



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:37 AM UTC

PDB ID : 3AT1 / pdb_00003at1
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
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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

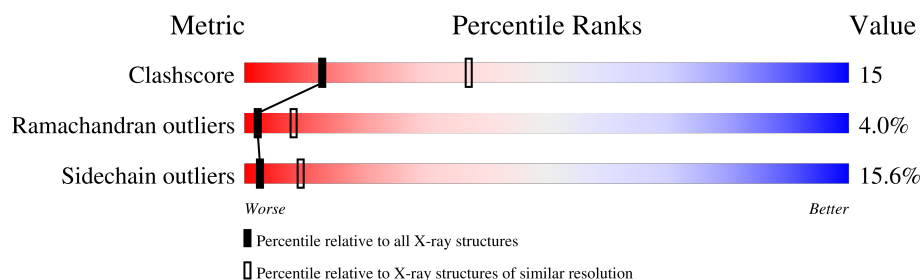
1 Overall quality at a glance

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	40% 39% 17% •
1	C	310	46% 34% 15% 5%
2	B	153	44% 35% 13% • 5%
2	D	153	47% 33% 13% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7124 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 (T 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

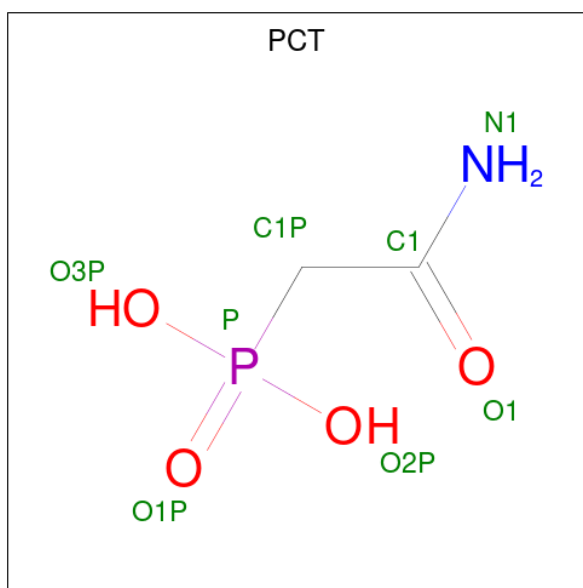
- Molecule 2 is a protein called ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN.

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 PHOSPHONOACETAMIDE (CCD ID: PCT) (formula: $C_2H_6NO_4P$).



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

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

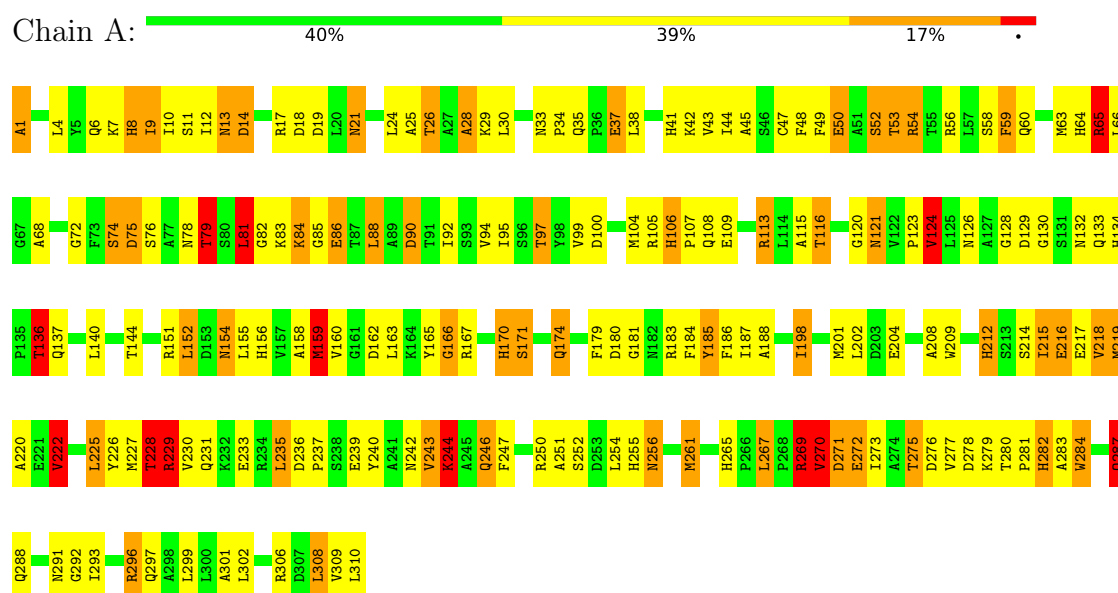
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

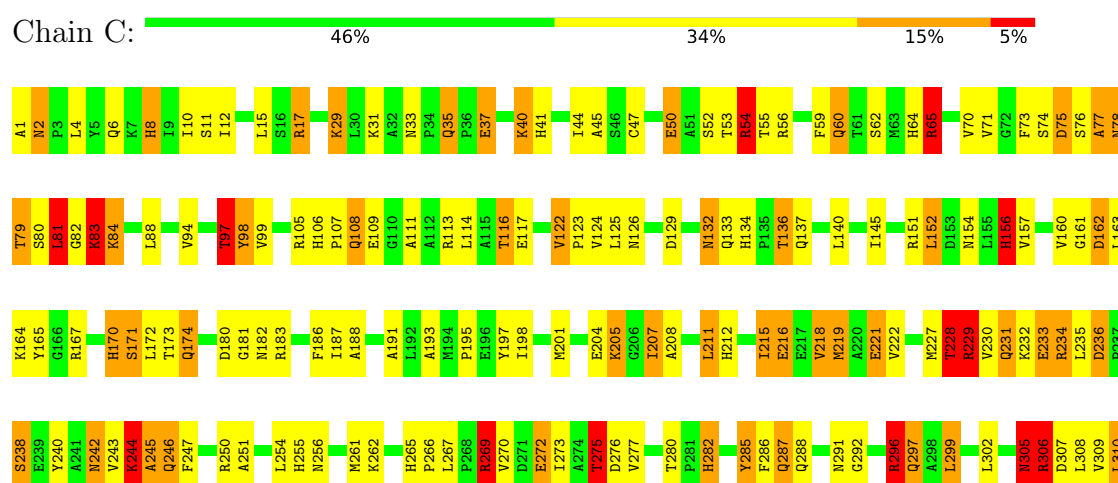
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

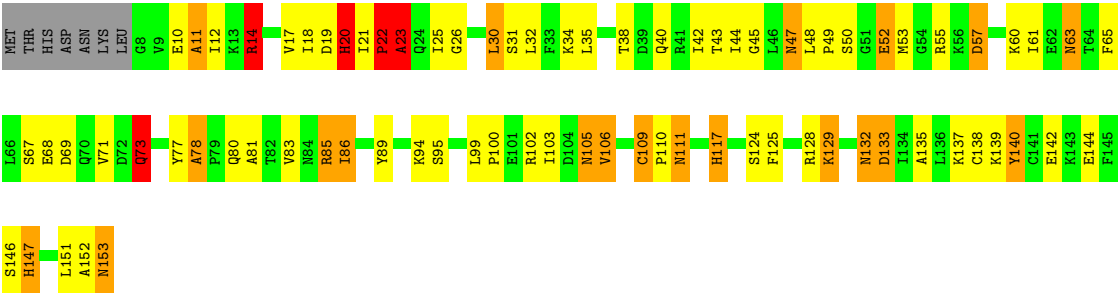


• Molecule 1: ASPARTATE CARBAMOYLTRANSFERASE (T STATE), CATALYTIC CHAIN



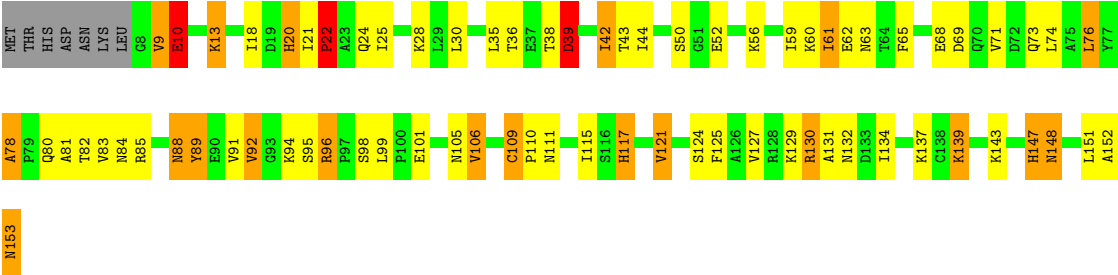
• Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN

