



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:16 AM UTC

PDB ID : 4U0T / pdb_00004u0t
Title : Crystal structure of ADC-7 beta-lactamase
Authors : Powers, R.A.; Wallar, B.J.
Deposited on : 2014-07-14
Resolution : 1.73 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

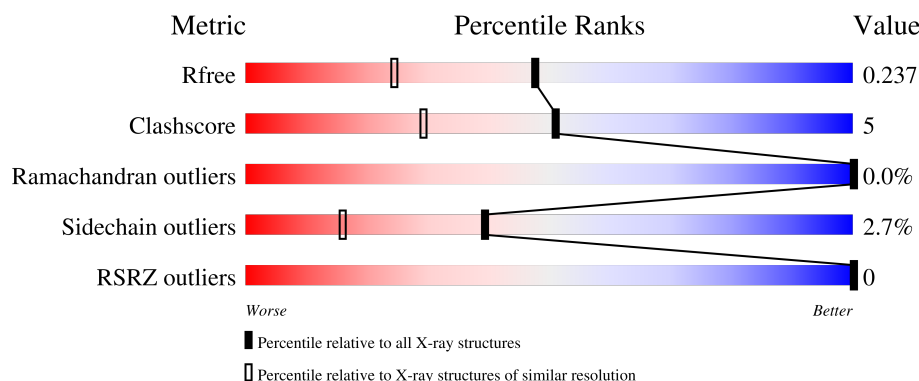
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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}	180053	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	360	 90% 9% ..
1	B	360	 84% 14% ..
1	C	360	 82% 14% ..
1	D	360	 76% 17% . .
1	E	360	 84% 13% ..

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Mol	Chain	Length	Quality of chain
1	F	360	 82% 15% ..
1	G	360	 83% 12% . .
1	H	360	 87% 9% . .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	C	401	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23766 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 ADC-7 beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	7	0
			2845	1833	467	534	11			
1	B	358	Total	C	N	O	S	0	8	0
			2857	1841	471	535	10			
1	C	352	Total	C	N	O	S	0	2	0
			2743	1767	452	515	9			
1	D	346	Total	C	N	O	S	0	3	0
			2684	1730	439	506	9			
1	E	354	Total	C	N	O	S	0	4	0
			2795	1801	465	520	9			
1	F	355	Total	C	N	O	S	0	1	0
			2768	1783	458	518	9			
1	G	348	Total	C	N	O	S	0	4	0
			2723	1757	446	511	9			
1	H	349	Total	C	N	O	S	0	1	0
			2711	1749	446	507	9			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	322	Total	O	0	9
			331	331		
3	B	335	Total	O	0	5
			340	340		
3	C	161	Total	O	0	2
			163	163		
3	D	163	Total	O	0	2
			165	165		

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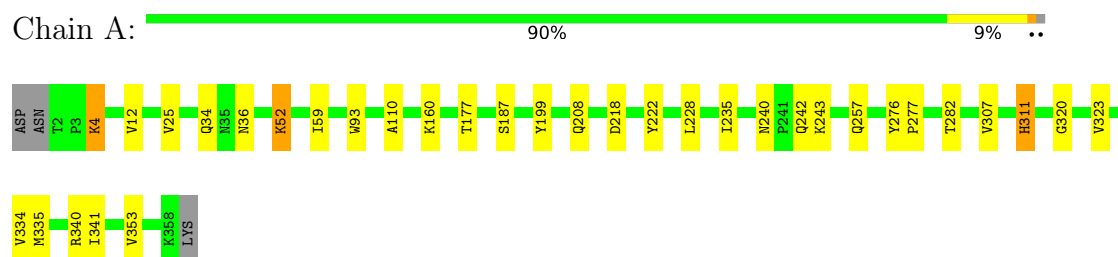
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	180	Total 180	O 180	0	0
3	F	157	Total 158	O 158	0	1
3	G	123	Total 124	O 124	0	1
3	H	139	Total 139	O 139	0	0

