



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:29 PM GMT

PDB ID : 1TUG  
Title : Aspartate Transcarbamoylase Catalytic Chain Mutant E50A Complex with Phosphonoacetamide, Malonate, and Cytidine-5-Prime-Triphosphate (CTP)  
Authors : Stieglitz, K.; Stec, B.; Baker, D.P.; Kantrowitz, E.R.  
Deposited on : 2004-06-24  
Resolution : 2.10 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

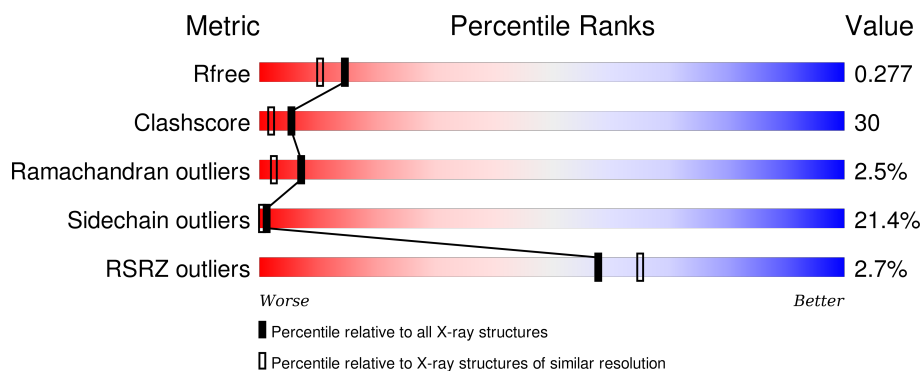
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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.

Mol	Chain	Length	Quality of chain
1	A	310	<div> <div>4%</div> <div>43% 43% 14%</div> </div>
1	C	310	<div> <div>%</div> <div>56% 32% 9%</div> </div>
2	B	153	<div> <div>3%</div> <div>27% 50% 20%</div> </div>
2	D	153	<div> <div>5%</div> <div>27% 50% 20%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MLI	C	1311	-	-	X	-
5	PCT	A	1314	-	-	-	X
5	PCT	C	1313	-	-	X	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8012 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 catalytic chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2411	1525	423	454	9			
1	C	310	Total	C	N	O	S	0	0	0
			2411	1525	423	454	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	ALA	GLU	ENGINEERED	UNP P0A786
C	50	ALA	GLU	ENGINEERED	UNP P0A786

- Molecule 2 is a protein called Aspartate carbamoyltransferase regulatory chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			
2	D	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			

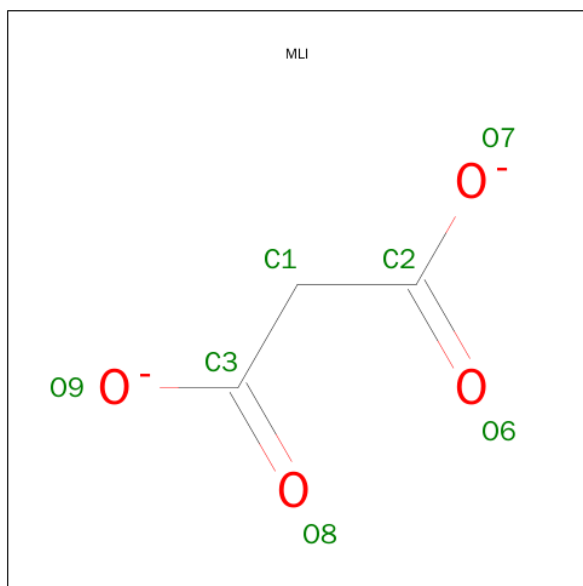
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	INITIATING METHIONINE	UNP P0A7F3
D	1	MET	-	INITIATING METHIONINE	UNP P0A7F3

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

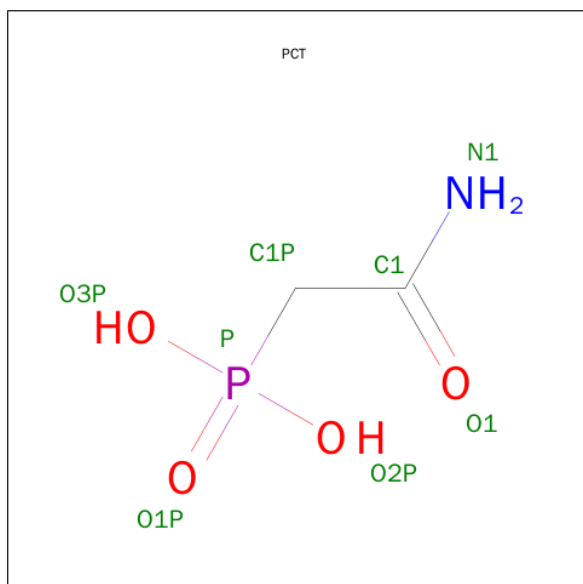
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is MALONATE ION (three-letter code: MLI) (formula:  $C_3H_2O_4$ ).



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

- Molecule 5 is PHOSPHONOACETAMIDE (three-letter code: PCT) (formula:  $C_2H_6NO_4P$ ).



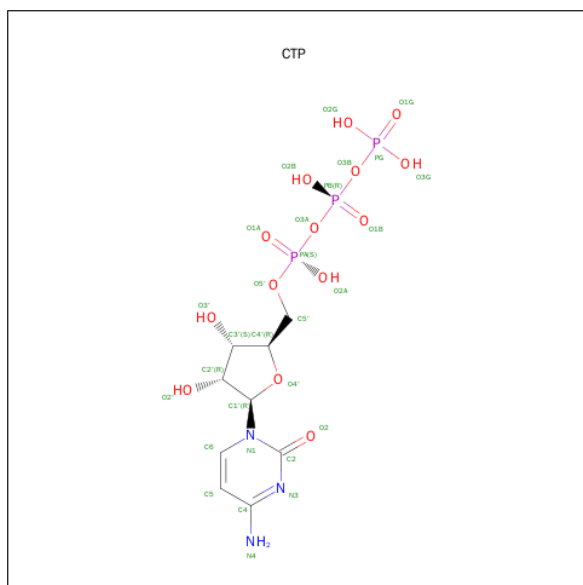
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			8	2	1	4	1		

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

- Molecule 6 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula:  $C_9H_{16}N_3O_{14}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
6	D	1	Total	C	N	O	P	0	0
			29	9	3	14	3		

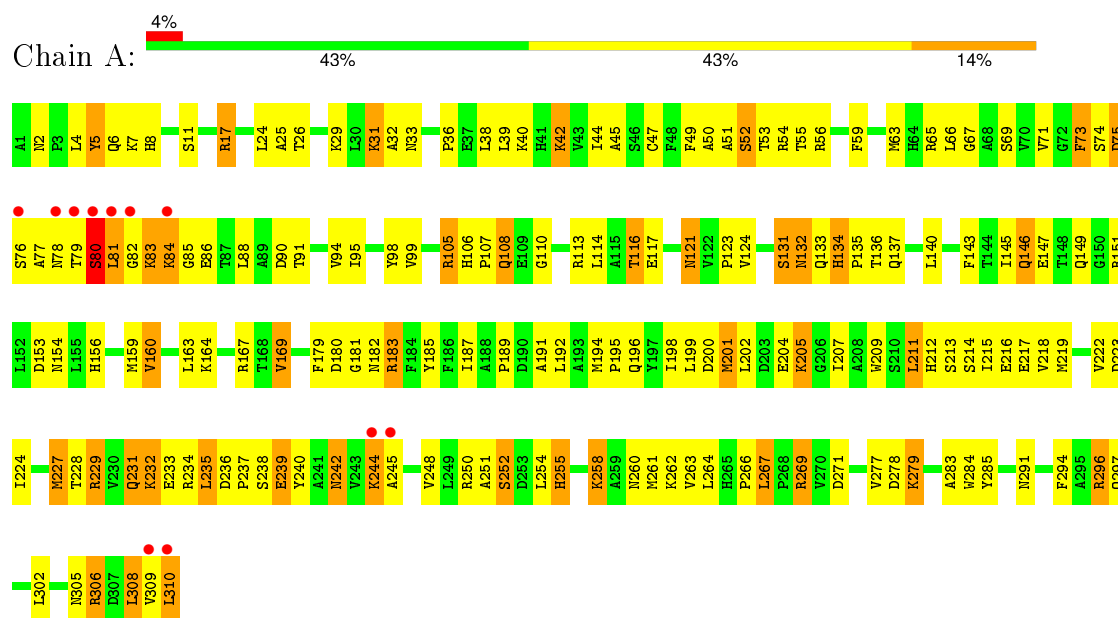
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	211	Total	O	0	0
			211	211		
7	B	101	Total	O	0	0
			101	101		
7	C	265	Total	O	0	0
			265	265		
7	D	121	Total	O	0	0
			121	121		