Chain B: 44% 35% 13% 5%



● Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN

Chain D: 47% 33% 13% 5%



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	122.40 Å 122.40 Å 142.20 Å 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}	0.181 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7124	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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: ZN, PCT

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	1.32	20/2461 (0.8%)	2.25	119/3339 (3.6%)
1	C	1.31	15/2461 (0.6%)	2.23	128/3339 (3.8%)
2	B	1.11	6/1155 (0.5%)	2.06	33/1561 (2.1%)
2	D	1.07	4/1155 (0.3%)	2.05	40/1561 (2.6%)
All	All	1.25	45/7232 (0.6%)	2.18	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	5
1	C	0	5
2	B	0	4
All	All	0	14

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	44	ILE	CA-CB	9.90	1.67	1.54
1	C	156	HIS	CD2-NE2	-8.18	1.28	1.37
1	C	64	HIS	CD2-NE2	-8.09	1.28	1.37
1	C	265	HIS	CD2-NE2	-7.84	1.29	1.37
1	A	212	HIS	CD2-NE2	-7.72	1.29	1.37
1	A	12	ILE	CA-CB	7.71	1.64	1.54
1	A	64	HIS	CD2-NE2	-7.66	1.29	1.37
1	C	41	HIS	CD2-NE2	-7.37	1.29	1.37
1	C	53	THR	CA-CB	7.13	1.65	1.53
1	A	156	HIS	CD2-NE2	-7.13	1.30	1.37
1	A	106	HIS	CD2-NE2	-6.99	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	9	ILE	CA-CB	6.79	1.60	1.53
1	A	265	HIS	CD2-NE2	-6.71	1.30	1.37
1	C	245	ALA	CA-C	6.70	1.57	1.53
1	A	134	HIS	CD2-NE2	-6.68	1.30	1.37
1	C	212	HIS	CD2-NE2	-6.55	1.30	1.37
1	A	124	VAL	CA-CB	6.45	1.64	1.55
2	B	147	HIS	CD2-NE2	-6.41	1.30	1.37
1	A	282	HIS	CD2-NE2	-6.39	1.30	1.37
2	D	117	HIS	CG-ND1	-6.39	1.31	1.38
2	B	12	ILE	CA-CB	6.32	1.63	1.54
2	B	20	HIS	CD2-NE2	-6.31	1.30	1.37
2	D	147	HIS	CD2-NE2	-6.28	1.30	1.37
1	C	60	GLN	CA-CB	-6.07	1.43	1.53
2	B	117	HIS	CD2-NE2	-6.02	1.31	1.37
1	C	170	HIS	CD2-NE2	-6.00	1.31	1.37
1	A	41	HIS	CD2-NE2	-5.91	1.31	1.37
2	D	117	HIS	CD2-NE2	-5.87	1.31	1.37
1	A	255	HIS	CD2-NE2	-5.85	1.31	1.37
1	C	282	HIS	CD2-NE2	-5.78	1.31	1.37
2	B	20	HIS	CB-CG	5.67	1.58	1.50
1	A	243	VAL	CA-CB	5.59	1.62	1.54
1	A	8	HIS	CD2-NE2	-5.56	1.31	1.37
2	D	20	HIS	CD2-NE2	-5.44	1.31	1.37
1	A	170	HIS	CD2-NE2	-5.42	1.31	1.37
2	B	140	TYR	CA-CB	-5.34	1.46	1.53
1	C	8	HIS	CD2-NE2	-5.33	1.31	1.37
1	C	64	HIS	CG-ND1	-5.27	1.32	1.38
1	A	212	HIS	CG-ND1	-5.24	1.32	1.38
1	A	280	THR	CA-CB	5.22	1.61	1.53
1	A	44	ILE	CA-CB	5.17	1.60	1.54
1	C	134	HIS	CD2-NE2	-5.15	1.32	1.37
1	C	106	HIS	CD2-NE2	-5.11	1.32	1.37
1	A	255	HIS	CG-ND1	-5.08	1.32	1.38
1	A	8	HIS	CG-ND1	-5.05	1.32	1.38

