



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:50 PM GMT

PDB ID : 2OTC  
Title : ORNITHINE TRANSCARBAMOYLASE COMPLEXED WITH N-(PHOSPHONACETYL)-L-ORNITHINE  
Authors : Ha, Y.; Allewell, N.M.  
Deposited on : 1997-06-15  
Resolution : 2.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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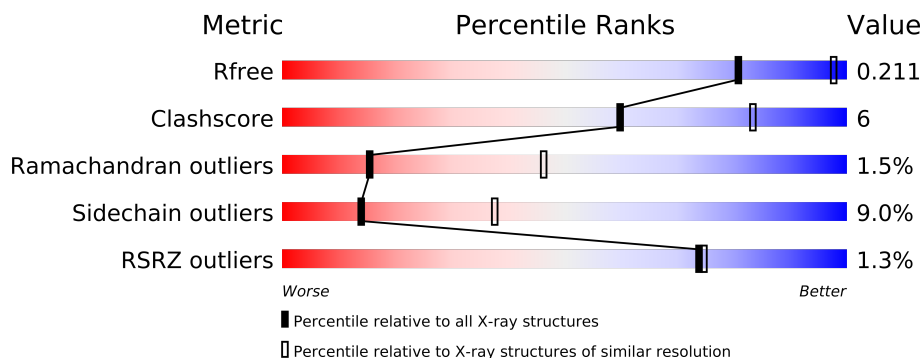
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	333	
1	B	333	
1	C	333	
1	D	333	
1	E	333	
1	F	333	
1	G	333	
1	H	333	
1	I	333	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23697 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ORNITHINE CARBAMOYLTRANSFERASE.

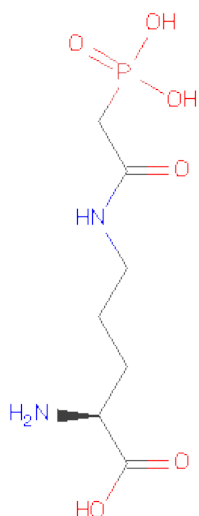
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2579	1627	441	495	16			
1	B	333	Total	C	N	O	S	0	0	0
			2579	1627	441	495	16			
1	C	333	Total	C	N	O	S	0	0	0
			2579	1627	441	495	16			
1	D	333	Total	C	N	O	S	0	0	0
			2579	1627	441	495	16			
1	E	333	Total	C	N	O	S	0	0	0
			2579	1627	441	495	16			
1	F	333	Total	C	N	O	S	0	0	0
			2579	1627	441	495	16			
1	G	333	Total	C	N	O	S	0	0	0
			2579	1627	441	495	16			
1	H	333	Total	C	N	O	S	0	0	0
			2579	1627	441	495	16			
1	I	333	Total	C	N	O	S	0	0	0
			2579	1627	441	495	16			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	121	ARG	SER	CONFLICT	UNP P04391
B	121	ARG	SER	CONFLICT	UNP P04391
C	121	ARG	SER	CONFLICT	UNP P04391
D	121	ARG	SER	CONFLICT	UNP P04391
E	121	ARG	SER	CONFLICT	UNP P04391
F	121	ARG	SER	CONFLICT	UNP P04391
G	121	ARG	SER	CONFLICT	UNP P04391
H	121	ARG	SER	CONFLICT	UNP P04391
I	121	ARG	SER	CONFLICT	UNP P04391

- Molecule 2 is N-(PHOSPHONOACETYL)-L-ORNITHINE (three-letter code: PAO)

(formula: C<sub>7</sub>H<sub>15</sub>N<sub>2</sub>O<sub>6</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	7	2	6	1		
2	B	1	Total	C	N	O	P	0	0
			16	7	2	6	1		
2	C	1	Total	C	N	O	P	0	0
			16	7	2	6	1		
2	D	1	Total	C	N	O	P	0	0
			16	7	2	6	1		
2	E	1	Total	C	N	O	P	0	0
			16	7	2	6	1		
2	F	1	Total	C	N	O	P	0	0
			16	7	2	6	1		
2	G	1	Total	C	N	O	P	0	0
			16	7	2	6	1		
2	H	1	Total	C	N	O	P	0	0
			16	7	2	6	1		
2	I	1	Total	C	N	O	P	0	0
			16	7	2	6	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	37	Total	O	0	0
			37	37		
3	B	38	Total	O	0	0
			38	38		

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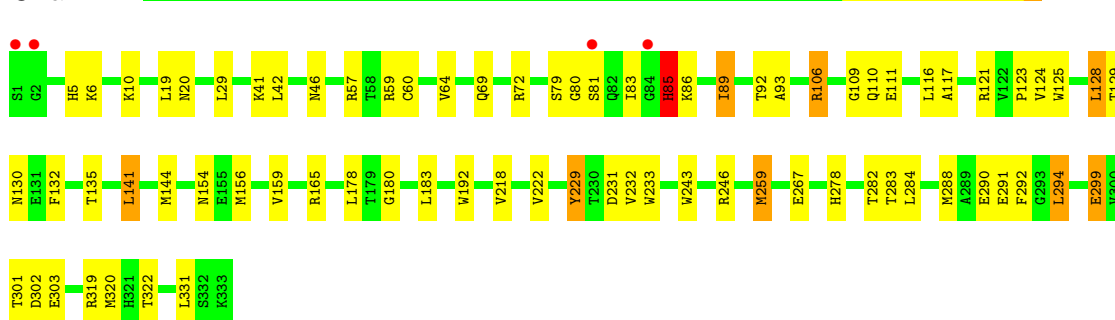
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	39	Total 39	O 39	0	0
3	D	38	Total 38	O 38	0	0
3	E	38	Total 38	O 38	0	0
3	F	38	Total 38	O 38	0	0
3	G	38	Total 38	O 38	0	0
3	H	38	Total 38	O 38	0	0
3	I	38	Total 38	O 38	0	0

### 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.

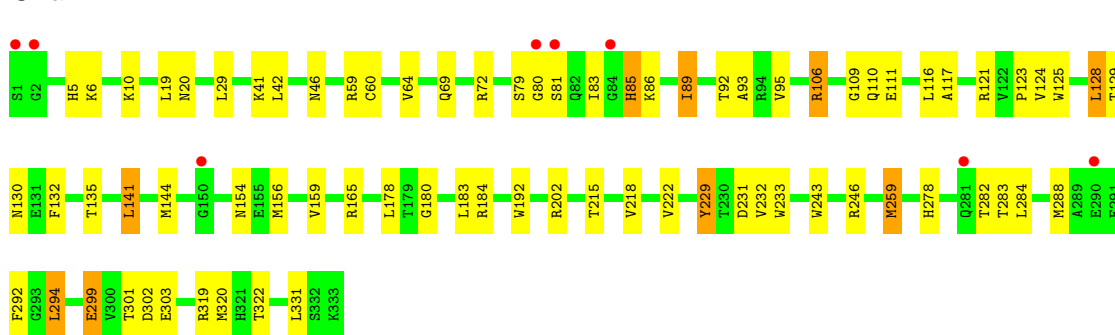
#### • Molecule 1: ORNITHINE CARBAMOYLTRANSFERASE

Chain A:



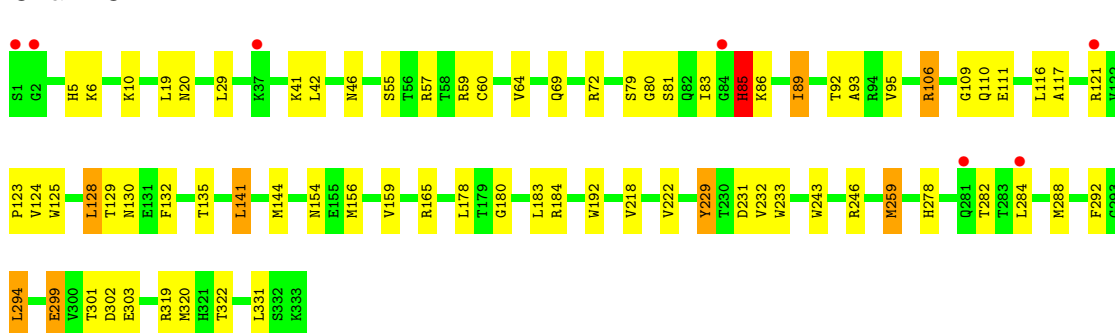
#### • Molecule 1: ORNITHINE CARBAMOYLTRANSFERASE

Chain B:



