PRO	N-CA-CB	-6.32	96.61	103.25
1	A	309	VAL	CA-C-N	6.32	133.07	121.70
1	A	309	VAL	C-N-CA	6.32	133.07	121.70
1	C	17	ARG	NE-CZ-NH2	6.31	124.88	119.20
1	C	291	ASN	OD1-CG-ND2	-6.31	116.29	122.60
2	D	24	GLN	OE1-CD-NE2	-6.29	116.31	122.60
2	D	14	ARG	NE-CZ-NH2	6.29	124.86	119.20
2	D	74	LEU	N-CA-C	-6.26	103.76	111.33
1	C	74	SER	N-CA-C	-6.22	105.73	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	48	PHE	CA-C-O	6.21	127.10	120.46
1	C	99	VAL	N-CA-C	6.19	117.75	108.96
1	C	159	MET	CA-CB-CG	-6.15	101.80	114.10
1	A	275	THR	N-CA-C	6.13	120.23	112.87
1	C	122	VAL	CA-C-N	6.13	125.89	119.76
1	C	122	VAL	C-N-CA	6.13	125.89	119.76
2	B	101	GLU	CA-CB-CG	6.13	126.36	114.10
2	D	105	ASN	N-CA-C	6.09	123.77	110.80
1	A	65	ARG	NE-CZ-NH2	6.09	124.68	119.20
1	C	100	ASP	N-CA-C	6.06	120.84	113.38
1	C	167	ARG	NE-CZ-NH1	-6.05	115.45	121.50
2	B	104	ASP	CA-CB-CG	6.04	118.64	112.60
1	C	260	ASN	CB-CG-ND2	6.03	125.44	116.40
1	A	246	GLN	N-CA-C	-6.02	104.40	110.97
2	B	133	ASP	CA-CB-CG	6.01	118.61	112.60
1	A	77	ALA	N-CA-C	6.01	118.61	111.33
2	D	88	ASN	OD1-CG-ND2	-5.98	116.62	122.60
2	D	48	LEU	O-C-N	-5.97	114.45	121.32
1	A	116	THR	N-CA-C	-5.96	104.72	112.23
1	C	132	ASN	OD1-CG-ND2	-5.95	116.65	122.60
1	C	129	ASP	CA-CB-CG	5.95	118.55	112.60
1	A	21	ASN	CA-CB-CG	-5.94	106.66	112.60
2	B	21	ILE	N-CA-CB	5.94	116.59	110.23
1	A	174	GLN	O-C-N	-5.91	115.42	122.15
2	D	127	VAL	N-CA-C	5.90	116.11	106.72
1	A	81	LEU	N-CA-C	-5.88	104.77	111.07
2	B	92	VAL	N-CA-CB	-5.88	99.85	110.95
1	C	2	ASN	CA-CB-CG	5.87	118.47	112.60
1	C	305	ASN	CA-CB-CG	-5.86	106.74	112.60
2	B	139	LYS	O-C-N	5.82	128.07	122.07
1	A	137	GLN	O-C-N	5.82	128.06	122.07
1	A	172	LEU	CA-C-O	-5.78	114.29	120.42
1	C	182	ASN	CB-CG-ND2	5.78	125.07	116.40
2	D	139	LYS	CB-CG-CD	-5.77	98.02	111.30
1	C	52	SER	N-CA-C	5.76	117.86	108.76
1	C	56	ARG	CB-CG-CD	-5.73	98.11	111.30
1	C	269	ARG	CG-CD-NE	-5.73	99.39	112.00
2	B	10	GLU	N-CA-C	5.73	118.11	109.23
2	D	128	ARG	NE-CZ-NH2	5.71	124.34	119.20
1	A	276	ASP	CA-CB-CG	5.71	118.31	112.60
1	A	187	ILE	N-CA-CB	-5.69	105.75	112.40
1	C	276	ASP	CA-CB-CG	5.68	118.28	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	103	ILE	N-CA-C	-5.68	100.24	108.36
1	A	288	GLN	OE1-CD-NE2	-5.67	116.93	122.60
2	D	61	ILE	CA-CB-CG2	-5.66	100.88	110.50
1	C	98	TYR	CB-CA-C	-5.64	99.89	109.03
1	A	157	VAL	N-CA-C	5.64	115.72	107.37
1	C	243	VAL	N-CA-CB	-5.64	102.87	110.54
1	A	162	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	297	GLN	CA-CB-CG	5.62	125.33	114.10
1	C	104	MET	N-CA-C	5.61	118.61	109.06
2	B	83	VAL	CA-C-N	-5.61	115.31	122.77