All (320) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	ASN	CA-CB-CG	-13.92	98.68	112.60
2	B	52	GLU	N-CA-C	13.57	127.01	110.19
1	A	269	ARG	NE-CZ-NH2	11.60	129.64	119.20
1	C	56	ARG	NE-CZ-NH2	11.10	129.19	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	77	ALA	N-CA-C	-10.59	99.42	110.97
1	C	60	GLN	OE1-CD-NE2	-10.53	112.07	122.60
1	A	54	ARG	NE-CZ-NH1	-10.41	111.09	121.50
1	A	56	ARG	NE-CZ-NH1	-10.30	111.20	121.50
1	C	113	ARG	CA-CB-CG	10.28	134.66	114.10
2	B	11	ALA	N-CA-C	9.94	131.98	110.80
1	C	287	GLN	OE1-CD-NE2	-9.92	112.68	122.60
2	D	106	VAL	N-CA-C	9.78	120.22	111.81
1	A	126	ASN	OD1-CG-ND2	-9.76	112.84	122.60
1	C	287	GLN	CG-CD-NE2	9.63	130.84	116.40
1	A	52	SER	N-CA-C	9.60	123.52	107.20
1	C	2	ASN	CA-CB-CG	9.57	122.17	112.60
1	A	14	ASP	CA-CB-CG	9.55	122.15	112.60
1	A	276	ASP	CA-CB-CG	9.20	121.80	112.60
1	A	275	THR	CA-CB-OG1	-9.01	96.08	109.60
1	C	245	ALA	N-CA-C	-8.95	100.16	108.75
2	D	20	HIS	CA-CB-CG	8.90	122.70	113.80
1	C	56	ARG	NE-CZ-NH1	-8.85	112.65	121.50
1	C	296	ARG	NE-CZ-NH1	-8.83	112.67	121.50
1	C	269	ARG	NE-CZ-NH2	8.77	127.10	119.20
1	A	231	GLN	OE1-CD-NE2	-8.75	113.85	122.60
2	B	153	ASN	OD1-CG-ND2	-8.74	113.86	122.60
1	A	222	VAL	N-CA-C	8.67	121.01	109.21
1	A	75	ASP	CA-CB-CG	8.65	121.25	112.60
1	A	56	ARG	NE-CZ-NH2	8.64	126.98	119.20
1	A	19	ASP	CA-CB-CG	8.62	121.22	112.60
1	A	54	ARG	NE-CZ-NH2	8.52	126.86	119.20
2	B	106	VAL	N-CA-CB	-8.45	97.37	111.98
1	A	6	GLN	OE1-CD-NE2	-8.42	114.18	122.60
1	A	167	ARG	CA-CB-CG	8.40	130.91	114.10
2	D	117	HIS	CA-CB-CG	-8.36	105.44	113.80
1	C	113	ARG	NE-CZ-NH2	8.35	126.71	119.20
2	B	132	ASN	CA-CB-CG	8.34	120.94	112.60
1	A	13	ASN	CA-CB-CG	8.33	120.93	112.60
1	C	111	ALA	N-CA-C	8.33	120.36	111.28
2	B	63	ASN	OD1-CG-ND2	-8.08	114.52	122.60
2	B	153	ASN	CB-CG-ND2	7.80	128.10	116.40
1	A	54	ARG	CA-C-O	-7.79	112.64	120.82
1	A	50	GLU	N-CA-C	-7.75	97.05	109.76
1	A	288	GLN	N-CA-CB	-7.73	98.42	109.94
1	C	172	LEU	N-CA-C	-7.72	102.86	111.82
1	C	122	VAL	CA-C-N	7.71	127.47	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	122	VAL	C-N-CA	7.71	127.47	119.76
1	A	90	ASP	N-CA-C	7.67	120.72	111.82
1	A	121	ASN	N-CA-C	7.58	121.36	112.72
1	C	236	ASP	CA-CB-CG	7.58	120.18	112.60
1	C	218	VAL	CA-CB-CG2	-7.57	97.54	110.40
1	C	8	HIS	O-C-N	-7.56	113.94	122.86
1	A	215	ILE	N-CA-C	-7.55	102.92	110.62
1	C	193	ALA	N-CA-C	7.50	121.07	110.50
1	A	208	ALA	N-CA-C	7.49	120.71	109.25
1	A	129	ASP	CA-CB-CG	7.43	120.03	112.60
2	D	22	PRO	N-CA-C	7.40	127.72	112.47
1	C	97	THR	N-CA-C	-7.35	103.27	111.28
1	C	50	GLU	N-CA-C	-7.34	97.77	109.59
1	C	60	GLN	CG-CD-NE2	7.29	127.33	116.40
2	D	139	LYS	O-C-N	7.28	129.66	122.09
1	A	65	ARG	NE-CZ-NH2	7.28	125.75	119.20
2	D	9	VAL	N-CA-C	-7.28	96.27	106.53
2	B	67	SER	CA-C-O	7.25	130.88	120.51
1	A	222	VAL	N-CA-CB	-7.19	100.41	110.26
1	C	17	ARG	NE-CZ-NH2	7.19	125.67	119.20
1	C	231	GLN	OE1-CD-NE2	-7.14	115.46	122.60
1	A	53	THR	N-CA-C	7.14	126.00	110.80
1	A	79	THR	N-CA-CB	7.13	122.54	110.49
1	C	244	LYS	N-CA-C	-7.09	95.69	110.80
1	C	50	GLU	CA-CB-CG	7.09	128.28	114.10
1	A	35	GLN	CA-CB-CG	-7.08	99.94	114.10
1	A	120	GLY	CA-C-N	-7.02	111.43	122.73
1	A	120	GLY	C-N-CA	-7.02	111.43	122.73
1	C	53	THR	O-C-N	-7.00	114.03	122.22
1	A	136	THR	OG1-CB-CG2	6.96	123.23	109.30
2	D	153	ASN	CA-CB-CG	6.95	119.55	112.60
1	C	171	SER	CA-CB-OG	-6.94	97.22	111.10
1	C	180	ASP	N-CA-C	6.92	120.78	109.85
2	D	152	ALA	O-C-N	6.89	129.42	122.12
1	A	174	GLN	OE1-CD-NE2	-6.89	115.71	122.60
1	C	269	ARG	NE-CZ-NH1	-6.85	114.65	121.50
1	C	275	THR	N-CA-CB	-6.84	98.93	110.49
1	C	136	THR	N-CA-CB	-6.82	100.09	110.12
1	C	126	ASN	OD1-CG-ND2	-6.82	115.78	122.60
1	C	232	LYS	CA-CB-CG	6.81	127.73	114.10
1	C	288	GLN	OE1-CD-NE2	-6.80	115.80	122.60
1	A	270	VAL	O-C-N	-6.79	114.08	122.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	132	ASN	OD1-CG-ND2	-6.79	115.81	122.60
2	D	92	VAL	CA-CB-CG2	-6.76	98.91	110.40
1	C	242	ASN	CA-CB-CG	6.75	119.35	112.60
1	A	18	ASP	CA-CB-CG	6.72	119.33	112.60
2	D	88	ASN	N-CA-C	-6.70	99.67	109.18
1	A	243	VAL	N-CA-C	6.63	123.13	109.34
2	D	69	ASP	CA-CB-CG	6.62	119.22	112.60
1	C	8	HIS	CA-C-O	-6.61	114.35	121.56
1	A	10	ILE	N-CA-C	6.61	117.95	111.67
1	A	54	ARG	CB-CA-C	-6.61	100.50	110.88
1	A	261	MET	CG-SD-CE	-6.60	86.39	100.90
1	C	116	THR	N-CA-CB	-6.57	100.46	110.12
2	D	36	THR	N-CA-C	6.56	121.02	112.89
1	A	287	GLN	CG-CD-NE2	6.55	126.23	116.40
2	D	61	ILE	CB-CA-C	-6.50	101.01	110.63
1	A	269	ARG	NE-CZ-NH1	-6.49	115.01	121.50
2	B	35	LEU	CA-C-O	6.49	127.43	120.10