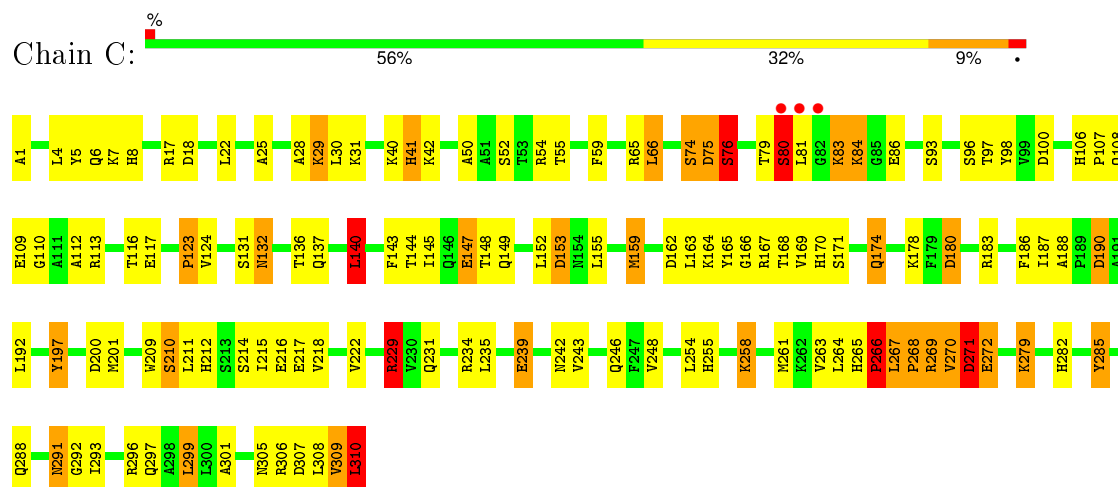
### 3 Residue-property plots

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.

- Molecule 1: Aspartate carbamoyltransferase catalytic chain

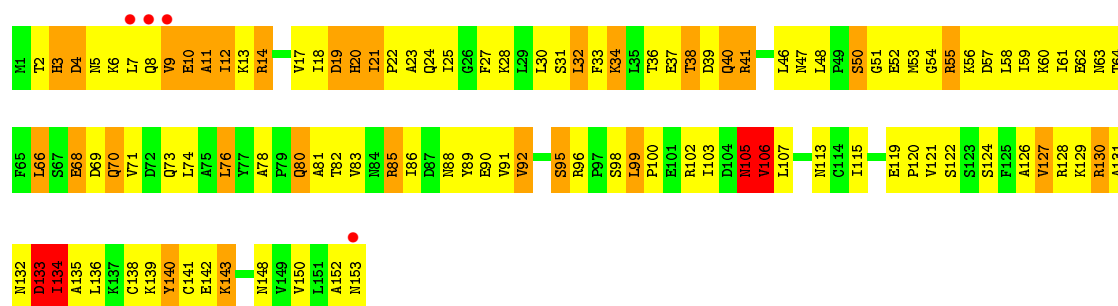


- Molecule 1: Aspartate carbamoyltransferase catalytic chain

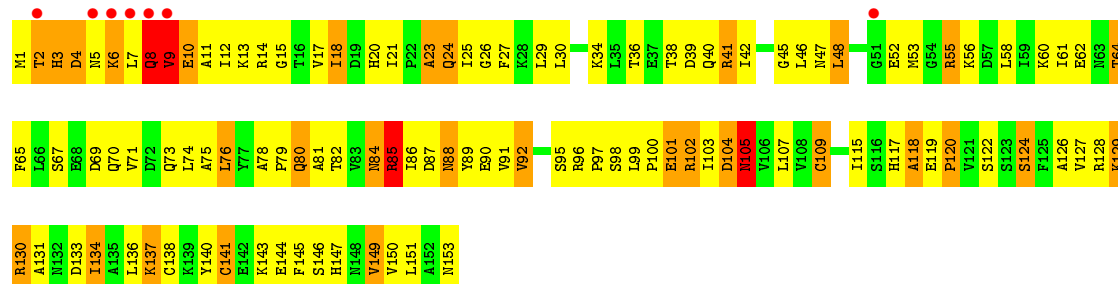


- Molecule 2: Aspartate carbamoyltransferase regulatory chain





• Molecule 2: Aspartate carbamoyltransferase regulatory chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.29 Å   122.29 Å   142.41 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	30.00 – 2.10 59.09 – 2.08	Depositor EDS
% Data completeness (in resolution range)	88.1 (30.00-2.10) 90.8 (59.09-2.08)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.86 (at 2.08 Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.230 , 0.272 0.231 , 0.277	Depositor DCC
$R_{free}$ test set	2653 reflections (3.95%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.6	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 435.6	EDS
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 67145 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	8012	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MLI, CTP, 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	0.71	9/2457 (0.4%)	1.27	19/3334 (0.6%)
1	C	0.70	7/2457 (0.3%)	1.24	24/3334 (0.7%)
2	B	0.93	7/1219 (0.6%)	1.13	8/1647 (0.5%)
2	D	0.90	10/1219 (0.8%)	1.57	28/1647 (1.7%)
All	All	0.78	33/7352 (0.4%)	1.29	79/9962 (0.8%)

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	4
2	B	0	1
2	D	0	6
All	All	0	14

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	133	ASP	C-N	-20.57	0.86	1.34
1	C	310	LEU	C-OXT	-15.38	0.94	1.23
2	D	153	ASN	C-OXT	15.01	1.51	1.23
1	C	271	ASP	C-N	13.87	1.66	1.34
2	B	134	ILE	C-N	-13.59	1.02	1.34
1	A	79	THR	C-N	13.00	1.64	1.34
1	A	80	SER	C-N	12.89	1.63	1.34
2	D	8	GLN	C-N	12.75	1.63	1.34
1	C	269	ARG	C-N	11.26	1.59	1.34
1	C	41	HIS	C-N	10.82	1.58	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	ALA	C-N	10.56	1.58	1.34
1	A	132	ASN	C-N	10.28	1.57	1.34
1	A	308	LEU	C-N	10.06	1.57	1.34
1	A	198	ILE	C-N	9.77	1.56	1.34
2	B	152	ALA	C-N	9.61	1.56	1.34
2	D	24	GLN	C-N	9.35	1.55	1.34
2	B	20	HIS	C-N	8.56	1.53	1.34
1	A	244	LYS	C-N	-8.50	1.14	1.34
2	B	105	ASN	C-N	-7.68	1.16	1.34
1	C	74	SER	C-N	7.67	1.51	1.34
2	B	19	ASP	C-N	6.79	1.49	1.34
2	B	140	TYR	C-N	6.57	1.49	1.34
2	D	120	PRO	N-CD	6.28	1.56	1.47
2	D	104	ASP	C-N	-6.13	1.20	1.34
1	A	269	ARG	C-N	6.08	1.48	1.34
2	D	6	LYS	C-O	5.89	1.34	1.23
2	D	6	LYS	N-CA	5.79	1.57	1.46
2	D	105	ASN	C-N	-5.66	1.21	1.34
1	A	131	SER	C-N	-5.33	1.21	1.34
1	C	267	LEU	C-N	5.24	1.44	1.34
2	D	4	ASP	C-N	5.11	1.45	1.34
1	C	132	ASN	C-N	5.07	1.45	1.34
2	D	119	GLU	C-N	5.01	1.43	1.34