2	B	83	VAL	C-N-CA	-5.61	115.31	122.77
2	B	34	LYS	CA-C-N	5.60	127.72	120.44
2	B	34	LYS	C-N-CA	5.60	127.72	120.44
1	A	49	PHE	O-C-N	-5.60	115.21	122.37
1	A	297	GLN	OE1-CD-NE2	-5.59	117.01	122.60
1	C	116	THR	N-CA-C	5.57	118.11	111.71
1	C	246	GLN	OE1-CD-NE2	-5.56	117.04	122.60
2	B	21	ILE	CB-CA-C	-5.55	105.78	110.94
2	D	57	ASP	CA-CB-CG	5.55	118.15	112.60
1	C	255	HIS	CA-CB-CG	5.54	119.34	113.80
1	C	269	ARG	CA-CB-CG	5.53	125.17	114.10
1	C	68	ALA	N-CA-C	5.52	117.65	110.53
1	A	58	SER	N-CA-C	-5.52	105.34	111.36
1	A	182	ASN	N-CA-C	-5.52	101.55	110.32
1	C	180	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	107	PRO	N-CA-C	5.49	120.79	114.20
1	C	61	THR	CA-C-O	-5.47	114.62	120.42
2	D	37	GLU	CB-CG-CD	5.47	121.89	112.60
2	B	105	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	A	65	ARG	NE-CZ-NH1	-5.45	116.05	121.50
2	D	9	VAL	O-C-N	5.45	129.38	122.57
1	A	61	THR	CA-C-O	-5.42	114.75	120.55
1	A	139	LEU	CA-C-O	-5.41	114.69	120.42
2	D	103	ILE	CB-CA-C	-5.41	103.07	110.96
1	C	53	THR	OG1-CB-CG2	5.38	120.06	109.30
1	A	248	VAL	O-C-N	-5.36	117.67	123.14
2	D	152	ALA	CA-C-O	5.35	128.16	120.51
1	A	194	MET	N-CA-C	5.34	116.14	109.57
1	A	211	LEU	O-C-N	-5.34	116.13	122.65
1	A	236	ASP	CA-CB-CG	-5.34	107.26	112.60
1	C	179	PHE	CA-C-O	5.34	127.77	121.58
1	C	59	PHE	CA-CB-CG	-5.34	108.46	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	68	GLU	CA-C-N	5.34	128.83	120.82
2	D	68	GLU	C-N-CA	5.34	128.83	120.82
2	B	60	LYS	N-CA-C	-5.30	99.64	108.34
1	C	217	GLU	CA-CB-CG	5.30	124.70	114.10
2	D	106	VAL	CB-CA-C	-5.30	102.60	111.29
1	C	77	ALA	N-CA-C	5.28	118.50	111.75
1	A	91	THR	CA-CB-CG2	5.27	119.45	110.50
1	C	144	THR	CA-CB-OG1	-5.27	101.70	109.60
2	B	98	SER	N-CA-C	-5.26	102.96	110.59
1	A	54	ARG	N-CA-C	5.26	117.44	111.02
1	A	60	GLN	O-C-N	-5.26	115.55	122.39
1	A	105	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	A	284	TRP	CE2-CD2-CG	-5.25	100.89	107.20
1	A	106	HIS	CB-CG-CD2	-5.25	124.38	131.20
1	C	284	TRP	CE2-CD2-CG	-5.24	100.91	107.20
2	D	66	LEU	N-CA-C	5.23	118.75	109.96
1	A	148	THR	O-C-N	-5.23	116.30	122.32
1	A	121	ASN	OD1-CG-ND2	-5.23	117.37	122.60
2	D	107	LEU	CD1-CG-CD2	-5.23	99.30	110.80
2	B	81	ALA	N-CA-C	-5.22	103.99	110.41
1	A	201	MET	CA-CB-CG	5.20	124.50	114.10
2	B	153	ASN	CA-CB-CG	5.20	117.80	112.60
1	C	102	ILE	CA-C-N	5.20	129.88	123.12
1	C	102	ILE	C-N-CA	5.20	129.88	123.12
1	C	188	ALA	CA-C-O	-5.20	114.92	120.28
2	D	46	LEU	CA-C-O	5.20	126.52	120.49
1	A	284	TRP	CD1-CG-CD2	5.18	114.59	106.30
1	C	49	PHE	N-CA-C	-5.18	106.80	113.02