1	A	10	ILE	CB-CG1-CD1	-6.48	100.19	113.80
1	C	75	ASP	CA-CB-CG	6.47	119.07	112.60
2	D	139	LYS	CB-CG-CD	-6.44	96.48	111.30
1	C	113	ARG	NE-CZ-NH1	-6.44	115.06	121.50
1	A	74	SER	N-CA-C	-6.41	99.58	109.52
2	B	73	GLN	OE1-CD-NE2	-6.41	116.19	122.60
1	C	246	GLN	OE1-CD-NE2	-6.41	116.19	122.60
2	D	73	GLN	OE1-CD-NE2	-6.40	116.20	122.60
1	C	307	ASP	CA-CB-CG	6.38	118.98	112.60
1	C	79	THR	N-CA-C	-6.38	99.26	108.07
1	A	1	ALA	N-CA-C	-6.38	93.14	111.00
2	B	106	VAL	CB-CA-C	6.38	120.39	110.95
1	A	33	ASN	CA-C-N	6.33	126.70	119.93
1	A	33	ASN	C-N-CA	6.33	126.70	119.93
1	C	37	GLU	CA-CB-CG	-6.31	101.48	114.10
1	A	269	ARG	CA-CB-CG	6.30	126.71	114.10
1	A	216	GLU	CA-CB-CG	6.30	126.70	114.10
1	A	228	THR	CA-CB-OG1	-6.30	100.15	109.60
1	A	244	LYS	CA-CB-CG	6.25	126.61	114.10
1	C	80	SER	N-CA-C	-6.25	97.49	108.23
1	C	265	HIS	CB-CG-CD2	-6.24	123.09	131.20
1	C	296	ARG	NE-CZ-NH2	6.23	124.80	119.20
1	A	84	LYS	N-CA-C	-6.21	101.27	110.46
2	B	94	LYS	CB-CG-CD	-6.20	97.05	111.30
2	B	23	ALA	N-CA-C	-6.19	97.62	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	222	VAL	N-CA-C	6.18	118.54	109.63
2	D	39	ASP	CA-CB-CG	-6.18	106.42	112.60
1	A	97	THR	CA-CB-OG1	-6.15	100.37	109.60
1	C	218	VAL	CA-CB-CG1	6.15	120.85	110.40
2	B	19	ASP	CA-CB-CG	6.14	118.74	112.60
1	C	116	THR	OG1-CB-CG2	6.13	121.57	109.30
1	C	105	ARG	NE-CZ-NH1	-6.12	115.38	121.50
1	A	144	THR	N-CA-C	-6.12	104.52	112.23
1	C	44	ILE	N-CA-C	-6.11	99.69	108.48
2	D	83	VAL	N-CA-C	-6.10	103.40	110.05
1	A	72	GLY	N-CA-C	6.10	119.10	110.74
1	C	307	ASP	N-CA-C	-6.08	95.00	107.70
1	C	197	TYR	CA-CB-CG	6.08	124.83	113.90
1	C	207	ILE	N-CA-C	6.07	117.75	108.71
1	A	154	ASN	OD1-CG-ND2	-6.07	116.53	122.60
1	A	184	PHE	N-CA-C	6.06	118.62	108.02
1	A	136	THR	N-CA-C	6.05	117.95	111.36
1	C	195	PRO	N-CA-C	6.05	120.73	111.11
1	C	132	ASN	OD1-CG-ND2	-6.05	116.55	122.60
1	C	129	ASP	CA-CB-CG	6.04	118.64	112.60
1	C	255	HIS	CA-CB-CG	-6.04	107.76	113.80
1	A	58	SER	CA-CB-OG	6.03	123.16	111.10
1	A	64	HIS	CA-CB-CG	-6.02	107.78	113.80
2	B	105	ASN	CA-CB-CG	-6.02	106.58	112.60
1	C	77	ALA	O-C-N	6.02	128.29	122.03
1	C	276	ASP	CA-CB-CG	6.00	118.60	112.60
1	C	275	THR	OG1-CB-CG2	5.99	121.28	109.30
1	A	284	TRP	CG-CD2-CE3	5.96	139.86	133.90
2	D	61	ILE	N-CA-CB	5.95	119.62	111.41
2	B	105	ASN	N-CA-C	5.94	123.45	110.80
1	C	45	ALA	N-CA-C	-5.91	100.04	109.96
1	C	250	ARG	NE-CZ-NH1	-5.90	115.60	121.50
1	A	38	LEU	N-CA-C	5.90	118.50	111.71
1	A	26	THR	CA-CB-OG1	-5.89	100.77	109.60
1	A	137	GLN	OE1-CD-NE2	-5.88	116.72	122.60
2	B	57	ASP	CA-CB-CG	5.86	118.46	112.60
1	A	162	ASP	CA-CB-CG	5.85	118.45	112.60
1	A	231	GLN	CG-CD-NE2	5.81	125.12	116.40
1	C	83	LYS	N-CA-C	5.81	116.22	108.38
1	C	62	SER	CA-C-O	-5.80	114.69	120.90
1	A	49	PHE	N-CA-C	-5.80	104.92	112.23
1	A	92	ILE	CA-C-O	-5.79	114.51	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	105	ASN	N-CA-C	5.78	123.12	110.80
1	A	308	LEU	N-CA-C	-5.77	99.33	108.73
2	D	92	VAL	CA-CB-CG1	5.77	120.21	110.40
2	D	10	GLU	N-CA-C	5.76	123.07	110.80
1	C	230	VAL	N-CA-C	-5.75	100.12	108.87
2	D	109	CYS	CA-C-N	5.75	125.60	119.28
2	D	109	CYS	C-N-CA	5.75	125.60	119.28
2	D	117	HIS	CA-C-O	-5.74	112.54	119.49
1	C	54	ARG	NE-CZ-NH2	5.74	124.36	119.20
1	A	21	ASN	OD1-CG-ND2	-5.73	116.87	122.60
2	B	85	ARG	N-CA-C	-5.73	99.39	108.73
1	C	188	ALA	O-C-N	-5.73	117.81	121.88
2	D	148	ASN	OD1-CG-ND2	-5.73	116.87	122.60
1	C	219	MET	N-CA-C	5.72	122.98	110.80
1	C	221	GLU	N-CA-C	5.72	120.39	112.90
1	C	251	ALA	N-CA-C	5.71	118.24	111.33
1	C	306	ARG	N-CA-C	5.71	122.97	110.80
1	C	173	THR	OG1-CB-CG2	-5.71	97.88	109.30
1	C	246	GLN	CG-CD-NE2	5.70	124.95	116.40
1	A	159	MET	CG-SD-CE	-5.68	88.41	100.90
2	D	73	GLN	CG-CD-NE2	5.67	124.91	116.40
1	C	272	GLU	N-CA-C	5.64	120.17	113.28
1	A	272	GLU	N-CA-C	5.64	122.81	110.80
1	A	95	ILE	CA-CB-CG1	-5.62	100.84	110.40
1	A	166	GLY	CA-C-N	5.62	128.08	120.38
1	A	166	GLY	C-N-CA	5.62	128.08	120.38
1	A	183	ARG	CA-CB-CG	5.61	125.31	114.10
1	A	251	ALA	CA-C-N	5.60	128.05	120.38
1	A	251	ALA	C-N-CA	5.60	128.05	120.38
1	C	53	THR	N-CA-CB	-5.59	101.60	110.22
1	C	88	LEU	N-CA-C	-5.58	105.19	111.28
1	C	116	THR	CA-CB-OG1	-5.58	101.22	109.60
2	B	57	ASP	N-CA-C	-5.58	102.49	110.59
1	C	35	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	A	273	ILE	N-CA-C	-5.57	98.42	107.28
1	C	113	ARG	N-CA-C	-5.57	105.21	112.23
1	C	232	LYS	N-CA-CB	-5.56	101.65	110.22
1	A	115	ALA	CA-C-N	5.55	129.49	120.60
1	A	115	ALA	C-N-CA	5.55	129.49	120.60
1	C	81	LEU	O-C-N	5.55	128.96	123.46
1	A	13	ASN	N-CA-CB	-5.54	101.39	110.14