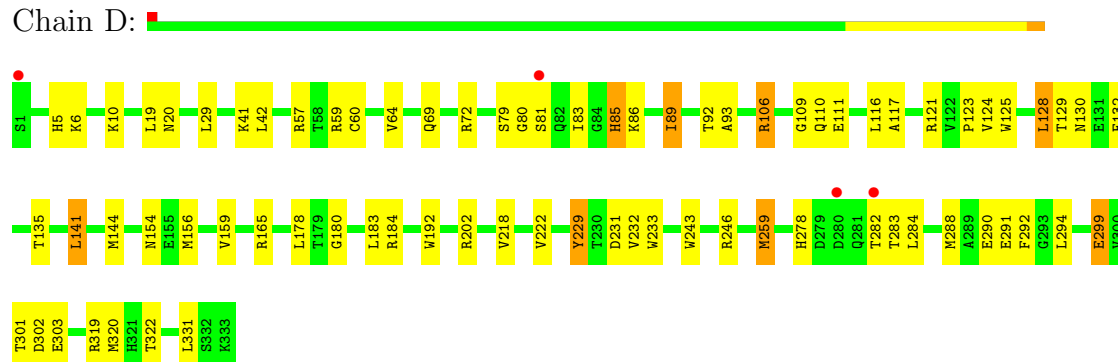
#### • Molecule 1: ORNITHINE CARBAMOYLTRANSFERASE

Chain C:



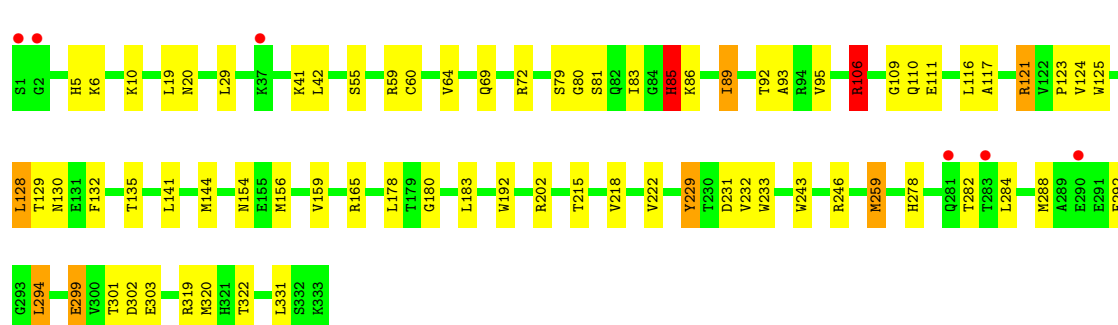
#### • Molecule 1: ORNITHINE CARBAMOYLTRANSFERASE

Chain D:



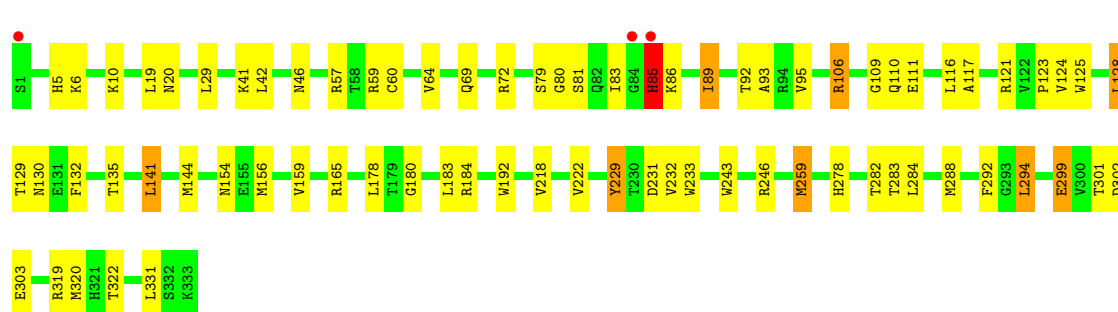
- Molecule 1: ORNITHINE CARBAMOYLTRANSFERASE

Chain E:



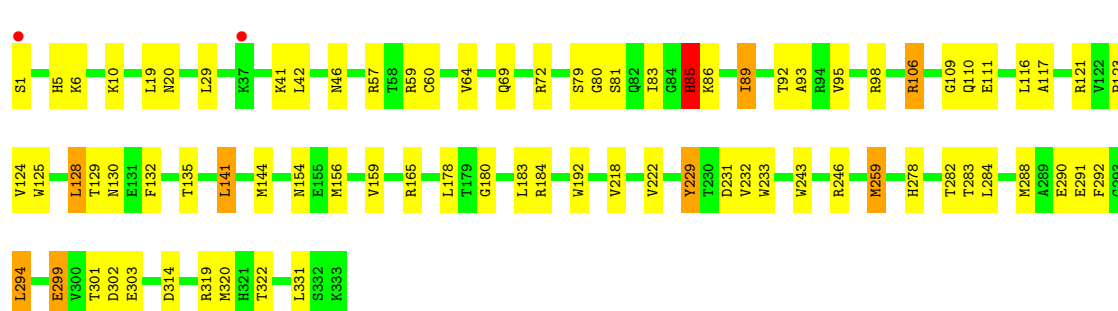
- Molecule 1: ORNITHINE CARBAMOYLTRANSFERASE

Chain F:

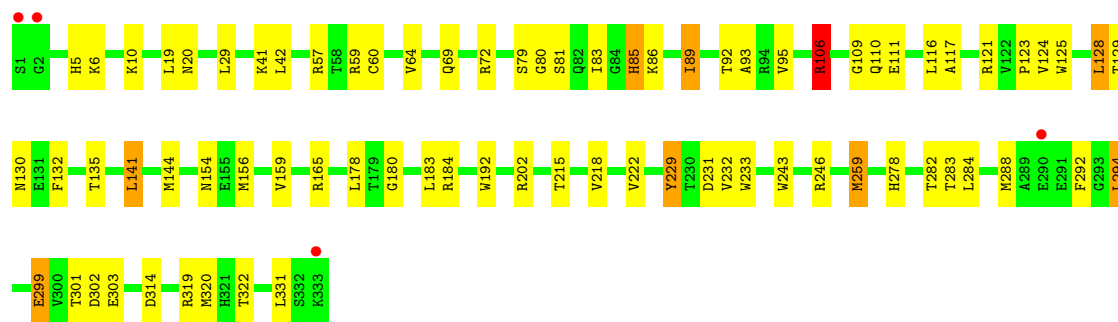


- Molecule 1: ORNITHINE CARBAMOYLTRANSFERASE

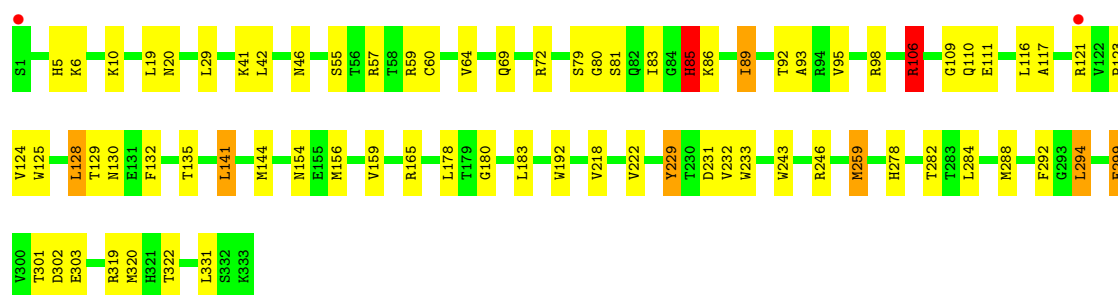
Chain G:



- Molecule 1: ORNITHINE CARBAMOYLTRANSFERASE

Chain H: 

- Molecule 1: ORNITHINE CARBAMOYLTRANSFERASE

Chain I: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.03Å 114.69Å 93.78Å 86.99° 93.11° 118.81°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	58.0 (15.00-2.80) 57.9 (15.00-2.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 2.81Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.213 , 0.230 0.194 , 0.211	Depositor DCC
$R_{free}$ test set	5466 reflections (11.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.7	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.21 , -10.0	EDS
Estimated twinning fraction	0.077 for -h,h+k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 53683 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	23697	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PAO

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	0.72	0/2627	1.25	16/3549 (0.5%)
1	B	0.72	0/2627	1.25	16/3549 (0.5%)
1	C	0.72	0/2627	1.25	16/3549 (0.5%)
1	D	0.72	0/2627	1.25	16/3549 (0.5%)
1	E	0.72	0/2627	1.25	17/3549 (0.5%)
1	F	0.71	0/2627	1.25	16/3549 (0.5%)
1	G	0.72	0/2627	1.25	16/3549 (0.5%)
1	H	0.72	0/2627	1.25	17/3549 (0.5%)
1	I	0.72	0/2627	1.24	17/3549 (0.5%)
All	All	0.72	0/23643	1.25	147/31941 (0.5%)

There are no bond length outliers.

