



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2017 – 07:38 PM EST

PDB ID : 2AT1  
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 : unknown  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

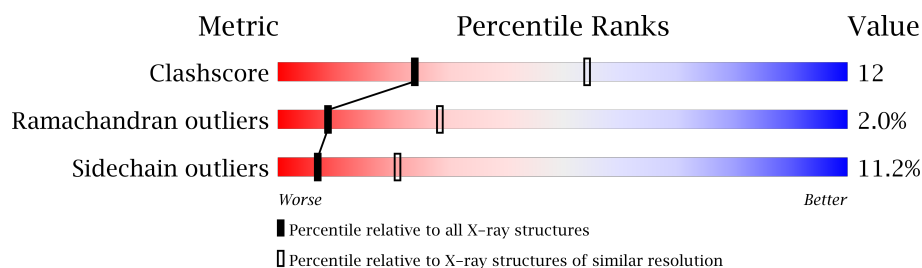
# 1 Overall quality at a glance

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	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

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

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MAL	A	312	X	X	-	-
3	MAL	C	312	X	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

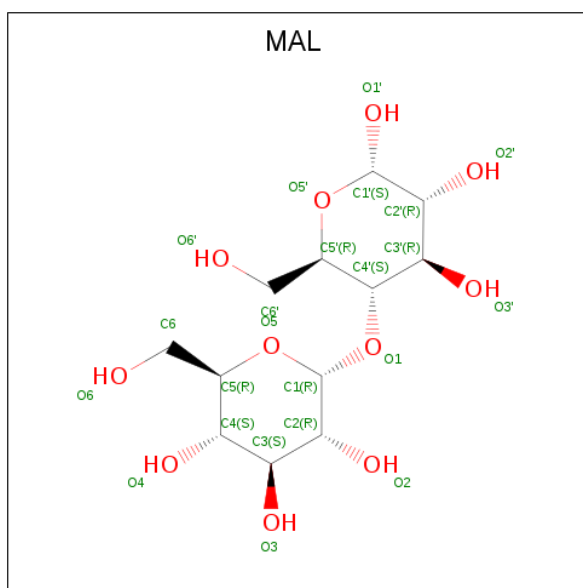
- Molecule 2 is a protein called ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN.

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:

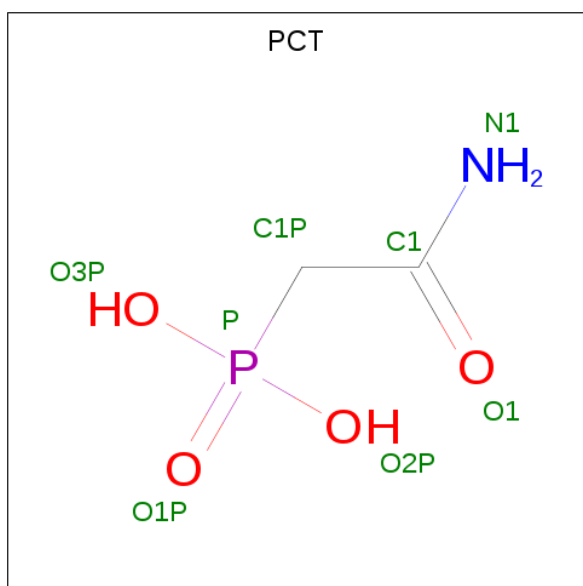
Chain	Residue	Modelled	Actual	Comment	Reference
B	8	GLY	GLN	CONFLICT	UNP P0A7F3
D	8	GLY	GLN	CONFLICT	UNP P0A7F3

- Molecule 3 is MALTOSE (three-letter code: MAL) (formula:  $C_{12}H_{22}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is PHOSPHONOACETAMIDE (three-letter code: PCT) (formula:  $C_2H_6NO_4P$ ).