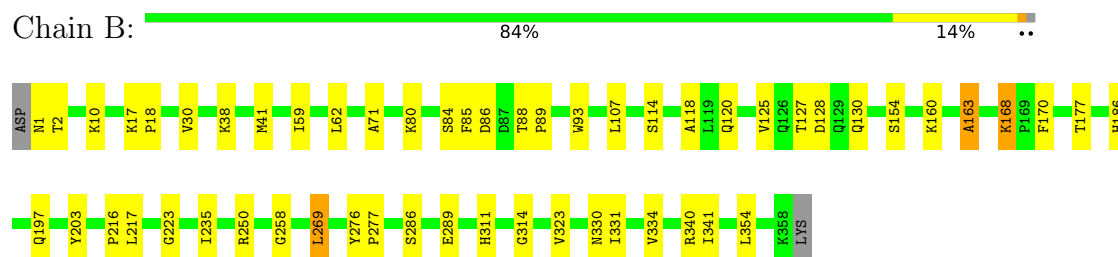
3 Residue-property plots

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

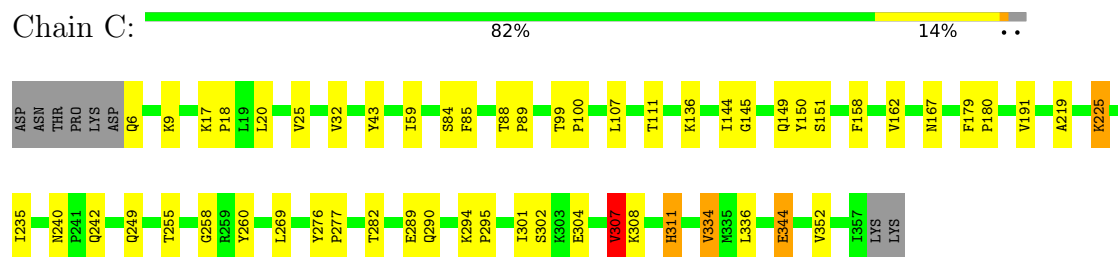
• Molecule 1: ADC-7 beta-lactamase



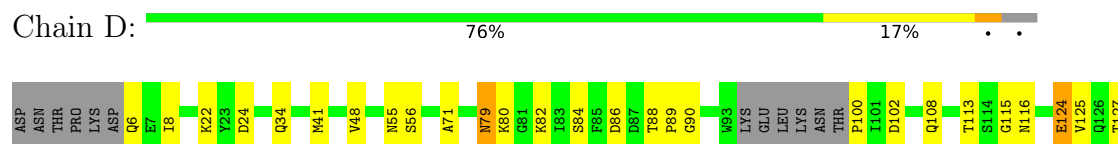
• Molecule 1: ADC-7 beta-lactamase

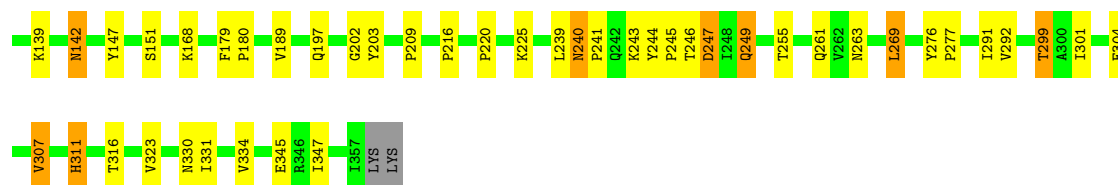


• Molecule 1: ADC-7 beta-lactamase



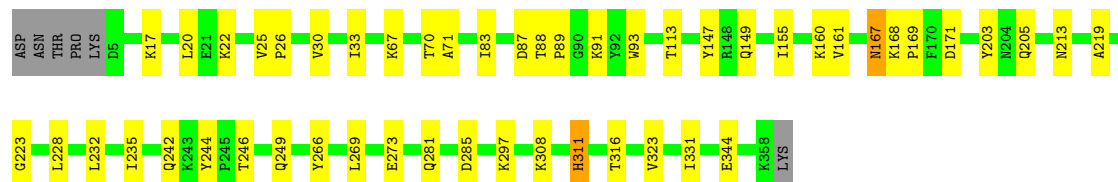
• Molecule 1: ADC-7 beta-lactamase





- Molecule 1: ADC-7 beta-lactamase

Chain E: 84% 13% ..