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	6	LYS	CB-CA-C	15.81	142.02	110.40
1	A	79	THR	O-C-N	15.43	147.38	122.70
2	D	105	ASN	O-C-N	-14.76	99.08	122.70
1	A	80	SER	O-C-N	-13.77	100.68	122.70
2	D	6	LYS	CA-C-N	11.68	142.89	117.20
2	D	9	VAL	O-C-N	-11.56	104.20	122.70
1	A	79	THR	CA-C-N	-10.72	93.61	117.20
1	C	140	LEU	CA-CB-CG	10.50	139.46	115.30
1	C	267	LEU	C-N-CD	10.45	150.35	128.40
1	A	80	SER	CA-C-N	9.51	138.12	117.20
2	B	133	ASP	C-N-CA	9.46	145.34	121.70
2	D	6	LYS	O-C-N	-9.36	107.73	122.70
2	D	85	ARG	CD-NE-CZ	9.19	136.47	123.60
1	C	76	SER	CA-C-O	9.03	139.05	120.10
2	D	104	ASP	O-C-N	-8.59	108.96	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4	ASP	O-C-N	8.49	136.29	122.70
1	A	80	SER	C-N-CA	8.48	142.91	121.70
1	C	76	SER	O-C-N	-8.45	109.19	122.70
2	D	24	GLN	O-C-N	-8.31	109.41	122.70
1	A	98	TYR	CB-CG-CD1	8.13	125.88	121.00
1	A	245	ALA	O-C-N	8.09	135.64	122.70
2	D	4	ASP	CA-C-N	-7.89	99.84	117.20
2	D	85	ARG	NE-CZ-NH2	7.85	124.22	120.30
2	D	104	ASP	C-N-CA	7.67	140.88	121.70
1	A	269	ARG	O-C-N	-7.62	110.51	122.70
2	B	152	ALA	O-C-N	7.61	134.87	122.70
1	A	84	LYS	O-C-N	7.55	136.03	123.20
1	A	79	THR	C-N-CA	-7.39	103.22	121.70
1	A	98	TYR	CB-CG-CD2	-7.35	116.59	121.00
1	C	131	SER	O-C-N	-7.33	110.97	122.70
2	D	120	PRO	O-C-N	-7.25	111.09	122.70
2	D	119	GLU	C-N-CD	7.11	143.33	128.40
1	C	54	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	C	113	ARG	CD-NE-CZ	6.46	132.65	123.60
1	A	245	ALA	CA-C-N	-6.42	103.07	117.20
1	A	5	TYR	CB-CG-CD2	-6.41	117.15	121.00
2	D	8	GLN	O-C-N	6.41	132.95	122.70
1	C	40	LYS	C-N-CA	6.29	137.43	121.70
2	D	96	ARG	CD-NE-CZ	6.24	132.33	123.60
1	C	54	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	84	LYS	CA-C-N	-6.09	104.03	116.20
1	C	266	PRO	C-N-CA	6.05	136.83	121.70
2	B	152	ALA	CA-C-N	-5.88	104.28	117.20
2	B	133	ASP	CA-C-N	5.85	130.07	117.20
1	C	268	PRO	CA-N-CD	-5.84	103.33	111.50
2	D	23	ALA	C-N-CA	5.83	136.27	121.70
1	A	98	TYR	CA-CB-CG	5.78	124.39	113.40
1	C	113	ARG	NE-CZ-NH2	5.76	123.18	120.30
2	D	105	ASN	C-N-CA	-5.75	107.32	121.70
1	A	296	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	C	229	ARG	CD-NE-CZ	5.73	131.63	123.60
1	C	80	SER	N-CA-CB	5.71	119.07	110.50
1	C	76	SER	CA-C-N	-5.71	104.64	117.20
2	D	6	LYS	C-N-CA	5.67	135.88	121.70
1	A	76	SER	CA-C-O	5.66	131.99	120.10
2	D	119	GLU	CA-C-N	-5.64	101.31	117.10
1	C	98	TYR	CA-CB-CG	5.61	124.05	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	79	THR	C-N-CA	5.58	135.64	121.70
2	D	6	LYS	N-CA-CB	-5.57	100.57	110.60
1	C	98	TYR	CB-CG-CD1	-5.49	117.71	121.00
2	B	19	ASP	O-C-N	5.46	131.44	122.70
2	D	104	ASP	CA-C-N	5.42	129.12	117.20
2	D	138	CYS	CA-CB-SG	5.42	123.75	114.00
1	A	105	ARG	NE-CZ-NH1	-5.40	117.60	120.30
2	B	11	ALA	C-N-CA	5.34	135.04	121.70
1	C	75	ASP	CB-CG-OD2	5.33	123.10	118.30
1	C	131	SER	CA-C-N	5.31	128.88	117.20
2	D	120	PRO	CA-N-CD	-5.31	104.07	111.50
1	A	83	LYS	O-C-N	-5.28	114.26	122.70
2	D	6	LYS	CA-C-O	-5.15	109.28	120.10
1	C	123	PRO	C-N-CA	5.15	134.57	121.70
2	D	6	LYS	CA-CB-CG	5.09	124.60	113.40
1	C	269	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	C	65	ARG	NE-CZ-NH2	-5.06	117.77	120.30
2	D	141	CYS	CA-CB-SG	5.05	123.08	114.00
2	D	8	GLN	CA-C-N	-5.02	106.16	117.20
2	B	133	ASP	O-C-N	-5.02	114.67	122.70
2	B	66	LEU	C-N-CA	5.01	134.22	121.70
1	C	197	TYR	CA-CB-CG	5.00	122.91	113.40

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	242	ASN	Mainchain
1	A	73	PHE	Mainchain
1	A	82	GLY	Mainchain
2	B	133	ASP	Peptide
1	C	266	PRO	Peptide
1	C	269	ARG	Mainchain
1	C	76	SER	Mainchain,Peptide
2	D	105	ASN	Mainchain
2	D	118	ALA	Mainchain
2	D	23	ALA	Mainchain
2	D	5	ASN	Mainchain,Peptide
2	D	9	VAL	Mainchain

## 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	2411	0	2420	149	0
1	C	2411	0	2421	91	0
2	B	1201	0	1216	116	0
2	D	1201	0	1218	92	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	7	0	2	0	0
4	C	7	0	2	4	0
5	A	8	0	4	3	0
5	C	8	0	4	5	0
6	B	29	0	12	7	0
6	D	29	0	12	7	0
7	A	211	0	0	26	0
7	B	101	0	0	13	0
7	C	265	0	0	20	0
7	D	121	0	0	14	0
All	All	8012	0	7311	436	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 30.

