



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:26 AM GMT

PDB ID : 3AT1  
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](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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

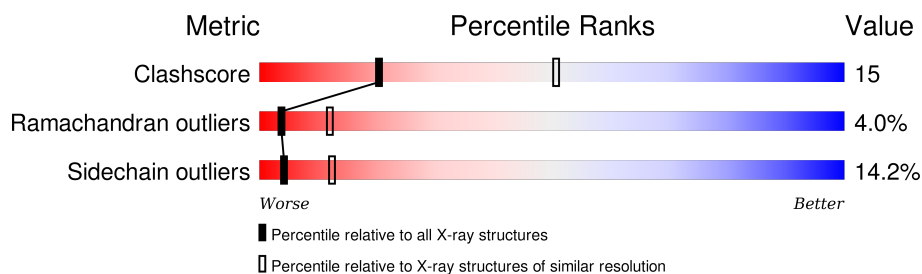
# 1 Overall quality at a glance

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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (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	

## 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			

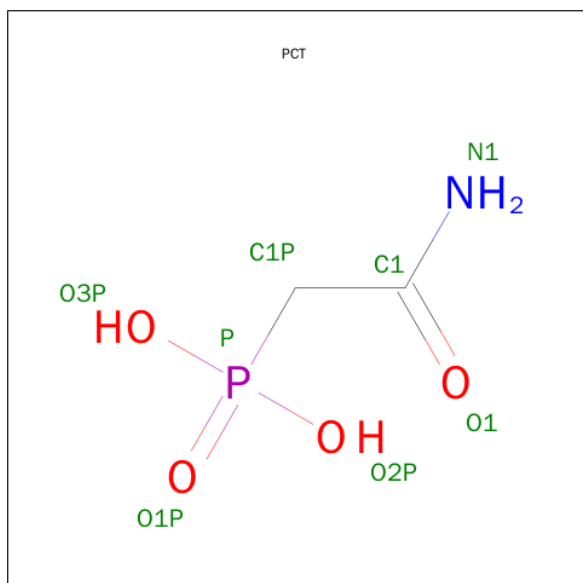
There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is PHOSPHONOACETAMIDE (three-letter code: PCT) (formula: C<sub>2</sub>H<sub>6</sub>NO<sub>4</sub>P).



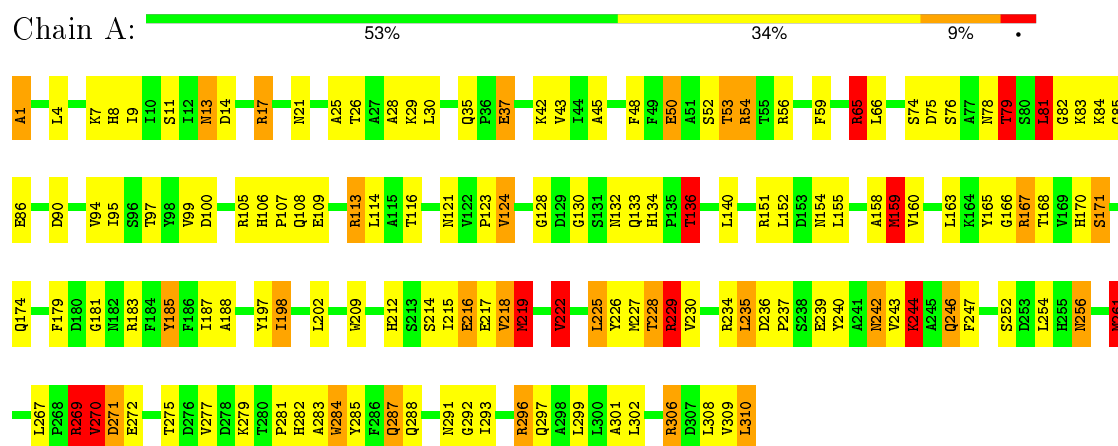
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			8	2	1	4	1		
4	C	1	Total	C	N	O	P	0	0
			8	2	1	4	1		