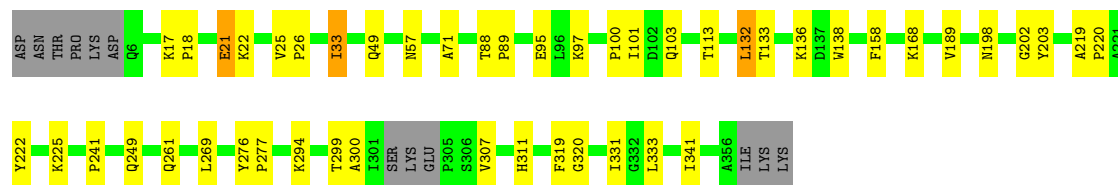
- Molecule 1: ADC-7 beta-lactamase

Chain F: 82% 15% ..



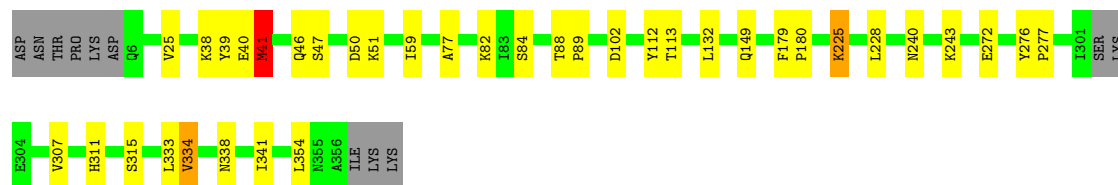
- Molecule 1: ADC-7 beta-lactamase

Chain G: 83% 12% ..



- Molecule 1: ADC-7 beta-lactamase

Chain H: 87% 9% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	81.00Å 88.57Å 105.88Å 67.29° 89.84° 89.40°	Depositor
Resolution (Å)	40.00 – 1.73 40.00 – 1.73	Depositor EDS
% Data completeness (in resolution range)	95.7 (40.00-1.73) 95.2 (40.00-1.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.194 , 0.239 0.195 , 0.237	Depositor DCC
R_{free} test set	13803 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 27.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.387 for h,-k,-l 0.001 for -h,k,k-l 0.000 for -h,-k,-k+l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	23766	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.86 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0227e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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

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	1.49	10/2935 (0.3%)	1.27	3/3988 (0.1%)
1	B	1.52	18/2951 (0.6%)	1.27	9/4012 (0.2%)
1	C	1.36	11/2816 (0.4%)	1.26	9/3835 (0.2%)
1	D	1.36	8/2759 (0.3%)	1.28	18/3763 (0.5%)
1	E	1.15	3/2871 (0.1%)	1.15	14/3902 (0.4%)
1	F	1.14	5/2838 (0.2%)	1.13	2/3859 (0.1%)
1	G	1.11	4/2801 (0.1%)	1.15	7/3812 (0.2%)
1	H	1.17	7/2780 (0.3%)	1.17	10/3785 (0.3%)
All	All	1.30	66/22751 (0.3%)	1.21	72/30956 (0.2%)