All (436) 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)
5:C:1313:PCT:H1P2	7:C:1461:HOH:O	1.31	1.25
1:A:67:GLY:HA2	7:A:1510:HOH:O	1.39	1.20
2:B:133:ASP:O	2:B:134:ILE:N	1.78	1.15
1:C:200:ASP:HB3	7:C:1516:HOH:O	1.49	1.11
1:C:234:ARG:NH1	4:C:1311:MLI:H11	1.65	1.11
1:C:234:ARG:HH11	4:C:1311:MLI:H11	0.94	1.07
2:B:133:ASP:CA	2:B:134:ILE:N	2.19	1.06
2:D:131:ALA:HB3	7:D:1272:HOH:O	1.56	1.05
2:B:133:ASP:C	2:B:134:ILE:CA	2.24	1.05
2:D:2:THR:HG21	6:D:1157:CTP:O3'	1.58	1.03
2:D:18:ILE:HG22	2:D:21:ILE:HD11	1.44	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:105:ASN:OD1	2:D:122:SER:HB2	1.64	0.96
2:D:17:VAL:HG22	2:D:60:LYS:HG2	1.47	0.96
1:A:235:LEU:HD13	1:A:240:TYR:HB2	1.48	0.95
1:A:26:THR:HA	1:A:29:LYS:HE3	1.49	0.93
2:B:129:LYS:HA	2:B:134:ILE:HG13	1.50	0.93
2:B:133:ASP:C	2:B:134:ILE:N	0.86	0.91
1:C:267:LEU:HD23	7:C:1474:HOH:O	1.70	0.91
1:C:197:TYR:HD1	7:C:1538:HOH:O	1.55	0.89
2:B:41:ARG:HB3	2:B:41:ARG:HH11	1.37	0.88
2:B:38:THR:HG23	2:B:40:GLN:H	1.37	0.88
1:A:73:PHE:HA	7:A:1464:HOH:O	1.76	0.86
1:C:8:HIS:HD2	1:C:124:VAL:H	1.25	0.84
2:B:89:TYR:C	6:B:1156:CTP:HN42	1.81	0.84
2:B:22:PRO:HB2	2:B:25:ILE:HD13	1.59	0.83
2:B:99:LEU:HD12	2:B:100:PRO:HD2	1.59	0.82
1:A:229:ARG:HH11	1:A:229:ARG:HB3	1.45	0.82
2:D:105:ASN:OD1	2:D:122:SER:CB	2.27	0.81
1:A:32:ALA:HA	7:A:1376:HOH:O	1.80	0.80
1:A:81:LEU:HA	1:A:86:GLU:HB3	1.62	0.78
1:A:252:SER:HB2	7:A:1448:HOH:O	1.84	0.78
2:D:27:PHE:HA	2:D:30:LEU:HD12	1.64	0.78
2:B:18:ILE:HG22	2:B:21:ILE:HD11	1.66	0.77
2:B:85:ARG:HH11	2:B:85:ARG:HB3	1.48	0.77
1:A:81:LEU:HD13	1:A:91:THR:HG23	1.65	0.77
1:A:113:ARG:O	1:A:116:THR:HB	1.85	0.76
2:B:107:LEU:HB2	7:B:1176:HOH:O	1.85	0.76
2:D:13:LYS:HD3	7:D:1221:HOH:O	1.85	0.75
1:C:229:ARG:HA	1:C:272:GLU:OE1	1.87	0.75
1:C:265:HIS:H	1:C:288:GLN:HE22	1.35	0.74
2:B:62:GLU:HG2	7:B:1213:HOH:O	1.87	0.74
2:D:41:ARG:HB2	2:D:41:ARG:HH11	1.53	0.74
1:C:234:ARG:NH1	4:C:1311:MLI:C1	2.49	0.74
1:A:231:GLN:O	1:A:234:ARG:HB2	1.87	0.73
2:B:129:LYS:CA	2:B:134:ILE:HG13	2.19	0.73
1:A:191:ALA:O	1:A:192:LEU:HD23	1.88	0.72
1:C:163:LEU:HG	1:C:188:ALA:HB2	1.71	0.71
2:B:17:VAL:HG22	2:B:60:LYS:HG2	1.72	0.71
1:A:51:ALA:HB2	1:A:75:ASP:HB2	1.72	0.71
1:A:81:LEU:HB3	1:A:91:THR:OG1	1.90	0.71
1:C:31:LYS:NZ	1:C:291:ASN:HD21	1.89	0.71
2:D:56:LYS:HE3	2:D:58:LEU:HD12	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:LEU:CD2	7:C:1474:HOH:O	2.32	0.70
1:C:266:PRO:HB2	1:C:267:LEU:HG	1.73	0.70
1:A:236:ASP:HB3	1:A:239:GLU:HB3	1.72	0.70
1:A:251:ALA:O	1:A:254:LEU:HB2	1.91	0.70
1:A:114:LEU:O	1:A:117:GLU:HG3	1.91	0.69
5:C:1313:PCT:N1	7:C:1474:HOH:O	2.24	0.69
2:D:17:VAL:HB	2:D:84:ASN:HD22	1.58	0.69
1:A:154:ASN:HA	1:A:181:GLY:O	1.93	0.69
2:D:55:ARG:HB3	2:D:55:ARG:HH11	1.59	0.68
1:A:231:GLN:HB3	1:A:234:ARG:HG3	1.76	0.68
1:A:255:HIS:HB3	7:A:1489:HOH:O	1.93	0.68
1:A:232:LYS:O	1:A:235:LEU:HD12	1.94	0.68
1:A:278:ASP:HB2	1:A:279:LYS:NZ	2.08	0.68
2:B:38:THR:HG23	2:B:40:GLN:N	2.09	0.67
1:A:279:LYS:HE2	1:A:279:LYS:N	2.09	0.67
2:D:102:ARG:HD3	7:D:1215:HOH:O	1.93	0.67
1:C:231:GLN:HB2	1:C:234:ARG:HD2	1.74	0.67
1:A:183:ARG:HH11	1:A:183:ARG:HB3	1.60	0.67
2:B:10:GLU:HA	2:D:8:GLN:NE2	2.09	0.67
2:B:12:ILE:HG13	2:B:86:ILE:HD11	1.76	0.66
1:A:201:MET:HE3	1:A:202:LEU:N	2.11	0.66
1:A:88:LEU:HD23	1:A:114:LEU:HD22	1.77	0.66
2:B:70:GLN:O	2:B:73:GLN:HB2	1.96	0.66
2:B:89:TYR:O	6:B:1156:CTP:N4	2.25	0.66
2:D:100:PRO:HB2	2:D:101:GLU:OE2	1.96	0.65
2:D:107:LEU:HB2	7:D:1164:HOH:O	1.96	0.65
1:A:74:SER:O	7:A:1454:HOH:O	2.14	0.65
1:C:153:ASP:HB3	1:C:180:ASP:H	1.61	0.65
1:A:154:ASN:HD22	1:A:181:GLY:HA3	1.63	0.64
1:C:234:ARG:HH11	4:C:1311:MLI:C1	1.89	0.64
2:D:25:ILE:O	2:D:29:LEU:HG	1.97	0.64
1:C:52:SER:HA	5:C:1313:PCT:O1P	1.98	0.64
1:A:26:THR:HG23	1:A:308:LEU:HD22	1.79	0.64
2:B:8:GLN:NE2	2:D:9:VAL:O	2.31	0.64
2:B:13:LYS:HG2	7:B:1174:HOH:O	1.98	0.63
2:B:95:SER:HB2	7:B:1177:HOH:O	1.97	0.63
2:D:45:GLY:HA3	2:D:48:LEU:HD21	1.80	0.63
2:B:76:LEU:HD23	2:B:103:ILE:HD11	1.79	0.63
1:A:235:LEU:HB3	7:A:1484:HOH:O	1.97	0.63
1:A:199:LEU:HD22	1:A:209:TRP:CH2	2.34	0.63
2:B:61:ILE:HG22	2:B:64:THR:HB	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:LYS:HD3	7:C:1390:HOH:O	1.98	0.63
2:B:40:GLN:HG2	2:B:62:GLU:O	1.99	0.62
2:B:48:LEU:O	2:B:55:ARG:HA	1.98	0.62
1:A:235:LEU:HD23	7:A:1484:HOH:O	2.00	0.62
1:C:112:ALA:O	1:C:116:THR:HG23	1.99	0.62
2:B:107:LEU:HD13	2:B:150:VAL:HG11	1.80	0.62
2:D:14:ARG:HG3	2:D:87:ASP:HA	1.82	0.62
2:B:10:GLU:HA	2:D:8:GLN:HE22	1.64	0.62
1:A:223:ASP:O	1:A:261:MET:HA	1.99	0.62
1:C:235:LEU:HD22	1:C:239:GLU:OE2	2.00	0.61
2:B:130:ARG:HB2	2:B:133:ASP:HB3	1.82	0.61
1:A:214:SER:O	1:A:217:GLU:HB2	1.99	0.61
2:D:11:ALA:HA	6:D:1157:CTP:N3	2.16	0.61
1:C:145:ILE:O	1:C:149:GLN:HB2	2.01	0.61
2:B:14:ARG:HG2	2:B:63:ASN:HA	1.83	0.61
1:C:309:VAL:HG23	7:C:1484:HOH:O	2.00	0.61
2:B:22:PRO:HA	7:B:1194:HOH:O	2.01	0.60
1:A:52:SER:OG	1:A:55:THR:HB	2.01	0.60
2:D:12:ILE:HD12	2:D:14:ARG:O	2.02	0.60
1:A:164:LYS:HG3	7:A:1459:HOH:O	2.02	0.60
2:D:102:ARG:HH21	2:D:124:SER:HB2	1.67	0.60
2:B:105:ASN:O	2:B:106:VAL:HG13	2.02	0.60
2:D:85:ARG:HD3	2:D:92:VAL:HG23	1.83	0.60
2:B:89:TYR:C	6:B:1156:CTP:N4	2.54	0.60
2:D:14:ARG:HA	2:D:86:ILE:O	2.02	0.59
1:A:11:SER:HA	1:A:133:GLN:HG3	1.84	0.59
2:B:129:LYS:CB	2:B:134:ILE:HG13	2.31	0.59
1:A:232:LYS:HD3	1:A:240:TYR:CZ	2.38	0.59
1:A:105:ARG:HH22	5:A:1314:PCT:HN11	1.50	0.59
1:A:131:SER:HB3	7:A:1492:HOH:O	2.01	0.59
1:C:93:SER:O	1:C:97:THR:HG23	2.03	0.59
1:A:182:ASN:O	1:A:207:ILE:HG23	2.03	0.58
2:D:15:GLY:HA2	2:D:64:THR:H	1.68	0.58
2:B:39:ASP:HB2	2:D:55:ARG:HH21	1.69	0.58
2:D:102:ARG:HB3	7:D:1170:HOH:O	2.03	0.58
2:D:79:PRO:HG2	2:D:80:GLN:HG3	1.85	0.58
2:D:133:ASP:HB3	7:D:1193:HOH:O	2.03	0.58
1:C:166:GLY:O	1:C:169:VAL:HG22	2.03	0.58
2:D:38:THR:CG2	2:D:42:ILE:HD11	2.33	0.58
1:A:17:ARG:HD3	1:A:179:PHE:CE1	2.39	0.58
2:B:88:ASN:O	2:B:89:TYR:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:LEU:HB2	7:C:1553:HOH:O	2.04	0.58
1:C:168:THR:HG23	7:C:1369:HOH:O	2.04	0.57
1:C:5:TYR:CE1	1:C:6:GLN:HG2	2.40	0.57
1:C:248:VAL:HG13	1:C:271:ASP:O	2.04	0.57
2:B:130:ARG:CG	2:B:133:ASP:HB3	2.35	0.57
2:B:21:ILE:HB	2:B:57:ASP:HB2	1.85	0.57
1:C:258:LYS:HB3	7:C:1535:HOH:O	2.05	0.57
1:C:50:ALA:HB2	1:C:107:PRO:HD3	1.86	0.57
2:D:11:ALA:HA	6:D:1157:CTP:O2	2.05	0.57
1:A:194:MET:SD	1:A:195:PRO:HD2	2.45	0.57
2:B:4:ASP:OD1	2:B:9:VAL:HG21	2.04	0.56
1:A:132:ASN:HD22	2:B:143:LYS:NZ	2.02	0.56
2:D:2:THR:CG2	6:D:1157:CTP:O3'	2.41	0.56
1:A:81:LEU:HD23	1:A:86:GLU:OE1	2.05	0.56
2:B:69:ASP:O	2:B:73:GLN:HG2	2.05	0.56
2:D:10:GLU:OE1	2:D:10:GLU:HA	2.05	0.56
1:A:205:LYS:HB2	1:A:205:LYS:HZ3	1.71	0.56
2:B:129:LYS:HA	2:B:134:ILE:HA	1.88	0.56
2:D:78:ALA:HB1	2:D:81:ALA:HB2	1.87	0.56
1:A:59:PHE:HZ	1:A:136:THR:HG21	1.71	0.56
1:A:183:ARG:CB	1:A:183:ARG:HH11	2.19	0.56
1:A:205:LYS:HB2	1:A:205:LYS:NZ	2.20	0.56
1:A:11:SER:HB2	1:A:133:GLN:HG3	1.86	0.56
2:B:30:LEU:HD21	2:B:59:ILE:HD13	1.88	0.56
2:B:107:LEU:HD13	2:B:150:VAL:CG1	2.36	0.56
1:A:33:ASN:HB3	7:A:1418:HOH:O	2.05	0.55
1:A:278:ASP:HB2	1:A:279:LYS:HZ3	1.69	0.55
1:A:163:LEU:O	1:A:195:PRO:HD3	2.07	0.55
2:D:127:VAL:HG22	2:D:136:LEU:CD2	2.36	0.55
1:C:1:ALA:HB2	1:C:306:ARG:HD3	1.87	0.55
2:D:11:ALA:HA	6:D:1157:CTP:C2	2.42	0.55
2:B:10:GLU:HG2	7:B:1239:HOH:O	2.07	0.55
1:A:187:ILE:HG13	1:A:212:HIS:HB2	1.89	0.55
1:C:270:VAL:O	1:C:272:GLU:N	2.40	0.55
2:D:8:GLN:NE2	2:D:8:GLN:HA	2.21	0.55
1:A:50:ALA:HB3	1:A:105:ARG:HG2	1.88	0.55
1:C:254:LEU:HD22	1:C:261:MET:CE	2.37	0.55
1:C:8:HIS:CD2	1:C:123:PRO:HA	2.42	0.55
2:B:78:ALA:HB1	2:B:81:ALA:HB2	1.88	0.55
1:A:239:GLU:HA	7:A:1393:HOH:O	2.07	0.55
2:B:13:LYS:HG3	2:B:14:ARG:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:126:ALA:O	2:D:136:LEU:HA	2.06	0.55
1:C:165:TYR:CD2	1:C:234:ARG:HD3	2.42	0.54
2:B:80:GLN:NE2	2:B:80:GLN:HA	2.21	0.54
2:B:130:ARG:CB	2:B:133:ASP:HB3	2.38	0.54
1:C:31:LYS:HZ2	1:C:291:ASN:HD21	1.54	0.54
1:A:8:HIS:CD2	7:A:1508:HOH:O	2.61	0.54
1:A:44:ILE:HD13	1:A:63:MET:HG2	1.90	0.54
1:A:169:VAL:CG1	1:A:228:THR:HG21	2.38	0.54
1:A:90:ASP:O	1:A:94:VAL:HG23	2.07	0.54
2:B:17:VAL:HG22	2:B:60:LYS:CG	2.37	0.54
2:D:103:ILE:HG13	2:D:127:VAL:HG21	1.90	0.54
1:A:216:GLU:HG2	7:A:1451:HOH:O	2.07	0.54
1:A:258:LYS:HD3	7:A:1379:HOH:O	2.07	0.53
5:C:1313:PCT:N1	7:C:1398:HOH:O	2.31	0.53
2:B:129:LYS:HG3	2:B:129:LYS:O	2.06	0.53
2:D:73:GLN:HA	2:D:73:GLN:OE1	2.07	0.53
1:C:282:HIS:HA	7:C:1462:HOH:O	2.07	0.53
2:B:86:ILE:HD13	6:B:1156:CTP:C4	2.44	0.53
2:D:102:ARG:HH21	2:D:124:SER:CB	2.21	0.53
1:C:30:LEU:HD23	7:C:1482:HOH:O	2.09	0.53
2:B:130:ARG:NE	2:B:135:ALA:HB2	2.24	0.52
1:A:31:LYS:NZ	1:A:291:ASN:HD21	2.07	0.52
1:A:231:GLN:HA	7:A:1498:HOH:O	2.09	0.52
1:A:121:ASN:HA	7:A:1321:HOH:O	2.09	0.52
2:B:141:CYS:O	2:B:143:LYS:HE2	2.09	0.52
2:D:137:LYS:HE3	7:D:1171:HOH:O	2.10	0.52
1:C:55:THR:OG1	5:C:1313:PCT:O1	2.26	0.52
1:C:31:LYS:HZ1	1:C:291:ASN:HD21	1.57	0.52
1:C:165:TYR:HD2	1:C:234:ARG:HD3	1.74	0.52
2:B:76:LEU:HD23	2:B:103:ILE:CD1	2.40	0.52
1:C:187:ILE:HG12	1:C:212:HIS:HB2	1.92	0.52
1:A:59:PHE:CZ	1:A:136:THR:HG21	2.45	0.51
1:A:47:CYS:HB3	1:A:49:PHE:CE1	2.45	0.51
1:A:121:ASN:HB3	7:A:1321:HOH:O	2.08	0.51
2:D:10:GLU:HB3	7:D:1275:HOH:O	2.10	0.51
2:D:146:SER:O	2:D:149:VAL:HG13	2.10	0.51
1:A:110:GLY:HA3	2:B:140:TYR:HB3	1.92	0.51
2:B:13:LYS:HG3	2:B:14:ARG:H	1.76	0.51
1:A:229:ARG:HH11	1:A:229:ARG:CB	2.21	0.51
1:A:11:SER:CB	1:A:133:GLN:HG3	2.41	0.51
2:D:55:ARG:CB	2:D:55:ARG:HH11	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ILE:HA	1:A:212:HIS:O	2.11	0.50
1:A:105:ARG:HD3	7:A:1427:HOH:O	2.12	0.50
2:B:3:HIS:O	2:B:9:VAL:HG23	2.11	0.50
