



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:27 PM GMT

PDB ID : 1AVQ  
Title : TOROIDAL STRUCTURE OF LAMBDA EXONUCLEASE DETERMINED  
AT 2.4 ANGSTROMS  
Authors : Kovall, R.A.; Matthews, B.W.  
Deposited on : 1997-09-18  
Resolution : 2.40 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

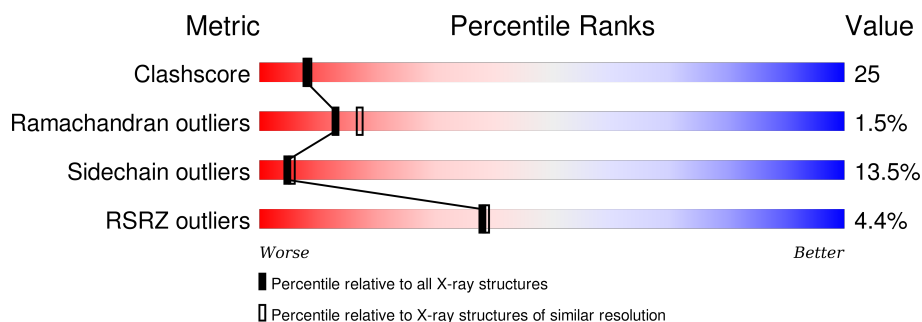
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	228	<div> <div>3%</div> <div>57% 30% 10% .</div> </div>
1	B	228	<div> <div>4%</div> <div>55% 32% 11% .</div> </div>
1	C	228	<div> <div>6%</div> <div>54% 32% 9% . .</div> </div>

## 2 Entry composition [i](#)

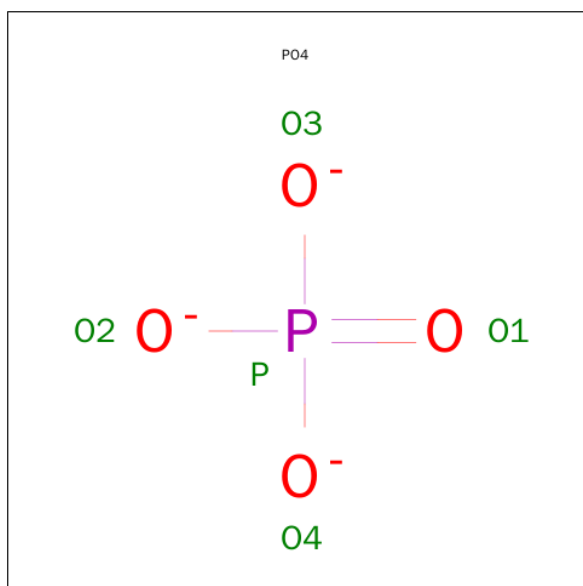
There are 4 unique types of molecules in this entry. The entry contains 5933 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 LAMBDA EXONUCLEASE.

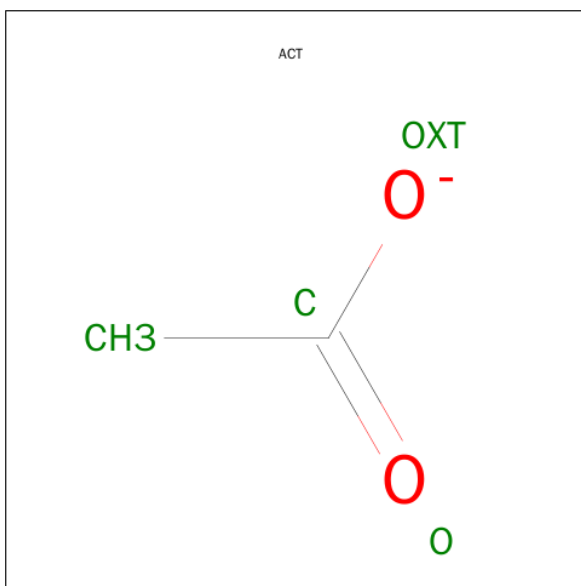
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1837	1169	313	341	14			
1	B	228	Total	C	N	O	S	0	0	0
			1837	1169	313	341	14			
1	C	225	Total	C	N	O	S	0	0	0
			1812	1155	308	336	13			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		

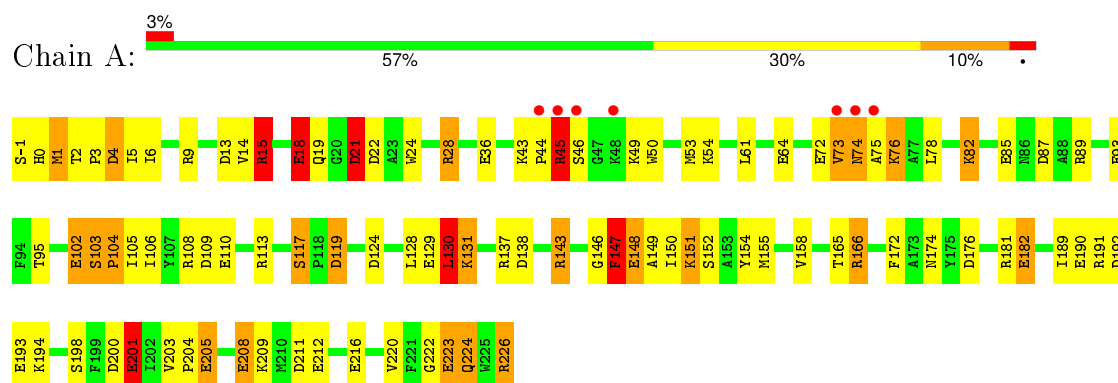
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	169	Total	O	0	0
			169	169		
4	B	131	Total	O	0	0
			131	131		
4	C	116	Total	O	0	0
			116	116		