1	C	191	ALA	N-CA-C	5.54	118.08	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	LEU	O-C-N	-5.53	114.96	121.32
1	C	157	VAL	N-CA-CB	-5.53	104.49	111.46
1	A	137	GLN	CG-CD-NE2	5.53	124.69	116.40
1	A	37	GLU	CA-CB-CG	5.52	125.14	114.10
2	B	21	ILE	N-CA-C	-5.52	96.96	108.88
1	C	54	ARG	NE-CZ-NH1	-5.52	115.98	121.50
2	B	34	LYS	CB-CG-CD	5.49	123.93	111.30
2	B	69	ASP	CA-CB-CG	5.48	118.08	112.60
1	C	52	SER	N-CA-CB	-5.48	102.57	112.27
1	A	275	THR	CA-CB-CG2	5.47	119.80	110.50
1	A	79	THR	CB-CA-C	-5.46	99.56	110.42
1	A	309	VAL	O-C-N	5.44	129.37	122.57
2	D	78	ALA	CA-C-N	5.43	125.10	119.56
2	D	78	ALA	C-N-CA	5.43	125.10	119.56
2	D	18	ILE	N-CA-C	-5.42	98.85	107.15
1	C	55	THR	N-CA-C	-5.42	105.45	111.36
2	D	39	ASP	CA-C-O	5.42	128.26	120.51
1	A	52	SER	CA-C-O	-5.41	114.62	120.09
1	A	88	LEU	N-CA-C	-5.41	105.38	111.28
1	A	28	ALA	O-C-N	5.39	127.84	122.12
1	C	17	ARG	NE-CZ-NH1	-5.38	116.12	121.50
1	C	285	TYR	O-C-N	-5.38	116.01	122.15
1	C	205	LYS	CG-CD-CE	5.38	123.66	111.30
1	C	152	LEU	CA-C-O	5.37	125.51	119.18
2	B	78	ALA	CA-C-N	5.37	125.03	119.56
2	B	78	ALA	C-N-CA	5.37	125.03	119.56
2	D	10	GLU	CB-CG-CD	5.35	121.70	112.60
2	B	128	ARG	NE-CZ-NH2	5.35	124.02	119.20
2	B	125	PHE	CA-CB-CG	-5.34	108.46	113.80
2	B	146	SER	N-CA-CB	5.34	118.12	110.06
1	C	33	ASN	CA-C-O	5.33	126.42	120.34
1	C	273	ILE	N-CA-C	-5.33	97.96	107.18
2	B	109	CYS	CA-CB-SG	-5.31	102.18	114.40
1	C	182	ASN	OD1-CG-ND2	-5.31	117.29	122.60
1	A	209	TRP	O-C-N	-5.31	115.35	122.94
2	B	133	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	278	ASP	CA-C-O	-5.29	115.25	120.70
1	C	229	ARG	NE-CZ-NH2	5.29	123.97	119.20
1	C	216	GLU	CA-C-O	-5.29	114.99	120.92
1	A	43	VAL	CG1-CB-CG2	-5.29	99.17	110.80
1	A	229	ARG	CA-CB-CG	5.28	124.66	114.10
1	A	279	LYS	CA-CB-CG	5.28	124.66	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	LEU	CA-C-O	5.28	124.52	119.08
1	A	269	ARG	CD-NE-CZ	5.27	131.78	124.40
1	C	40	LYS	CA-CB-CG	5.27	124.64	114.10
1	A	54	ARG	N-CA-CB	5.26	117.64	110.01
1	C	29	LYS	CA-C-N	5.26	127.33	120.28
1	C	29	LYS	C-N-CA	5.26	127.33	120.28
1	C	53	THR	CA-C-O	-5.26	114.16	120.10
1	A	34	PRO	O-C-N	-5.25	116.44	122.85
2	D	24	GLN	OE1-CD-NE2	-5.25	117.35	122.60
2	D	117	HIS	N-CA-C	5.25	118.79	112.38
1	A	284	TRP	CE2-CD2-CG	-5.25	100.90	107.20
1	C	99	VAL	O-C-N	5.25	128.22	122.76
2	D	121	VAL	N-CA-CB	-5.24	102.12	111.92
1	C	145	ILE	N-CA-C	-5.23	105.44	110.72
1	C	174	GLN	CA-CB-CG	5.23	124.55	114.10
2	B	45	GLY	N-CA-C	-5.22	102.72	110.71
1	C	269	ARG	N-CA-C	-5.21	100.69	109.07
1	C	231	GLN	CG-CD-NE2	5.20	124.20	116.40
1	C	136	THR	OG1-CB-CG2	5.19	119.69	109.30
1	C	232	LYS	CA-C-O	5.18	125.96	120.10
1	A	60	GLN	OE1-CD-NE2	-5.18	117.42	122.60
1	C	234	ARG	N-CA-C	-5.18	106.55	112.92
2	D	130	ARG	CA-C-O	5.18	126.07	120.32
1	A	275	THR	N-CA-C	5.18	119.07	112.34
1	A	284	TRP	CB-CG-CD1	-5.17	119.15	126.90
2	D	106	VAL	CA-CB-CG2	-5.17	101.62	110.40
1	C	204	GLU	CA-CB-CG	5.16	124.42	114.10
1	C	71	VAL	O-C-N	-5.15	117.32	123.04
1	A	86	GLU	CA-CB-CG	-5.15	103.80	114.10
1	C	136	THR	N-CA-C	5.14	116.89	111.28
1	C	10	ILE	N-CA-CB	-5.14	103.23	111.82
1	A	250	ARG	CA-CB-CG	5.14	124.38	114.10
1	A	68	ALA	N-CA-C	5.14	117.16	110.43
2	B	132	ASN	N-CA-C	-5.13	99.86	110.80
1	A	113	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	C	65	ARG	CB-CG-CD	5.12	123.09	111.30
1	C	116	THR	N-CA-C	5.12	116.86	111.28
2	D	129	LYS	N-CA-C	-5.11	101.79	109.15
1	A	275	THR	OG1-CB-CG2	5.11	119.51	109.30
1	C	113	ARG	N-CA-CB	-5.10	102.45	110.30
1	A	84	LYS	CA-C-N	5.09	131.40	121.41
1	A	84	LYS	C-N-CA	5.09	131.40	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	80	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	C	47	CYS	CA-C-N	-5.08	115.79	122.85
1	C	47	CYS	C-N-CA	-5.08	115.79	122.85
1	A	231	GLN	N-CA-C	-5.08	100.13	108.41
1	C	52	SER	CA-C-N	5.05	127.56	120.28
1	C	52	SER	C-N-CA	5.05	127.56	120.28
1	C	215	ILE	CB-CG1-CD1	5.05	124.42	113.80
1	C	305	ASN	OD1-CG-ND2	-5.05	117.55	122.60
1	A	35	GLN	CA-C-N	5.05	126.15	119.84
1	A	35	GLN	C-N-CA	5.05	126.15	119.84
1	C	228	THR	CA-CB-OG1	-5.04	102.03	109.60
1	C	297	GLN	O-C-N	5.04	127.54	122.09
1	C	108	GLN	N-CA-C	5.03	117.95	109.95
1	A	204	GLU	CB-CG-CD	5.03	121.14	112.60
1	A	47	CYS	N-CA-CB	-5.02	101.97	110.46
1	C	215	ILE	CA-C-O	5.02	126.27	121.05
1	A	65	ARG	NE-CZ-NH1	-5.02	116.48	121.50
2	D	21	ILE	CA-C-N	5.01	126.11	119.84
2	D	21	ILE	C-N-CA	5.01	126.11	119.84
2	B	47	ASN	OD1-CG-ND2	-5.01	117.59	122.60
1	A	180	ASP	N-CA-C	5.01	117.89	110.48
1	C	79	THR	CB-CA-C	-5.01	102.89	114.41