1:C:7:LYS:HA	7:C:1549:HOH:O	2.12	0.50
1:A:31:LYS:HG3	1:A:294:PHE:CD2	2.46	0.50
1:A:45:ALA:HA	1:A:71:VAL:O	2.12	0.50
1:A:132:ASN:HD22	2:B:143:LYS:HZ1	1.57	0.50
1:C:254:LEU:HD22	1:C:261:MET:HE1	1.93	0.50
2:B:27:PHE:HD2	7:D:1172:HOH:O	1.94	0.50
1:A:223:ASP:O	1:A:224:ILE:HD13	2.12	0.50
2:D:41:ARG:NH1	2:D:41:ARG:HB2	2.23	0.50
2:D:78:ALA:O	2:D:97:PRO:HG3	2.12	0.50
1:A:199:LEU:HD22	1:A:209:TRP:CZ3	2.47	0.49
2:B:133:ASP:O	2:B:133:ASP:OD2	2.30	0.49
1:A:244:LYS:HG3	1:A:248:VAL:HG12	1.95	0.49
2:D:91:VAL:HG22	2:D:91:VAL:O	2.11	0.49
1:A:4:LEU:O	1:A:7:LYS:HB2	2.12	0.49
1:C:301:ALA:O	1:C:305:ASN:HB2	2.12	0.49
2:B:126:ALA:O	2:B:136:LEU:HA	2.12	0.49
1:C:136:THR:HG22	1:C:299:LEU:CD2	2.43	0.49
1:C:144:THR:O	1:C:148:THR:HG23	2.12	0.49
1:A:218:VAL:O	1:A:222:VAL:HG13	2.12	0.48
2:D:101:GLU:HB2	7:D:1170:HOH:O	2.13	0.48
2:D:104:ASP:OD2	2:D:124:SER:HB2	2.13	0.48
1:A:236:ASP:N	1:A:239:GLU:HG2	2.28	0.48
2:D:145:PHE:HB2	2:D:150:VAL:HG22	1.95	0.48
2:B:8:GLN:HE21	2:D:10:GLU:HA	1.79	0.48
1:A:121:ASN:HA	7:A:1487:HOH:O	2.13	0.48
2:B:115:ILE:HG13	2:B:115:ILE:O	2.13	0.48
1:C:308:LEU:HB3	1:C:310:LEU:HD22	1.94	0.48
2:B:50:SER:HB3	2:B:54:GLY:C	2.34	0.48
1:C:164:LYS:HE2	1:C:165:TYR:CZ	2.49	0.48
1:A:52:SER:OG	1:A:52:SER:O	2.30	0.48
1:C:265:HIS:ND1	1:C:266:PRO:HD2	2.28	0.48
1:A:236:ASP:HB3	1:A:239:GLU:CB	2.43	0.48
1:C:293:ILE:O	1:C:297:GLN:HG3	2.14	0.48
2:B:96:ARG:HB3	2:B:96:ARG:NH1	2.28	0.48
1:A:136:THR:HB	1:A:296:ARG:HE	1.78	0.48
2:D:67:SER:OG	2:D:70:GLN:HG3	2.14	0.48
2:B:71:VAL:O	2:B:74:LEU:HG	2.14	0.47
1:A:8:HIS:CE1	1:A:123:PRO:HA	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:SER:HA	1:A:84:LYS:HB2	1.95	0.47
2:D:20:HIS:HD2	2:D:82:THR:HG23	1.78	0.47
1:A:156:HIS:HB3	1:A:185:TYR:HE1	1.78	0.47
1:A:24:LEU:HD22	1:A:143:PHE:HB2	1.97	0.47
2:B:50:SER:HB3	2:B:54:GLY:O	2.14	0.47
2:D:109:CYS:O	2:D:117:HIS:CE1	2.68	0.47
1:A:29:LYS:HB3	1:A:310:LEU:HD22	1.96	0.47
6:B:1156:CTP:O3G	6:B:1156:CTP:O2B	2.33	0.47
2:D:136:LEU:HD12	2:D:147:HIS:HA	1.97	0.47
1:C:159:MET:HG3	1:C:186:PHE:CE1	2.50	0.47
1:A:306:ARG:HG2	7:A:1429:HOH:O	2.13	0.47
1:A:106:HIS:CG	1:A:107:PRO:HD2	2.49	0.47
2:B:107:LEU:CD1	2:B:136:LEU:HD13	2.45	0.47
2:B:121:VAL:HB	2:B:140:TYR:OH	2.15	0.47
2:D:3:HIS:O	2:D:4:ASP:HB2	2.15	0.47
1:A:145:ILE:HG12	1:A:224:ILE:HG13	1.96	0.47
1:A:25:ALA:HB2	7:A:1479:HOH:O	2.15	0.47
2:D:21:ILE:N	2:D:21:ILE:HD13	2.30	0.46
2:D:145:PHE:HB2	2:D:150:VAL:CG2	2.45	0.46
1:C:152:LEU:HA	1:C:155:LEU:HD11	1.97	0.46
1:C:137:GLN:HA	1:C:140:LEU:HD13	1.97	0.46
1:C:174:GLN:HG2	1:C:201:MET:HE3	1.97	0.46
2:D:11:ALA:CA	6:D:1157:CTP:N3	2.79	0.46
1:A:232:LYS:H	1:A:232:LYS:HG2	1.38	0.46
2:B:76:LEU:HA	2:B:76:LEU:HD13	1.66	0.46
1:C:5:TYR:CD2	1:C:306:ARG:HA	2.51	0.46
2:D:67:SER:O	2:D:71:VAL:HG23	2.15	0.46
2:B:86:ILE:HD13	6:B:1156:CTP:N3	2.31	0.46
1:A:11:SER:CA	1:A:133:GLN:HG3	2.46	0.46
1:C:110:GLY:HA3	2:D:140:TYR:HB3	1.96	0.46
2:B:8:GLN:NE2	2:D:10:GLU:HA	2.31	0.46
1:C:42:LYS:HA	1:C:100:ASP:OD2	2.16	0.46
1:A:227:MET:HE3	1:A:227:MET:HA	1.98	0.46
2:B:8:GLN:HB3	2:D:10:GLU:HG2	1.98	0.46
2:B:50:SER:N	2:B:54:GLY:O	2.49	0.46
2:D:99:LEU:CD1	2:D:134:ILE:HD12	2.46	0.46
2:B:47:ASN:OD1	2:B:55:ARG:NH1	2.49	0.46
1:C:83:LYS:HG2	1:C:83:LYS:H	1.43	0.46
2:B:124:SER:HB3	2:B:139:LYS:HD2	1.97	0.45
2:B:139:LYS:NZ	7:B:1257:HOH:O	2.48	0.45
1:A:134:HIS:CD2	5:A:1314:PCT:HN12	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ASP:OD1	1:A:179:PHE:HB3	2.17	0.45
1:A:17:ARG:NH2	1:A:180:ASP:OD1	2.50	0.45
2:D:73:GLN:NE2	7:D:1173:HOH:O	2.50	0.45
2:B:23:ALA:O	2:B:24:GLN:HB2	2.15	0.45
2:D:144:GLU:HB3	7:D:1252:HOH:O	2.16	0.45
1:A:234:ARG:NE	7:A:1525:HOH:O	2.50	0.45
2:D:102:ARG:NE	2:D:104:ASP:OD2	2.49	0.45
1:C:30:LEU:HA	7:C:1482:HOH:O	2.17	0.45
1:A:277:VAL:O	1:A:283:ALA:HB2	2.17	0.45
2:B:41:ARG:NH1	2:B:62:GLU:OE2	2.50	0.45
1:C:291:ASN:HD22	1:C:291:ASN:HA	1.50	0.45
2:B:2:THR:O	2:B:4:ASP:N	2.50	0.45
1:C:255:HIS:CD2	1:C:255:HIS:H	2.34	0.45
2:B:138:CYS:O	2:B:142:GLU:HA	2.17	0.45
2:B:128:ARG:O	2:B:135:ALA:N	2.49	0.45
1:C:7:LYS:NZ	7:C:1375:HOH:O	2.49	0.45
1:A:56:ARG:NH1	7:A:1482:HOH:O	2.50	0.45
1:C:267:LEU:HB3	1:C:268:PRO:HD2	1.97	0.45
2:B:22:PRO:HG3	7:B:1175:HOH:O	2.16	0.45
1:A:209:TRP:HZ3	1:A:211:LEU:HD21	1.81	0.45
2:B:47:ASN:ND2	2:D:39:ASP:HA	2.32	0.45
2:B:127:VAL:HG12	2:B:127:VAL:O	2.17	0.45
1:C:84:LYS:HG3	1:C:84:LYS:O	2.17	0.45
1:A:232:LYS:HA	1:A:235:LEU:HD11	1.99	0.45
2:B:32:LEU:HD23	2:B:106:VAL:CG1	2.47	0.45
1:A:137:GLN:OE1	1:A:140:LEU:HD22	2.16	0.45
2:B:131:ALA:O	2:B:132:ASN:HB3	2.17	0.44
2:D:48:LEU:O	2:D:56:LYS:N	2.49	0.44
1:A:258:LYS:HB3	1:A:260:ASN:OD1	2.16	0.44
1:C:263:VAL:C	1:C:264:LEU:HD23	2.37	0.44
2:B:148:ASN:HA	7:B:1199:HOH:O	2.16	0.44
1:A:266:PRO:O	1:A:267:LEU:HB2	2.17	0.44
2:D:2:THR:CB	6:D:1157:CTP:O2B	2.65	0.44
2:D:101:GLU:N	2:D:101:GLU:OE2	2.50	0.44
2:B:46:LEU:HB2	2:D:42:ILE:HB	1.98	0.44
2:D:17:VAL:CB	2:D:84:ASN:HD22	2.29	0.44
2:D:14:ARG:CG	2:D:87:ASP:HA	2.47	0.44
1:A:66:LEU:HD21	1:A:297:GLN:HE21	1.82	0.44
2:D:103:ILE:HG13	2:D:127:VAL:CG2	2.46	0.44
1:C:170:HIS:O	1:C:174:GLN:HG3	2.16	0.44
1:C:25:ALA:O	1:C:28:ALA:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:GLU:HG2	1:C:132:ASN:HB2	1.99	0.44
1:A:236:ASP:HB3	1:A:239:GLU:HG2	1.99	0.44
2:B:80:GLN:HB2	7:B:1175:HOH:O	2.16	0.44
1:C:305:ASN:ND2	7:C:1410:HOH:O	2.50	0.44
1:C:143:PHE:O	1:C:147:GLU:HB3	2.18	0.44
1:A:219:MET:HE3	1:A:254:LEU:HD23	1.99	0.43
2:D:26:GLY:O	2:D:30:LEU:HG	2.17	0.43
2:D:137:LYS:HD2	7:D:1171:HOH:O	2.18	0.43
2:B:96:ARG:HB3	2:B:96:ARG:HH11	1.84	0.43
2:B:10:GLU:HG3	2:B:10:GLU:H	1.36	0.43
2:B:34:LYS:NZ	7:B:1165:HOH:O	2.50	0.43
2:B:36:THR:O	2:B:38:THR:N	2.50	0.43
1:A:263:VAL:C	1:A:264:LEU:HD23	2.39	0.43
1:A:236:ASP:OD2	1:A:239:GLU:HB3	2.18	0.43
2:B:86:ILE:HG22	2:B:91:VAL:HA	1.99	0.43
2:D:38:THR:HG21	2:D:42:ILE:HD11	1.99	0.43
1:C:299:LEU:HD12	1:C:299:LEU:HA	1.54	0.43
2:B:71:VAL:HG22	2:B:83:VAL:HG21	1.99	0.43
1:A:160:VAL:HB	1:A:227:MET:HE3	2.00	0.43
1:C:200:ASP:CB	7:C:1516:HOH:O	2.30	0.43
2:B:85:ARG:O	2:B:92:VAL:HG23	2.18	0.43
1:C:285:TYR:HA	1:C:288:GLN:HE21	1.82	0.43
2:B:14:ARG:HG2	2:B:63:ASN:HD22	1.84	0.43
1:A:146:GLN:HG3	1:A:147:GLU:N	2.27	0.43
2:B:27:PHE:CD1	2:D:36:THR:HG21	2.53	0.43
1:A:227:MET:HE2	1:A:227:MET:HB3	1.90	0.43
1:C:162:ASP:OD2	1:C:192:LEU:HD22	2.18	0.43
1:A:77:ALA:O	1:A:83:LYS:HD3	2.19	0.43
1:A:232:LYS:HD3	1:A:240:TYR:OH	2.19	0.43
1:A:145:ILE:HG22	1:A:146:GLN:N	2.33	0.43
1:A:222:VAL:HG23	1:A:261:MET:HG3	2.01	0.43
1:A:26:THR:HG23	1:A:308:LEU:CD2	2.48	0.43
2:B:28:LYS:O	2:B:32:LEU:HB2	2.19	0.43
2:B:21:ILE:N	2:B:21:ILE:HD13	2.34	0.42
1:A:105:ARG:HD3	1:A:105:ARG:HH11	1.63	0.42
1:C:29:LYS:HG2	7:C:1491:HOH:O	2.18	0.42
1:A:196:GLN:NE2	1:A:200:ASP:OD1	2.46	0.42
1:A:134:HIS:N	1:A:135:PRO:HD3	2.34	0.42
2:B:68:GLU:H	2:B:68:GLU:HG3	1.66	0.42
1:A:54:ARG:HB3	5:A:1314:PCT:O2P	2.19	0.42
1:C:254:LEU:HD22	1:C:261:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ASN:ND2	1:A:5:TYR:HB2	2.34	0.42
1:A:236:ASP:HB3	1:A:239:GLU:CG	2.50	0.42
1:A:164:LYS:HB2	1:A:192:LEU:C	2.39	0.42
1:A:65:ARG:NE	7:A:1512:HOH:O	2.50	0.42
1:A:54:ARG:NH1	1:A:54:ARG:HB2	2.34	0.42
2:D:71:VAL:HA	2:D:74:LEU:CD1	2.50	0.42
1:A:36:PRO:HA	1:A:65:ARG:O	2.19	0.42
1:C:4:LEU:HD23	1:C:4:LEU:HA	1.88	0.42
1:C:66:LEU:HA	1:C:66:LEU:HD12	1.89	0.42
2:D:133:ASP:HB2	2:D:147:HIS:HE1	1.84	0.42
1:C:209:TRP:CZ3	1:C:211:LEU:HD21	2.54	0.42
2:D:76:LEU:HD23	2:D:151:LEU:HD21	2.00	0.42
1:C:263:VAL:O	1:C:264:LEU:HD23	2.19	0.42
1:A:160:VAL:HB	1:A:227:MET:CE	2.50	0.41
2:B:19:ASP:OD1	2:B:20:HIS:N	2.50	0.41
1:A:17:ARG:HB3	7:A:1399:HOH:O	2.19	0.41
1:A:262:LYS:HD2	1:A:284:TRP:CD2	2.56	0.41
2:B:80:GLN:OE1	2:B:96:ARG:NH2	2.50	0.41
1:C:210:SER:C	1:C:211:LEU:HD23	2.40	0.41
1:A:39:LEU:HD22	1:A:42:LYS:HD2	2.02	0.41
1:A:235:LEU:HB2	1:A:239:GLU:CG	2.51	0.41
2:B:119:GLU:HB3	2:B:120:PRO:HD2	2.03	0.41
1:C:218:VAL:O	1:C:222:VAL:HG13	2.20	0.41
1:C:106:HIS:CE1	1:C:107:PRO:HG2	2.55	0.41
1:A:33:ASN:O	1:A:310:LEU:HD21	2.19	0.41
2:B:11:ALA:O	6:B:1156:CTP:O2	2.38	0.41
2:D:65:PHE:HA	7:D:1207:HOH:O	2.19	0.41
1:C:190:ASP:OD1	1:C:190:ASP:N	2.50	0.41
2:D:115:ILE:HG13	2:D:115:ILE:O	2.21	0.41
2:D:129:LYS:HG2	2:D:129:LYS:HZ3	1.77	0.41
1:A:77:ALA:O	1:A:83:LYS:CD	2.68	0.41
1:C:214:SER:O	1:C:217:GLU:HG3	2.21	0.41
1:A:236:ASP:HA	1:A:237:PRO:HD2	1.91	0.41
1:A:271:ASP:N	1:A:271:ASP:OD2	2.53	0.41
2:D:88:ASN:O	2:D:90:GLU:N	2.54	0.41
1:A:45:ALA:HB2	1:A:99:VAL:HG11	2.03	0.41
1:A:95:ILE:O	1:A:95:ILE:HG22	2.20	0.41
2:B:33:PHE:CE2	2:B:73:GLN:HB3	2.56	0.40
1:C:153:ASP:HB2	1:C:180:ASP:O	2.21	0.40
1:C:235:LEU:HA	1:C:235:LEU:HD23	1.85	0.40
2:D:46:LEU:O	2:D:47:ASN:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:ARG:CB	2:B:41:ARG:HH11	2.20	0.40
1:C:308:LEU:HD13	1:C:308:LEU:HA	1.81	0.40
1:A:189:PRO:O	1:A:192:LEU:N	2.50	0.40
2:D:130:ARG:HB2	2:D:133:ASP:O	2.21	0.40
2:B:141:CYS:SG	2:B:143:LYS:HG2	2.61	0.40
2:B:34:LYS:HA	7:B:1167:HOH:O	2.21	0.40
1:A:2:ASN:ND2	1:A:305:ASN:O	2.55	0.40
1:A:201:MET:HE2	1:A:201:MET:HB3	1.85	0.40
1:A:66:LEU:CD2	1:A:297:GLN:HE21	2.34	0.40
1:C:292:GLY:O	1:C:296:ARG:HB2	2.20	0.40
2:D:13:LYS:HG3	2:D:88:ASN:HA	2.04	0.40
1:C:5:TYR:CZ	1:C:6:GLN:HG2	2.57	0.40
1:A:132:ASN:ND2	2:B:143:LYS:NZ	2.70	0.40
1:A:108:GLN:HG3	2:B:113:ASN:O	2.21	0.40
2:B:153:ASN:C	7:B:1232:HOH:O	2.59	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%)	284 (92%)	22 (7%)	2 (1%)	30	24
1	C	308/310 (99%)	286 (93%)	17 (6%)	5 (2%)	12	6
2	B	151/153 (99%)	123 (82%)	21 (14%)	7 (5%)	3	1
2	D	151/153 (99%)	124 (82%)	18 (12%)	9 (6%)	2	0
All	All	918/926 (99%)	817 (89%)	78 (8%)	23 (2%)	7	2