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

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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

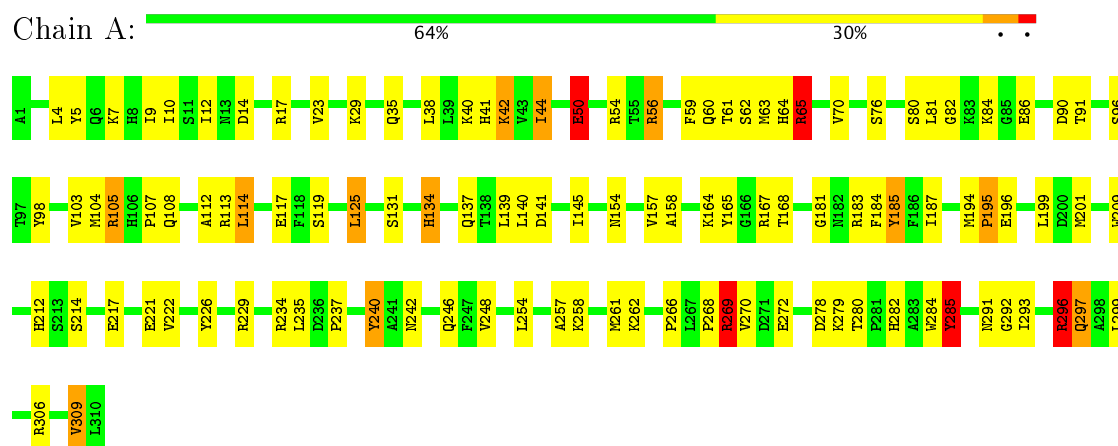
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		
5	D	1	Total	Zn	0	0
			1	1		

### 3 Residue-property plots

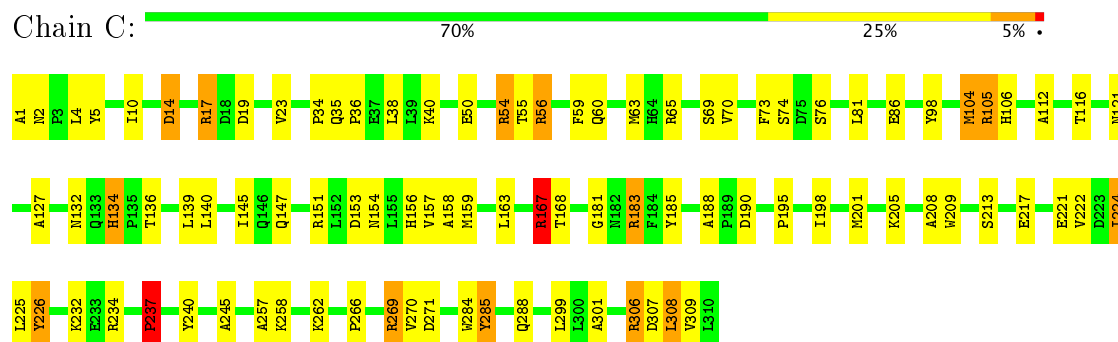
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

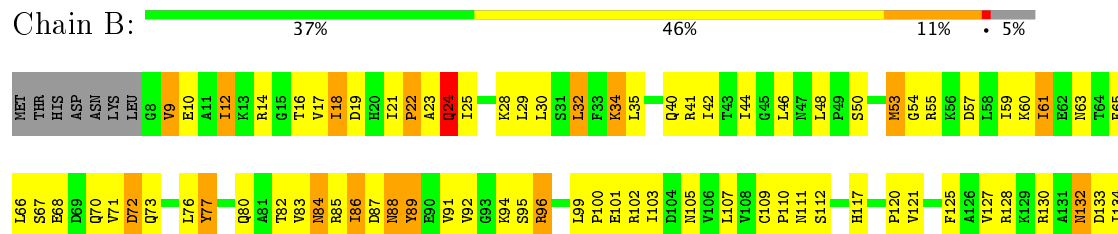
#### • Molecule 1: ASPARTATE CARBAMOYLTRANSFERASE (R STATE), CATALYTIC CHAIN