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	C	0	1
1	F	0	1
All	All	0	2

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	338	ASN	N-CA	8.74	1.55	1.46
1	G	222	TYR	C-O	8.37	1.30	1.23
1	A	25	VAL	N-CA	7.64	1.52	1.46
1	C	258	GLY	N-CA	7.38	1.53	1.45
1	D	323[A]	VAL	C-O	7.10	1.31	1.24
1	D	323[B]	VAL	C-O	7.10	1.31	1.24
1	F	42	TYR	N-CA	7.04	1.54	1.46
1	B	258	GLY	C-O	6.62	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	32	VAL	C-O	-6.55	1.17	1.24
1	H	47	SER	N-CA	6.55	1.54	1.46
1	D	301	ILE	C-O	6.47	1.31	1.24
1	C	302	SER	C-O	6.45	1.29	1.23
1	B	286	SER	N-CA	-6.41	1.38	1.46
1	B	250	ARG	C-O	-6.39	1.16	1.24
1	A	340	ARG	C-O	6.29	1.31	1.23
1	B	217	LEU	CA-C	-6.27	1.45	1.53
1	C	301	ILE	C-O	6.27	1.30	1.24
1	A	282	THR	CA-C	-6.26	1.44	1.52
1	D	41	MET	N-CA	6.24	1.53	1.46
1	F	40	GLU	N-CA	6.20	1.53	1.46
1	E	228	LEU	C-O	-6.07	1.18	1.24
1	H	46	GLN	C-N	-6.03	1.26	1.33
1	B	38	LYS	CA-C	-5.98	1.45	1.52
1	C	240	ASN	CA-CB	-5.97	1.46	1.53
1	B	2	THR	CA-C	-5.95	1.46	1.52
1	C	344	GLU	CD-OE2	5.91	1.36	1.25
1	B	59	ILE	CA-CB	-5.86	1.47	1.54
1	B	163	ALA	N-CA	5.78	1.53	1.46
1	A	353	VAL	N-CA	5.75	1.53	1.46
1	A	320	GLY	C-O	5.74	1.30	1.23
1	H	46	GLN	C-O	-5.74	1.17	1.24
1	H	41	MET	CA-C	5.74	1.59	1.52
1	B	120	GLN	N-CA	5.74	1.52	1.45
1	B	203	TYR	N-CA	-5.73	1.38	1.46
1	H	47	SER	C-O	-5.73	1.17	1.23
1	D	347	ILE	N-CA	-5.71	1.39	1.46
1	G	319	PHE	N-CA	5.71	1.53	1.45
1	H	334	VAL	C-O	-5.63	1.18	1.24
1	B	314	GLY	C-O	-5.59	1.17	1.24
1	B	62	LEU	C-O	5.55	1.31	1.24
1	A	228	LEU	N-CA	-5.54	1.41	1.46
1	A	187	SER	C-O	5.54	1.31	1.24
1	C	352	VAL	N-CA	-5.46	1.40	1.46
1	B	154	SER	C-O	-5.43	1.17	1.24
1	E	30	VAL	C-O	-5.42	1.18	1.24
1	C	282	THR	CA-C	5.39	1.59	1.52
1	D	55	ASN	C-O	5.38	1.29	1.23
1	A	222	TYR	N-CA	-5.29	1.42	1.47
1	G	320	GLY	CA-C	5.26	1.56	1.51
1	D	299	THR	N-CA	-5.26	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	340	ARG	C-O	5.25	1.29	1.23
1	F	341	ILE	C-O	-5.22	1.19	1.24
1	F	126	GLN	CA-C	5.20	1.57	1.52
1	F	47	SER	N-CA	5.20	1.52	1.46
1	D	24	ASP	CA-C	-5.18	1.46	1.53
1	B	118	ALA	N-CA	-5.16	1.39	1.45
1	B	177	THR	CA-C	-5.15	1.48	1.52
1	C	334	VAL	CA-C	5.15	1.58	1.52
1	B	340	ARG	CA-C	-5.11	1.46	1.52
1	C	191	VAL	C-O	-5.11	1.18	1.24
1	C	336	LEU	CA-C	5.10	1.58	1.52
1	A	110	ALA	N-CA	5.08	1.52	1.46
1	E	70	THR	C-O	5.08	1.29	1.24
1	B	10	LYS	C-O	-5.07	1.18	1.24
1	A	177	THR	CA-C	-5.03	1.48	1.52
1	G	158	PHE	C-O	-5.03	1.18	1.24