### 3 Residue-property plots

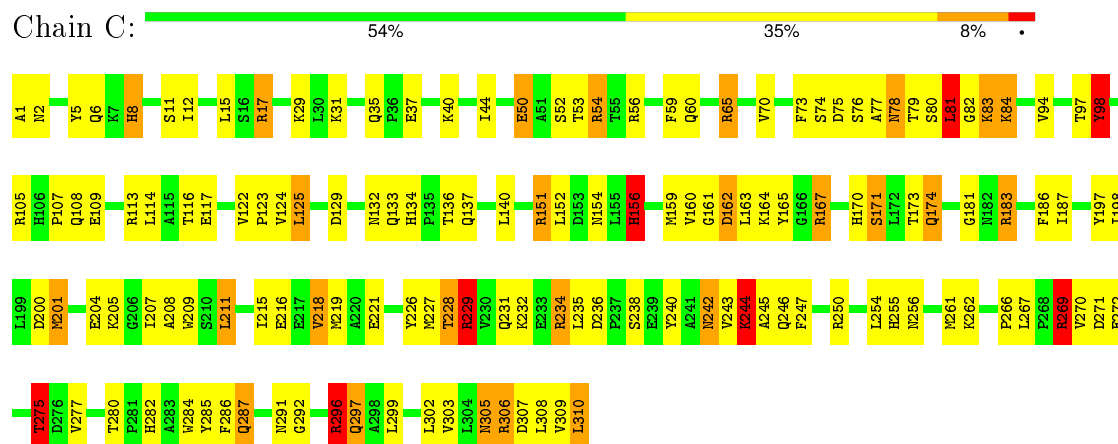
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

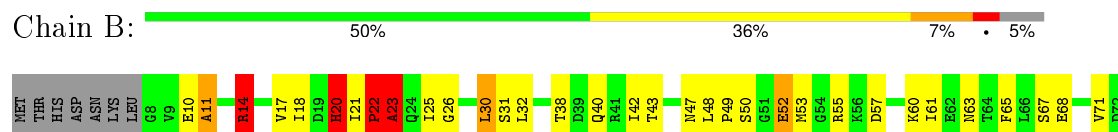
#### • Molecule 1: ASPARTATE CARBAMOYLTRANSFERASE (T STATE), CATALYTIC CHAIN



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

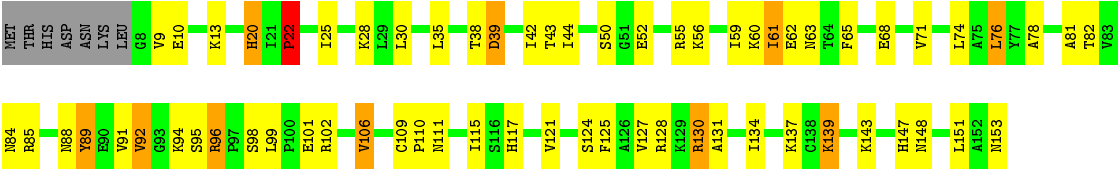


#### • Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN





● Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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	0.98	0/2461	1.87	57/3339 (1.7%)
1	C	0.97	1/2461 (0.0%)	1.89	62/3339 (1.9%)
2	B	0.85	0/1155	1.72	18/1561 (1.2%)
2	D	0.84	0/1155	1.59	13/1561 (0.8%)
All	All	0.94	1/7232 (0.0%)	1.81	150/9800 (1.5%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	44	ILE	CA-CB	5.66	1.67	1.54