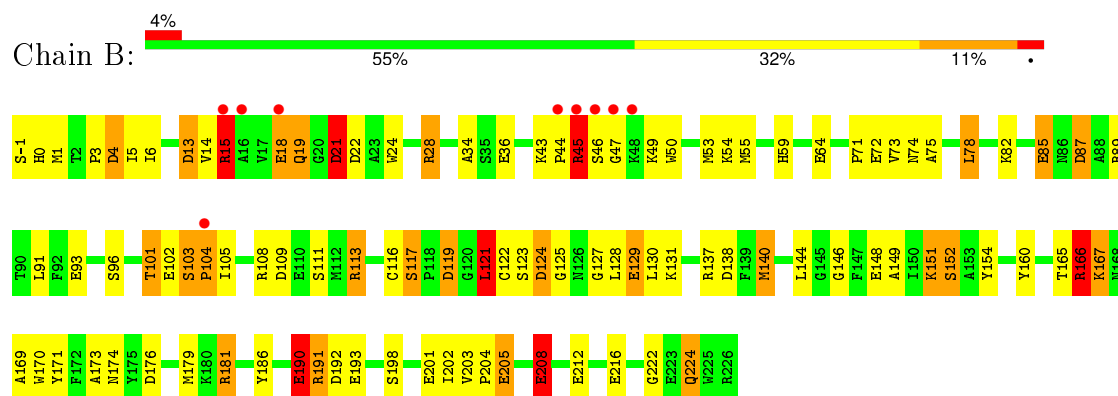
### 3 Residue-property plots

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.

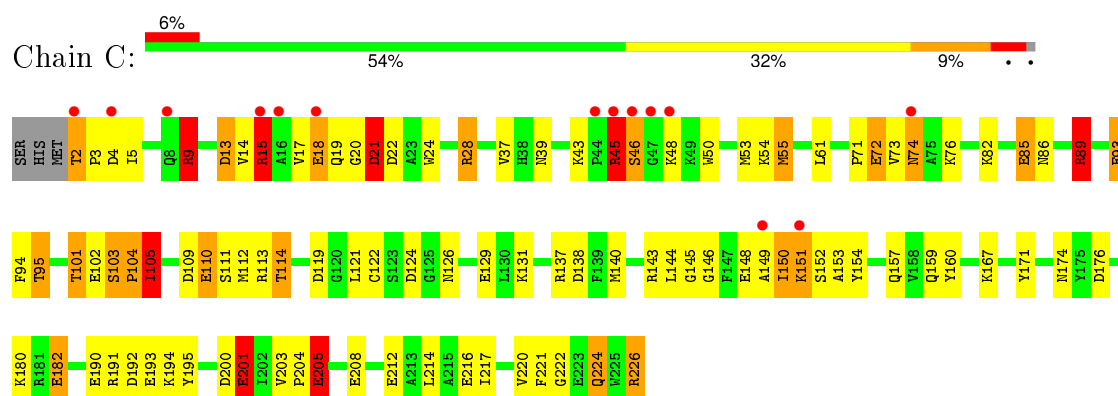
#### • Molecule 1: LAMBDA EXONUCLEASE



#### • Molecule 1: LAMBDA EXONUCLEASE



#### • Molecule 1: LAMBDA EXONUCLEASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	156.70 Å   156.70 Å   131.70 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	30.00 – 2.40 29.93 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.0 (30.00-2.40) 98.2 (29.93-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.31 (at 2.42 Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, $R_{free}$	0.198 , (Not available) 0.193 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	28.7	Xtriage
Anisotropy	0.663	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 102.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 62855 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5933	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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: PO4, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.28	19/1883 (1.0%)	1.73	50/2542 (2.0%)
1	B	1.22	16/1883 (0.8%)	1.62	34/2542 (1.3%)
1	C	1.27	14/1857 (0.8%)	1.63	34/2509 (1.4%)
All	All	1.26	49/5623 (0.9%)	1.66	118/7593 (1.6%)

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	72	GLU	CD-OE1	10.40	1.37	1.25
1	B	208	GLU	CD-OE2	9.18	1.35	1.25
1	A	201	GLU	CD-OE2	8.74	1.35	1.25
1	A	129	GLU	CD-OE1	8.64	1.35	1.25
1	A	216	GLU	CD-OE1	8.55	1.35	1.25
1	A	182	GLU	CD-OE1	8.42	1.34	1.25
1	B	102	GLU	CD-OE1	8.26	1.34	1.25
1	C	110	GLU	CD-OE2	8.23	1.34	1.25
1	B	216	GLU	CD-OE1	7.93	1.34	1.25
1	A	148	GLU	CD-OE2	7.91	1.34	1.25
1	A	208	GLU	CD-OE2	7.68	1.34	1.25
1	C	102	GLU	CD-OE1	7.65	1.34	1.25
1	A	102	GLU	CD-OE2	7.64	1.34	1.25
1	B	148	GLU	CD-OE2	7.62	1.34	1.25
1	C	201	GLU	CD-OE1	7.55	1.33	1.25
1	B	85	GLU	CD-OE1	7.52	1.33	1.25
1	A	205	GLU	CD-OE2	7.36	1.33	1.25
1	C	85	GLU	CD-OE2	7.31	1.33	1.25
1	B	201	GLU	CD-OE1	7.29	1.33	1.25
1	C	148	GLU	CD-OE2	7.26	1.33	1.25
1	A	72	GLU	CD-OE2	7.19	1.33	1.25
1	A	64	GLU	CD-OE2	7.16	1.33	1.25
1	C	190	GLU	CD-OE2	7.12	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	208	GLU	CD-OE2	7.11	1.33	1.25
1	C	18	GLU	CD-OE2	7.09	1.33	1.25
1	B	36	GLU	CD-OE2	7.05	1.33	1.25
1	B	72	GLU	CD-OE1	6.80	1.33	1.25
1	A	18	GLU	CD-OE2	6.52	1.32	1.25
1	C	216	GLU	CD-OE1	6.52	1.32	1.25
1	B	205	GLU	CD-OE2	6.46	1.32	1.25
1	B	93	GLU	CD-OE2	6.29	1.32	1.25
1	B	212	GLU	CD-OE2	6.25	1.32	1.25
1	A	190	GLU	CD-OE2	6.24	1.32	1.25
1	C	212	GLU	CD-OE2	6.22	1.32	1.25
1	B	18	GLU	CD-OE2	5.73	1.31	1.25
1	C	205	GLU	CD-OE2	5.72	1.31	1.25
1	A	85	GLU	CD-OE2	5.60	1.31	1.25
1	A	212	GLU	CD-OE2	5.56	1.31	1.25
1	A	36	GLU	CD-OE2	5.56	1.31	1.25
1	B	190	GLU	CD-OE2	5.55	1.31	1.25
1	B	193	GLU	CD-OE1	5.55	1.31	1.25
1	B	64	GLU	CD-OE2	5.51	1.31	1.25
1	C	93	GLU	CD-OE2	5.51	1.31	1.25
1	C	129	GLU	CD-OE2	-5.50	1.19	1.25
1	B	129	GLU	CD-OE1	5.44	1.31	1.25
1	A	223	GLU	CD-OE1	5.36	1.31	1.25
1	A	193	GLU	CD-OE1	5.33	1.31	1.25
1	A	93	GLU	CD-OE2	5.29	1.31	1.25
1	A	193	GLU	CD-OE2	-5.13	1.20	1.25