1	A	246	GLN	CA-C-N	-5.17	115.89	122.77
1	A	246	GLN	C-N-CA	-5.17	115.89	122.77
1	A	209	TRP	O-C-N	-5.17	116.18	123.11
1	C	93	SER	CA-C-O	-5.17	115.39	120.82
1	A	145	ILE	O-C-N	-5.16	116.85	121.91
2	D	96	ARG	N-CA-C	-5.16	103.68	110.39
2	D	153	ASN	CB-CG-ND2	5.15	124.13	116.40
1	C	193	ALA	N-CA-C	5.15	117.50	110.55
1	A	61	THR	CA-CB-OG1	-5.14	101.89	109.60
1	A	284	TRP	CG-CD1-NE1	-5.12	103.54	110.20
1	C	282	HIS	N-CA-C	-5.12	107.58	113.88
1	C	268	PRO	CA-C-N	-5.12	114.77	122.81
1	C	268	PRO	C-N-CA	-5.12	114.77	122.81
1	A	105	ARG	O-C-N	-5.12	116.58	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	HIS	CB-CG-CD2	-5.11	124.56	131.20
2	B	147	HIS	CB-CG-CD2	-5.11	124.56	131.20
1	A	215	ILE	N-CA-C	-5.11	105.52	110.42
1	C	209	TRP	CB-CG-CD1	-5.11	119.24	126.90
1	A	55	THR	CA-C-O	-5.10	115.45	120.70
1	A	261	MET	O-C-N	5.10	129.14	122.87
2	B	82	THR	CB-CA-C	5.09	117.98	110.14
1	C	294	PHE	O-C-N	-5.09	116.34	122.15
1	A	53	THR	CA-C-N	5.09	127.86	120.79
1	A	53	THR	C-N-CA	5.09	127.86	120.79
1	A	14	ASP	O-C-N	-5.08	115.36	122.37
2	D	24	GLN	CG-CD-NE2	5.08	124.02	116.40
1	A	305	ASN	CA-CB-CG	-5.07	107.53	112.60
1	A	138	THR	OG1-CB-CG2	5.07	119.43	109.30
1	A	36	PRO	N-CA-C	5.06	121.15	113.81
1	C	207	ILE	O-C-N	-5.05	116.93	122.69
1	C	172	LEU	CA-C-O	-5.05	115.07	120.42
1	C	209	TRP	CE2-CD2-CG	-5.05	101.14	107.20
1	A	8	HIS	CA-CB-CG	5.05	118.85	113.80
1	C	137	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	C	21	ASN	OD1-CG-ND2	-5.03	117.57	122.60
1	A	154	ASN	OD1-CG-ND2	-5.03	117.57	122.60
1	C	124	VAL	N-CA-C	-5.03	101.13	108.17
1	A	95	ILE	CA-CB-CG1	-5.03	101.86	110.40
1	A	17	ARG	NE-CZ-NH2	5.02	123.72	119.20
2	D	61	ILE	CA-CB-CG1	5.01	118.93	110.40
1	A	306	ARG	O-C-N	5.01	127.23	122.07
2	B	63	ASN	CB-CA-C	-5.01	104.80	112.11
1	A	303	VAL	O-C-N	-5.00	115.49	122.05

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	TYR	Sidechain
1	A	285	TYR	Sidechain
1	A	5	TYR	Sidechain
2	B	77	TYR	Sidechain
2	B	89	TYR	Sidechain
1	C	185	TYR	Sidechain
1	C	226	TYR	Sidechain
1	C	240	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	C	285	TYR	Sidechain
1	C	5	TYR	Sidechain
1	C	73	PHE	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	58	0
1	C	2415	0	2422	35	0
2	B	1138	0	1154	63	0
2	D	1138	0	1154	34	0
3	E	7	0	0	2	0
3	F	7	0	0	1	0
4	A	8	0	4	0	0
4	C	8	0	4	1	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
All	All	7138	0	7160	184	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 13.

All (184) 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:B:17:VAL:HG13	2:B:60:LYS:HG2	1.55	0.86