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	ARG	NE-CZ-NH2	18.68	129.64	120.30
1	A	54	ARG	NE-CZ-NH1	-18.41	111.09	120.30
1	A	56	ARG	NE-CZ-NH1	-18.19	111.20	120.30
1	C	56	ARG	NE-CZ-NH2	17.77	129.19	120.30
1	C	56	ARG	NE-CZ-NH1	-15.30	112.65	120.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	296	ARG	NE-CZ-NH1	-15.26	112.67	120.30
1	C	269	ARG	NE-CZ-NH2	13.59	127.10	120.30
1	A	56	ARG	NE-CZ-NH2	13.35	126.98	120.30
1	A	54	ARG	NE-CZ-NH2	13.13	126.86	120.30
1	C	113	ARG	NE-CZ-NH2	12.83	126.71	120.30
1	C	269	ARG	NE-CZ-NH1	-11.30	114.65	120.30
1	A	65	ARG	NE-CZ-NH2	10.90	125.75	120.30
1	C	17	ARG	NE-CZ-NH2	10.74	125.67	120.30
1	A	269	ARG	NE-CZ-NH1	-10.58	115.01	120.30
1	C	113	ARG	NE-CZ-NH1	-10.48	115.06	120.30
1	C	105	ARG	NE-CZ-NH1	-9.84	115.38	120.30
1	C	113	ARG	CA-CB-CG	9.67	134.66	113.40
1	C	250	ARG	NE-CZ-NH1	-9.40	115.60	120.30
1	C	296	ARG	NE-CZ-NH2	9.01	124.80	120.30
1	C	218	VAL	CA-CB-CG2	-8.91	97.54	110.90
1	C	54	ARG	NE-CZ-NH1	-8.63	115.98	120.30
1	A	261	MET	CG-SD-CE	-8.63	86.39	100.20
1	C	17	ARG	NE-CZ-NH1	-8.37	116.12	120.30
1	C	54	ARG	NE-CZ-NH2	8.13	124.36	120.30
1	A	284	TRP	CE2-CD2-CG	-8.00	100.90	107.30
2	D	92	VAL	CA-CB-CG2	-7.99	98.91	110.90
1	A	167	ARG	CA-CB-CG	7.96	130.91	113.40
2	B	11	ALA	N-CA-C	7.77	131.98	111.00
1	A	65	ARG	NE-CZ-NH1	-7.64	116.48	120.30
2	B	67	SER	CA-C-N	-7.59	100.50	117.20
1	A	113	ARG	NE-CZ-NH1	-7.54	116.53	120.30
1	A	209	TRP	CD1-CG-CD2	7.48	112.28	106.30
1	C	284	TRP	CE2-CD2-CG	-7.46	101.33	107.30
1	A	284	TRP	CD1-CG-CD2	7.44	112.25	106.30
2	B	128	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	A	159	MET	CG-SD-CE	-7.37	88.41	100.20
1	C	98	TYR	CB-CG-CD2	-7.36	116.59	121.00
1	A	43	VAL	CG1-CB-CG2	-7.33	99.17	110.90
1	C	229	ARG	NE-CZ-NH2	7.33	123.97	120.30
1	A	209	TRP	CE2-CD2-CG	-7.09	101.63	107.30
1	A	167	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	A	113	ARG	NE-CZ-NH2	7.03	123.81	120.30
1	C	129	ASP	CB-CG-OD1	6.90	124.51	118.30
1	A	288	GLN	N-CA-CB	-6.76	98.42	110.60
1	C	50	GLU	CA-CB-CG	6.76	128.28	113.40
1	C	167	ARG	NE-CZ-NH2	6.74	123.67	120.30
2	B	102	ARG	NE-CZ-NH1	-6.73	116.93	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	284	TRP	CD1-CG-CD2	6.71	111.67	106.30