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	3	HIS
2	B	12	ILE
2	B	106	VAL
2	D	6	LYS
2	D	9	VAL
2	D	24	GLN
2	B	51	GLY
2	B	105	ASN
1	C	41	HIS
2	D	89	TYR
2	D	118	ALA
1	A	85	GLY
1	C	80	SER
1	C	271	ASP
1	C	76	SER
2	D	52	GLU
1	A	75	ASP
2	B	37	GLU
2	B	134	ILE
2	D	7	LEU
2	D	75	ALA
2	D	120	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	260/260 (100%)	208 (80%)	52 (20%)	1	0
1	C	260/260 (100%)	217 (84%)	43 (16%)	3	1
2	B	137/137 (100%)	98 (72%)	39 (28%)	0	0
2	D	137/137 (100%)	101 (74%)	36 (26%)	0	0
All	All	794/794 (100%)	624 (79%)	170 (21%)	1	0

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	17	ARG
1	A	31	LYS
1	A	38	LEU
1	A	40	LYS
1	A	42	LYS
1	A	52	SER
1	A	53	THR
1	A	69	SER
1	A	78	ASN
1	A	80	SER
1	A	81	LEU
1	A	108	GLN
1	A	116	THR
1	A	121	ASN
1	A	124	VAL
1	A	134	HIS
1	A	146	GLN
1	A	149	GLN
1	A	151	ARG
1	A	159	MET
1	A	160	VAL
1	A	167	ARG
1	A	169	VAL
1	A	183	ARG
1	A	201	MET
1	A	204	GLU
1	A	205	LYS
1	A	211	LEU
1	A	213	SER
1	A	215	ILE
1	A	227	MET
1	A	229	ARG
1	A	231	GLN
1	A	232	LYS
1	A	233	GLU
1	A	235	LEU
1	A	238	SER
1	A	239	GLU
1	A	242	ASN
1	A	250	ARG
1	A	252	SER
1	A	255	HIS