2:D:146:SER:HB3	2:D:149:VAL:HG23	1.58	0.85
2:D:102:ARG:HH21	2:D:102:ARG:HB3	1.42	0.82
1:C:10:ILE:HD11	1:C:116:THR:HG21	1.67	0.75
2:B:14:ARG:HG3	2:B:87:ASP:HA	1.68	0.74
2:B:46:LEU:HB2	2:D:42:ILE:HD13	1.69	0.73
1:A:154:ASN:HA	1:A:181:GLY:O	1.90	0.71
2:B:40:GLN:HE21	2:B:63:ASN:HB2	1.56	0.70
2:D:107:LEU:HD23	2:D:150:VAL:HG11	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:GLN:NE2	2:B:63:ASN:HB2	2.08	0.69
1:C:63:MET:SD	1:C:70:VAL:HG22	2.32	0.69
1:C:56:ARG:HG2	1:C:56:ARG:HH21	1.58	0.67
1:C:154:ASN:HA	1:C:181:GLY:O	1.94	0.67
1:C:10:ILE:HD11	1:C:116:THR:CG2	2.25	0.67
2:B:67:SER:H	2:B:70:GLN:HB2	1.60	0.66
1:C:1:ALA:HA	1:C:306:ARG:HG2	1.78	0.65
2:B:84:ASN:HD21	2:B:91:VAL:HG13	1.62	0.64
2:B:137:LYS:HG3	2:B:144:GLU:HG2	1.80	0.64
1:A:292:GLY:O	1:A:296:ARG:HB2	1.98	0.63
1:A:134:HIS:CD2	1:A:137:GLN:HB2	2.34	0.63
2:B:9:VAL:HG12	2:B:10:GLU:H	1.64	0.63
2:D:76:LEU:HD21	2:D:134:ILE:HG21	1.80	0.63
2:B:30:LEU:HD13	2:B:59:ILE:HG12	1.82	0.62
1:C:227:MET:HE2	1:C:249:LEU:HB2	1.81	0.61
2:D:130:ARG:HD2	2:D:135:ALA:HB2	1.82	0.60
2:D:49:PRO:O	2:D:56:LYS:HG2	2.02	0.59
1:A:4:LEU:HD23	1:A:7:LYS:HD3	1.82	0.59
1:A:167:ARG:HD2	3:E:2:GLC:C4	2.33	0.59
2:B:42:ILE:HB	2:D:46:LEU:HB2	1.84	0.59
2:B:110:PRO:HG2	2:B:145:PHE:CD2	2.38	0.58
2:D:72:ASP:HB3	2:D:100:PRO:HG3	1.84	0.58
1:A:134:HIS:HB2	1:A:167:ARG:HD3	1.85	0.58
2:D:16:THR:OG1	2:D:65:PHE:HA	2.04	0.58
1:A:38:LEU:HD21	1:A:309:VAL:HG21	1.86	0.57
2:B:30:LEU:HD11	2:B:59:ILE:HG21	1.87	0.57
2:B:66:LEU:HD12	2:B:71:VAL:HG22	1.86	0.56
1:A:219:MET:HE2	1:A:261:MET:HE2	1.86	0.56
2:B:30:LEU:HA	2:B:35:LEU:HD12	1.87	0.56
1:A:35:GLN:HG3	1:A:38:LEU:HD22	1.88	0.55
1:C:226:TYR:OH	1:C:266:PRO:HG3	2.06	0.55
1:A:50:GLU:HG3	1:A:107:PRO:HD3	1.89	0.55
1:C:105:ARG:HG3	1:C:106:HIS:N	2.22	0.55
1:C:54:ARG:HE	4:C:311:PCT:H1P2	1.72	0.55
1:C:50:GLU:HB3	1:C:105:ARG:HG2	1.89	0.55
2:B:25:ILE:HG12	2:B:28:LYS:NZ	2.23	0.54
1:A:44:ILE:HD13	1:A:63:MET:HG2	1.90	0.54
2:B:50:SER:HB3	2:B:53:MET:O	2.06	0.54
2:B:25:ILE:HA	2:B:28:LYS:HG3	1.90	0.54
1:C:195:PRO:HG2	1:C:198:ILE:HD12	1.90	0.54
1:A:61:THR:O	1:A:65:ARG:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:MET:SD	1:A:70:VAL:HG22	2.48	0.54
2:B:23:ALA:O	2:B:24:GLN:HB2	2.06	0.53
1:A:137:GLN:O	1:A:140:LEU:HG	2.08	0.53
1:C:104:MET:HE2	1:C:112:ALA:HA	1.89	0.53
2:B:84:ASN:ND2	2:B:91:VAL:HG22	2.24	0.53
1:C:158:ALA:HB2	1:C:222:VAL:HG11	1.89	0.53
1:A:254:LEU:HD12	1:A:280:THR:HG21	1.92	0.52
1:A:254:LEU:HD13	1:A:282:HIS:HD2	1.74	0.52
2:D:102:ARG:HB3	2:D:102:ARG:NH2	2.17	0.52
1:A:164:LYS:HD3	1:A:165:TYR:CE2	2.44	0.52