1	A	121	ASN	CA-CB-CG	-6.69	98.68	113.40
2	B	20	HIS	CA-C-N	-6.68	102.50	117.20
1	C	218	VAL	CA-CB-CG1	6.64	120.85	110.90
1	A	284	TRP	CG-CD2-CE3	6.62	139.86	133.90
1	A	1	ALA	N-CA-C	-6.61	93.14	111.00
1	C	53	THR	CA-C-N	6.61	131.74	117.20
1	C	8	HIS	CA-C-N	6.58	131.68	117.20
2	B	109	CYS	CA-CB-SG	-6.57	102.18	114.00
1	C	209	TRP	CE2-CD2-CG	-6.56	102.05	107.30
1	C	232	LYS	CA-CB-CG	6.51	127.73	113.40
1	A	136	THR	CA-CB-CG2	-6.47	103.34	112.40
1	A	79	THR	N-CA-CB	6.44	122.54	110.30
2	B	106	VAL	N-CA-CB	-6.42	97.37	111.50
2	B	85	ARG	NE-CZ-NH2	6.42	123.51	120.30
2	B	130	ARG	NE-CZ-NH1	-6.40	117.10	120.30
1	A	197	TYR	CB-CG-CD1	-6.36	117.18	121.00
1	A	306	ARG	NE-CZ-NH2	6.34	123.47	120.30
2	D	55	ARG	NE-CZ-NH1	-6.26	117.17	120.30
2	D	92	VAL	CA-CB-CG1	6.20	120.21	110.90
2	D	106	VAL	CA-CB-CG2	-6.19	101.62	110.90
1	A	275	THR	CA-CB-OG1	-6.15	96.08	109.00
1	A	35	GLN	CA-CB-CG	-6.12	99.94	113.40
2	B	23	ALA	N-CA-CB	6.08	118.62	110.10
2	D	130	ARG	NE-CZ-NH2	6.06	123.33	120.30
1	A	270	VAL	CA-C-N	6.06	130.54	117.20
1	A	269	ARG	CA-CB-CG	6.05	126.71	113.40
1	A	216	GLU	CA-CB-CG	6.04	126.70	113.40
1	A	284	TRP	CB-CG-CD1	-6.04	119.15	127.00
1	A	309	VAL	CA-C-N	-6.04	103.92	117.20
1	C	151	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	C	197	TYR	CA-CB-CG	6.02	124.83	113.40
2	D	22	PRO	N-CA-C	6.01	127.72	112.10
1	A	244	LYS	CA-CB-CG	6.00	126.61	113.40
1	C	275	THR	N-CA-CB	-5.99	98.93	110.30
1	A	17	ARG	NE-CZ-NH2	5.96	123.28	120.30
2	B	52	GLU	N-CA-C	5.93	127.01	111.00
1	C	209	TRP	CD1-CG-CD2	5.93	111.04	106.30
1	C	307	ASP	N-CA-C	-5.93	95.00	111.00
1	C	287	GLN	CG-CD-NE2	5.89	130.84	116.70
1	C	125	LEU	CA-CB-CG	5.87	128.79	115.30
1	A	234	ARG	NE-CZ-NH1	-5.85	117.37	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	A	269	ARG	CD-NE-CZ	5.84	131.78	123.60
2	D	139	LYS	CB-CG-CD	-5.82	96.48	111.60
2	B	130	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	C	303	VAL	CA-CB-CG2	-5.78	102.23	110.90
1	A	136	THR	OG1-CB-CG2	5.75	123.23	110.00
1	A	168	THR	CA-CB-CG2	-5.71	104.41	112.40
2	D	128	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	C	244	LYS	N-CA-C	-5.67	95.69	111.00
1	C	303	VAL	CG1-CB-CG2	-5.66	101.85	110.90