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	ARG	NE-CZ-NH2	-13.52	113.54	120.30
1	B	103	SER	C-N-CD	-12.89	92.23	120.60
1	A	89	ARG	NE-CZ-NH2	-12.89	113.86	120.30
1	B	28	ARG	NE-CZ-NH1	12.67	126.63	120.30
1	C	138	ASP	CB-CG-OD2	-11.96	107.54	118.30
1	A	166	ARG	NE-CZ-NH1	11.44	126.02	120.30
1	A	143	ARG	NE-CZ-NH2	-11.29	114.65	120.30
1	A	103	SER	C-N-CD	-10.46	97.59	120.60
1	B	28	ARG	NE-CZ-NH2	-10.38	115.11	120.30
1	A	89	ARG	NE-CZ-NH1	10.11	125.35	120.30
1	B	192	ASP	CB-CG-OD1	9.76	127.08	118.30
1	C	124	ASP	CB-CG-OD2	-9.65	109.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	15	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	A	143	ARG	NE-CZ-NH1	9.29	124.94	120.30
1	C	138	ASP	CB-CG-OD1	9.13	126.52	118.30
1	C	28	ARG	NE-CZ-NH1	9.13	124.86	120.30
1	B	192	ASP	CB-CG-OD2	-8.99	110.20	118.30
1	A	21	ASP	CB-CA-C	-8.93	92.53	110.40
1	A	119	ASP	CB-CG-OD2	8.70	126.13	118.30
1	B	176	ASP	CB-CG-OD2	-8.62	110.55	118.30
1	B	22	ASP	CB-CG-OD2	-8.32	110.82	118.30
1	A	137	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	B	124	ASP	CB-CG-OD2	-8.27	110.86	118.30
1	A	13	ASP	CB-CG-OD1	8.25	125.73	118.30
1	A	119	ASP	CB-CG-OD1	-8.21	110.91	118.30
1	A	28	ARG	NE-CZ-NH1	8.07	124.34	120.30
1	C	192	ASP	CB-CG-OD2	-8.04	111.07	118.30
1	C	22	ASP	CB-CG-OD2	-8.04	111.07	118.30
1	C	45	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	A	147	PHE	N-CA-CB	-7.88	96.42	110.60
1	A	22	ASP	CB-CG-OD1	7.82	125.34	118.30
1	A	176	ASP	CB-CG-OD1	7.78	125.30	118.30
1	C	95	THR	CA-CB-CG2	-7.74	101.57	112.40
1	B	176	ASP	CB-CG-OD1	7.53	125.07	118.30
1	B	21	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	C	119	ASP	CB-CG-OD1	-7.49	111.56	118.30
1	B	13	ASP	CB-CG-OD1	7.35	124.91	118.30
1	C	200	ASP	CB-CG-OD2	-7.30	111.72	118.30
1	A	4	ASP	CB-CG-OD2	-7.27	111.75	118.30
1	B	138	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	B	13	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	A	192	ASP	CB-CG-OD2	-7.15	111.87	118.30
1	A	176	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	C	109	ASP	CB-CG-OD2	-7.08	111.92	118.30
1	B	108	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	C	176	ASP	CB-CG-OD2	-7.04	111.96	118.30
1	A	130	LEU	CB-CA-C	-7.03	96.84	110.20
1	A	21	ASP	CB-CG-OD2	-7.03	111.97	118.30
1	A	87	ASP	CB-CG-OD1	6.98	124.58	118.30
1	B	109	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	C	103	SER	C-N-CD	-6.91	105.40	120.60
1	B	119	ASP	CB-CG-OD1	-6.86	112.13	118.30
1	B	89	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	C	124	ASP	CB-CG-OD1	6.83	124.45	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	A	137	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	A	21	ASP	CB-CG-OD1	6.69	124.33	118.30
1	A	191	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	A	108	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	A	192	ASP	CB-CG-OD1	6.60	124.24	118.30
1	B	166	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	C	109	ASP	CB-CG-OD1	6.54	124.19	118.30
1	A	13	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	A	102	GLU	CG-CD-OE2	-6.42	105.47	118.30
1	A	200	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	B	181	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	A	189	ILE	CA-CB-CG1	-6.36	98.91	111.00
1	B	87	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	B	15	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	191	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	A	1	MET	CG-SD-CE	-6.17	90.33	100.20
1	A	28	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	A	103	SER	N-CA-CB	6.14	119.70	110.50
1	C	4	ASP	CB-CG-OD2	6.07	123.77	118.30
1	C	114	THR	CA-CB-CG2	-6.06	103.92	112.40
1	A	131	LYS	CB-CA-C	-6.05	98.30	110.40
1	B	124	ASP	CB-CG-OD1	6.03	123.72	118.30
1	C	192	ASP	CB-CG-OD1	5.96	123.67	118.30
1	C	226	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	C	9	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	B	22	ASP	CB-CG-OD1	5.94	123.64	118.30
1	C	13	ASP	CB-CG-OD1	5.89	123.60	118.30
1	B	137	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	B	113	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	A	109	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	C	9	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	B	121	LEU	N-CA-CB	5.77	121.94	110.40
1	A	9	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	C	4	ASP	CB-CG-OD1	-5.74	113.14	118.30
1	B	166	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	A	22	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	C	220	VAL	CA-CB-CG1	-5.69	102.37	110.90
1	B	87	ASP	CB-CG-OD1	5.68	123.41	118.30
1	B	21	ASP	CB-CA-C	-5.65	99.11	110.40
1	A	9	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	A	113	ARG	NE-CZ-NH2	-5.60	117.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	119	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	138	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	45	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	A	138	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	A	87	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	A	82	LYS	CB-CA-C	5.38	121.15	110.40
1	B	191	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	C	150	ILE	CA-CB-CG2	5.34	121.59	110.90
1	C	220	VAL	CG1-CB-CG2	-5.33	102.38	110.90
1	C	176	ASP	CB-CG-OD1	5.32	123.09	118.30
1	C	21	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	B	4	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	C	89	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	182	GLU	CB-CA-C	-5.22	99.96	110.40
1	C	174	ASN	N-CA-CB	5.18	119.93	110.60
1	A	211	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	A	15	ARG	N-CA-CB	5.12	119.81	110.60
1	B	140	MET	CG-SD-CE	-5.11	92.02	100.20
1	B	0	HIS	CA-CB-CG	-5.05	105.01	113.60
1	C	171	TYR	CB-CA-C	-5.03	100.34	110.40
1	B	138	ASP	CB-CG-OD1	5.02	122.82	118.30
1	C	22	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	1837	0	1784	75	0
1	B	1837	0	1784	102	0
1	C	1812	0	1760	91	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
2	C	5	0	0	0	0
3	A	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	3	0	0
3	C	8	0	6	1	0
4	A	169	0	0	5	0
4	B	131	0	0	5	0
4	C	116	0	0	4	0
All	All	5933	0	5340	268	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 25.