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	125	TRP	CD1-CG-CD2	8.73	113.28	106.30
1	G	125	TRP	CD1-CG-CD2	8.71	113.27	106.30
1	I	125	TRP	CD1-CG-CD2	8.71	113.27	106.30
1	A	125	TRP	CD1-CG-CD2	8.71	113.26	106.30
1	C	125	TRP	CD1-CG-CD2	8.70	113.26	106.30
1	D	125	TRP	CD1-CG-CD2	8.70	113.26	106.30
1	F	125	TRP	CD1-CG-CD2	8.70	113.26	106.30
1	B	125	TRP	CD1-CG-CD2	8.69	113.25	106.30
1	H	125	TRP	CD1-CG-CD2	8.68	113.25	106.30
1	G	243	TRP	CD1-CG-CD2	8.00	112.70	106.30
1	D	243	TRP	CD1-CG-CD2	7.98	112.69	106.30
1	H	243	TRP	CD1-CG-CD2	7.96	112.67	106.30
1	C	243	TRP	CD1-CG-CD2	7.96	112.66	106.30
1	A	243	TRP	CD1-CG-CD2	7.95	112.66	106.30
1	E	243	TRP	CD1-CG-CD2	7.95	112.66	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	125	TRP	CE2-CD2-CG	-7.94	100.95	107.30
1	I	125	TRP	CE2-CD2-CG	-7.93	100.96	107.30
1	D	125	TRP	CE2-CD2-CG	-7.92	100.96	107.30
1	I	243	TRP	CD1-CG-CD2	7.92	112.63	106.30
1	F	243	TRP	CD1-CG-CD2	7.91	112.63	106.30
1	B	125	TRP	CE2-CD2-CG	-7.91	100.97	107.30
1	F	125	TRP	CE2-CD2-CG	-7.91	100.97	107.30
1	A	125	TRP	CE2-CD2-CG	-7.90	100.98	107.30
1	E	125	TRP	CE2-CD2-CG	-7.89	100.98	107.30
1	G	125	TRP	CE2-CD2-CG	-7.86	101.01	107.30
1	B	243	TRP	CD1-CG-CD2	7.86	112.59	106.30
1	H	125	TRP	CE2-CD2-CG	-7.83	101.03	107.30
1	E	243	TRP	CE2-CD2-CG	-7.70	101.14	107.30
1	D	243	TRP	CE2-CD2-CG	-7.70	101.14	107.30
1	A	243	TRP	CE2-CD2-CG	-7.69	101.15	107.30
1	C	243	TRP	CE2-CD2-CG	-7.69	101.15	107.30
1	G	243	TRP	CE2-CD2-CG	-7.69	101.15	107.30
1	I	243	TRP	CE2-CD2-CG	-7.69	101.15	107.30
1	C	192	TRP	CE2-CD2-CG	-7.69	101.15	107.30
1	F	243	TRP	CE2-CD2-CG	-7.68	101.16	107.30
1	G	233	TRP	CE2-CD2-CG	-7.68	101.16	107.30
1	H	243	TRP	CE2-CD2-CG	-7.67	101.16	107.30
1	B	243	TRP	CE2-CD2-CG	-7.66	101.18	107.30
1	D	233	TRP	CE2-CD2-CG	-7.65	101.18	107.30
1	F	233	TRP	CE2-CD2-CG	-7.65	101.18	107.30
1	H	192	TRP	CE2-CD2-CG	-7.65	101.18	107.30
1	E	192	TRP	CE2-CD2-CG	-7.65	101.18	107.30
1	A	233	TRP	CE2-CD2-CG	-7.64	101.19	107.30
1	I	233	TRP	CE2-CD2-CG	-7.64	101.19	107.30
1	E	233	TRP	CE2-CD2-CG	-7.63	101.20	107.30
1	A	192	TRP	CE2-CD2-CG	-7.62	101.20	107.30
1	C	233	TRP	CE2-CD2-CG	-7.61	101.21	107.30
1	B	192	TRP	CE2-CD2-CG	-7.61	101.21	107.30
1	B	233	TRP	CE2-CD2-CG	-7.61	101.21	107.30
1	F	192	TRP	CE2-CD2-CG	-7.61	101.21	107.30
1	C	233	TRP	CD1-CG-CD2	7.61	112.39	106.30
1	I	192	TRP	CE2-CD2-CG	-7.61	101.22	107.30
1	D	192	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	B	233	TRP	CD1-CG-CD2	7.59	112.37	106.30
1	G	233	TRP	CD1-CG-CD2	7.58	112.36	106.30
1	D	233	TRP	CD1-CG-CD2	7.57	112.36	106.30
1	G	192	TRP	CE2-CD2-CG	-7.57	101.25	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	233	TRP	CE2-CD2-CG	-7.57	101.25	107.30
1	A	233	TRP	CD1-CG-CD2	7.56	112.35	106.30
1	I	233	TRP	CD1-CG-CD2	7.56	112.34	106.30
1	F	233	TRP	CD1-CG-CD2	7.55	112.34	106.30
1	E	192	TRP	CD1-CG-CD2	7.54	112.33	106.30
1	E	233	TRP	CD1-CG-CD2	7.54	112.33	106.30
1	H	233	TRP	CD1-CG-CD2	7.53	112.33	106.30
1	H	192	TRP	CD1-CG-CD2	7.49	112.29	106.30
1	G	192	TRP	CD1-CG-CD2	7.49	112.29	106.30
1	C	192	TRP	CD1-CG-CD2	7.48	112.28	106.30
1	A	192	TRP	CD1-CG-CD2	7.47	112.28	106.30
1	I	192	TRP	CD1-CG-CD2	7.47	112.28	106.30
1	F	192	TRP	CD1-CG-CD2	7.46	112.27	106.30
1	D	192	TRP	CD1-CG-CD2	7.46	112.27	106.30
1	B	192	TRP	CD1-CG-CD2	7.45	112.26	106.30
1	E	319	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	C	319	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	319	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	H	319	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	D	319	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	B	319	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	G	319	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	I	319	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	F	319	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	H	85	HIS	CA-C-N	-6.14	103.70	117.20
1	F	85	HIS	CA-C-N	-6.13	103.71	117.20
1	B	85	HIS	CA-C-N	-6.13	103.72	117.20
1	D	85	HIS	CA-C-N	-6.13	103.72	117.20
1	C	85	HIS	CA-C-N	-6.12	103.72	117.20
1	I	85	HIS	CA-C-N	-6.12	103.74	117.20
1	A	85	HIS	CA-C-N	-6.12	103.74	117.20
1	G	85	HIS	CA-C-N	-6.12	103.74	117.20
1	E	85	HIS	CA-C-N	-6.11	103.76	117.20
1	D	319	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	E	319	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	H	319	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	319	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	319	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	G	319	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	I	319	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	C	319	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	B	246	ARG	NE-CZ-NH1	5.39	123.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	319	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	F	246	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	G	125	TRP	CG-CD2-CE3	5.37	138.73	133.90
1	E	125	TRP	CG-CD2-CE3	5.36	138.73	133.90
1	D	125	TRP	CG-CD2-CE3	5.36	138.72	133.90
1	E	246	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	246	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	125	TRP	CG-CD2-CE3	5.34	138.71	133.90
1	I	125	TRP	CG-CD2-CE3	5.33	138.70	133.90
1	H	246	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	C	125	TRP	CG-CD2-CE3	5.32	138.69	133.90
1	F	125	TRP	CG-CD2-CE3	5.32	138.69	133.90
1	I	246	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	125	TRP	CG-CD2-CE3	5.31	138.68	133.90
1	D	246	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	H	125	TRP	CG-CD2-CE3	5.30	138.67	133.90
1	C	246	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	I	229	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	A	229	TYR	CB-CG-CD2	-5.26	117.84	121.00
1	B	229	TYR	CB-CG-CD2	-5.26	117.84	121.00
1	G	246	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	E	243	TRP	CG-CD2-CE3	5.25	138.62	133.90
1	E	229	TYR	CB-CG-CD2	-5.24	117.85	121.00
1	H	243	TRP	CG-CD2-CE3	5.24	138.61	133.90
1	F	229	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	G	229	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	G	243	TRP	CG-CD2-CE3	5.22	138.60	133.90
1	C	229	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	D	243	TRP	CG-CD2-CE3	5.22	138.60	133.90
1	F	243	TRP	CG-CD2-CE3	5.21	138.59	133.90
1	H	229	TYR	CB-CG-CD2	-5.21	117.87	121.00
1	A	243	TRP	CG-CD2-CE3	5.21	138.59	133.90
1	C	243	TRP	CG-CD2-CE3	5.20	138.58	133.90
1	D	229	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	I	243	TRP	CG-CD2-CE3	5.19	138.57	133.90
1	H	192	TRP	CG-CD2-CE3	5.19	138.57	133.90
1	F	192	TRP	CG-CD2-CE3	5.18	138.56	133.90
1	C	192	TRP	CG-CD2-CE3	5.18	138.56	133.90
1	G	192	TRP	CG-CD2-CE3	5.17	138.56	133.90
1	E	192	TRP	CG-CD2-CE3	5.17	138.55	133.90
1	I	192	TRP	CG-CD2-CE3	5.16	138.55	133.90
1	A	192	TRP	CG-CD2-CE3	5.16	138.54	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	243	TRP	CG-CD2-CE3	5.16	138.54	133.90
1	B	192	TRP	CG-CD2-CE3	5.15	138.53	133.90
1	D	192	TRP	CG-CD2-CE3	5.13	138.52	133.90
1	E	106	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	H	106	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	I	106	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2579	0	2542	36	2
1	B	2579	0	2542	33	2
1	C	2579	0	2542	35	0
1	D	2579	0	2542	35	3
1	E	2579	0	2542	30	3
1	F	2579	0	2542	35	0
1	G	2579	0	2542	38	3
1	H	2579	0	2542	35	2
1	I	2579	0	2542	34	0
2	A	16	0	12	0	0
2	B	16	0	12	0	0
2	C	16	0	12	0	0
2	D	16	0	12	0	0
2	E	16	0	12	0	0
2	F	16	0	12	0	0
2	G	16	0	12	0	0
2	H	16	0	12	0	0
2	I	16	0	12	0	0
3	A	37	0	0	0	1
3	B	38	0	0	0	1
3	C	39	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	38	0	0	0	1
3	E	38	0	0	0	1
3	F	38	0	0	0	0
3	G	38	0	0	0	1
3	H	38	0	0	0	2
3	I	38	0	0	0	0
All	All	23697	0	22986	279	11