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	TYR	Sidechain
1	A	185	TYR	Sidechain
1	A	226	TYR	Sidechain
1	A	240	TYR	Sidechain
1	A	59	PHE	Sidechain
2	B	140	TYR	Sidechain
2	B	48	LEU	Peptide
2	B	77	TYR	Sidechain
2	B	89	TYR	Sidechain
1	C	156	HIS	Sidechain
1	C	240	TYR	Sidechain
1	C	285	TYR	Sidechain
1	C	286	PHE	Sidechain
1	C	98	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	91	0
1	C	2415	0	2422	70	0
2	B	1138	0	1154	28	0
2	D	1138	0	1154	28	0
3	A	8	0	4	2	0
3	C	8	0	4	3	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
All	All	7124	0	7160	215	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 15.

All (215) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LEU:HA	1:A:7:LYS:HD3	1.51	0.92
1:A:136:THR:HB	1:A:296:ARG:NH2	1.84	0.92
1:C:280:THR:HG22	1:C:282:HIS:H	1.41	0.84
1:A:8:HIS:HD2	1:A:124:VAL:H	1.26	0.82
1:A:81:LEU:HD22	1:A:81:LEU:H	1.46	0.81
1:A:136:THR:HB	1:A:296:ARG:HH21	1.46	0.79
1:C:94:VAL:O	1:C:97:THR:HB	1.86	0.76
1:A:9:ILE:HG13	1:A:299:LEU:HD11	1.68	0.74
1:C:50:GLU:HA	1:C:76:SER:OG	1.89	0.72
1:C:163:LEU:O	1:C:170:HIS:HE1	1.72	0.72
2:B:14:ARG:HA	2:B:86:ILE:O	1.88	0.72
1:A:140:LEU:HD22	1:A:292:GLY:HA2	1.71	0.71
2:D:65:PHE:HB3	2:D:85:ARG:NH2	2.08	0.68
1:C:50:GLU:HB2	1:C:107:PRO:HD3	1.76	0.68
2:D:10:GLU:HA	2:D:60:LYS:NZ	2.10	0.67
1:C:229:ARG:CZ	1:C:231:GLN:HA	2.24	0.67
1:C:1:ALA:HA	1:C:306:ARG:HD2	1.77	0.66
1:A:225:LEU:HB2	1:A:261:MET:HE2	1.78	0.66
1:A:292:GLY:O	1:A:296:ARG:HB2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:PHE:HB3	1:A:63:MET:HE3	1.79	0.65
1:A:106:HIS:HD2	1:A:108:GLN:H	1.44	0.64
1:C:8:HIS:HD2	1:C:124:VAL:H	1.45	0.64
2:B:38:THR:HG22	2:B:40:GLN:H	1.64	0.62
1:C:292:GLY:O	1:C:296:ARG:HB2	2.00	0.62
1:C:234:ARG:O	1:C:235:LEU:HD23	1.99	0.62
1:A:163:LEU:HG	1:A:188:ALA:HB2	1.80	0.62
1:C:65:ARG:HB2	1:C:297:GLN:NE2	2.15	0.62
1:C:229:ARG:NH1	1:C:231:GLN:HA	2.15	0.62
1:A:50:GLU:HB2	1:A:107:PRO:HD3	1.81	0.61
1:A:11:SER:OG	1:A:13:ASN:HB3	1.99	0.61
1:A:66:LEU:HG	1:A:297:GLN:HE21	1.66	0.61
1:C:31:LYS:NZ	1:C:291:ASN:HD21	1.99	0.60
1:C:261:MET:O	1:C:282:HIS:HD2	1.84	0.60
1:A:54:ARG:HD2	3:A:311:PCT:H1P2	1.84	0.60
2:D:82:THR:HG23	2:D:96:ARG:HH22	1.66	0.59
1:C:54:ARG:HB3	3:C:311:PCT:O2P	2.02	0.59
1:C:132:ASN:OD1	1:C:133:GLN:HG2	2.01	0.59
1:A:225:LEU:HD12	1:A:261:MET:HE1	1.85	0.59
1:C:160:VAL:HG11	1:C:215:ILE:HD11	1.85	0.59
1:A:154:ASN:HA	1:A:181:GLY:O	2.04	0.58
2:B:71:VAL:HG13	2:B:83:VAL:HG21	1.86	0.58
1:A:261:MET:O	1:A:282:HIS:HD2	1.87	0.58
1:A:219:MET:HG3	1:A:256:ASN:HD21	1.68	0.58
2:B:73:GLN:OE1	2:B:103:ILE:HG23	2.03	0.57
2:D:76:LEU:HD11	2:D:134:ILE:HD13	1.85	0.57
1:A:113:ARG:O	1:A:116:THR:HB	2.03	0.57
2:D:10:GLU:HA	2:D:60:LYS:HZ1	1.69	0.57
1:A:82:GLY:HA2	1:A:86:GLU:HB3	1.86	0.56
1:A:48:PHE:CD2	1:A:105:ARG:HB3	2.41	0.56
1:A:8:HIS:CD2	1:A:124:VAL:H	2.16	0.55
1:A:65:ARG:HB3	1:A:297:GLN:NE2	2.21	0.55
1:C:8:HIS:HD2	1:C:124:VAL:N	2.03	0.55
1:C:77:ALA:O	1:C:78:ASN:HB2	2.06	0.55
1:A:302:LEU:HA	1:A:308:LEU:HD21	1.88	0.55
1:C:65:ARG:HB2	1:C:297:GLN:HE21	1.72	0.55
1:C:302:LEU:HD23	1:C:308:LEU:HD12	1.89	0.54
1:A:171:SER:HA	1:A:174:GLN:HE21	1.72	0.54
1:A:287:GLN:H	1:A:287:GLN:HE21	1.55	0.54
1:C:186:PHE:HB2	1:C:211:LEU:HD12	1.89	0.54
1:A:214:SER:HB3	1:A:216:GLU:HG2	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:TRP:HA	1:A:287:GLN:NE2	2.22	0.54
2:D:50:SER:HB2	2:D:56:LYS:HG2	1.89	0.54
1:C:73:PHE:CE1	1:C:81:LEU:HD11	2.42	0.54
2:D:111:ASN:O	2:D:117:HIS:HE1	1.91	0.53
2:D:62:GLU:HG2	2:D:63:ASN:ND2	2.23	0.53
1:A:254:LEU:HD11	1:A:277:VAL:HG13	1.91	0.53
1:C:205:LYS:HD3	1:C:207:ILE:HD11	1.91	0.53
2:B:18:ILE:HG23	2:B:83:VAL:HG22	1.90	0.53
1:C:227:MET:O	1:C:266:PRO:HD2	2.08	0.53
1:A:45:ALA:HB2	1:A:99:VAL:HG21	1.91	0.52
1:A:229:ARG:HD3	1:A:230:VAL:O	2.09	0.52
1:C:12:ILE:HA	1:C:15:LEU:HD12	1.90	0.52
1:A:13:ASN:HB2	1:A:174:GLN:OE1	2.09	0.52
2:D:30:LEU:HD23	2:D:35:LEU:HB2	1.91	0.52
1:A:132:ASN:CG	1:A:133:GLN:HG2	2.35	0.52
2:D:111:ASN:O	2:D:117:HIS:CE1	2.62	0.52
2:B:65:PHE:CD2	2:B:85:ARG:HG3	2.45	0.51
1:A:160:VAL:O	1:A:228:THR:HG22	2.10	0.51
1:C:187:ILE:HG22	1:C:247:PHE:HE1	1.75	0.51
2:B:42:ILE:HG12	2:B:61:ILE:HG23	1.92	0.51
2:B:78:ALA:HB1	2:B:81:ALA:HB2	1.93	0.51
1:A:109:GLU:HG3	1:A:130:GLY:HA3	1.93	0.51
2:B:65:PHE:CE2	2:B:85:ARG:HG3	2.45	0.51
1:C:198:ILE:O	1:C:201:MET:HB3	2.11	0.51
2:B:135:ALA:HB1	2:B:144:GLU:HG2	1.93	0.51
1:C:79:THR:HG1	1:C:81:LEU:HB2	1.76	0.50
1:A:151:ARG:NH2	1:A:154:ASN:O	2.45	0.50
1:A:187:ILE:HG22	1:A:247:PHE:CE2	2.46	0.50
2:B:40:GLN:HG3	2:B:63:ASN:HB2	1.92	0.50
1:A:8:HIS:HD2	1:A:124:VAL:N	2.01	0.50
1:A:214:SER:HB3	1:A:216:GLU:CD	2.37	0.50
1:A:301:ALA:HB1	1:A:308:LEU:HD11	1.94	0.50
1:C:163:LEU:O	1:C:170:HIS:CE1	2.61	0.50
1:A:308:LEU:HB3	1:A:310:LEU:HG	1.93	0.49
2:D:38:THR:CG2	2:D:42:ILE:HD11	2.42	0.49
1:A:219:MET:HG3	1:A:256:ASN:ND2	2.26	0.49
1:A:302:LEU:HD23	1:A:308:LEU:HD23	1.94	0.49
2:B:111:ASN:O	2:B:117:HIS:HE1	1.95	0.49
2:B:129:LYS:HG2	2:B:133:ASP:OD2	2.12	0.49
1:C:151:ARG:NH2	1:C:154:ASN:O	2.46	0.49
1:A:235:LEU:HG	1:A:239:GLU:CD	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:HIS:CD2	1:A:123:PRO:HA	2.48	0.48