All (268) 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:45:ARG:H	1:A:45:ARG:NH1	1.45	1.14
1:B:1:MET:HE3	1:B:5:ILE:HB	1.27	1.13
1:A:45:ARG:HH11	1:A:45:ARG:N	1.47	1.12
1:C:45:ARG:HH11	1:C:45:ARG:HB3	1.18	1.08
1:B:75:ALA:HA	1:B:78:LEU:HD12	1.35	1.06
1:B:224:GLN:HE21	1:B:224:GLN:N	1.61	0.98
1:A:222:GLY:H	1:A:224:GLN:HE22	1.14	0.95
1:B:224:GLN:H	1:B:224:GLN:NE2	1.65	0.94
1:B:21:ASP:HB2	1:B:24:TRP:HB2	1.51	0.93
1:C:151:LYS:HG2	1:C:153:ALA:H	1.34	0.93
1:A:224:GLN:HE21	1:A:224:GLN:H	1.05	0.91
1:A:1:MET:HE1	1:A:6:ILE:HG13	1.51	0.91
1:C:224:GLN:H	1:C:224:GLN:HE21	1.20	0.88
1:C:151:LYS:HE3	1:C:154:TYR:CD2	2.10	0.87
1:C:15:ARG:HG2	1:C:15:ARG:HH11	1.40	0.85
1:A:1:MET:HE3	1:A:5:ILE:HB	1.57	0.85
1:C:222:GLY:H	1:C:224:GLN:HE22	1.25	0.84
1:C:103:SER:OG	1:C:104:PRO:HD2	1.77	0.83
1:B:1:MET:HE1	1:B:6:ILE:HG13	1.61	0.82
1:B:45:ARG:HD2	1:B:45:ARG:N	1.95	0.81
1:C:15:ARG:NH1	1:C:15:ARG:HG2	1.94	0.80
1:C:45:ARG:HH11	1:C:45:ARG:CB	1.93	0.78
1:B:73:VAL:O	1:B:78:LEU:HD11	1.83	0.78
1:B:1:MET:CE	1:B:5:ILE:HB	2.10	0.78
1:A:224:GLN:NE2	1:A:224:GLN:H	1.81	0.78
1:A:15:ARG:HH11	1:A:15:ARG:HG2	1.49	0.78
1:C:103:SER:HB2	1:C:121:LEU:CD1	2.15	0.77
1:C:45:ARG:N	1:C:45:ARG:HD2	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:TYR:O	1:A:158:VAL:HG23	1.86	0.76
1:A:1:MET:CE	1:A:6:ILE:HG13	2.16	0.76
1:C:2:THR:N	1:C:3:PRO:HD3	2.01	0.76
1:B:15:ARG:HG2	1:B:15:ARG:HH11	1.50	0.76
1:A:103:SER:OG	1:A:104:PRO:HD2	1.87	0.74
1:A:75:ALA:O	1:A:78:LEU:HB2	1.87	0.74
1:A:45:ARG:HD2	1:A:46:SER:H	1.52	0.74
1:B:91:LEU:O	1:B:91:LEU:HD12	1.88	0.73
1:B:28:ARG:NH1	1:B:117:SER:HB2	2.04	0.73
1:C:50:TRP:CE2	1:C:54:LYS:HE2	2.24	0.73
1:A:147:PHE:O	1:A:150:ILE:HG13	1.90	0.72
1:B:45:ARG:HH11	1:B:45:ARG:H	1.37	0.72
1:B:203:VAL:HB	1:B:204:PRO:HD3	1.69	0.72
1:C:50:TRP:CD2	1:C:54:LYS:HE2	2.25	0.72
1:B:224:GLN:HE21	1:B:224:GLN:H	0.80	0.71
1:B:103:SER:HB2	1:B:121:LEU:HD12	1.73	0.70
1:B:204:PRO:O	1:B:208:GLU:HG2	1.91	0.70
1:A:45:ARG:N	1:A:45:ARG:HD2	2.06	0.70
1:B:222:GLY:H	1:B:224:GLN:HE22	1.39	0.70
1:C:151:LYS:HD3	1:C:153:ALA:HB3	1.75	0.69
1:A:155:MET:HA	1:A:155:MET:HE2	1.74	0.69
1:C:45:ARG:NH1	1:C:45:ARG:HB3	2.01	0.68
1:C:222:GLY:H	1:C:224:GLN:NE2	1.91	0.68
1:A:203:VAL:HB	1:A:204:PRO:HD3	1.74	0.68
1:C:151:LYS:HD2	1:C:154:TYR:H	1.59	0.67
1:B:28:ARG:HH12	1:B:117:SER:HB2	1.58	0.67
1:A:222:GLY:N	1:A:224:GLN:HE22	1.92	0.67
1:B:103:SER:HB2	1:B:121:LEU:CD1	2.24	0.66
1:B:1:MET:HE2	1:B:6:ILE:HD12	1.75	0.66
1:C:151:LYS:HG2	1:C:152:SER:N	2.09	0.66
1:A:45:ARG:HB3	1:A:45:ARG:NH1	2.11	0.66
1:B:1:MET:CE	1:B:6:ILE:HG13	2.25	0.66
1:A:224:GLN:HE21	1:A:224:GLN:N	1.87	0.66
1:C:73:VAL:HG12	1:C:74:ASN:CG	2.16	0.65
1:B:119:ASP:OD2	1:B:130:LEU:N	2.29	0.64
1:A:74:ASN:HA	1:A:76:LYS:NZ	2.13	0.64
1:B:146:GLY:O	1:B:149:ALA:HB3	1.97	0.64
1:C:73:VAL:HG12	1:C:74:ASN:OD1	1.97	0.64
1:A:21:ASP:HB2	1:A:24:TRP:HB2	1.79	0.64
1:A:43:LYS:HB3	1:A:44:PRO:HD2	1.78	0.63
1:B:1:MET:HE2	1:B:6:ILE:CD1	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:GLU:O	1:C:21:ASP:HB2	1.98	0.63
1:A:146:GLY:O	1:A:149:ALA:HB3	1.98	0.63
1:C:55:MET:HA	1:C:55:MET:HE3	1.81	0.63
1:B:13:ASP:OD1	1:B:15:ARG:HD2	1.99	0.62
1:C:71:PRO:HD2	4:C:322:HOH:O	2.00	0.62
1:C:45:ARG:CD	1:C:46:SER:H	2.13	0.61
1:B:21:ASP:CB	1:B:24:TRP:HB2	2.27	0.61
1:A:6:ILE:HD13	1:A:14:VAL:HG11	1.82	0.61
1:A:45:ARG:CD	1:A:46:SER:H	2.13	0.61
1:A:15:ARG:NH1	1:A:15:ARG:HG2	2.12	0.61
1:C:9:ARG:NH2	1:C:110:GLU:O	2.28	0.61
1:C:45:ARG:HD2	1:C:46:SER:H	1.65	0.61
1:B:3:PRO:HD3	4:B:318:HOH:O	2.02	0.60
1:C:9:ARG:HD2	4:C:263:HOH:O	2.02	0.59
1:A:45:ARG:H	1:A:45:ARG:HH11	0.70	0.59
1:B:15:ARG:CG	1:B:15:ARG:HH11	2.15	0.59
1:C:151:LYS:CD	1:C:153:ALA:HB3	2.33	0.58
1:A:222:GLY:H	1:A:224:GLN:NE2	1.94	0.58
1:A:143:ARG:O	1:A:143:ARG:HD2	2.03	0.58
1:A:19:GLN:HG2	4:A:342:HOH:O	2.03	0.58
1:B:74:ASN:O	1:B:78:LEU:HG	2.03	0.57