2:B:111:ASN:O	2:B:117:HIS:HE1	1.93	0.52
2:D:50:SER:N	2:D:54:GLY:O	2.43	0.52
2:B:111:ASN:O	2:B:117:HIS:CE1	2.63	0.51
1:A:194:MET:SD	1:A:195:PRO:HD2	2.50	0.51
2:D:111:ASN:O	2:D:117:HIS:HE1	1.92	0.51
1:A:214:SER:HB3	1:A:217:GLU:HG3	1.93	0.51
2:B:25:ILE:HG12	2:B:28:LYS:HZ3	1.76	0.51
2:B:30:LEU:HD12	2:B:35:LEU:HD13	1.92	0.51
1:C:55:THR:HG21	1:C:127:ALA:HB1	1.91	0.51
1:C:219:MET:HE1	1:C:249:LEU:HD11	1.92	0.51
1:A:56:ARG:HE	1:A:60:GLN:NE2	2.08	0.51
2:B:44:ILE:HB	2:D:44:ILE:HD13	1.93	0.51
1:C:23:VAL:HG11	1:C:139:LEU:HD13	1.92	0.51
2:D:102:ARG:HH21	2:D:102:ARG:CB	2.19	0.51
2:D:19:ASP:O	2:D:81:ALA:HA	2.11	0.50
1:C:183:ARG:HD2	1:C:208:ALA:HB3	1.93	0.50
1:C:157:VAL:HG13	1:C:224:ILE:HG22	1.94	0.50
2:D:102:ARG:HA	2:D:125:PHE:O	2.12	0.50
1:C:4:LEU:HD21	1:C:19:ASP:HB3	1.93	0.50
1:A:196:GLU:HA	1:A:199:LEU:HD12	1.93	0.50
2:B:136:LEU:HD12	2:B:150:VAL:HG21	1.94	0.50
2:D:107:LEU:HD12	2:D:107:LEU:H	1.77	0.50
2:D:124:SER:HB3	2:D:139:LYS:HD2	1.93	0.50
1:A:103:VAL:HG22	1:A:125:LEU:HD23	1.94	0.49
1:A:35:GLN:HB2	1:A:38:LEU:HB2	1.94	0.49
1:C:104:MET:CE	1:C:112:ALA:HA	2.43	0.49
2:B:99:LEU:HD22	2:B:127:VAL:HG11	1.95	0.49
1:A:185:TYR:HD2	1:A:212:HIS:NE2	2.10	0.48
2:D:13:LYS:HG3	2:D:88:ASN:HA	1.94	0.48
1:A:29:LYS:HD2	1:A:309:VAL:O	2.13	0.48
2:B:53:MET:SD	2:B:54:GLY:N	2.87	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:LEU:HB2	2:D:42:ILE:CD1	2.42	0.48
1:C:34:PRO:O	1:C:36:PRO:HD3	2.12	0.48
2:B:14:ARG:HA	2:B:86:ILE:HG22	1.93	0.48
1:A:167:ARG:NH2	3:E:2:GLC:O3	2.45	0.48
1:A:187:ILE:HG12	1:A:212:HIS:HB2	1.96	0.48
2:B:16:THR:OG1	2:B:65:PHE:HA	2.14	0.48
2:D:14:ARG:HG2	2:D:63:ASN:HA	1.94	0.48
2:D:107:LEU:HD12	2:D:107:LEU:N	2.29	0.48
1:A:254:LEU:HD13	1:A:282:HIS:CD2	2.49	0.48
2:B:71:VAL:HG22	2:B:83:VAL:HG21	1.95	0.48
1:C:145:ILE:HG12	1:C:224:ILE:HD13	1.96	0.48
1:A:183:ARG:NH2	1:A:184:PHE:O	2.46	0.48
2:B:22:PRO:HB2	2:B:25:ILE:HD12	1.95	0.48
1:A:114:LEU:CD2	2:B:121:VAL:HG11	2.44	0.47
1:A:248:VAL:HG22	1:A:272:GLU:HA	1.96	0.47
2:B:91:VAL:HG11	2:B:94:LYS:HZ2	1.79	0.47
2:D:77:TYR:HE1	2:D:151:LEU:HD22	1.79	0.47
1:A:96:SER:OG	1:A:119:SER:HA	2.15	0.47
1:A:62:SER:HB3	1:A:297:GLN:HB3	1.97	0.47
1:A:168:THR:HG21	1:A:266:PRO:HB3	1.95	0.47
1:A:219:MET:HE1	1:A:225:LEU:HD22	1.97	0.47
2:B:127:VAL:HA	2:B:136:LEU:HD23	1.97	0.47
2:B:134:ILE:O	2:B:147:HIS:HB3	2.14	0.47
2:D:77:TYR:CE1	2:D:151:LEU:HD22	2.50	0.47
1:A:81:LEU:C	1:A:81:LEU:HD23	2.41	0.46
1:A:137:GLN:HG2	1:A:168:THR:HG22	1.97	0.46
2:D:10:GLU:HG3	2:D:11:ALA:H	1.81	0.46
1:C:301:ALA:HB1	1:C:308:LEU:HD11	1.98	0.46
2:B:23:ALA:HB3	2:B:55:ARG:HH21	1.81	0.45