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	240	ASN	CB-CA-C	-8.62	99.92	111.21
1	D	307	VAL	CB-CA-C	7.40	121.27	110.77
1	D	139	LYS	CA-C-N	7.23	127.23	119.78
1	D	139	LYS	C-N-CA	7.23	127.23	119.78
1	D	168	LYS	CA-C-N	-7.19	112.59	119.85
1	D	168	LYS	C-N-CA	-7.19	112.59	119.85
1	D	240[A]	ASN	CA-C-N	-7.15	112.34	119.56
1	D	240[A]	ASN	C-N-CA	-7.15	112.34	119.56
1	D	240[B]	ASN	CA-C-N	-7.15	112.34	119.56
1	D	240[B]	ASN	C-N-CA	-7.15	112.34	119.56
1	H	25	VAL	CA-C-N	-7.11	111.16	119.05
1	H	25	VAL	C-N-CA	-7.11	111.16	119.05
1	D	79	ASN	N-CA-C	7.07	120.02	111.82
1	B	341	ILE	CA-C-N	-6.54	113.02	119.76
1	B	341	ILE	C-N-CA	-6.54	113.02	119.76
1	E	167	ASN	N-CA-C	6.51	120.40	111.54
1	C	145	GLY	N-CA-C	6.44	122.74	115.08
1	E	161	VAL	N-CA-C	6.39	116.54	110.53
1	A	36	ASN	N-CA-C	6.30	120.75	113.38
1	H	113	THR	N-CA-C	6.27	120.24	112.59
1	F	25	VAL	CA-C-N	-6.21	112.09	118.85
1	F	25	VAL	C-N-CA	-6.21	112.09	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	307	VAL	CB-CA-C	6.19	119.37	110.33
1	H	228	LEU	CA-C-N	-6.12	112.18	118.85
1	H	228	LEU	C-N-CA	-6.12	112.18	118.85
1	G	189	VAL	N-CA-C	-6.06	105.82	111.45
1	D	220	PRO	N-CA-C	6.05	121.42	113.86
1	E	168	LYS	CA-C-N	-6.02	113.58	119.78
1	E	168	LYS	C-N-CA	-6.02	113.58	119.78
1	C	219	ALA	CA-C-N	-5.98	113.58	120.04
1	C	219	ALA	C-N-CA	-5.98	113.58	120.04
1	D	292	VAL	N-CA-C	5.96	116.74	110.72
1	E	205	GLN	N-CA-C	-5.91	105.56	112.89
1	D	304	GLU	CA-C-N	-5.85	113.91	119.76
1	D	304	GLU	C-N-CA	-5.85	113.91	119.76
1	A	218	ASP	N-CA-C	5.80	117.61	111.28
1	E	25	VAL	CA-C-N	-5.75	112.58	118.85
1	E	25	VAL	C-N-CA	-5.75	112.58	118.85
1	G	202	GLY	N-CA-C	-5.74	103.82	112.89
1	D	316	THR	N-CA-C	-5.63	101.83	109.95
1	G	168	LYS	CB-CA-C	-5.63	99.62	108.91
1	B	80	LYS	N-CA-C	5.58	119.95	113.20
1	C	151	SER	N-CA-C	5.56	117.69	108.13
1	H	272	GLU	N-CA-C	-5.51	100.72	109.76
1	D	189	VAL	N-CA-C	-5.50	105.75	111.58
1	E	244	TYR	CA-C-N	-5.49	114.05	119.92
1	E	244	TYR	C-N-CA	-5.49	114.05	119.92
1	D	151	SER	N-CA-C	5.44	117.49	108.13
1	E	246	THR	N-CA-C	5.43	120.34	111.37
1	G	113	THR	N-CA-C	5.43	119.22	112.59
1	B	170	PHE	N-CA-C	5.42	117.19	111.28
1	D	56	SER	N-CA-C	5.40	118.97	112.38
1	B	168	LYS	CA-C-N	-5.39	114.69	120.03
1	B	168	LYS	C-N-CA	-5.39	114.69	120.03
1	G	25	VAL	CB-CA-C	-5.33	104.65	110.78
1	H	334	VAL	CB-CA-C	-5.32	102.69	110.62
1	A	12	VAL	CB-CA-C	5.27	118.92	112.02
1	H	315	SER	CB-CA-C	-5.25	104.23	110.94
1	E	213	ASN	CA-C-N	5.11	125.39	119.93
1	E	213	ASN	C-N-CA	5.11	125.39	119.93
1	H	341	ILE	CA-C-N	-5.10	114.52	119.78
1	H	341	ILE	C-N-CA	-5.10	114.52	119.78
1	E	232	LEU	N-CA-C	-5.09	105.81	111.36
1	B	114	SER	O-C-N	5.09	128.17	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	316	THR	N-CA-C	-5.08	102.64	109.95
1	G	341	ILE	CA-C-N	-5.07	114.54	119.76
1	G	341	ILE	C-N-CA	-5.07	114.54	119.76
1	C	304	GLU	CA-C-N	-5.06	114.70	119.76
1	C	304	GLU	C-N-CA	-5.06	114.70	119.76
1	B	2	THR	CA-C-N	-5.04	114.76	119.90
1	B	2	THR	C-N-CA	-5.04	114.76	119.90
1	C	289	GLU	CA-C-O	5.02	126.05	120.63