1:C:103:SER:HB2	1:C:121:LEU:HD12	1.85	0.57
1:C:50:TRP:CG	1:C:54:LYS:HE2	2.38	0.57
1:A:201:GLU:O	1:A:205:GLU:HG3	2.04	0.57
1:C:103:SER:HB2	1:C:121:LEU:HD11	1.86	0.57
1:A:181:ARG:HA	4:A:312:HOH:O	2.04	0.57
1:B:119:ASP:HB2	1:B:128:LEU:O	2.04	0.56
1:C:146:GLY:O	1:C:149:ALA:HB3	2.06	0.56
1:B:21:ASP:HB3	1:B:24:TRP:H	1.70	0.56
1:A:220:VAL:O	1:A:223:GLU:HG3	2.06	0.56
1:A:4:ASP:HB2	4:A:274:HOH:O	2.05	0.56
1:C:151:LYS:HG2	1:C:153:ALA:N	2.14	0.55
1:B:71:PRO:HD2	4:B:230:HOH:O	2.05	0.55
1:B:165:THR:O	1:B:166:ARG:HB2	2.06	0.55
1:B:104:PRO:HB2	1:B:105:ILE:HG22	1.88	0.55
1:B:44:PRO:HG3	1:B:49:LYS:O	2.07	0.55
1:B:55:MET:HE3	1:B:55:MET:CA	2.36	0.55
1:C:18:GLU:O	1:C:21:ASP:N	2.35	0.55
1:B:21:ASP:O	1:B:24:TRP:HB3	2.06	0.55
1:C:131:LYS:HE3	1:C:154:TYR:CZ	2.42	0.55
1:B:45:ARG:HD2	1:B:46:SER:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:LYS:HB3	3:C:228:ACT:H3	1.89	0.55
1:C:104:PRO:O	1:C:105:ILE:HB	2.05	0.55
1:A:74:ASN:HA	1:A:76:LYS:HZ1	1.71	0.54
1:C:151:LYS:CG	1:C:153:ALA:H	2.15	0.54
1:A:45:ARG:CB	1:A:45:ARG:HH11	2.20	0.54
1:C:50:TRP:CD1	1:C:54:LYS:HE2	2.42	0.54
1:C:151:LYS:HE3	1:C:154:TYR:CE2	2.42	0.54
1:C:143:ARG:HH21	1:C:182:GLU:HG3	1.73	0.54
1:B:122:CYS:O	1:B:125:GLY:N	2.34	0.53
1:B:21:ASP:HB2	1:B:24:TRP:CB	2.32	0.53
1:B:101:THR:O	1:B:121:LEU:N	2.29	0.53
1:B:55:MET:HE3	1:B:55:MET:HA	1.89	0.53
1:C:85:GLU:HG3	1:C:86:ASN:N	2.23	0.53
1:C:71:PRO:HD2	4:C:258:HOH:O	2.09	0.53
1:B:151:LYS:HG2	1:B:154:TYR:CD2	2.44	0.53
1:B:18:GLU:O	1:B:21:ASP:HB2	2.09	0.53
1:C:104:PRO:HG2	1:C:105:ILE:H	1.75	0.52
1:C:24:TRP:O	1:C:28:ARG:HG3	2.09	0.52
1:B:73:VAL:HG12	1:B:74:ASN:ND2	2.24	0.52
1:B:50:TRP:CG	1:B:54:LYS:HD3	2.44	0.52
1:C:143:ARG:HG3	1:C:143:ARG:O	2.07	0.52
1:A:45:ARG:CA	1:A:45:ARG:HH11	2.21	0.51
1:B:127:GLY:HA3	1:B:170:TRP:CZ3	2.45	0.51
1:B:45:ARG:CD	1:B:46:SER:N	2.73	0.51
1:B:71:PRO:HG2	4:B:347:HOH:O	2.10	0.51
1:B:75:ALA:HA	1:B:78:LEU:CD1	2.25	0.51
1:A:151:LYS:O	1:A:154:TYR:N	2.44	0.51
1:B:103:SER:OG	1:B:104:PRO:HD2	2.11	0.51
1:B:34:ALA:HA	1:B:160:TYR:CD2	2.46	0.50
1:B:73:VAL:O	1:B:74:ASN:C	2.48	0.50
1:B:140:MET:HE1	1:B:144:LEU:HG	1.93	0.50
1:A:45:ARG:HB3	1:A:45:ARG:HH11	1.77	0.50
1:A:45:ARG:HD3	1:A:46:SER:OG	2.12	0.50
1:B:45:ARG:CD	1:B:46:SER:H	2.24	0.50
1:C:20:GLY:O	1:C:21:ASP:C	2.50	0.50
1:C:39:ASN:O	1:C:54:LYS:HB2	2.12	0.50
1:A:21:ASP:HB2	1:A:24:TRP:CB	2.41	0.50
1:C:89:ARG:HG3	1:C:89:ARG:HH11	1.76	0.50
1:C:17:VAL:HG12	1:C:18:GLU:N	2.27	0.50
1:A:45:ARG:CD	1:A:46:SER:N	2.76	0.49
1:C:151:LYS:O	1:C:154:TYR:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:ASP:O	1:C:24:TRP:HB3	2.12	0.49
1:C:95:THR:HG22	1:C:95:THR:O	2.11	0.49
1:B:167:LYS:O	1:B:191:ARG:HD2	2.12	0.49
1:B:18:GLU:O	1:B:19:GLN:C	2.51	0.49
1:C:151:LYS:O	1:C:154:TYR:HB2	2.13	0.49
1:A:103:SER:O	1:A:104:PRO:C	2.50	0.48
1:B:129:GLU:OE1	1:B:129:GLU:HA	2.13	0.48
1:A:209:LYS:HA	1:A:209:LYS:HD2	1.32	0.48
1:B:14:VAL:HG13	1:B:15:ARG:N	2.27	0.48
1:B:103:SER:HA	1:B:104:PRO:HD3	1.54	0.48
1:A:21:ASP:HB3	1:A:24:TRP:H	1.77	0.48
1:A:181:ARG:O	1:A:182:GLU:HB2	2.13	0.48
1:B:151:LYS:HE3	4:B:338:HOH:O	2.14	0.47
1:B:140:MET:CE	1:B:144:LEU:HG	2.44	0.47
1:A:18:GLU:HG3	4:A:392:HOH:O	2.14	0.47
1:A:155:MET:HE2	1:A:155:MET:CA	2.38	0.47
1:B:96:SER:HA	1:B:186:TYR:OH	2.13	0.47
1:B:103:SER:O	1:B:104:PRO:C	2.52	0.47
1:B:140:MET:HE1	1:B:144:LEU:CD1	2.44	0.47
1:B:128:LEU:HD12	1:B:171:TYR:HB2	1.97	0.47
1:C:93:GLU:O	1:C:94:PHE:C	2.53	0.47
1:A:45:ARG:CG	1:A:46:SER:N	2.78	0.47
1:C:151:LYS:HD2	1:C:154:TYR:N	2.29	0.47
1:C:101:THR:HG23	1:C:121:LEU:O	2.15	0.47
1:A:203:VAL:N	1:A:204:PRO:CD	2.77	0.47
1:C:55:MET:CA	1:C:55:MET:CE	2.93	0.47
1:B:73:VAL:CG1	1:B:74:ASN:N	2.78	0.46
1:C:13:ASP:OD1	1:C:15:ARG:HG3	2.15	0.46
1:B:140:MET:HE1	1:B:144:LEU:CG	2.46	0.46
1:B:111:SER:OG	1:B:113:ARG:HG2	2.16	0.46
1:C:193:GLU:HB3	4:C:259:HOH:O	2.15	0.46
1:A:50:TRP:CE2	1:A:54:LYS:HE2	2.51	0.46