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

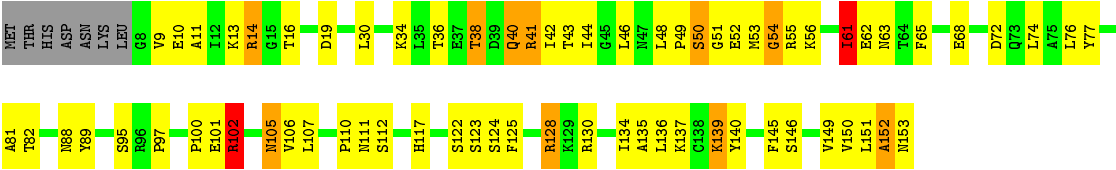


#### • Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN





● Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.20 Å 122.20 Å 156.60 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, $R_{free}$	0.170 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7138	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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: ZN, MAL, 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	0.98	1/2461 (0.0%)	1.76	41/3339 (1.2%)
1	C	0.98	1/2461 (0.0%)	1.67	34/3339 (1.0%)
2	B	0.93	0/1155	1.56	10/1561 (0.6%)
2	D	0.83	0/1155	1.62	14/1561 (0.9%)
All	All	0.95	2/7232 (0.0%)	1.68	99/9800 (1.0%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	50	GLU	CD-OE2	-11.27	1.13	1.25
1	C	76	SER	CA-CB	-5.01	1.45	1.52