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	6	GLN	Peptide
1	F	357	ILE	Peptide

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	2845	0	2838	23	0
1	B	2857	0	2849	31	0
1	C	2743	0	2692	38	0
1	D	2684	0	2606	41	0
1	E	2795	0	2780	20	0
1	F	2768	0	2727	30	0
1	G	2723	0	2669	26	0
1	H	2711	0	2648	22	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
3	A	331	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	340	0	0	10	0
3	C	163	0	0	3	0
3	D	165	0	0	2	0
3	E	180	0	0	1	0
3	F	158	0	0	2	0
3	G	124	0	0	2	0
3	H	139	0	0	3	0
All	All	23766	0	21809	229	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 5.

All (229) 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:C:107:LEU:O	1:C:111[B]:THR:HG22	1.40	1.19
1:B:235[A]:ILE:HD11	1:B:323[A]:VAL:HG11	1.34	1.09
1:B:235[A]:ILE:HD11	1:B:323[A]:VAL:CG1	1.91	1.01
1:D:240[B]:ASN:OD1	1:D:243:LYS:HE3	1.68	0.94
1:G:132:LEU:C	1:G:132:LEU:HD23	1.99	0.87
1:E:235:ILE:HD11	1:E:323[A]:VAL:CG2	2.05	0.86
1:C:111[B]:THR:HG1	1:C:260:TYR:HE2	1.24	0.85
1:C:235:ILE:CD1	1:C:334:VAL:HG23	2.07	0.85
1:C:235:ILE:HD11	1:C:334:VAL:CG2	2.07	0.85
1:A:335[B]:MET:HE1	1:A:341:ILE:HD11	1.60	0.83
1:B:186[A]:HIS:CD2	3:B:501:HOH:O	2.33	0.81
1:C:111[B]:THR:OG1	1:C:260:TYR:HE2	1.63	0.79
1:D:239:LEU:C	1:D:240[B]:ASN:HD22	1.89	0.79
1:C:242:GLN:HA	1:C:249:GLN:NE2	1.98	0.79
1:F:235:ILE:HD11	1:F:323:VAL:CG1	2.14	0.78
1:F:79:ASN:OD1	1:F:250:ARG:NH1	2.15	0.78
1:D:115:GLY:O	1:D:142:ASN:HB2	1.83	0.77
1:D:261:GLN:HG2	1:D:299:THR:HG23	1.69	0.75
1:B:1:ASN:HB3	3:B:506:HOH:O	1.86	0.73
1:C:235:ILE:HD11	1:C:334:VAL:HG23	1.66	0.73
1:D:240[B]:ASN:OD1	1:D:243:LYS:CE	2.37	0.73
1:E:235:ILE:HD11	1:E:323[A]:VAL:HG23	1.68	0.72
1:A:235[B]:ILE:CD1	1:A:334:VAL:HG23	2.20	0.72
1:F:20:LEU:HD22	1:F:25:VAL:HB	1.73	0.71
1:C:111[B]:THR:OG1	1:C:260:TYR:CE2	2.43	0.70
1:C:235:ILE:CD1	1:C:334:VAL:CG2	2.69	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:235:ILE:HD11	1:F:323:VAL:HG13	1.74	0.67
2:B:401:PO4:O4	3:B:776:HOH:O	2.13	0.66
1:C:290:GLN:NE2	1:H:50:ASP:OD1	2.29	0.66
1:B:186[A]:HIS:HD2	3:B:501:HOH:O	1.75	0.66
1:H:132:LEU:HD23	1:H:132:LEU:C	2.21	0.65