1:C:163:LEU:HG	1:C:188:ALA:HB2	1.97	0.45
1:A:158:ALA:HA	1:A:185:TYR:HB2	1.98	0.45
1:A:293:ILE:O	1:A:297:GLN:HG2	2.16	0.45
2:B:91:VAL:HG11	2:B:94:LYS:NZ	2.32	0.45
1:C:2:ASN:N	1:C:306:ARG:O	2.50	0.45
2:B:70:GLN:O	2:B:73:GLN:HB2	2.16	0.45
2:D:61:ILE:H	2:D:61:ILE:HD12	1.81	0.45
2:B:48:LEU:O	2:B:55:ARG:HA	2.17	0.45
1:A:219:MET:CE	1:A:261:MET:HE2	2.47	0.44
2:D:107:LEU:HD23	2:D:136:LEU:HD13	2.00	0.44
1:A:76:SER:O	1:A:82:GLY:HA3	2.17	0.44
2:B:107:LEU:HD13	2:B:150:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:ILE:HG22	2:B:29:LEU:HG	1.98	0.44
1:A:80:SER:HB3	1:A:84:LYS:HB2	2.00	0.44
2:D:38:THR:HG23	2:D:40:GLN:H	1.81	0.44
1:A:269:ARG:NH1	1:A:278:ASP:OD2	2.51	0.44
1:C:140:LEU:HD13	1:C:288:GLN:O	2.17	0.44
2:B:10:GLU:HG3	2:B:41:ARG:HH22	1.82	0.44
2:B:18:ILE:HD11	2:B:61:ILE:HD11	2.00	0.44
2:B:72:ASP:HB3	2:B:100:PRO:HB3	2.00	0.44
2:B:133:ASP:HB2	2:B:147:HIS:CE1	2.53	0.44
1:C:154:ASN:HD22	1:C:181:GLY:HA3	1.83	0.44
2:D:13:LYS:CG	2:D:88:ASN:HA	2.48	0.43
1:A:141:ASP:O	1:A:145:ILE:HG13	2.19	0.43
1:A:226:TYR:CZ	1:A:266:PRO:HD3	2.52	0.43
2:D:49:PRO:HA	2:D:54:GLY:O	2.17	0.43
1:A:229:ARG:HB2	1:A:268:PRO:O	2.18	0.43
2:D:14:ARG:HG3	2:D:65:PHE:CE1	2.54	0.43
1:A:291:ASN:HD22	1:A:291:ASN:HA	1.59	0.43
1:A:23:VAL:HG11	1:A:139:LEU:HD22	2.01	0.43
1:A:235:LEU:HB2	1:A:240:TYR:HE2	1.83	0.43
2:B:23:ALA:HA	2:B:57:ASP:CG	2.44	0.43
2:D:110:PRO:HB2	2:D:145:PHE:CE2	2.54	0.42
1:C:245:ALA:HB3	1:C:271:ASP:OD1	2.18	0.42
1:A:222:VAL:O	1:A:258:LYS:HD3	2.19	0.42
2:B:110:PRO:HG2	2:B:145:PHE:CE2	2.54	0.42
2:B:16:THR:HG21	2:B:66:LEU:HG	2.02	0.42
2:B:16:THR:HG23	2:B:83:VAL:HG13	2.00	0.42
2:B:102:ARG:HA	2:B:125:PHE:O	2.19	0.42
2:B:30:LEU:CD1	2:B:59:ILE:HG12	2.47	0.42
2:B:109:CYS:HA	2:B:110:PRO:HD2	1.80	0.42
1:C:136:THR:HG22	1:C:299:LEU:CD2	2.49	0.42
1:A:9:ILE:HG13	1:A:299:LEU:HD11	2.01	0.41
1:A:262:LYS:HD3	1:A:262:LYS:HA	1.86	0.41
2:B:21:ILE:O	2:B:57:ASP:N	2.52	0.41
2:B:28:LYS:O	2:B:32:LEU:HB2	2.20	0.41
1:A:10:ILE:HD12	1:A:112:ALA:HB1	2.02	0.41
2:B:80:GLN:HA	2:B:96:ARG:HH22	1.86	0.41
1:A:114:LEU:HD21	2:B:121:VAL:HG11	2.03	0.41
1:A:269:ARG:HA	1:A:272:GLU:OE2	2.20	0.41
2:B:29:LEU:HD21	2:B:77:TYR:HB2	2.02	0.41
2:B:147:HIS:CE1	2:B:148:ASN:OD1	2.73	0.41
2:B:18:ILE:HD12	2:B:18:ILE:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:LYS:HA	2:B:144:GLU:HA	2.01	0.41
1:C:158:ALA:HB3	1:C:225:LEU:HD12	2.03	0.41
2:D:14:ARG:HG3	2:D:65:PHE:HE1	1.86	0.41
1:C:134:HIS:HD2	1:C:168:THR:HG22	1.84	0.41
1:A:12:ILE:HD13	1:A:12:ILE:HA	1.79	0.40
1:A:229:ARG:HH21	1:A:229:ARG:HD2	1.74	0.40