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (279) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:267:GLU:OE2	1:D:202:ARG:NH1	2.03	0.91
1:F:89:ILE:H	1:F:89:ILE:HD13	1.50	0.77
1:D:89:ILE:H	1:D:89:ILE:HD13	1.50	0.76
1:I:89:ILE:HD13	1:I:89:ILE:H	1.50	0.76
1:E:89:ILE:H	1:E:89:ILE:HD13	1.50	0.76
1:A:89:ILE:H	1:A:89:ILE:HD13	1.50	0.75
1:G:89:ILE:H	1:G:89:ILE:HD13	1.50	0.75
1:B:89:ILE:H	1:B:89:ILE:HD13	1.50	0.75
1:C:89:ILE:H	1:C:89:ILE:HD13	1.50	0.75
1:H:89:ILE:HD13	1:H:89:ILE:H	1.50	0.75
1:F:81:SER:HB2	1:F:83:ILE:HG22	1.74	0.70
1:E:81:SER:HB2	1:E:83:ILE:HG22	1.74	0.70
1:H:81:SER:HB2	1:H:83:ILE:HG22	1.74	0.70
1:I:81:SER:HB2	1:I:83:ILE:HG22	1.74	0.70
1:B:81:SER:HB2	1:B:83:ILE:HG22	1.74	0.69
1:A:81:SER:HB2	1:A:83:ILE:HG22	1.74	0.69
1:D:81:SER:HB2	1:D:83:ILE:HG22	1.74	0.69
1:G:81:SER:HB2	1:G:83:ILE:HG22	1.74	0.68
1:C:81:SER:HB2	1:C:83:ILE:HG22	1.74	0.68
1:E:284:LEU:H	1:E:284:LEU:HD23	1.65	0.62
1:A:284:LEU:H	1:A:284:LEU:HD23	1.65	0.62
1:F:284:LEU:H	1:F:284:LEU:HD23	1.65	0.62
1:G:284:LEU:HD23	1:G:284:LEU:H	1.65	0.62
1:D:284:LEU:H	1:D:284:LEU:HD23	1.64	0.61
1:H:284:LEU:HD23	1:H:284:LEU:H	1.65	0.61
1:B:284:LEU:H	1:B:284:LEU:HD23	1.65	0.61
1:I:284:LEU:H	1:I:284:LEU:HD23	1.65	0.61
1:C:284:LEU:H	1:C:284:LEU:HD23	1.65	0.61
1:A:267:GLU:CD	1:D:202:ARG:HH11	2.04	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:83:ILE:HD13	1:E:92:THR:HG21	1.85	0.59
1:F:83:ILE:HD13	1:F:92:THR:HG21	1.85	0.58
1:G:83:ILE:HD13	1:G:92:THR:HG21	1.85	0.58
1:H:144:MET:HB3	1:H:156:MET:HE1	1.85	0.58
1:B:83:ILE:HD13	1:B:92:THR:HG21	1.85	0.58
1:C:83:ILE:HD13	1:C:92:THR:HG21	1.85	0.58
1:A:83:ILE:HD13	1:A:92:THR:HG21	1.85	0.58
1:D:83:ILE:HD13	1:D:92:THR:HG21	1.85	0.58
1:F:144:MET:HB3	1:F:156:MET:HE1	1.86	0.57
1:I:83:ILE:HD13	1:I:92:THR:HG21	1.85	0.57
1:E:60:CYS:O	1:E:64:VAL:HG12	2.05	0.57
1:A:60:CYS:O	1:A:64:VAL:HG12	2.05	0.57
1:H:83:ILE:HD13	1:H:92:THR:HG21	1.85	0.57
1:B:60:CYS:O	1:B:64:VAL:HG12	2.05	0.57
1:G:60:CYS:O	1:G:64:VAL:HG12	2.05	0.57
1:F:60:CYS:O	1:F:64:VAL:HG12	2.05	0.57
1:I:60:CYS:O	1:I:64:VAL:HG12	2.05	0.56
1:D:60:CYS:O	1:D:64:VAL:HG12	2.05	0.56
1:G:85:HIS:HB3	1:H:283:THR:OG1	2.06	0.56
1:C:60:CYS:O	1:C:64:VAL:HG12	2.05	0.55
1:G:46:ASN:ND2	1:H:64:VAL:HG23	2.21	0.55
1:G:144:MET:HB3	1:G:156:MET:HE1	1.88	0.55
1:H:60:CYS:O	1:H:64:VAL:HG12	2.05	0.55
1:A:85:HIS:HB3	1:B:283:THR:OG1	2.07	0.54
1:G:19:LEU:HD22	1:G:178:LEU:HD23	1.90	0.54
1:H:19:LEU:HD22	1:H:178:LEU:HD23	1.90	0.54
1:C:19:LEU:HD22	1:C:178:LEU:HD23	1.90	0.54
1:I:19:LEU:HD22	1:I:178:LEU:HD23	1.90	0.54
1:I:144:MET:HB3	1:I:156:MET:HE1	1.88	0.54
1:E:19:LEU:HD22	1:E:178:LEU:HD23	1.90	0.53
1:A:106:ARG:HD2	1:A:128:LEU:HB3	1.90	0.53
1:H:106:ARG:HD2	1:H:128:LEU:HB3	1.90	0.53
1:D:222:VAL:HG11	1:D:259:MET:SD	2.49	0.53
1:F:19:LEU:HD22	1:F:178:LEU:HD23	1.90	0.53
1:C:106:ARG:HD2	1:C:128:LEU:HB3	1.91	0.53
1:B:144:MET:HB3	1:B:156:MET:HE1	1.91	0.53
1:B:106:ARG:HD2	1:B:128:LEU:HB3	1.90	0.53
1:B:222:VAL:HG11	1:B:259:MET:SD	2.49	0.53
1:B:19:LEU:HD22	1:B:178:LEU:HD23	1.90	0.53
1:C:222:VAL:HG11	1:C:259:MET:SD	2.49	0.53
1:F:106:ARG:HD2	1:F:128:LEU:HB3	1.90	0.53
1:F:222:VAL:HG11	1:F:259:MET:SD	2.49	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:222:VAL:HG11	1:G:259:MET:SD	2.49	0.53
1:H:222:VAL:HG11	1:H:259:MET:SD	2.49	0.53
1:I:222:VAL:HG11	1:I:259:MET:SD	2.49	0.53
1:D:106:ARG:HD2	1:D:128:LEU:HB3	1.90	0.52
1:A:19:LEU:HD22	1:A:178:LEU:HD23	1.90	0.52
1:A:222:VAL:HG11	1:A:259:MET:SD	2.49	0.52
1:D:19:LEU:HD22	1:D:178:LEU:HD23	1.90	0.52
1:F:89:ILE:H	1:F:89:ILE:CD1	2.22	0.52
1:E:222:VAL:HG11	1:E:259:MET:SD	2.49	0.52
1:E:144:MET:HB3	1:E:156:MET:HE1	1.92	0.52
1:D:144:MET:HB3	1:D:156:MET:HE1	1.92	0.52
1:I:106:ARG:HD2	1:I:128:LEU:HB3	1.90	0.52
1:E:42:LEU:H	1:E:69:GLN:HG3	1.75	0.52
1:A:42:LEU:H	1:A:69:GLN:HG3	1.75	0.52
1:G:57:ARG:HH11	1:I:95:VAL:HG21	1.74	0.52
1:G:106:ARG:HD2	1:G:128:LEU:HB3	1.90	0.52
1:E:106:ARG:HD2	1:E:128:LEU:HB3	1.90	0.51
1:F:42:LEU:H	1:F:69:GLN:HG3	1.75	0.51
1:C:144:MET:HB3	1:C:156:MET:HE1	1.92	0.51
1:G:42:LEU:H	1:G:69:GLN:HG3	1.75	0.51
1:C:89:ILE:H	1:C:89:ILE:CD1	2.22	0.51
1:C:42:LEU:H	1:C:69:GLN:HG3	1.75	0.51
1:H:81:SER:HA	1:I:55:SER:O	2.11	0.51
1:A:89:ILE:H	1:A:89:ILE:CD1	2.22	0.50
1:D:42:LEU:H	1:D:69:GLN:HG3	1.75	0.50
1:I:42:LEU:H	1:I:69:GLN:HG3	1.75	0.50
1:B:42:LEU:H	1:B:69:GLN:HG3	1.75	0.50
1:H:42:LEU:H	1:H:69:GLN:HG3	1.75	0.50
1:H:95:VAL:HG21	1:I:57:ARG:HH11	1.77	0.50
1:B:95:VAL:HG21	1:C:57:ARG:HH11	1.77	0.49
1:I:89:ILE:CD1	1:I:89:ILE:H	2.22	0.49
1:D:57:ARG:HH11	1:F:95:VAL:HG21	1.77	0.49
1:A:57:ARG:NH1	1:C:95:VAL:HG21	2.28	0.49
1:D:89:ILE:CD1	1:D:89:ILE:H	2.22	0.49
1:E:89:ILE:CD1	1:E:89:ILE:H	2.22	0.49
1:G:57:ARG:NH1	1:I:95:VAL:HG21	2.28	0.48
1:E:129:THR:HG23	1:E:132:PHE:H	1.79	0.48
1:A:129:THR:HG23	1:A:132:PHE:H	1.79	0.48
1:F:129:THR:HG23	1:F:132:PHE:H	1.79	0.48
1:H:129:THR:HG23	1:H:132:PHE:H	1.79	0.48
1:D:129:THR:HG23	1:D:132:PHE:H	1.79	0.48
1:A:144:MET:HB3	1:A:156:MET:HE1	1.95	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:129:THR:HG23	1:C:132:PHE:H	1.79	0.47
1:A:57:ARG:HH11	1:C:95:VAL:HG21	1.79	0.47
1:E:95:VAL:HG21	1:F:57:ARG:HH11	1.79	0.47
1:G:232:VAL:HA	1:G:299:GLU:HG2	1.97	0.47
1:E:232:VAL:HA	1:E:299:GLU:HG2	1.97	0.47
1:C:232:VAL:HA	1:C:299:GLU:HG2	1.97	0.47
1:F:232:VAL:HA	1:F:299:GLU:HG2	1.97	0.47
1:B:129:THR:HG23	1:B:132:PHE:H	1.79	0.47
1:H:232:VAL:HA	1:H:299:GLU:HG2	1.97	0.47
1:A:283:THR:OG1	1:C:85:HIS:HB3	2.14	0.47
1:I:129:THR:HG23	1:I:132:PHE:H	1.79	0.47
1:G:95:VAL:HG21	1:H:57:ARG:HH11	1.80	0.46
1:A:46:ASN:ND2	1:B:64:VAL:HG23	2.30	0.46
1:B:89:ILE:H	1:B:89:ILE:CD1	2.22	0.46
1:B:232:VAL:HA	1:B:299:GLU:HG2	1.97	0.46
1:G:64:VAL:HG23	1:I:46:ASN:ND2	2.31	0.46
1:G:129:THR:HG23	1:G:132:PHE:H	1.79	0.46
1:C:159:VAL:HG21	1:C:222:VAL:HA	1.98	0.46
1:D:232:VAL:HA	1:D:299:GLU:HG2	1.97	0.46
1:A:232:VAL:HA	1:A:299:GLU:HG2	1.97	0.46
1:D:81:SER:HA	1:E:55:SER:O	2.16	0.45
1:I:159:VAL:HG21	1:I:222:VAL:HA	1.98	0.45
1:H:159:VAL:HG21	1:H:222:VAL:HA	1.98	0.45
1:D:283:THR:OG1	1:F:85:HIS:HB3	2.16	0.45
1:E:159:VAL:HG21	1:E:222:VAL:HA	1.98	0.45