1:C:225:LYS:HD3	1:C:225:LYS:N	2.11	0.65
1:A:4:LYS:HE3	1:A:34:GLN:OE1	1.96	0.65
1:A:240:ASN:OD1	3:A:735:HOH:O	2.14	0.65
1:A:235[B]:ILE:HD11	1:A:334:VAL:HG23	1.78	0.64
1:C:235:ILE:HD11	1:C:334:VAL:HG22	1.80	0.63
1:E:235:ILE:HD11	1:E:323[A]:VAL:HG21	1.78	0.63
1:H:276:TYR:O	1:H:307:VAL:HG13	1.98	0.63
1:C:242:GLN:HA	1:C:249:GLN:CD	2.24	0.63
1:C:290:GLN:HB3	1:C:294:LYS:HE3	1.81	0.62
1:D:125:VAL:O	1:D:216:PRO:HG3	1.99	0.62
1:C:107:LEU:HD23	1:C:111[B]:THR:HG21	1.80	0.62
1:B:235[B]:ILE:CD1	1:B:334:VAL:HG23	2.30	0.61
1:B:186[A]:HIS:HE1	3:B:505:HOH:O	1.83	0.60
1:B:323[B]:VAL:HG12	1:B:334:VAL:HG22	1.83	0.60
1:D:261:GLN:HG2	1:D:299:THR:CG2	2.32	0.60
1:H:333:LEU:HD23	1:H:333:LEU:C	2.27	0.60
1:C:235:ILE:HD12	1:C:334:VAL:HG23	1.80	0.60
1:B:223:GLY:HA2	3:B:707:HOH:O	2.00	0.60
1:F:88:THR:HB	1:F:89:PRO:HD2	1.84	0.59
1:F:71:ALA:HB1	1:F:269:LEU:HB3	1.84	0.59
1:C:20:LEU:HD11	1:C:43:TYR:HB3	1.84	0.59
1:H:40:GLU:C	1:H:41:MET:HE3	2.27	0.59
1:D:90:GLY:N	1:D:102:ASP:OD2	2.35	0.59
1:C:107:LEU:O	1:C:111[B]:THR:CG2	2.33	0.58
1:E:242:GLN:HA	1:E:249:GLN:OE1	2.04	0.58
1:E:281:GLN:NE2	1:E:285:ASP:OD1	2.36	0.58
1:A:257:GLN:HG3	3:A:533[A]:HOH:O	2.03	0.57
1:A:235[B]:ILE:HD11	1:A:334:VAL:CG2	2.33	0.57
1:B:235[A]:ILE:CD1	1:B:323[A]:VAL:CG1	2.77	0.57
1:A:257:GLN:HG3	3:A:533[B]:HOH:O	2.04	0.57
1:C:107:LEU:HD23	1:C:111[B]:THR:CG2	2.35	0.57
1:C:167:ASN:ND2	3:C:501:HOH:O	2.37	0.57
1:D:84:SER:OG	1:D:86:ASP:OD1	2.22	0.57
1:E:93:TRP:CZ2	1:E:160:LYS:HE2	2.39	0.57
1:A:52:LYS:HD2	3:A:591:HOH:O	2.05	0.57
1:G:241:PRO:O	1:G:249:GLN:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:ALA:HB1	1:E:269:LEU:HB3	1.87	0.57
1:D:71:ALA:HB1	1:D:269:LEU:HB3	1.85	0.57
1:F:96:LEU:O	1:F:99:THR:HG22	2.05	0.56
1:A:235[B]:ILE:HD12	1:A:334:VAL:HG23	1.87	0.56
1:H:276:TYR:CD1	1:H:277:PRO:HA	2.41	0.56
1:F:344:GLU:H	1:F:344:GLU:CD	2.14	0.56
1:B:235[B]:ILE:HD12	1:B:334:VAL:HG23	1.87	0.55
1:F:237:ALA:HA	1:F:244:TYR:CE1	2.41	0.55
1:H:276:TYR:O	1:H:307:VAL:CG1	2.55	0.55
1:G:299:THR:HG22	1:G:300:ALA:O	2.06	0.55
1:F:276:TYR:CD1	1:F:277:PRO:HA	2.41	0.55
1:G:22:LYS:NZ	3:G:604:HOH:O	2.32	0.54