1:C:134:HIS:CD2	1:C:168:THR:HG22	2.56	0.40
1:A:113:ARG:HH21	1:A:113:ARG:HD2	1.73	0.40
2:B:137:LYS:HE3	2:B:142:GLU:O	2.21	0.40
1:C:201:MET:HG2	1:C:205:LYS:NZ	2.36	0.40
1:C:167:ARG:HD2	3:F:2:GLC:C4	2.52	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%)	285 (92%)	21 (7%)	2 (1%)	21	51
1	C	308/310 (99%)	289 (94%)	15 (5%)	4 (1%)	9	31
2	B	144/153 (94%)	122 (85%)	17 (12%)	5 (4%)	3	10
2	D	144/153 (94%)	117 (81%)	20 (14%)	7 (5%)	1	6
All	All	904/926 (98%)	813 (90%)	73 (8%)	18 (2%)	6	21

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	9	VAL
2	B	34	LYS
2	D	50	SER
2	D	54	GLY

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Mol	Chain	Res	Type
2	D	105	ASN
1	A	41	HIS
2	B	24	GLN
2	B	132	ASN
2	D	51	GLY
2	D	152	ALA
2	B	88	ASN
1	C	270	VAL
2	D	68	GLU
1	C	132	ASN
1	C	237	PRO
1	A	270	VAL
2	D	48	LEU
1	C	35	GLN

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%)	241 (92%)	20 (8%)	12	36
1	C	261/261 (100%)	233 (89%)	28 (11%)	6	21
2	B	129/136 (95%)	106 (82%)	23 (18%)	2	6
2	D	129/136 (95%)	107 (83%)	22 (17%)	2	7
All	All	780/794 (98%)	687 (88%)	93 (12%)	5	17

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LYS
1	A	50	GLU
1	A	59	PHE
1	A	65	ARG
1	A	104	MET
1	A	105	ARG
1	A	108	GLN

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Mol	Chain	Res	Type
1	A	117	GLU
1	A	125	LEU
1	A	131	SER
1	A	195	PRO
1	A	221	GLU
1	A	237	PRO
1	A	242	ASN
1	A	246	GLN
1	A	269	ARG
1	A	279	LYS
1	A	285	TYR
1	A	296	ARG
1	A	310	LEU
2	B	12	ILE
2	B	19	ASP
2	B	22	PRO
2	B	24	GLN
2	B	30	LEU
2	B	32	LEU
2	B	53	MET
2	B	61	ILE
2	B	68	GLU
2	B	72	ASP
2	B	76	LEU
2	B	82	THR
2	B	85	ARG
2	B	86	ILE
2	B	88	ASN
2	B	95	SER
2	B	103	ILE
2	B	105	ASN
2	B	112	SER
2	B	120	PRO
2	B	128	ARG
2	B	132	ASN
2	B	153	ASN
1	C	14	ASP
1	C	15	LEU
1	C	17	ARG
1	C	38	LEU
1	C	40	LYS
1	C	56	ARG

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Mol	Chain	Res	Type
1	C	59	PHE
1	C	65	ARG
1	C	69	SER
1	C	74	SER
1	C	81	LEU
1	C	83	LYS
1	C	104	MET
1	C	121	ASN
1	C	140	LEU
1	C	147	GLN
1	C	167	ARG
1	C	190	ASP
1	C	213	SER
1	C	221	GLU
1	C	224	ILE
1	C	232	LYS
1	C	237	PRO
1	C	256	ASN
1	C	258	LYS
1	C	262	LYS
1	C	285	TYR
1	C	307	ASP
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	43	THR
2	D	52	GLU
2	D	55	ARG
2	D	61	ILE
2	D	62	GLU
2	D	82	THR
2	D	95	SER
2	D	97	PRO
2	D	101	GLU
2	D	102	ARG
2	D	105	ASN
2	D	112	SER
2	D	123	SER
2	D	128	ARG

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Mol	Chain	Res	Type
2	D	137	LYS
2	D	153	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	13	ASN
1	A	60	GLN
1	A	78	ASN
1	A	108	GLN