1:A:226:ARG:HD2	1:A:226:ARG:HA	1.50	0.46
1:B:19:GLN:HA	1:B:24:TRP:CD1	2.50	0.46
1:C:103:SER:HA	1:C:104:PRO:HD3	1.84	0.46
1:B:15:ARG:CG	1:B:15:ARG:NH1	2.77	0.46
1:A:78:LEU:HD23	1:A:78:LEU:HA	1.64	0.46
1:C:9:ARG:HG3	1:C:9:ARG:O	2.15	0.46
1:A:119:ASP:HB3	1:A:130:LEU:HD22	1.97	0.46
1:C:122:CYS:HB2	1:C:126:ASN:O	2.16	0.46
1:B:202:ILE:HA	1:B:205:GLU:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:PRO:CG	1:C:105:ILE:H	2.28	0.46
1:C:55:MET:HB3	1:C:55:MET:HE2	1.62	0.46
1:C:201:GLU:O	1:C:205:GLU:HG3	2.16	0.46
1:C:140:MET:CE	1:C:144:LEU:HD11	2.45	0.46
1:C:17:VAL:CG1	1:C:18:GLU:N	2.79	0.45
1:B:151:LYS:O	1:B:152:SER:C	2.53	0.45
1:A:128:LEU:HD11	1:A:130:LEU:HD13	1.97	0.45
1:B:73:VAL:HG12	1:B:74:ASN:HD22	1.81	0.45
1:B:91:LEU:C	1:B:91:LEU:HD12	2.36	0.45
1:C:151:LYS:HE3	1:C:154:TYR:CG	2.50	0.45
1:A:203:VAL:CB	1:A:204:PRO:HD3	2.45	0.45
1:A:28:ARG:NH1	1:A:117:SER:HB2	2.32	0.45
1:C:111:SER:O	1:C:112:MET:HB2	2.16	0.45
1:C:15:ARG:H	1:C:15:ARG:HG3	1.55	0.45
1:A:73:VAL:O	1:A:74:ASN:C	2.53	0.45
1:B:127:GLY:HA3	1:B:170:TRP:CE3	2.52	0.45
1:B:82:LYS:HD2	1:B:85:GLU:OE1	2.16	0.45
1:C:45:ARG:CG	1:C:46:SER:N	2.79	0.45
1:B:140:MET:HE1	1:B:144:LEU:HD11	1.97	0.45
1:B:18:GLU:HB2	1:B:21:ASP:OD1	2.16	0.44
1:B:116:CYS:HA	2:B:227:PO4:O3	2.18	0.44
1:C:37:VAL:HG11	1:C:160:TYR:HB2	1.99	0.44
1:A:104:PRO:HB2	1:A:105:ILE:HG22	1.99	0.44
1:C:113:ARG:HD2	1:C:221:PHE:CE2	2.52	0.44
1:B:208:GLU:H	1:B:208:GLU:HG2	1.68	0.44
1:A:165:THR:O	1:A:166:ARG:HB2	2.18	0.44
1:B:130:LEU:HD13	1:B:173:ALA:HB3	2.00	0.43
1:C:45:ARG:CD	1:C:46:SER:N	2.80	0.43
1:C:103:SER:CB	1:C:121:LEU:HD11	2.46	0.43
1:C:21:ASP:HB2	1:C:24:TRP:HB2	2.00	0.43
1:C:55:MET:CE	1:C:55:MET:HA	2.46	0.43
1:B:222:GLY:H	1:B:224:GLN:NE2	2.10	0.43
1:A:1:MET:HG3	1:A:2:THR:N	2.32	0.43
1:B:14:VAL:CG1	1:B:15:ARG:N	2.82	0.43
1:B:82:LYS:HD2	1:B:82:LYS:HA	1.93	0.43
1:B:169:ALA:HB2	1:B:190:GLU:OE1	2.19	0.43
1:B:73:VAL:HG12	1:B:74:ASN:N	2.33	0.43
1:B:18:GLU:N	1:B:21:ASP:OD1	2.45	0.43
1:A:226:ARG:HH11	1:A:226:ARG:HD3	1.65	0.43
1:B:101:THR:N	1:B:121:LEU:O	2.42	0.43
1:C:203:VAL:HB	1:C:204:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ALA:CB	1:B:186:TYR:HB3	2.49	0.42
1:C:167:LYS:O	1:C:191:ARG:HD2	2.19	0.42
1:B:205:GLU:HA	1:B:208:GLU:HG3	2.00	0.42
1:A:2:THR:HB	1:A:3:PRO:HD2	2.02	0.42
1:A:104:PRO:HB2	1:A:105:ILE:H	1.42	0.42
1:C:50:TRP:CE2	1:C:54:LYS:CE	2.98	0.42
1:A:43:LYS:HB3	1:A:44:PRO:CD	2.48	0.42
1:C:50:TRP:NE1	1:C:54:LYS:HE2	2.34	0.42
1:B:173:ALA:HB2	1:B:186:TYR:HB3	2.00	0.42
1:B:55:MET:HE2	1:B:59:HIS:CE1	2.55	0.42
1:B:122:CYS:HB3	1:B:124:ASP:OD1	2.20	0.42
1:A:150:ILE:HG21	1:A:172:PHE:CE1	2.54	0.41
1:C:140:MET:CE	1:C:144:LEU:CD1	2.98	0.41
1:B:1:MET:CE	1:B:6:ILE:CG1	2.97	0.41
1:B:53:MET:HE3	4:B:319:HOH:O	2.19	0.41
1:A:45:ARG:CD	1:A:45:ARG:N	2.79	0.41
1:B:140:MET:HB3	1:B:140:MET:HE2	1.58	0.41
1:C:113:ARG:C	1:C:114:THR:HG23	2.41	0.41
1:C:214:LEU:HA	1:C:214:LEU:HD23	1.92	0.41
1:A:45:ARG:NH1	1:A:45:ARG:N	2.29	0.41
1:A:95:THR:HG21	4:A:370:HOH:O	2.19	0.41
1:A:-1:SER:HB3	1:A:110:GLU:HG2	2.03	0.41
1:A:6:ILE:HG21	1:A:14:VAL:HG13	2.03	0.41
1:C:159:GLN:HG3	1:C:195:TYR:CD2	2.56	0.41
1:C:151:LYS:HB3	1:C:151:LYS:HE2	1.40	0.41
1:B:44:PRO:HG2	1:B:47:GLY:O	2.21	0.41
1:B:179:MET:HB3	1:B:181:ARG:O	2.21	0.41
1:A:45:ARG:HD2	1:A:46:SER:N	2.28	0.40
1:C:145:GLY:HA3	1:C:149:ALA:HB2	2.02	0.40
1:A:105:ILE:HG13	1:A:106:ILE:N	2.36	0.40
1:C:137:ARG:HH11	1:C:137:ARG:HD3	1.75	0.40
1:B:203:VAL:CB	1:B:204:PRO:HD3	2.43	0.40
1:A:203:VAL:N	1:A:204:PRO:HD2	2.36	0.40
1:C:73:VAL:HG12	1:C:74:ASN:ND2	2.36	0.40
1:B:82:LYS:HE3	1:B:85:GLU:OE1	2.22	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	226/228 (99%)	220 (97%)	3 (1%)	3 (1%)	15	21
1	B	226/228 (99%)	218 (96%)	5 (2%)	3 (1%)	15	21
1	C	223/228 (98%)	210 (94%)	9 (4%)	4 (2%)	11	13
All	All	675/684 (99%)	648 (96%)	17 (2%)	10 (2%)	13	17