1:C:11:SER:HB2	1:C:133:GLN:HG3	1.95	0.48
2:D:124:SER:HB3	2:D:139:LYS:HB2	1.96	0.48
1:A:52:SER:HB3	3:A:311:PCT:O3P	2.13	0.48
1:A:158:ALA:HB2	1:A:222:VAL:HG21	1.95	0.48
2:B:138:CYS:O	2:B:142:GLU:HA	2.14	0.48
1:A:26:THR:O	1:A:29:LYS:HB2	2.14	0.48
1:A:243:VAL:HG23	1:A:246:GLN:HG3	1.95	0.48
1:A:212:HIS:NE2	1:A:218:VAL:HG13	2.29	0.48
2:B:102:ARG:HD2	2:B:124:SER:OG	2.14	0.48
1:C:8:HIS:CD2	1:C:124:VAL:H	2.29	0.48
2:D:22:PRO:HG2	2:D:25:ILE:HG13	1.95	0.48
1:A:171:SER:O	1:A:174:GLN:HB2	2.14	0.47
2:B:71:VAL:HG22	2:B:83:VAL:HG11	1.96	0.47
1:C:73:PHE:CZ	1:C:81:LEU:HD11	2.49	0.47
2:D:137:LYS:HA	2:D:143:LYS:O	2.14	0.47
2:D:20:HIS:HB3	2:D:81:ALA:HA	1.97	0.47
1:C:60:GLN:HG2	1:C:70:VAL:HG11	1.96	0.47
1:C:277:VAL:O	1:C:280:THR:HB	2.14	0.47
1:A:30:LEU:HD13	1:A:297:GLN:HB3	1.97	0.47
1:A:185:TYR:CD2	1:A:218:VAL:HG11	2.49	0.47
1:A:214:SER:HB3	1:A:216:GLU:CG	2.45	0.47
1:C:160:VAL:O	1:C:228:THR:HB	2.14	0.47
2:B:40:GLN:NE2	2:B:63:ASN:HD22	2.12	0.47
2:D:99:LEU:HD21	2:D:134:ILE:HG12	1.96	0.47
1:C:187:ILE:HG22	1:C:247:PHE:CE1	2.49	0.47
1:C:254:LEU:HD13	1:C:280:THR:HG21	1.96	0.47
1:A:214:SER:O	1:A:217:GLU:HB2	2.16	0.46
1:A:236:ASP:O	1:A:239:GLU:HB3	2.16	0.46
1:A:81:LEU:HD22	1:A:81:LEU:N	2.23	0.46
2:B:111:ASN:O	2:B:117:HIS:CE1	2.68	0.46
1:C:154:ASN:HA	1:C:181:GLY:O	2.16	0.46
1:C:156:HIS:HD2	1:C:221:GLU:HB3	1.81	0.46
1:C:161:GLY:HA3	1:C:228:THR:HG22	1.97	0.46
1:A:128:GLY:HA2	1:A:133:GLN:O	2.16	0.46
2:B:22:PRO:HB2	2:B:25:ILE:HG13	1.98	0.46
2:B:109:CYS:HA	2:B:110:PRO:HD3	1.78	0.46
1:C:229:ARG:HD3	1:C:231:GLN:OE1	2.16	0.46
1:C:305:ASN:HB2	1:C:308:LEU:HG	1.97	0.45
1:A:1:ALA:HA	1:A:306:ARG:O	2.16	0.45
1:C:171:SER:HA	1:C:174:GLN:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:GLU:H	1:C:233:GLU:CD	2.25	0.45
1:A:160:VAL:HG22	1:A:187:ILE:HD13	1.98	0.45
1:A:261:MET:O	1:A:282:HIS:CD2	2.68	0.45
1:C:205:LYS:HB3	1:C:207:ILE:HD12	1.98	0.45
1:A:212:HIS:HD2	1:A:217:GLU:HB3	1.81	0.45
1:C:183:ARG:HG2	1:C:208:ALA:HB3	1.97	0.45
1:C:137:GLN:O	1:C:140:LEU:HG	2.16	0.45
1:C:238:SER:O	1:C:242:ASN:HB2	2.16	0.44
1:A:158:ALA:HA	1:A:185:TYR:O	2.18	0.44
2:B:17:VAL:HG22	2:B:60:LYS:HG2	2.00	0.44
1:A:270:VAL:HG13	1:A:271:ASP:H	1.83	0.44
1:C:162:ASP:OD1	1:C:165:TYR:HB2	2.17	0.44
2:D:147:HIS:CE1	2:D:148:ASN:OD1	2.71	0.44
1:A:84:LYS:O	1:A:86:GLU:N	2.50	0.44
1:A:163:LEU:O	1:A:170:HIS:HE1	2.00	0.44
1:C:164:LYS:HD3	1:C:165:TYR:CE2	2.53	0.44
2:D:13:LYS:NZ	2:D:88:ASN:HA	2.33	0.44
2:D:71:VAL:HA	2:D:74:LEU:HD12	1.99	0.44
1:A:160:VAL:HG22	1:A:187:ILE:HB	1.99	0.44
1:C:79:THR:OG1	1:C:81:LEU:HB2	2.18	0.44
2:D:44:ILE:HG23	2:D:59:ILE:HG12	2.00	0.44
1:A:277:VAL:O	1:A:283:ALA:HB2	2.18	0.44
1:C:29:LYS:HD2	1:C:310:LEU:HD13	2.00	0.44
2:B:147:HIS:O	2:B:151:LEU:HB2	2.18	0.43
1:C:243:VAL:HB	1:C:245:ALA:O	2.17	0.43
2:B:26:GLY:O	2:B:30:LEU:HD22	2.18	0.43
2:D:109:CYS:HA	2:D:125:PHE:HZ	1.84	0.43
1:A:152:LEU:HA	1:A:155:LEU:HD11	2.01	0.43
2:B:99:LEU:HD12	2:B:100:PRO:HD2	2.01	0.43
1:A:159:MET:HB3	1:A:163:LEU:HD22	2.01	0.43
1:C:160:VAL:HA	1:C:187:ILE:O	2.18	0.42
1:A:8:HIS:CD2	1:A:124:VAL:HG13	2.53	0.42
1:A:160:VAL:HG11	1:A:215:ILE:HD11	2.01	0.42
2:B:23:ALA:HB2	2:B:55:ARG:HB2	2.02	0.42
2:D:25:ILE:O	2:D:28:LYS:HB3	2.18	0.42
1:A:4:LEU:HD23	1:A:7:LYS:CE	2.50	0.42
1:A:159:MET:HE2	1:A:186:PHE:HE1	1.84	0.42
1:C:31:LYS:HZ1	1:C:291:ASN:HD21	1.66	0.42
1:C:54:ARG:HD2	3:C:311:PCT:C1P	2.49	0.42
1:C:205:LYS:CD	1:C:207:ILE:HD11	2.49	0.42
1:C:54:ARG:HD2	3:C:311:PCT:H1P1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ILE:O	1:A:202:LEU:HG	2.19	0.42
1:A:140:LEU:HD22	1:A:292:GLY:CA	2.43	0.42
1:C:108:GLN:NE2	2:D:115:ILE:HD12	2.34	0.42
1:C:183:ARG:NH2	1:C:208:ALA:HB1	2.35	0.42
1:C:299:LEU:HD12	1:C:299:LEU:HA	1.84	0.42
1:A:42:LYS:HA	1:A:100:ASP:OD2	2.20	0.42
1:A:50:GLU:HB3	1:A:105:ARG:HG2	2.01	0.42
1:A:187:ILE:HG22	1:A:247:PHE:CD2	2.55	0.42
1:A:218:VAL:C	1:A:220:ALA:H	2.29	0.41
1:A:269:ARG:HA	1:A:272:GLU:OE2	2.20	0.41
1:C:109:GLU:HG3	1:C:132:ASN:HB2	2.03	0.41
1:A:17:ARG:HG3	1:A:179:PHE:CE1	2.55	0.41
2:D:22:PRO:HD2	2:D:78:ALA:HB1	2.02	0.41
2:D:109:CYS:HA	2:D:110:PRO:HD3	1.86	0.41
2:D:127:VAL:HG13	2:D:134:ILE:HG21	2.02	0.41
2:B:20:HIS:CE1	2:B:52:GLU:O	2.74	0.41
2:B:47:ASN:ND2	2:D:39:ASP:HA	2.36	0.41
1:A:90:ASP:O	1:A:94:VAL:HG23	2.21	0.41
1:C:82:GLY:O	1:C:83:LYS:HD3	2.21	0.41
1:C:122:VAL:HA	1:C:123:PRO:HD3	1.79	0.41
1:C:269:ARG:HA	1:C:272:GLU:OE1	2.21	0.41
2:D:147:HIS:O	2:D:151:LEU:HB2	2.21	0.41
1:A:242:ASN:HB3	1:A:243:VAL:H	1.67	0.41
1:C:75:ASP:O	1:C:76:SER:HB2	2.21	0.41
1:C:229:ARG:NH2	1:C:231:GLN:HG3	2.36	0.41
1:C:97:THR:HG22	1:C:98:TYR:CD2	2.55	0.40
1:A:25:ALA:O	1:A:28:ALA:HB3	2.21	0.40
1:A:88:LEU:HD11	1:A:104:MET:HE1	2.03	0.40
1:A:4:LEU:O	1:A:7:LYS:HB2	2.22	0.40
1:A:154:ASN:OD1	1:A:181:GLY:HA3	2.21	0.40
1:A:225:LEU:HD22	1:A:227:MET:SD	2.62	0.40
2:B:22:PRO:HB2	2:B:25:ILE:CG1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	273 (89%)	23 (8%)	12 (4%)	2	8
1	C	308/310 (99%)	282 (92%)	19 (6%)	7 (2%)	5	18
2	B	144/153 (94%)	117 (81%)	15 (10%)	12 (8%)	0	1
2	D	144/153 (94%)	122 (85%)	17 (12%)	5 (4%)	3	10
All	All	904/926 (98%)	794 (88%)	74 (8%)	36 (4%)	2	8