2	B	24	GLN
2	B	40	GLN
2	B	47	ASN
2	B	70	GLN
2	B	84	ASN
2	B	117	HIS
2	B	153	ASN
1	C	60	GLN
1	C	64	HIS
1	C	133	GLN
1	C	134	HIS
1	C	154	ASN
1	C	174	GLN
1	C	242	ASN
1	C	297	GLN
2	D	117	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	4.02	3 (60%)	5,5,17	2.16	3 (60%)
3	GLC	F	2	3	5,5,12	3.90	3 (60%)	5,5,17	2.74	3 (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	GLC	E	2	3	2/2/1/5	1/3/3/22	-
3	GLC	F	2	3	2/2/1/5	2/3/3/22	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	GLC	C4-C3	-6.89	1.22	1.51
3	F	2	GLC	C4-C3	-6.62	1.23	1.51
3	E	2	GLC	O3-C3	-4.74	1.23	1.43
3	F	2	GLC	O3-C3	-4.65	1.24	1.43
3	F	2	GLC	O5-C1	-3.23	1.25	1.42
3	E	2	GLC	O5-C1	-3.10	1.26	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	GLC	C1-C2-C3	-4.30	102.51	114.08
3	E	2	GLC	O3-C3-C2	2.98	122.71	109.56
3	F	2	GLC	O3-C3-C4	2.75	121.29	109.45
3	F	2	GLC	O3-C3-C2	2.70	121.47	109.56
3	E	2	GLC	O5-C1-C2	2.40	119.22	111.34
3	E	2	GLC	O3-C3-C4	2.20	118.93	109.45

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:

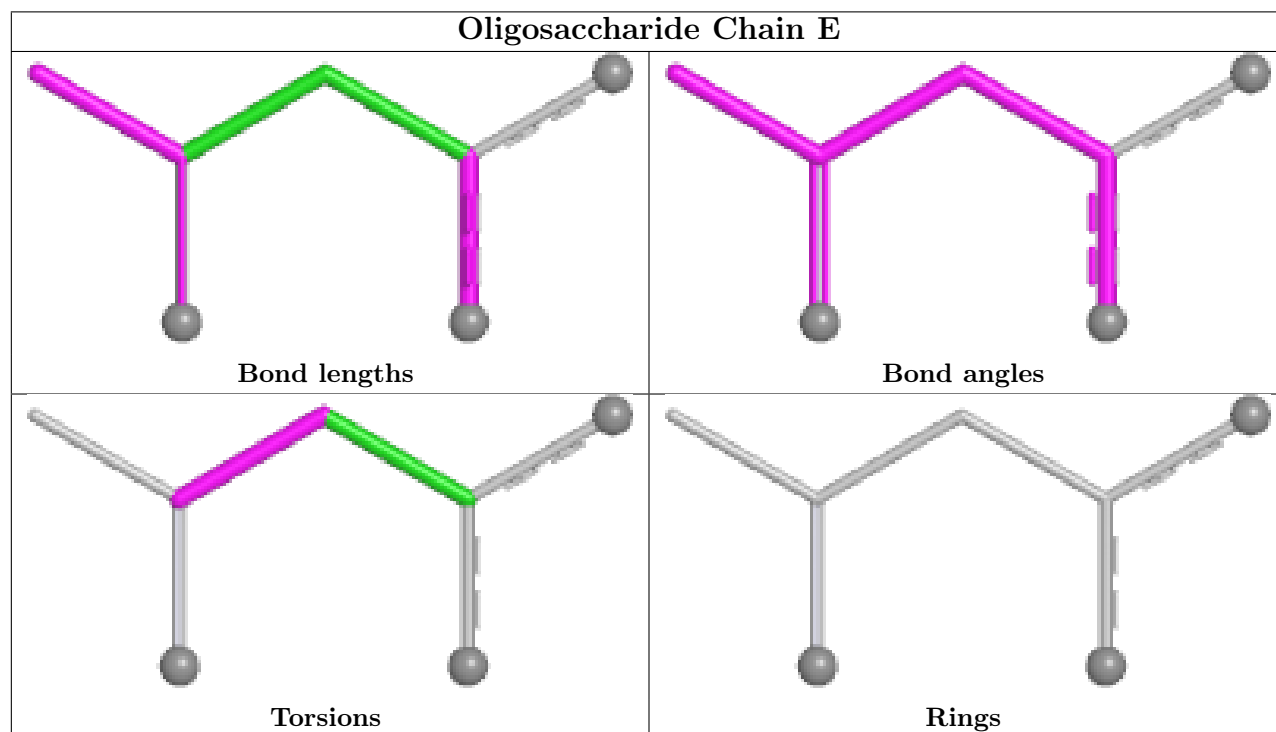
Mol	Chain	Res	Type	Atoms
3	E	2	GLC	C1-C2-C3-C4
3	F	2	GLC	C1-C2-C3-O3
3	F	2	GLC	C1-C2-C3-C4

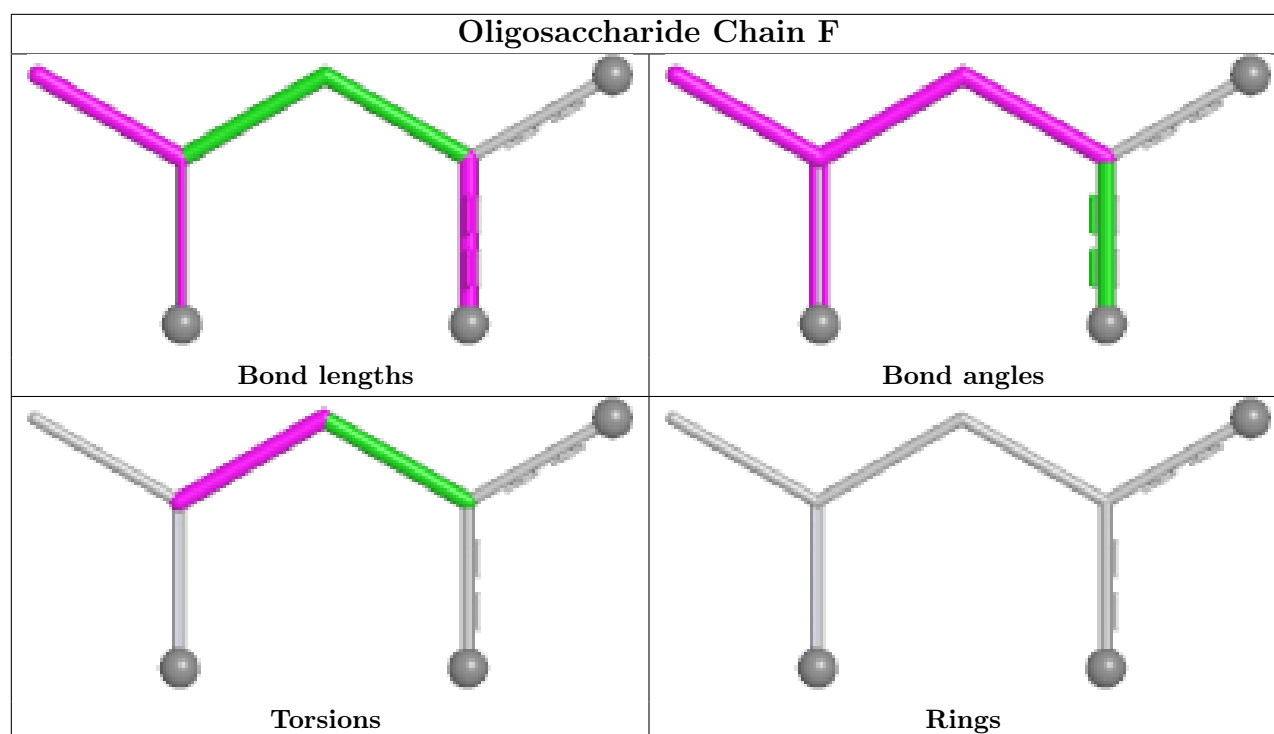
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2	GLC	2	0
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 [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	$\# Z > 2$
4	PCT	C	311	-	7,7,7	2.38	2 (28%)	9,10,10	1.81	2 (22%)
4	PCT	A	311	-	7,7,7	2.68	3 (42%)	9,10,10	2.22	5 (55%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCT	C	311	-	-	4/4/5/5	-
4	PCT	A	311	-	-	4/4/5/5	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	311	PCT	P-O1P	4.66	1.59	1.50
4	A	311	PCT	P-O1P	4.53	1.59	1.50
4	A	311	PCT	P-C1P	4.06	1.86	1.79
4	C	311	PCT	P-C1P	3.37	1.85	1.79
4	A	311	PCT	P-O3P	2.94	1.61	1.55

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	311	PCT	O1-C1-C1P	4.21	124.30	119.86
4	A	311	PCT	O1P-P-C1P	-3.58	102.83	111.10
4	A	311	PCT	O1-C1-C1P	3.31	123.35	119.86
4	A	311	PCT	O3P-P-C1P	2.35	111.78	106.84
4	A	311	PCT	O2P-P-C1P	-2.35	101.91	106.84
4	C	311	PCT	O2P-P-C1P	-2.22	102.18	106.84
4	A	311	PCT	C1P-C1-N1	-2.14	112.85	115.41

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	311	PCT	C1-C1P-P-O1P
4	C	311	PCT	C1-C1P-P-O1P
4	A	311	PCT	C1-C1P-P-O2P
4	A	311	PCT	C1-C1P-P-O3P
4	C	311	PCT	C1-C1P-P-O2P
4	C	311	PCT	C1-C1P-P-O3P
4	A	311	PCT	O1-C1-C1P-P
4	C	311	PCT	O1-C1-C1P-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	311	PCT	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.