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	ASP
1	A	104	PRO
1	B	104	PRO
1	B	45	ARG
1	C	105	ILE
1	A	152	SER
1	B	123	SER
1	C	21	ASP
1	C	104	PRO
1	C	150	ILE

### 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	194/194 (100%)	168 (87%)	26 (13%)	5	6
1	B	194/194 (100%)	172 (89%)	22 (11%)	7	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	191/194 (98%)	161 (84%)	30 (16%)	3	3
All	All	579/582 (100%)	501 (86%)	78 (14%)	5	5

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	15	ARG
1	A	18	GLU
1	A	21	ASP
1	A	45	ARG
1	A	49	LYS
1	A	53	MET
1	A	61	LEU
1	A	73	VAL
1	A	74	ASN
1	A	76	LYS
1	A	82	LYS
1	A	102	GLU
1	A	117	SER
1	A	130	LEU
1	A	131	LYS
1	A	147	PHE
1	A	148	GLU
1	A	151	LYS
1	A	174	ASN
1	A	194	LYS
1	A	198	SER
1	A	201	GLU
1	A	208	GLU
1	A	224	GLN
1	A	226	ARG
1	B	-1	SER
1	B	4	ASP
1	B	15	ARG
1	B	19	GLN
1	B	21	ASP
1	B	43	LYS
1	B	45	ARG
1	B	78	LEU
1	B	87	ASP
1	B	101	THR