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	ARG	NE-CZ-NH1	-19.64	110.48	120.30
1	A	56	ARG	NE-CZ-NH2	15.06	127.83	120.30
1	A	54	ARG	NE-CZ-NH2	13.90	127.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	ARG	NE-CZ-NH2	12.44	126.52	120.30
1	A	54	ARG	NE-CZ-NH1	-11.25	114.68	120.30
1	C	151	ARG	NE-CZ-NH2	11.10	125.85	120.30
1	A	284	TRP	CD1-CG-CD2	10.37	114.59	106.30
2	D	102	ARG	NE-CZ-NH2	10.13	125.36	120.30
1	C	167	ARG	NE-CZ-NH1	-9.71	115.45	120.30
1	A	98	TYR	CB-CG-CD2	-9.49	115.31	121.00
1	C	17	ARG	NE-CZ-NH2	9.16	124.88	120.30
2	D	14	ARG	NE-CZ-NH2	9.12	124.86	120.30
1	A	65	ARG	NE-CZ-NH2	8.76	124.68	120.30
1	C	284	TRP	CD1-CG-CD2	8.75	113.30	106.30
1	A	65	ARG	NE-CZ-NH1	-8.50	116.05	120.30
2	D	128	ARG	NE-CZ-NH2	8.08	124.34	120.30
1	A	284	TRP	CE2-CD2-CG	-8.01	100.89	107.30
1	C	284	TRP	CE2-CD2-CG	-7.99	100.91	107.30
1	A	309	VAL	O-C-N	7.93	135.40	122.70
1	C	209	TRP	CD1-CG-CD2	7.78	112.52	106.30
1	C	209	TRP	CE2-CD2-CG	-7.70	101.14	107.30
1	C	234	ARG	NE-CZ-NH1	-7.44	116.58	120.30
1	A	105	ARG	NE-CZ-NH2	7.26	123.93	120.30
2	B	89	TYR	CB-CG-CD2	-7.09	116.74	121.00
1	A	17	ARG	NE-CZ-NH2	6.84	123.72	120.30
1	C	159	MET	CA-CB-CG	-6.76	101.80	113.30
1	C	86	GLU	CA-CB-CG	6.60	127.93	113.40
1	A	201	MET	CA-CB-CG	6.59	124.50	113.30
1	A	284	TRP	CG-CD1-NE1	-6.56	103.54	110.10
1	A	56	ARG	CG-CD-NE	-6.54	98.06	111.80
1	A	309	VAL	CA-C-N	-6.52	102.85	117.20
1	C	105	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	A	114	LEU	CB-CG-CD2	-6.51	99.93	111.00
1	A	209	TRP	CE2-CD2-CG	-6.47	102.12	107.30
1	A	296	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	A	209	TRP	CD1-CG-CD2	6.40	111.42	106.30
1	A	234	ARG	NE-CZ-NH2	6.38	123.49	120.30
1	C	65	ARG	NE-CZ-NH2	6.37	123.49	120.30
2	B	34	LYS	N-CA-C	6.35	128.14	111.00
2	D	14	ARG	NE-CZ-NH1	-6.33	117.14	120.30
2	B	96	ARG	NE-CZ-NH1	-6.28	117.16	120.30
1	C	183	ARG	NE-CZ-NH2	6.13	123.36	120.30
1	C	308	LEU	CA-CB-CG	6.12	129.38	115.30
2	B	84	ASN	CA-CB-CG	-6.11	99.95	113.40
1	A	234	ARG	NE-CZ-NH1	-6.08	117.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	152	ALA	N-CA-C	6.00	127.19	111.00
1	C	54	ARG	NE-CZ-NH2	5.97	123.29	120.30
1	C	209	TRP	CB-CG-CD1	-5.97	119.24	127.00
1	C	269	ARG	CG-CD-NE	-5.91	99.39	111.80
1	C	60	GLN	CA-CB-CG	-5.89	100.44	113.40
2	B	101	GLU	CA-CB-CG	5.89	126.36	113.40
2	B	130	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	C	56	ARG	NE-CZ-NH2	5.79	123.20	120.30
1	C	104	MET	CA-CB-CG	5.75	123.07	113.30
2	D	152	ALA	CA-C-N	-5.72	104.61	117.20
1	A	285	TYR	CB-CG-CD2	-5.70	117.58	121.00
1	C	306	ARG	NE-CZ-NH2	5.65	123.12	120.30
1	A	86	GLU	OE1-CD-OE2	5.64	130.07	123.30
2	D	53	MET	CA-C-N	-5.60	105.00	116.20
1	C	151	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	A	134	HIS	CA-CB-CG	5.51	122.97	113.60
1	A	90	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	157	VAL	CG1-CB-CG2	-5.47	102.15	110.90
1	A	257	ALA	O-C-N	5.46	131.44	122.70
1	C	237	PRO	N-CA-CB	-5.44	96.61	102.60
1	A	14	ASP	CA-C-N	5.42	129.13	117.20
1	A	297	GLN	CA-CB-CG	5.42	125.33	113.40
2	D	122	SER	N-CA-CB	-5.40	102.41	110.50
1	C	105	ARG	NE-CZ-NH2	5.39	123.00	120.30
1	A	44	ILE	CG1-CB-CG2	-5.38	99.56	111.40
2	D	9	VAL	CA-C-N	-5.37	105.39	117.20
1	C	269	ARG	CA-CB-CG	5.35	125.17	113.40
1	A	42	LYS	O-C-N	-5.35	114.14	122.70
1	C	14	ASP	CB-CG-OD1	-5.31	113.52	118.30
1	A	284	TRP	CB-CG-CD1	-5.30	120.11	127.00
2	B	92	VAL	N-CA-CB	-5.30	99.85	111.50
1	A	64	HIS	CB-CA-C	-5.28	99.85	110.40
1	A	185	TYR	CB-CG-CD1	-5.26	117.84	121.00
1	C	98	TYR	CB-CA-C	-5.25	99.89	110.40
2	D	139	LYS	CB-CG-CD	-5.22	98.02	111.60
1	A	306	ARG	NE-CZ-NH2	5.22	122.91	120.30
2	D	41	ARG	NE-CZ-NH2	5.21	122.90	120.30
1	C	284	TRP	CG-CD1-NE1	-5.20	104.90	110.10
1	C	56	ARG	CB-CG-CD	-5.19	98.11	111.60
2	D	140	TYR	CB-CG-CD1	-5.15	117.91	121.00
1	C	156	HIS	N-CA-C	-5.15	97.10	111.00
1	A	257	ALA	CA-C-N	-5.14	105.89	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	153	ASP	CB-CG-OD1	5.14	122.93	118.30
1	C	217	GLU	CA-CB-CG	5.14	124.70	113.40
2	D	74	LEU	CA-CB-CG	5.11	127.05	115.30
1	A	104	MET	CG-SD-CE	-5.09	92.05	100.20
1	C	257	ALA	CB-CA-C	-5.09	102.46	110.10
1	C	309	VAL	N-CA-C	-5.08	97.29	111.00
2	D	106	VAL	CA-CB-CG1	-5.07	103.29	110.90
2	B	12	ILE	CA-C-N	-5.06	106.06	117.20
1	A	91	THR	CA-CB-CG2	5.04	119.45	112.40
2	B	18	ILE	N-CA-C	-5.02	97.45	111.00
1	A	114	LEU	CB-CG-CD1	5.01	119.53	111.00
2	D	61	ILE	CA-CB-CG2	-5.01	100.88	110.90