1:B:159:VAL:HG21	1:B:222:VAL:HA	1.98	0.45
1:I:232:VAL:HA	1:I:299:GLU:HG2	1.97	0.45
1:A:159:VAL:HG21	1:A:222:VAL:HA	1.98	0.45
1:I:5:HIS:HA	1:I:123:PRO:HG3	1.99	0.45
1:B:5:HIS:HA	1:B:123:PRO:HG3	1.99	0.45
1:D:5:HIS:HA	1:D:123:PRO:HG3	1.99	0.45
1:C:129:THR:CG2	1:C:132:PHE:H	2.30	0.45
1:F:231:ASP:O	1:F:299:GLU:HG2	2.17	0.45
1:B:129:THR:CG2	1:B:132:PHE:H	2.30	0.45
1:I:129:THR:CG2	1:I:132:PHE:H	2.30	0.45
1:B:231:ASP:O	1:B:299:GLU:HG2	2.17	0.45
1:I:231:ASP:O	1:I:299:GLU:HG2	2.17	0.45
1:B:81:SER:HA	1:C:55:SER:O	2.17	0.44
1:D:129:THR:CG2	1:D:132:PHE:H	2.30	0.44
1:G:129:THR:CG2	1:G:132:PHE:H	2.30	0.44
1:C:5:HIS:HA	1:C:123:PRO:HG3	1.99	0.44
1:C:231:ASP:O	1:C:299:GLU:HG2	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:159:VAL:HG21	1:D:222:VAL:HA	1.98	0.44
1:H:129:THR:CG2	1:H:132:PHE:H	2.30	0.44
1:H:231:ASP:O	1:H:299:GLU:HG2	2.17	0.44
1:H:5:HIS:HA	1:H:123:PRO:HG3	1.99	0.44
1:E:5:HIS:HA	1:E:123:PRO:HG3	1.99	0.44
1:F:159:VAL:HG21	1:F:222:VAL:HA	1.98	0.44
1:G:159:VAL:HG21	1:G:222:VAL:HA	1.98	0.44
1:E:231:ASP:O	1:E:299:GLU:HG2	2.17	0.44
1:D:231:ASP:O	1:D:299:GLU:HG2	2.17	0.44
1:G:283:THR:OG1	1:I:85:HIS:HB3	2.18	0.44
1:H:93:ALA:HB2	1:H:116:LEU:HD12	1.99	0.44
1:G:93:ALA:HB2	1:G:116:LEU:HD12	1.99	0.44
1:I:93:ALA:HB2	1:I:116:LEU:HD12	1.99	0.44
1:H:278:HIS:O	1:H:302:ASP:HB2	2.18	0.44
1:A:5:HIS:HA	1:A:123:PRO:HG3	1.99	0.44
1:G:98:ARG:NH2	1:H:314:ASP:HA	2.33	0.44
1:G:231:ASP:O	1:G:299:GLU:HG2	2.17	0.44
1:A:231:ASP:O	1:A:299:GLU:HG2	2.17	0.44
1:G:5:HIS:HA	1:G:123:PRO:HG3	1.99	0.44
1:C:93:ALA:HB2	1:C:116:LEU:HD12	1.99	0.44
1:D:278:HIS:O	1:D:302:ASP:HB2	2.18	0.44
1:A:93:ALA:HB2	1:A:116:LEU:HD12	1.99	0.44
1:A:129:THR:CG2	1:A:132:PHE:H	2.30	0.44
1:F:129:THR:CG2	1:F:132:PHE:H	2.30	0.44
1:A:278:HIS:O	1:A:302:ASP:HB2	2.18	0.44
1:F:5:HIS:HA	1:F:123:PRO:HG3	1.99	0.44
1:D:93:ALA:HB2	1:D:116:LEU:HD12	1.99	0.44
1:I:278:HIS:O	1:I:302:ASP:HB2	2.18	0.44
1:E:129:THR:CG2	1:E:132:PHE:H	2.30	0.43
1:E:154:ASN:HA	1:E:180:GLY:O	2.19	0.43
1:B:93:ALA:HB2	1:B:116:LEU:HD12	1.99	0.43
1:A:267:GLU:CD	1:D:202:ARG:NH1	2.64	0.43
1:B:46:ASN:ND2	1:C:64:VAL:HG23	2.33	0.43
1:A:301:THR:HG22	1:A:303:GLU:HB3	2.01	0.43
1:B:154:ASN:HA	1:B:180:GLY:O	2.19	0.43
1:B:301:THR:HG22	1:B:303:GLU:HB3	2.01	0.43
1:E:93:ALA:HB2	1:E:116:LEU:HD12	1.99	0.43
1:F:93:ALA:HB2	1:F:116:LEU:HD12	1.99	0.43
1:F:301:THR:HG22	1:F:303:GLU:HB3	2.01	0.43
1:F:109:GLY:H	1:F:130:ASN:H	1.67	0.43
1:D:301:THR:HG22	1:D:303:GLU:HB3	2.01	0.43
1:A:154:ASN:HA	1:A:180:GLY:O	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:301:THR:HG22	1:H:303:GLU:HB3	2.01	0.43
1:B:278:HIS:O	1:B:302:ASP:HB2	2.18	0.43
1:E:278:HIS:O	1:E:302:ASP:HB2	2.18	0.43
1:F:278:HIS:O	1:F:302:ASP:HB2	2.18	0.43
1:A:109:GLY:H	1:A:130:ASN:H	1.67	0.43
1:G:278:HIS:O	1:G:302:ASP:HB2	2.18	0.43
1:C:278:HIS:O	1:C:302:ASP:HB2	2.18	0.43
1:G:89:ILE:H	1:G:89:ILE:CD1	2.22	0.43
1:A:218:VAL:O	1:A:222:VAL:HG22	2.19	0.43
1:C:154:ASN:HA	1:C:180:GLY:O	2.19	0.43
1:H:109:GLY:H	1:H:130:ASN:H	1.67	0.43
1:H:154:ASN:HA	1:H:180:GLY:O	2.19	0.43
1:B:218:VAL:O	1:B:222:VAL:HG22	2.19	0.42
1:E:110:GLN:HG2	1:E:129:THR:HG21	2.01	0.42
1:E:301:THR:HG22	1:E:303:GLU:HB3	2.01	0.42
1:I:301:THR:HG22	1:I:303:GLU:HB3	2.01	0.42
1:H:218:VAL:O	1:H:222:VAL:HG22	2.19	0.42
1:E:218:VAL:O	1:E:222:VAL:HG22	2.19	0.42
1:G:109:GLY:H	1:G:130:ASN:H	1.67	0.42
1:G:154:ASN:HA	1:G:180:GLY:O	2.19	0.42
1:I:109:GLY:H	1:I:130:ASN:H	1.67	0.42
1:G:218:VAL:O	1:G:222:VAL:HG22	2.19	0.42
1:E:109:GLY:H	1:E:130:ASN:H	1.67	0.42
1:C:110:GLN:HG2	1:C:129:THR:HG21	2.01	0.42
1:I:154:ASN:HA	1:I:180:GLY:O	2.19	0.42
1:I:218:VAL:O	1:I:222:VAL:HG22	2.19	0.42
1:D:110:GLN:HG2	1:D:129:THR:HG21	2.01	0.42
1:D:154:ASN:HA	1:D:180:GLY:O	2.19	0.42
1:E:95:VAL:HG21	1:F:57:ARG:NH1	2.34	0.42
1:F:154:ASN:HA	1:F:180:GLY:O	2.19	0.42
1:D:109:GLY:H	1:D:130:ASN:H	1.67	0.42
1:C:109:GLY:H	1:C:130:ASN:H	1.67	0.42
1:D:57:ARG:NH1	1:F:95:VAL:HG21	2.34	0.42
1:F:117:ALA:HA	1:F:124:VAL:HG21	2.02	0.42
1:I:117:ALA:HA	1:I:124:VAL:HG21	2.02	0.42
1:B:109:GLY:H	1:B:130:ASN:H	1.67	0.42
1:E:85:HIS:HB3	1:F:283:THR:OG1	2.20	0.42
1:G:301:THR:HG22	1:G:303:GLU:HB3	2.01	0.42
1:H:117:ALA:HA	1:H:124:VAL:HG21	2.02	0.42
1:D:218:VAL:O	1:D:222:VAL:HG22	2.19	0.42
1:C:218:VAL:O	1:C:222:VAL:HG22	2.19	0.42
1:H:110:GLN:HG2	1:H:129:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:110:GLN:HG2	1:G:129:THR:HG21	2.01	0.41
1:G:117:ALA:HA	1:G:124:VAL:HG21	2.02	0.41
1:C:301:THR:HG22	1:C:303:GLU:HB3	2.01	0.41
1:F:218:VAL:O	1:F:222:VAL:HG22	2.19	0.41
1:B:110:GLN:HG2	1:B:129:THR:HG21	2.01	0.41
1:A:64:VAL:HG23	1:C:46:ASN:ND2	2.36	0.41
1:F:141:LEU:HD12	1:F:144:MET:CE	2.51	0.41
1:D:64:VAL:HG23	1:F:46:ASN:ND2	2.36	0.41
1:G:141:LEU:HD12	1:G:144:MET:CE	2.51	0.41
1:A:117:ALA:HA	1:A:124:VAL:HG21	2.02	0.41
1:B:117:ALA:HA	1:B:124:VAL:HG21	2.02	0.41
1:D:141:LEU:HD12	1:D:144:MET:CE	2.51	0.41
1:F:292:PHE:HB2	1:F:294:LEU:HD22	2.03	0.41
1:A:110:GLN:HG2	1:A:129:THR:HG21	2.01	0.41
1:A:141:LEU:HD12	1:A:144:MET:CE	2.51	0.41
1:H:292:PHE:HB2	1:H:294:LEU:HD22	2.03	0.41
1:B:292:PHE:HB2	1:B:294:LEU:HD22	2.03	0.41
1:I:292:PHE:HB2	1:I:294:LEU:HD22	2.03	0.41
1:C:141:LEU:HD12	1:C:144:MET:CE	2.51	0.41
1:G:95:VAL:HG21	1:H:57:ARG:NH1	2.36	0.41
1:H:89:ILE:H	1:H:89:ILE:CD1	2.22	0.41
1:D:159:VAL:HG22	1:D:184:ARG:HB2	2.03	0.41
1:F:159:VAL:HG22	1:F:184:ARG:HB2	2.03	0.41
1:I:110:GLN:HG2	1:I:129:THR:HG21	2.01	0.41
1:C:117:ALA:HA	1:C:124:VAL:HG21	2.02	0.41
1:E:292:PHE:HB2	1:E:294:LEU:HD22	2.03	0.41
1:H:141:LEU:HD12	1:H:144:MET:CE	2.51	0.41
1:F:110:GLN:HG2	1:F:129:THR:HG21	2.01	0.41
1:B:141:LEU:HD12	1:B:144:MET:CE	2.51	0.40
1:C:292:PHE:HB2	1:C:294:LEU:HD22	2.03	0.40
1:D:117:ALA:HA	1:D:124:VAL:HG21	2.02	0.40
1:I:141:LEU:HD12	1:I:144:MET:CE	2.51	0.40
1:C:159:VAL:HG22	1:C:184:ARG:HB2	2.03	0.40
1:G:292:PHE:HB2	1:G:294:LEU:HD22	2.03	0.40
1:B:159:VAL:HG22	1:B:184:ARG:HB2	2.03	0.40
1:G:159:VAL:HG22	1:G:184:ARG:HB2	2.03	0.40
1:A:292:PHE:HB2	1:A:294:LEU:HD22	2.03	0.40
1:E:117:ALA:HA	1:E:124:VAL:HG21	2.02	0.40
1:H:159:VAL:HG22	1:H:184:ARG:HB2	2.03	0.40
1:G:314:ASP:HA	1:I:98:ARG:NH2	2.37	0.40