2	B	94	LYS	CB-CG-CD	-5.60	97.05	111.60
1	C	81	LEU	CB-CG-CD1	-5.57	101.53	111.00
1	A	53	THR	N-CA-C	5.55	126.00	111.00
1	A	284	TRP	NE1-CE2-CZ2	-5.55	124.30	130.40
2	D	102	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	A	229	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	C	8	HIS	O-C-N	-5.47	113.94	122.70
1	C	183	ARG	NE-CZ-NH2	5.46	123.03	120.30
2	D	9	VAL	N-CA-C	-5.46	96.27	111.00
2	B	77	TYR	CB-CG-CD1	-5.43	117.74	121.00
1	C	53	THR	O-C-N	-5.42	114.03	122.70
1	C	37	GLU	CA-CB-CG	-5.42	101.48	113.40
1	A	183	ARG	CA-CB-CG	5.41	125.31	113.40
1	A	270	VAL	O-C-N	-5.39	114.08	122.70
2	D	130	ARG	CA-C-N	-5.38	105.36	117.20
1	C	136	THR	N-CA-CB	-5.37	100.09	110.30
1	A	219	MET	CA-CB-CG	5.36	122.41	113.30
2	D	20	HIS	CA-CB-CG	5.35	122.70	113.60
1	A	95	ILE	CA-CB-CG1	-5.35	100.84	111.00
2	B	140	TYR	CB-CG-CD1	-5.35	117.79	121.00
1	A	37	GLU	CA-CB-CG	5.34	125.14	113.40
1	C	200	ASP	CB-CG-OD2	-5.33	113.50	118.30
2	D	61	ILE	CB-CA-C	-5.29	101.01	111.60
1	A	275	THR	CA-CB-CG2	5.28	119.80	112.40
1	C	52	SER	N-CA-CB	-5.28	102.57	110.50
1	C	173	THR	OG1-CB-CG2	-5.27	97.88	110.00
1	C	201	MET	CA-CB-CG	5.26	122.24	113.30
2	B	21	ILE	N-CA-C	-5.20	96.96	111.00
1	C	116	THR	N-CA-CB	-5.18	100.46	110.30
1	C	171	SER	CA-CB-OG	-5.18	97.22	111.20
1	A	81	LEU	CA-CB-CG	5.17	127.20	115.30
1	A	50	GLU	N-CA-C	-5.17	97.05	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	159	MET	CA-CB-CG	5.14	122.03	113.30
2	B	67	SER	CA-C-O	5.13	130.88	120.10
1	C	5	TYR	CB-CG-CD1	-5.13	117.92	121.00
1	A	54	ARG	CG-CD-NE	-5.12	101.04	111.80
1	A	229	ARG	CA-CB-CG	5.12	124.66	113.40
1	A	279	LYS	CA-CB-CG	5.12	124.66	113.40
1	A	13	ASN	N-CA-CB	-5.12	101.39	110.60
1	C	40	LYS	CA-CB-CG	5.11	124.64	113.40
2	B	146	SER	N-CA-CB	5.08	118.12	110.50
1	C	174	GLN	CA-CB-CG	5.07	124.55	113.40
1	C	151	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	C	226	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	C	303	VAL	CA-CB-CG1	5.05	118.47	110.90
1	A	222	VAL	N-CA-CB	-5.04	100.41	111.50
1	C	116	THR	OG1-CB-CG2	5.03	121.57	110.00
1	C	151	ARG	CG-CD-NE	-5.02	101.27	111.80
1	C	204	GLU	CA-CB-CG	5.01	124.42	113.40
1	C	80	SER	N-CA-C	-5.00	97.49	111.00
1	C	197	TYR	CB-CG-CD1	-5.00	118.00	121.00