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Mol	Chain	Res	Type
1	A	258	LYS
1	A	267	LEU
1	A	269	ARG
1	A	279	LYS
1	A	285	TYR
1	A	302	LEU
1	A	306	ARG
1	A	309	VAL
1	A	310	LEU
2	B	4	ASP
2	B	5	ASN
2	B	6	LYS
2	B	7	LEU
2	B	9	VAL
2	B	10	GLU
2	B	14	ARG
2	B	21	ILE
2	B	31	SER
2	B	32	LEU
2	B	34	LYS
2	B	38	THR
2	B	40	GLN
2	B	41	ARG
2	B	50	SER
2	B	52	GLU
2	B	53	MET
2	B	55	ARG
2	B	56	LYS
2	B	58	LEU
2	B	66	LEU
2	B	68	GLU
2	B	70	GLN
2	B	76	LEU
2	B	80	GLN
2	B	82	THR
2	B	85	ARG
2	B	90	GLU
2	B	92	VAL
2	B	95	SER
2	B	98	SER
2	B	99	LEU
2	B	102	ARG

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Mol	Chain	Res	Type
2	B	105	ASN
2	B	106	VAL
2	B	122	SER
2	B	127	VAL
2	B	130	ARG
2	B	143	LYS
1	C	17	ARG
1	C	18	ASP
1	C	29	LYS
1	C	59	PHE
1	C	66	LEU
1	C	74	SER
1	C	75	ASP
1	C	80	SER
1	C	81	LEU
1	C	83	LYS
1	C	84	LYS
1	C	86	GLU
1	C	96	SER
1	C	108	GLN
1	C	117	GLU
1	C	140	LEU
1	C	147	GLU
1	C	153	ASP
1	C	159	MET
1	C	167	ARG
1	C	171	SER
1	C	174	GLN
1	C	178	LYS
1	C	180	ASP
1	C	183	ARG
1	C	190	ASP
1	C	210	SER
1	C	215	ILE
1	C	216	GLU
1	C	229	ARG
1	C	239	GLU
1	C	242	ASN
1	C	243	VAL
1	C	246	GLN
1	C	258	LYS
1	C	272	GLU