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
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	56	0
1	C	2415	0	2422	33	0
2	B	1138	0	1154	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1138	0	1154	35	0
3	A	7	0	0	2	0
3	C	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	178	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 12.

All (178) 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:HB3	2:D:102:ARG:HH21	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
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:154:ASN:HA	1:C:181:GLY:O	1.94	0.67
1:C:56:ARG:HH21	1:C:56:ARG:HG2	1.58	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:137:LYS:HG3	2:B:144:GLU:HG2	1.80	0.64
2:B:84:ASN:HD21	2:B:91:VAL:HG13	1.62	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ARG:HD2	3:A:312:MAL: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
2:B:23:ALA:O	2:B:24:GLN:HB2	2.06	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
1:A:63:MET:SD	1:A:70:VAL:HG22	2.48	0.54
1:A:137:GLN:O	1:A:140:LEU:HG	2.08	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:VAL:HG11	1:C:139:LEU:HD13	1.92	0.51
2:D:102:ARG:CB	2:D:102:ARG:HH21	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
1:C:104:MET:HE2	1:C:112:ALA:HA	1.92	0.50
2:B:136:LEU:HD12	2:B:150:VAL:HG21	1.94	0.50
2:D:107:LEU:H	2:D:107:LEU:HD12	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
2:D:16:THR:HG1	2:D:65:PHE:HA	1.75	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
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:A:312:MAL: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:N	2:D:107:LEU:HD12	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: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:168:THR:HG21	1:A:266:PRO:HB3	1.95	0.47
1:A:62:SER:HB3	1:A:297:GLN:HB3	1.97	0.47
2:B:127:VAL:HA	2:B:136:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:254:LEU:HD22	1:A:261:MET:HE1	1.97	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
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
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: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
2:B:18:ILE:HD11	2:B:61:ILE:HD11	2.00	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:ARG:HA	2:B:125:PHE:O	2.19	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:109:CYS:HA	2:B:110:PRO:HD2	1.80	0.42
2:B:30:LEU:CD1	2:B:59:ILE:HG12	2.47	0.42
1:C:136:THR:HG22	1:C:299:LEU:CD2	2.49	0.42
1:A:262:LYS:HD3	1:A:262:LYS:HA	1.86	0.41
1:A:9:ILE:HG13	1:A:299:LEU:HD11	2.01	0.41
1:A:81:LEU:C	1:A:81:LEU:HD23	2.41	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:H	2:B:18:ILE:HD12	1.86	0.41
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:HA	1:A:12:ILE:HD13	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:C:312:MAL:C4	2.52	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%)	285 (92%)	21 (7%)	2 (1%)	28	62
1	C	308/310 (99%)	289 (94%)	15 (5%)	4 (1%)	14	41
2	B	144/153 (94%)	122 (85%)	17 (12%)	5 (4%)	4	14
2	D	144/153 (94%)	117 (81%)	20 (14%)	7 (5%)	2	8
All	All	904/926 (98%)	813 (90%)	73 (8%)	18 (2%)	9	28

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
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%)	242 (93%)	19 (7%)	16	42
1	C	261/261 (100%)	238 (91%)	23 (9%)	12	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	693 (89%)	87 (11%)	7	21