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	THR
1	A	76	SER
1	A	85	GLY
2	B	23	ALA
2	B	50	SER
1	C	78	ASN
1	C	275	THR
2	D	22	PRO
2	D	68	GLU
2	D	89	TYR
1	A	79	THR
1	A	81	LEU
1	A	83	LYS
1	A	166	GLY
1	A	219	MET
2	B	68	GLU
1	C	219	MET
1	C	244	LYS
1	C	267	LEU
2	D	91	VAL
1	A	244	LYS
2	B	14	ARG
2	B	49	PRO
1	C	84	LYS
2	D	131	ALA
1	A	78	ASN
2	B	132	ASN
1	A	270	VAL

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Mol	Chain	Res	Type
2	B	11	ALA
2	B	105	ASN
2	B	152	ALA
2	B	20	HIS
2	B	129	LYS
1	A	267	LEU
2	B	22	PRO
1	C	270	VAL

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%)	223 (85%)	38 (15%)	3	11
1	C	261/261 (100%)	217 (83%)	44 (17%)	2	7
2	B	129/136 (95%)	111 (86%)	18 (14%)	3	12
2	D	129/136 (95%)	107 (83%)	22 (17%)	2	7
All	All	780/794 (98%)	658 (84%)	122 (16%)	2	9

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	21	ASN
1	A	24	LEU
1	A	37	GLU
1	A	65	ARG
1	A	74	SER
1	A	75	ASP
1	A	79	THR
1	A	81	LEU
1	A	97	THR
1	A	116	THR
1	A	121	ASN
1	A	124	VAL

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Mol	Chain	Res	Type
1	A	136	THR
1	A	159	MET
1	A	171	SER
1	A	198	ILE
1	A	201	MET
1	A	218	VAL
1	A	222	VAL
1	A	225	LEU
1	A	228	THR
1	A	229	ARG
1	A	233	GLU
1	A	235	LEU
1	A	237	PRO
1	A	244	LYS
1	A	246	GLN
1	A	252	SER
1	A	256	ASN
1	A	269	ARG
1	A	271	ASP
1	A	275	THR
1	A	281	PRO
1	A	287	GLN
1	A	291	ASN
1	A	293	ILE
1	A	296	ARG
2	B	10	GLU
2	B	14	ARG
2	B	22	PRO
2	B	30	LEU
2	B	31	SER
2	B	32	LEU
2	B	43	THR
2	B	44	ILE
2	B	53	MET
2	B	57	ASP
2	B	73	GLN
2	B	86	ILE
2	B	95	SER
2	B	106	VAL
2	B	111	ASN
2	B	137	LYS
2	B	139	LYS

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Mol	Chain	Res	Type
2	B	153	ASN
1	C	2	ASN
1	C	4	LEU
1	C	6	GLN
1	C	17	ARG
1	C	35	GLN
1	C	37	GLU
1	C	40	LYS
1	C	54	ARG
1	C	59	PHE
1	C	65	ARG
1	C	74	SER
1	C	81	LEU
1	C	83	LYS
1	C	84	LYS
1	C	97	THR
1	C	114	LEU
1	C	116	THR
1	C	117	GLU
1	C	125	LEU
1	C	136	THR
1	C	152	LEU
1	C	162	ASP
1	C	167	ARG
1	C	211	LEU
1	C	216	GLU
1	C	218	VAL
1	C	228	THR
1	C	229	ARG
1	C	233	GLU
1	C	236	ASP
1	C	238	SER
1	C	244	LYS
1	C	246	GLN
1	C	256	ASN
1	C	262	LYS
1	C	269	ARG
1	C	275	THR
1	C	287	GLN
1	C	296	ARG
1	C	299	LEU
1	C	305	ASN

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Mol	Chain	Res	Type
1	C	306	ARG
1	C	309	VAL
1	C	310	LEU
2	D	9	VAL
2	D	10	GLU
2	D	13	LYS
2	D	39	ASP
2	D	42	ILE
2	D	43	THR
2	D	52	GLU
2	D	61	ILE
2	D	76	LEU
2	D	80	GLN
2	D	84	ASN
2	D	89	TYR
2	D	92	VAL
2	D	94	LYS
2	D	95	SER
2	D	96	ARG
2	D	98	SER
2	D	101	GLU
2	D	106	VAL
2	D	121	VAL
2	D	130	ARG
2	D	153	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	21	ASN
1	A	60	GLN
1	A	106	HIS
1	A	121	ASN
1	A	146	GLN
1	A	174	GLN
1	A	255	HIS
1	A	287	GLN
1	A	297	GLN
2	B	40	GLN
2	B	47	ASN
2	B	117	HIS

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Mol	Chain	Res	Type
1	C	8	HIS
1	C	106	HIS
1	C	108	GLN
1	C	154	ASN
1	C	156	HIS
1	C	170	HIS
1	C	256	ASN
1	C	282	HIS
1	C	291	ASN
1	C	297	GLN
1	C	305	ASN
2	D	40	GLN
2	D	63	ASN
2	D	70	GLN
2	D	73	GLN
2	D	105	ASN
2	D	117	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	PCT	C	311	-	7,7,7	2.13	2 (28%)	9,10,10	1.70	1 (11%)
3	PCT	A	311	-	7,7,7	2.05	2 (28%)	9,10,10	2.30	4 (44%)

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	PCT	C	311	-	-	2/4/5/5	-
3	PCT	A	311	-	-	1/4/5/5	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	311	PCT	P-O1P	4.75	1.59	1.50
3	A	311	PCT	P-O1P	4.10	1.58	1.50
3	A	311	PCT	P-C1P	2.91	1.84	1.79
3	C	311	PCT	P-C1P	2.42	1.83	1.79

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	311	PCT	O1-C1-C1P	4.28	124.37	119.86
3	A	311	PCT	C1P-C1-N1	-3.91	110.75	115.41
3	C	311	PCT	O1-C1-C1P	3.90	123.97	119.86
3	A	311	PCT	O3P-P-C1P	2.30	111.67	106.84
3	A	311	PCT	O1P-P-C1P	-2.20	106.01	111.10

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	311	PCT	O1-C1-C1P-P
3	C	311	PCT	C1-C1P-P-O2P
3	A	311	PCT	O1-C1-C1P-P

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	311	PCT	3	0
3	A	311	PCT	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.