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Mol	Chain	Res	Type
1	C	279	LYS
1	C	285	TYR
1	C	291	ASN
1	C	299	LEU
1	C	307	ASP
1	C	309	VAL
1	C	310	LEU
2	D	1	MET
2	D	2	THR
2	D	3	HIS
2	D	8	GLN
2	D	10	GLU
2	D	18	ILE
2	D	34	LYS
2	D	40	GLN
2	D	41	ARG
2	D	48	LEU
2	D	53	MET
2	D	55	ARG
2	D	61	ILE
2	D	62	GLU
2	D	64	THR
2	D	69	ASP
2	D	76	LEU
2	D	80	GLN
2	D	84	ASN
2	D	85	ARG
2	D	88	ASN
2	D	92	VAL
2	D	95	SER
2	D	98	SER
2	D	101	GLU
2	D	102	ARG
2	D	109	CYS
2	D	124	SER
2	D	128	ARG
2	D	129	LYS
2	D	130	ARG
2	D	134	ILE
2	D	137	LYS
2	D	141	CYS
2	D	143	LYS

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Mol	Chain	Res	Type
2	D	149	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	21	ASN
1	A	132	ASN
1	A	154	ASN
1	A	156	HIS
1	A	212	HIS
1	A	255	HIS
1	A	291	ASN
1	A	297	GLN
1	A	305	ASN
2	B	3	HIS
2	B	63	ASN
2	B	73	GLN
2	B	105	ASN
1	C	8	HIS
1	C	33	ASN
1	C	108	GLN
1	C	137	GLN
1	C	174	GLN
1	C	255	HIS
1	C	288	GLN
1	C	291	ASN
1	C	305	ASN
2	D	40	GLN
2	D	63	ASN
2	D	70	GLN
2	D	80	GLN
2	D	84	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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	MLI	A	1312	-	0,6,6	0.00	-	0,7,7	0.00	-
5	PCT	A	1314	-	7,7,7	3.00	4 (57%)	9,10,10	1.37	2 (22%)
6	CTP	B	1156	-	21,30,30	2.09	4 (19%)	31,47,47	3.52	12 (38%)
4	MLI	C	1311	-	0,6,6	0.00	-	0,7,7	0.00	-
5	PCT	C	1313	-	7,7,7	3.08	4 (57%)	9,10,10	1.38	1 (11%)
6	CTP	D	1157	-	21,30,30	2.11	5 (23%)	31,47,47	3.55	13 (41%)

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	MLI	A	1312	-	-	0/0/4/4	0/0/0/0
5	PCT	A	1314	-	-	0/4/5/5	0/0/0/0
6	CTP	B	1156	-	-	0/18/38/38	0/2/2/2
4	MLI	C	1311	-	-	0/0/4/4	0/0/0/0
5	PCT	C	1313	-	-	0/4/5/5	0/0/0/0
6	CTP	D	1157	-	-	0/18/38/38	0/2/2/2

All (17) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1157	CTP	PB-O1B	2.06	1.58	1.51
6	D	1157	CTP	PG-O3G	2.19	1.62	1.54
5	C	1313	PCT	P-O2P	2.29	1.60	1.54
6	B	1156	CTP	PG-O3G	2.30	1.63	1.54
5	A	1314	PCT	P-O2P	2.32	1.60	1.54
6	D	1157	CTP	PA-O1A	2.44	1.60	1.51
6	B	1156	CTP	PA-O1A	2.67	1.60	1.51
6	B	1156	CTP	PG-O1G	3.07	1.61	1.51
5	A	1314	PCT	P-O3P	3.10	1.62	1.54
6	D	1157	CTP	PG-O1G	3.14	1.61	1.51
5	C	1313	PCT	P-O3P	3.18	1.62	1.54
5	C	1313	PCT	P-O1P	4.44	1.60	1.50
5	A	1314	PCT	P-O1P	4.67	1.60	1.50
5	A	1314	PCT	P-C1P	4.97	1.86	1.79
5	C	1313	PCT	P-C1P	5.32	1.87	1.79
6	B	1156	CTP	C4-N3	7.25	1.49	1.35
6	D	1157	CTP	C4-N3	7.29	1.49	1.35

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1156	CTP	PB-O3A-PA	-10.46	103.35	132.73
6	D	1157	CTP	PB-O3A-PA	-8.70	108.30	132.73
6	B	1156	CTP	C6-N1-C2	-7.24	109.56	121.28
6	D	1157	CTP	C6-N1-C2	-5.90	111.73	121.28
6	D	1157	CTP	O3G-PG-O3B	-5.71	79.19	105.09
6	B	1156	CTP	PB-O3B-PG	-5.28	114.95	132.67
6	D	1157	CTP	PB-O3B-PG	-4.68	116.99	132.67
6	B	1156	CTP	C5-C4-N3	-4.32	116.35	121.80
6	D	1157	CTP	C5-C4-N3	-3.59	117.28	121.80
6	D	1157	CTP	O2G-PG-O1G	-3.17	100.36	110.58
6	B	1156	CTP	O2G-PG-O1G	-2.93	101.16	110.58
6	D	1157	CTP	O2A-PA-O5'	-2.30	96.87	108.46
6	B	1156	CTP	C5'-C4'-C3'	-2.15	106.66	115.21
5	A	1314	PCT	O1P-P-C1P	-2.06	105.84	110.92
6	D	1157	CTP	O3G-PG-O1G	2.11	117.38	110.58
6	D	1157	CTP	O2A-PA-O3A	2.14	114.82	105.09
6	B	1156	CTP	C2-N3-C4	2.15	118.64	115.61
6	B	1156	CTP	O3G-PG-O1G	2.18	117.60	110.58
5	C	1313	PCT	O1-C1-C1P	2.21	122.46	119.90
5	A	1314	PCT	O3P-P-O2P	2.26	114.75	108.13
6	D	1157	CTP	O4'-C4'-C3'	2.42	110.03	105.15
6	D	1157	CTP	C5-C6-N1	3.46	129.07	120.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1156	CTP	C5-C6-N1	4.25	130.99	120.58
6	B	1156	CTP	O3A-PA-O5'	4.40	114.61	102.94
6	D	1157	CTP	O3A-PA-O5'	4.60	115.14	102.94
6	B	1156	CTP	O2G-PG-O3B	6.37	133.99	105.09
6	B	1156	CTP	O2B-PB-O3A	7.07	137.19	105.09
6	D	1157	CTP	O2B-PB-O3A	11.01	155.02	105.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1314	PCT	3	0
6	B	1156	CTP	7	0
4	C	1311	MLI	4	0
5	C	1313	PCT	5	0
6	D	1157	CTP	7	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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	310/310 (100%)	-0.66	11 (3%) 48 57	7, 25, 95, 158	0
1	C	310/310 (100%)	-0.83	3 (0%) 84 87	6, 18, 86, 158	0
2	B	153/153 (100%)	-0.34	4 (2%) 59 66	14, 45, 157, 158	0
2	D	153/153 (100%)	-0.20	7 (4%) 36 45	13, 47, 156, 158	0
All	All	926/926 (100%)	-0.59	25 (2%) 58 65	6, 30, 133, 158	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	81	LEU	10.7
1	A	80	SER	7.6
1	A	82	GLY	6.3
2	D	5	ASN	6.3
2	D	7	LEU	6.2
1	C	81	LEU	5.7
1	A	310	LEU	4.6
1	A	244	LYS	4.0
2	B	9	VAL	4.0
2	D	6	LYS	3.8
1	A	79	THR	3.8
2	D	8	GLN	3.6
1	A	76	SER	3.2
1	A	309	VAL	3.2
2	B	8	GLN	3.2
1	C	82	GLY	2.8
2	D	51	GLY	2.8
1	C	80	SER	2.8
2	B	153	ASN	2.5
1	A	245	ALA	2.5
1	A	78	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	2	THR	2.4
1	A	84	LYS	2.2
2	D	9	VAL	2.1
2	B	7	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	PCT	A	1314	8/8	0.73	0.36	13.67	52,72,78,92	8
5	PCT	C	1313	8/8	0.84	0.21	3.56	39,53,79,86	8
6	CTP	D	1157	29/29	0.89	0.16	0.50	56,79,88,90	29
6	CTP	B	1156	29/29	0.82	0.15	0.33	25,40,73,80	0
3	ZN	D	155	1/1	0.98	0.06	-0.78	121,121,121,121	1
3	ZN	B	154	1/1	1.00	0.05	-0.90	19,19,19,19	0
4	MLI	A	1312	7/7	0.47	0.82	-	36,56,74,76	7
4	MLI	C	1311	7/7	0.35	0.65	-	80,81,87,87	7

## 6.5 Other polymers [i](#)

There are no such residues in this entry.