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	86	0
1	C	2415	0	2422	68	0
2	B	1138	0	1154	28	0
2	D	1138	0	1154	29	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	8	0	4	2	0
4	C	8	0	4	3	0
All	All	7124	0	7160	209	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 (209) 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:H	1:A:81:LEU:HD22	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:292:GLY:O	1:A:296:ARG:HB2	1.96	0.66
1:A:106:HIS:HD2	1:A:108:GLN:H	1.44	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:HIS:HD2	1:C:124:VAL:H	1.45	0.64
1:C:292:GLY:O	1:C:296:ARG:HB2	2.00	0.62
2:B:38:THR:HG22	2:B:40:GLN:H	1.64	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:229:ARG:NH1	1:C:231:GLN:HA	2.15	0.62
1:C:65:ARG:HB2	1:C:297:GLN:NE2	2.15	0.62
1:A:225:LEU:HD12	1:A:261:MET:HE1	1.81	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:261:MET:O	1:C:282:HIS:HD2	1.84	0.60
1:C:31:LYS:NZ	1:C:291:ASN:HD21	1.99	0.60
1:A:54:ARG:HD2	4: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	4:C:311:PCT:O2P	2.02	0.59
1:C:132:ASN:OD1	1:C:133:GLN:HG2	2.01	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
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:C:8:HIS:HD2	1:C:124:VAL:N	2.03	0.55
1:A:65:ARG:HB3	1:A:297:GLN:NE2	2.21	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:C:186:PHE:HB2	1:C:211:LEU:HD12	1.89	0.54
1:A:287:GLN:HE21	1:A:287:GLN:H	1.55	0.54
1:A:214:SER:HB3	1:A:216:GLU:HG2	1.87	0.54
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:187:ILE:HG22	1:C:247:PHE:HE1	1.75	0.51
1:A:160:VAL:O	1:A:228:THR:HG22	2.10	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
2:B:65:PHE:CE2	2:B:85:ARG:HG3	2.45	0.51
1:A:109:GLU:HG3	1:A:130:GLY:HA3	1.93	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: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:C:163:LEU:O	1:C:170:HIS:CE1	2.61	0.50
1:A:301:ALA:HB1	1:A:308:LEU:HD11	1.94	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: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	4: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:243:VAL:HG23	1:A:246:GLN:HG3	1.95	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:THR:O	1:A:29:LYS:HB2	2.14	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:277:VAL:O	1:C:280:THR:HB	2.14	0.47
1:A:132:ASN:CG	1:A:133:GLN:HG2	2.35	0.47
1:C:60:GLN:HG2	1:C:70:VAL:HG11	1.96	0.47
1:A:30:LEU:HD13	1:A:297:GLN:HB3	1.97	0.47
1:C:160:VAL:O	1:C:228:THR:HB	2.14	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
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:254:LEU:HD13	1:C:280:THR:HG21	1.96	0.47
1:C:187:ILE:HG22	1:C:247:PHE:CE1	2.49	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
1:C:229:ARG:HD3	1:C:231:GLN:OE1	2.16	0.46
2:B:109:CYS:HA	2:B:110:PRO:HD3	1.78	0.46
2:B:22:PRO:HB2	2:B:25:ILE:HG13	1.98	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
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:A:214:SER:HB3	1:A:216:GLU:CD	2.37	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:147:HIS:CE1	2:D:148:ASN:OD1	2.71	0.44
1:C:162:ASP:OD1	1:C:165:TYR:HB2	2.17	0.44
1:A:163:LEU:O	1:A:170:HIS:HE1	2.00	0.44
1:A:84:LYS:O	1:A:86:GLU:N	2.50	0.44
1:A:235:LEU:HG	1:A:239:GLU:CD	2.38	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
2:D:10:GLU:HA	2:D:60:LYS:HZ3	1.81	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:D:109:CYS:HA	2:D:125:PHE:HZ	1.84	0.43
2:B:26:GLY:O	2:B:30:LEU:HD22	2.18	0.43
2:B:99:LEU:HD12	2:B:100:PRO:HD2	2.01	0.43
1:A:152:LEU:HA	1:A:155:LEU:HD11	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:D:25:ILE:O	2:D:28:LYS:HB3	2.18	0.42
2:B:23:ALA:HB2	2:B:55:ARG:HB2	2.02	0.42
1:A:4:LEU:HD23	1:A:7:LYS:CE	2.50	0.42
1:C:54:ARG:HD2	4: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	4:C:311:PCT:H1P1	2.01	0.42
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:183:ARG:NH2	1:C:208:ALA:HB1	2.35	0.42
1:C:108:GLN:NE2	2:D:115:ILE:HD12	2.34	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:GLU:HB3	1:A:105:ARG:HG2	2.01	0.42
1:C:31:LYS:HZ1	1:C:291:ASN:HD21	1.66	0.42
1:A:187:ILE:HG22	1:A:247:PHE:CD2	2.55	0.42
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
2:D:13:LYS:HZ1	2:D:88:ASN:HA	1.86	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
1:A:17:ARG:HG3	1:A:179:PHE:CE1	2.55	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
2:D:147:HIS:O	2:D:151:LEU:HB2	2.21	0.41
1:C:269:ARG:HA	1:C:272:GLU:OE1	2.21	0.41
1:A:90:ASP:O	1:A:94:VAL:HG23	2.21	0.41
1:C:122:VAL:HA	1:C:123:PRO:HD3	1.79	0.41
1:C:82:GLY:O	1:C:83:LYS:HD3	2.21	0.41
1:C:75:ASP:O	1:C:76:SER:HB2	2.21	0.41
1:A:242:ASN:HB3	1:A:243:VAL:H	1.67	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: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 [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%)	273 (89%)	23 (8%)	12 (4%)	4	12
1	C	308/310 (99%)	282 (92%)	19 (6%)	7 (2%)	8	26
2	B	144/153 (94%)	117 (81%)	15 (10%)	12 (8%)	1	2
2	D	144/153 (94%)	122 (85%)	17 (12%)	5 (4%)	4	15
All	All	904/926 (98%)	794 (88%)	74 (8%)	36 (4%)	4	12