All (11) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:290:GLU:OE1	1:H:202:ARG:NH2[1.566]	1.31	0.89
1:B:202:ARG:NH2	1:G:290:GLU:OE1[1.455]	1.67	0.53
3:B:350:HOH:O	3:G:354:HOH:O[1.455]	1.68	0.52
3:D:354:HOH:O	3:H:350:HOH:O[1.566]	1.74	0.46
1:D:291:GLU:OE1	1:H:215:THR:OG1[1.566]	1.82	0.38
1:A:291:GLU:OE1	1:E:215:THR:OG1[1.445]	1.95	0.25
1:B:215:THR:OG1	1:G:291:GLU:OE1[1.455]	1.98	0.22
1:A:290:GLU:OE1	1:E:202:ARG:NH2[1.445]	2.00	0.20
1:D:292:PHE:CE1	3:H:353:HOH:O[1.566]	2.03	0.17
3:A:354:HOH:O	3:E:350:HOH:O[1.445]	2.11	0.09
1:E:121:ARG:NE	1:G:1:SER:CA[1.666]	2.18	0.02

## 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	331/333 (99%)	313 (95%)	13 (4%)	5 (2%)	15	46
1	B	331/333 (99%)	313 (95%)	13 (4%)	5 (2%)	15	46
1	C	331/333 (99%)	313 (95%)	13 (4%)	5 (2%)	15	46
1	D	331/333 (99%)	313 (95%)	13 (4%)	5 (2%)	15	46
1	E	331/333 (99%)	313 (95%)	13 (4%)	5 (2%)	15	46
1	F	331/333 (99%)	313 (95%)	13 (4%)	5 (2%)	15	46
1	G	331/333 (99%)	313 (95%)	13 (4%)	5 (2%)	15	46
1	H	331/333 (99%)	313 (95%)	13 (4%)	5 (2%)	15	46
1	I	331/333 (99%)	313 (95%)	13 (4%)	5 (2%)	15	46
All	All	2979/2997 (99%)	2817 (95%)	117 (4%)	45 (2%)	15	46