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Mol	Chain	Res	Type
1	B	117	SER
1	B	121	LEU
1	B	131	LYS
1	B	151	LYS
1	B	152	SER
1	B	166	ARG
1	B	167	LYS
1	B	174	ASN
1	B	190	GLU
1	B	198	SER
1	B	208	GLU
1	B	224	GLN
1	C	2	THR
1	C	5	ILE
1	C	9	ARG
1	C	14	VAL
1	C	15	ARG
1	C	19	GLN
1	C	21	ASP
1	C	43	LYS
1	C	45	ARG
1	C	46	SER
1	C	48	LYS
1	C	53	MET
1	C	55	MET
1	C	61	LEU
1	C	72	GLU
1	C	74	ASN
1	C	76	LYS
1	C	82	LYS
1	C	89	ARG
1	C	101	THR
1	C	105	ILE
1	C	151	LYS
1	C	157	GLN
1	C	180	LYS
1	C	182	GLU
1	C	201	GLU
1	C	205	GLU
1	C	217	ILE
1	C	224	GLN
1	C	226	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	74	ASN
1	A	174	ASN
1	A	224	GLN
1	B	19	GLN
1	B	74	ASN
1	B	185	HIS
1	B	224	GLN
1	C	224	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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	$\# Z  > 2$
2	PO4	A	227	-	4,4,4	1.50	0	6,6,6	0.29	0
3	ACT	A	228	-	1,3,3	1.41	0	0,3,3	0.00	-
2	PO4	B	227	-	4,4,4	1.56	1 (25%)	6,6,6	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ACT	B	228	-	1,3,3	2.14	1 (100%)	0,3,3	0.00	-
2	PO4	C	227	-	4,4,4	1.20	0	6,6,6	0.31	0
3	ACT	C	228	-	1,3,3	2.83	1 (100%)	0,3,3	0.00	-
3	ACT	C	229	-	1,3,3	1.19	0	0,3,3	0.00	-

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
2	PO4	A	227	-	-	0/0/0/0	0/0/0/0
3	ACT	A	228	-	-	0/0/0/0	0/0/0/0
2	PO4	B	227	-	-	0/0/0/0	0/0/0/0
3	ACT	B	228	-	-	0/0/0/0	0/0/0/0
2	PO4	C	227	-	-	0/0/0/0	0/0/0/0
3	ACT	C	228	-	-	0/0/0/0	0/0/0/0
3	ACT	C	229	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	227	PO4	P-O4	-2.05	1.46	1.53
3	B	228	ACT	CH3-C	2.14	1.51	1.48
3	C	228	ACT	CH3-C	2.83	1.52	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	227	PO4	1	0
3	C	228	ACT	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	228/228 (100%)	-0.21	7 (3%)	52	52	19, 30, 71, 100	0
1	B	228/228 (100%)	-0.02	9 (3%)	43	44	23, 38, 73, 100	0
1	C	225/228 (98%)	-0.01	14 (6%)	24	25	16, 35, 77, 98	0
All	All	681/684 (99%)	-0.08	30 (4%)	38	39	16, 34, 75, 100	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	46	SER	5.3
1	C	46	SER	5.2
1	C	4	ASP	4.1
1	A	45	ARG	4.1
1	B	45	ARG	3.9
1	C	15	ARG	3.9
1	C	2	THR	3.6
1	A	46	SER	3.5
1	B	47	GLY	3.4
1	A	75	ALA	3.4
1	C	74	ASN	3.3
1	C	47	GLY	3.2
1	B	48	LYS	3.1
1	C	45	ARG	3.0
1	C	48	LYS	2.8
1	B	104	PRO	2.8
1	B	15	ARG	2.8
1	A	48	LYS	2.8
1	C	18	GLU	2.7
1	B	16	ALA	2.6
1	C	8	GLN	2.5
1	B	18	GLU	2.5
1	A	44	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	73	VAL	2.3
1	A	74	ASN	2.3
1	B	44	PRO	2.2
1	C	44	PRO	2.2
1	C	16	ALA	2.2
1	C	149	ALA	2.2
1	C	151	LYS	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(Å <sup>2</sup> )	Q<0.9
2	PO4	B	227	5/5	1.00	0.16	0.38	25,30,46,62	0
2	PO4	C	227	5/5	0.99	0.15	0.21	27,35,47,55	0
2	PO4	A	227	5/5	1.00	0.15	-0.21	27,42,44,47	0
3	ACT	C	229	4/4	0.95	0.14	-0.33	42,42,42,42	0
3	ACT	B	228	4/4	0.77	0.23	-	70,70,70,70	4
3	ACT	A	228	4/4	0.92	0.20	-	40,40,40,40	4
3	ACT	C	228	4/4	0.74	0.22	-	73,73,73,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.