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LYS
1	A	42	LYS
1	A	50	GLU
1	A	59	PHE
1	A	65	ARG
1	A	105	ARG
1	A	108	GLN
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
2	B	12	ILE
2	B	19	ASP
2	B	22	PRO
2	B	24	GLN
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

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Mol	Chain	Res	Type
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	148	ASN
2	B	153	ASN
1	C	14	ASP
1	C	17	ARG
1	C	38	LEU
1	C	40	LYS
1	C	59	PHE
1	C	69	SER
1	C	74	SER
1	C	81	LEU
1	C	121	ASN
1	C	134	HIS
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	258	LYS
1	C	262	LYS
1	C	269	ARG
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

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	60	GLN
1	A	147	GLN
1	A	154	ASN
1	A	291	ASN
2	B	40	GLN
2	B	47	ASN
2	B	63	ASN
2	B	84	ASN
2	B	117	HIS
2	B	153	ASN
1	C	13	ASN
1	C	60	GLN
1	C	134	HIS
1	C	154	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	2.51	3 (42%)	8,10,10	2.03	3 (37%)
3	MAL	A	312	-	6,6,24	4.89	5 (83%)	5,7,35	4.85	5 (100%)
4	PCT	C	311	-	7,7,7	2.23	2 (28%)	8,10,10	1.72	1 (12%)
3	MAL	C	312	-	6,6,24	4.73	4 (66%)	5,7,35	4.34	5 (100%)

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	-	-	0/4/5/5	0/0/0/0
3	MAL	A	312	-	2/2/2/10	0/4/4/48	0/0/0/2
4	PCT	C	311	-	-	0/4/5/5	0/0/0/0
3	MAL	C	312	-	2/2/2/10	0/4/4/48	0/0/0/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	312	MAL	O1-C1	-6.69	1.24	1.40
3	A	312	MAL	O1-C1	-6.67	1.24	1.40
3	A	312	MAL	C4-C3	-6.25	1.22	1.51
3	C	312	MAL	O5-C1	-6.08	1.25	1.40
3	C	312	MAL	C4-C3	-6.00	1.23	1.51
3	A	312	MAL	O5-C1	-5.80	1.26	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	312	MAL	O3-C3	-4.14	1.23	1.43
3	C	312	MAL	O3-C3	-4.06	1.24	1.43
3	A	312	MAL	C2-C1	2.80	1.54	1.51
4	A	311	PCT	P-O3P	2.81	1.61	1.54
4	C	311	PCT	P-C1P	3.14	1.85	1.79
4	A	311	PCT	P-C1P	3.77	1.86	1.79
4	A	311	PCT	P-O1P	4.23	1.59	1.50
4	C	311	PCT	P-O1P	4.35	1.59	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	311	PCT	O1P-P-C1P	-3.42	102.83	110.97
4	A	311	PCT	C1P-C1-N1	-2.14	112.85	115.37
3	A	312	MAL	O3-C3-C4	2.06	118.93	109.46
3	C	312	MAL	C4-C3-C2	2.18	117.24	112.56
3	C	312	MAL	O3-C3-C4	2.58	121.29	109.46
3	A	312	MAL	C4-C3-C2	2.70	118.35	112.56
4	A	311	PCT	O1-C1-C1P	3.36	123.35	119.77
4	C	311	PCT	O1-C1-C1P	4.25	124.30	119.77
3	C	312	MAL	O1-C1-C2	4.29	117.56	109.13
3	C	312	MAL	O5-C1-C2	4.35	117.67	109.13
3	A	312	MAL	O1-C1-C2	5.00	118.94	109.13
3	A	312	MAL	O5-C1-C2	5.14	119.22	109.13
3	C	312	MAL	O3-C3-C2	6.72	121.47	109.26
3	A	312	MAL	O3-C3-C2	7.41	122.71	109.26

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	312	MAL	C3
3	A	312	MAL	C1
3	C	312	MAL	C3
3	C	312	MAL	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	312	MAL	2	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	311	PCT	1	0
3	C	312	MAL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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.