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	128	LEU
1	B	85	HIS

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Mol	Chain	Res	Type
1	B	128	LEU
1	C	85	HIS
1	C	128	LEU
1	D	85	HIS
1	D	128	LEU
1	E	85	HIS
1	E	128	LEU
1	F	85	HIS
1	F	128	LEU
1	G	85	HIS
1	G	128	LEU
1	H	85	HIS
1	H	128	LEU
1	I	85	HIS
1	I	128	LEU
1	A	79	SER
1	A	86	LYS
1	B	79	SER
1	B	86	LYS
1	C	79	SER
1	C	86	LYS
1	D	79	SER
1	D	86	LYS
1	E	79	SER
1	E	86	LYS
1	F	79	SER
1	F	86	LYS
1	G	79	SER
1	G	86	LYS
1	H	79	SER
1	H	86	LYS
1	I	79	SER
1	I	86	LYS
1	A	80	GLY
1	B	80	GLY
1	C	80	GLY
1	D	80	GLY
1	E	80	GLY
1	F	80	GLY
1	G	80	GLY
1	H	80	GLY
1	I	80	GLY

### 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	268/270 (99%)	244 (91%)	24 (9%)	14	37
1	B	268/270 (99%)	244 (91%)	24 (9%)	14	37
1	C	268/270 (99%)	244 (91%)	24 (9%)	14	37
1	D	268/270 (99%)	244 (91%)	24 (9%)	14	37
1	E	268/270 (99%)	244 (91%)	24 (9%)	14	37
1	F	268/270 (99%)	244 (91%)	24 (9%)	14	37
1	G	268/270 (99%)	244 (91%)	24 (9%)	14	37
1	H	268/270 (99%)	244 (91%)	24 (9%)	14	37
1	I	268/270 (99%)	244 (91%)	24 (9%)	14	37
All	All	2412/2430 (99%)	2196 (91%)	216 (9%)	14	37

All (216) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	10	LYS
1	A	20	ASN
1	A	29	LEU
1	A	41	LYS
1	A	59	ARG
1	A	72	ARG
1	A	89	ILE
1	A	106	ARG
1	A	111	GLU
1	A	121	ARG
1	A	135	THR
1	A	141	LEU
1	A	165	ARG
1	A	183	LEU
1	A	229	TYR
1	A	259	MET
1	A	282	THR
1	A	288	MET

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Mol	Chain	Res	Type
1	A	294	LEU
1	A	299	GLU
1	A	320	MET
1	A	322	THR
1	A	331	LEU
1	B	6	LYS
1	B	10	LYS
1	B	20	ASN
1	B	29	LEU
1	B	41	LYS
1	B	59	ARG
1	B	72	ARG
1	B	89	ILE
1	B	106	ARG
1	B	111	GLU
1	B	121	ARG
1	B	135	THR
1	B	141	LEU
1	B	165	ARG
1	B	183	LEU
1	B	229	TYR
1	B	259	MET
1	B	282	THR
1	B	288	MET
1	B	294	LEU
1	B	299	GLU
1	B	320	MET
1	B	322	THR
1	B	331	LEU
1	C	6	LYS
1	C	10	LYS
1	C	20	ASN
1	C	29	LEU
1	C	41	LYS
1	C	59	ARG
1	C	72	ARG
1	C	89	ILE
1	C	106	ARG
1	C	111	GLU
1	C	121	ARG
1	C	135	THR
1	C	141	LEU

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Mol	Chain	Res	Type
1	C	165	ARG
1	C	183	LEU
1	C	229	TYR
1	C	259	MET
1	C	282	THR
1	C	288	MET
1	C	294	LEU
1	C	299	GLU
1	C	320	MET
1	C	322	THR
1	C	331	LEU
1	D	6	LYS
1	D	10	LYS
1	D	20	ASN
1	D	29	LEU
1	D	41	LYS
1	D	59	ARG
1	D	72	ARG
1	D	89	ILE
1	D	106	ARG
1	D	111	GLU
1	D	121	ARG
1	D	135	THR
1	D	141	LEU
1	D	165	ARG
1	D	183	LEU
1	D	229	TYR
1	D	259	MET
1	D	282	THR
1	D	288	MET
1	D	294	LEU
1	D	299	GLU
1	D	320	MET
1	D	322	THR
1	D	331	LEU
1	E	6	LYS
1	E	10	LYS
1	E	20	ASN
1	E	29	LEU
1	E	41	LYS
1	E	59	ARG
1	E	72	ARG

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Mol	Chain	Res	Type
1	E	89	ILE
1	E	106	ARG
1	E	111	GLU
1	E	121	ARG
1	E	135	THR
1	E	141	LEU
1	E	165	ARG
1	E	183	LEU
1	E	229	TYR
1	E	259	MET
1	E	282	THR
1	E	288	MET
1	E	294	LEU
1	E	299	GLU
1	E	320	MET
1	E	322	THR
1	E	331	LEU
1	F	6	LYS
1	F	10	LYS
1	F	20	ASN
1	F	29	LEU
1	F	41	LYS
1	F	59	ARG
1	F	72	ARG
1	F	89	ILE
1	F	106	ARG
1	F	111	GLU
1	F	121	ARG
1	F	135	THR
1	F	141	LEU
1	F	165	ARG
1	F	183	LEU
1	F	229	TYR
1	F	259	MET
1	F	282	THR
1	F	288	MET
1	F	294	LEU
1	F	299	GLU
1	F	320	MET
1	F	322	THR
1	F	331	LEU
1	G	6	LYS

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Mol	Chain	Res	Type
1	G	10	LYS
1	G	20	ASN
1	G	29	LEU
1	G	41	LYS
1	G	59	ARG
1	G	72	ARG
1	G	89	ILE
1	G	106	ARG
1	G	111	GLU
1	G	121	ARG
1	G	135	THR
1	G	141	LEU
1	G	165	ARG
1	G	183	LEU
1	G	229	TYR
1	G	259	MET
1	G	282	THR
1	G	288	MET
1	G	294	LEU
1	G	299	GLU
1	G	320	MET
1	G	322	THR
1	G	331	LEU
1	H	6	LYS
1	H	10	LYS
1	H	20	ASN
1	H	29	LEU
1	H	41	LYS
1	H	59	ARG
1	H	72	ARG
1	H	89	ILE
1	H	106	ARG
1	H	111	GLU
1	H	121	ARG
1	H	135	THR
1	H	141	LEU
1	H	165	ARG
1	H	183	LEU
1	H	229	TYR
1	H	259	MET
1	H	282	THR
1	H	288	MET

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Mol	Chain	Res	Type
1	H	294	LEU
1	H	299	GLU
1	H	320	MET
1	H	322	THR
1	H	331	LEU
1	I	6	LYS
1	I	10	LYS
1	I	20	ASN
1	I	29	LEU
1	I	41	LYS
1	I	59	ARG
1	I	72	ARG
1	I	89	ILE
1	I	106	ARG
1	I	111	GLU
1	I	121	ARG
1	I	135	THR
1	I	141	LEU
1	I	165	ARG
1	I	183	LEU
1	I	229	TYR
1	I	259	MET
1	I	282	THR
1	I	288	MET
1	I	294	LEU
1	I	299	GLU
1	I	320	MET
1	I	322	THR
1	I	331	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	167	ASN
1	A	265	ASN
1	B	46	ASN
1	B	167	ASN
1	B	265	ASN
1	C	46	ASN
1	C	167	ASN
1	C	265	ASN