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
2	B	11	ALA
2	B	105	ASN
2	B	152	ALA
2	B	20	HIS
2	B	129	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	267	LEU
2	B	22	PRO
1	C	270	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	261/261 (100%)	222 (85%)	39 (15%)	4	11
1	C	261/261 (100%)	220 (84%)	41 (16%)	3	9
2	B	129/136 (95%)	115 (89%)	14 (11%)	8	23
2	D	129/136 (95%)	112 (87%)	17 (13%)	5	14
All	All	780/794 (98%)	669 (86%)	111 (14%)	4	12

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	21	ASN
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	114	LEU
1	A	124	VAL
1	A	134	HIS
1	A	136	THR
1	A	159	MET
1	A	167	ARG
1	A	171	SER
1	A	198	ILE
1	A	218	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	222	VAL
1	A	225	LEU
1	A	228	THR
1	A	229	ARG
1	A	235	LEU
1	A	237	PRO
1	A	242	ASN
1	A	244	LYS
1	A	246	GLN
1	A	252	SER
1	A	256	ASN
1	A	261	MET
1	A	269	ARG
1	A	271	ASP
1	A	281	PRO
1	A	285	TYR
1	A	287	GLN
1	A	291	ASN
1	A	293	ILE
1	A	296	ARG
1	A	310	LEU
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	53	MET
2	B	57	ASP
2	B	73	GLN
2	B	95	SER
2	B	106	VAL
2	B	139	LYS
2	B	153	ASN
1	C	2	ASN
1	C	6	GLN
1	C	17	ARG
1	C	35	GLN
1	C	59	PHE
1	C	65	ARG
1	C	74	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	81	LEU
1	C	83	LYS
1	C	84	LYS
1	C	114	LEU
1	C	117	GLU
1	C	125	LEU
1	C	134	HIS
1	C	152	LEU
1	C	156	HIS
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	234	ARG
1	C	236	ASP
1	C	242	ASN
1	C	244	LYS
1	C	246	GLN
1	C	255	HIS
1	C	256	ASN
1	C	262	LYS
1	C	269	ARG
1	C	271	ASP
1	C	275	THR
1	C	287	GLN
1	C	296	ARG
1	C	297	GLN
1	C	305	ASN
1	C	306	ARG
1	C	309	VAL
1	C	310	LEU
2	D	39	ASP
2	D	43	THR
2	D	52	GLU
2	D	61	ILE
2	D	76	LEU
2	D	84	ASN
2	D	89	TYR
2	D	92	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) 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	287	GLN
1	A	297	GLN
2	B	40	GLN
1	C	8	HIS
1	C	60	GLN
1	C	106	HIS
1	C	108	GLN
1	C	154	ASN
1	C	156	HIS
1	C	170	HIS
1	C	174	GLN
1	C	256	ASN
1	C	282	HIS
1	C	291	ASN
1	C	297	GLN
2	D	40	GLN
2	D	63	ASN
2	D	73	GLN
2	D	117	HIS
2	D	132	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	A	311	-	7,7,7	1.96	2 (28%)	9,10,10	2.13	3 (33%)
4	PCT	C	311	-	7,7,7	1.99	2 (28%)	9,10,10	1.57	1 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCT	A	311	-	-	0/4/5/5	0/0/0/0
4	PCT	C	311	-	-	0/4/5/5	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	311	PCT	P-C1P	2.58	1.83	1.79

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	311	PCT	P-C1P	3.10	1.84	1.79
4	A	311	PCT	P-O1P	3.64	1.58	1.50
4	C	311	PCT	P-O1P	4.22	1.59	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	311	PCT	C1P-C1-N1	-3.72	110.75	115.25
4	A	311	PCT	O3P-P-C1P	2.12	111.67	107.01
4	C	311	PCT	O1-C1-C1P	3.50	123.97	119.90
4	A	311	PCT	O1-C1-C1P	3.85	124.37	119.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	311	PCT	2	0
4	C	311	PCT	3	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.