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Mol	Chain	Res	Type
1	D	167	ASN
1	D	265	ASN
1	E	46	ASN
1	E	167	ASN
1	E	265	ASN
1	F	46	ASN
1	F	167	ASN
1	F	265	ASN
1	G	46	ASN
1	G	167	ASN
1	G	265	ASN
1	H	46	ASN
1	H	167	ASN
1	H	265	ASN
1	I	46	ASN
1	I	167	ASN
1	I	265	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

9 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	PAO	A	334	-	15,15,15	1.62	3 (20%)	20,20,20	1.03	2 (10%)
2	PAO	B	334	-	15,15,15	1.62	3 (20%)	20,20,20	1.03	2 (10%)
2	PAO	C	334	-	15,15,15	1.62	3 (20%)	20,20,20	1.03	2 (10%)
2	PAO	D	334	-	15,15,15	1.61	3 (20%)	20,20,20	1.03	2 (10%)
2	PAO	E	334	-	15,15,15	1.62	3 (20%)	20,20,20	1.03	2 (10%)
2	PAO	F	334	-	15,15,15	1.62	3 (20%)	20,20,20	1.03	2 (10%)
2	PAO	G	334	-	15,15,15	1.62	3 (20%)	20,20,20	1.03	2 (10%)
2	PAO	H	334	-	15,15,15	1.62	3 (20%)	20,20,20	1.03	2 (10%)
2	PAO	I	334	-	15,15,15	1.62	3 (20%)	20,20,20	1.03	2 (10%)

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	PAO	A	334	-	-	0/16/16/16	0/0/0/0
2	PAO	B	334	-	-	0/16/16/16	0/0/0/0
2	PAO	C	334	-	-	0/16/16/16	0/0/0/0
2	PAO	D	334	-	-	0/16/16/16	0/0/0/0
2	PAO	E	334	-	-	0/16/16/16	0/0/0/0
2	PAO	F	334	-	-	0/16/16/16	0/0/0/0
2	PAO	G	334	-	-	0/16/16/16	0/0/0/0
2	PAO	H	334	-	-	0/16/16/16	0/0/0/0
2	PAO	I	334	-	-	0/16/16/16	0/0/0/0

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	334	PAO	P-O1P	4.50	1.60	1.50
2	C	334	PAO	P-O1P	4.49	1.60	1.50
2	A	334	PAO	P-O1P	4.49	1.60	1.50
2	H	334	PAO	P-O1P	4.48	1.60	1.50
2	D	334	PAO	P-O1P	4.48	1.60	1.50
2	F	334	PAO	P-O1P	4.48	1.60	1.50
2	G	334	PAO	P-O1P	4.47	1.60	1.50
2	I	334	PAO	P-O1P	4.46	1.60	1.50
2	B	334	PAO	P-O1P	4.45	1.60	1.50
2	G	334	PAO	P-O3P	3.11	1.60	1.54
2	F	334	PAO	P-O3P	3.11	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	334	PAO	P-O3P	3.11	1.60	1.54
2	E	334	PAO	P-O3P	3.09	1.60	1.54
2	A	334	PAO	P-O3P	3.09	1.60	1.54
2	C	334	PAO	P-O3P	3.09	1.60	1.54
2	I	334	PAO	P-O3P	3.08	1.60	1.54
2	H	334	PAO	P-O3P	3.07	1.60	1.54
2	D	334	PAO	P-O3P	3.05	1.60	1.54
2	G	334	PAO	P-O2P	2.36	1.59	1.54
2	B	334	PAO	P-O2P	2.35	1.59	1.54
2	I	334	PAO	P-O2P	2.35	1.59	1.54
2	H	334	PAO	P-O2P	2.35	1.59	1.54
2	E	334	PAO	P-O2P	2.35	1.59	1.54
2	A	334	PAO	P-O2P	2.33	1.59	1.54
2	D	334	PAO	P-O2P	2.33	1.59	1.54
2	F	334	PAO	P-O2P	2.31	1.59	1.54
2	C	334	PAO	P-O2P	2.30	1.59	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	334	PAO	P-C1P-C1	-2.58	109.28	113.58
2	D	334	PAO	P-C1P-C1	-2.57	109.30	113.58
2	C	334	PAO	P-C1P-C1	-2.56	109.31	113.58
2	B	334	PAO	P-C1P-C1	-2.56	109.31	113.58
2	F	334	PAO	P-C1P-C1	-2.56	109.32	113.58
2	A	334	PAO	P-C1P-C1	-2.56	109.32	113.58
2	E	334	PAO	P-C1P-C1	-2.55	109.32	113.58
2	G	334	PAO	P-C1P-C1	-2.55	109.33	113.58
2	I	334	PAO	P-C1P-C1	-2.54	109.35	113.58
2	I	334	PAO	O3P-P-C1P	2.17	111.31	106.85
2	G	334	PAO	O3P-P-C1P	2.17	111.30	106.85
2	D	334	PAO	O3P-P-C1P	2.17	111.30	106.85
2	E	334	PAO	O3P-P-C1P	2.16	111.29	106.85
2	A	334	PAO	O3P-P-C1P	2.16	111.29	106.85
2	H	334	PAO	O3P-P-C1P	2.16	111.28	106.85
2	B	334	PAO	O3P-P-C1P	2.15	111.27	106.85
2	F	334	PAO	O3P-P-C1P	2.15	111.27	106.85
2	C	334	PAO	O3P-P-C1P	2.15	111.26	106.85

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.



## 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	333/333 (100%)	-0.66	4 (1%) 75 76	3, 23, 61, 93	0
1	B	333/333 (100%)	-0.54	8 (2%) 56 57	3, 23, 61, 93	0
1	C	333/333 (100%)	-0.60	7 (2%) 60 61	3, 23, 61, 93	0
1	D	333/333 (100%)	-0.57	4 (1%) 75 76	3, 23, 61, 93	0
1	E	333/333 (100%)	-0.58	6 (1%) 65 66	3, 23, 61, 93	0
1	F	333/333 (100%)	-0.66	3 (0%) 81 81	3, 23, 61, 93	0
1	G	333/333 (100%)	-0.64	2 (0%) 86 88	3, 23, 61, 93	0
1	H	333/333 (100%)	-0.65	4 (1%) 75 76	3, 23, 61, 93	0
1	I	333/333 (100%)	-0.65	2 (0%) 86 88	3, 23, 61, 93	0
All	All	2997/2997 (100%)	-0.62	40 (1%) 74 75	3, 23, 65, 93	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1	SER	10.0
1	G	1	SER	9.0
1	C	1	SER	8.4
1	A	1	SER	8.2
1	B	1	SER	8.1
1	F	1	SER	7.9
1	I	1	SER	7.1
1	B	2	GLY	6.3
1	H	1	SER	6.0
1	D	1	SER	5.5
1	C	84	GLY	4.4
1	A	81	SER	3.9
1	B	290	GLU	3.7
1	E	37	LYS	3.5
1	B	281	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	2	GLY	3.3
1	F	84	GLY	3.2
1	G	37	LYS	3.1
1	E	290	GLU	3.0
1	E	2	GLY	3.0
1	E	283	THR	3.0
1	C	284	LEU	2.9
1	E	281	GLN	2.9
1	D	280	ASP	2.9
1	B	80	GLY	2.9
1	H	290	GLU	2.7
1	D	282	THR	2.6
1	B	84	GLY	2.6
1	B	150	GLY	2.4
1	C	121	ARG	2.3
1	A	2	GLY	2.3
1	C	281	GLN	2.3
1	B	81	SER	2.3
1	I	121	ARG	2.2
1	F	85	HIS	2.2
1	A	84	GLY	2.1
1	C	37	LYS	2.1
1	C	2	GLY	2.1
1	D	81	SER	2.1
1	H	333	LYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PAO	A	334	16/16	0.13	0.52	2,5,13,16	0
2	PAO	H	334	16/16	0.12	0.12	2,5,13,16	0
2	PAO	F	334	16/16	0.12	0.10	2,5,13,16	0
2	PAO	B	334	16/16	0.11	-0.08	2,5,13,16	0
2	PAO	E	334	16/16	0.11	-0.18	2,5,13,16	0
2	PAO	G	334	16/16	0.11	-0.19	2,5,13,16	0
2	PAO	I	334	16/16	0.10	-0.36	2,5,13,16	0
2	PAO	D	334	16/16	0.10	-0.60	2,5,13,16	0
2	PAO	C	334	16/16	0.09	-0.68	2,5,13,16	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.