1:B:127:THR:OG1	1:B:130:GLN:HG3	2.07	0.54
1:D:48[A]:VAL:HG22	1:D:203:TYR:OH	2.06	0.54
1:D:179:PHE:HB2	1:D:180:PRO:HD3	1.90	0.54
1:G:33:ILE:O	1:G:331:ILE:HA	2.08	0.54
1:A:307[A]:VAL:HG12	3:A:514:HOH:O	2.07	0.54
1:C:107:LEU:HD23	1:C:107:LEU:C	2.33	0.53
1:F:235:ILE:HD11	1:F:323:VAL:HG11	1.88	0.53
1:G:276:TYR:CD1	1:G:277:PRO:HA	2.43	0.53
1:C:107:LEU:CD2	1:C:111[B]:THR:HG21	2.38	0.53
1:E:88:THR:HB	1:E:89:PRO:HD2	1.91	0.53
1:G:21:GLU:O	1:G:21:GLU:HG3	2.07	0.53
1:G:132:LEU:HD23	1:G:133:THR:N	2.23	0.53
1:D:255:THR:HA	1:D:269:LEU:HB2	1.91	0.53
1:D:276:TYR:CD1	1:D:277:PRO:HA	2.43	0.53
1:E:219:ALA:HA	1:E:223:GLY:HA3	1.90	0.53
1:H:59:ILE:CG2	1:H:225:LYS:HB2	2.39	0.53
1:B:93:TRP:CZ3	1:B:160:LYS:HD3	2.45	0.52
1:D:88:THR:HB	1:D:89:PRO:HD2	1.92	0.52
1:A:242:GLN:HG2	1:A:243:LYS:HD3	1.90	0.52
1:D:6:GLN:HA	3:D:589:HOH:O	2.09	0.52
1:F:12:VAL:HG21	1:F:41:MET:HE3	1.90	0.52
1:C:290:GLN:O	1:C:294:LYS:HG2	2.11	0.51
1:H:38:LYS:NZ	3:H:526:HOH:O	2.42	0.51
1:E:93:TRP:CZ3	1:E:160:LYS:HD3	2.46	0.51
1:D:142:ASN:ND2	1:D:147:TYR:CD1	2.79	0.51
1:H:51:LYS:NZ	3:H:501:HOH:O	2.41	0.51
1:D:22:LYS:NZ	1:D:345:GLU:OE2	2.40	0.51
1:A:4:LYS:CE	1:A:34:GLN:OE1	2.60	0.50
1:C:17:LYS:N	1:C:18:PRO:CD	2.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:TYR:HB3	1:C:307:VAL:HG22	1.94	0.50
1:F:96:LEU:O	1:F:99:THR:CG2	2.59	0.50
1:B:128:ASP:HB3	3:B:729:HOH:O	2.11	0.50
1:C:276:TYR:CD1	1:C:277:PRO:HA	2.46	0.50
1:C:107:LEU:O	1:C:107:LEU:HD23	2.12	0.49
1:D:102:ASP:OD1	1:D:102:ASP:O	2.30	0.49
1:E:169:PRO:HB2	1:E:171:ASP:OD1	2.12	0.49
1:B:163:ALA:HB1	1:B:168:LYS:O	2.13	0.49
1:G:132:LEU:C	1:G:132:LEU:CD2	2.78	0.49
1:C:20:LEU:HD23	1:C:25:VAL:HB	1.94	0.48
1:F:265:MET:HG2	1:F:266:TYR:N	2.28	0.48
1:B:235[B]:ILE:HD11	1:B:334:VAL:CG2	2.43	0.48
1:D:241:PRO:O	1:D:249:GLN:HG3	2.13	0.48
1:F:144:ILE:HD11	3:F:534:HOH:O	2.14	0.48
1:D:113:THR:HA	1:D:147:TYR:O	2.13	0.48
1:B:88:THR:HB	1:B:89:PRO:HD2	1.96	0.48
1:D:100:PRO:C	1:D:102:ASP:N	2.69	0.48
1:G:333:LEU:C	1:G:333:LEU:HD23	2.39	0.48
1:H:39:TYR:CD1	1:H:39:TYR:N	2.81	0.47
1:D:124:GLU:CD	1:D:124:GLU:H	2.20	0.47
1:D:244:TYR:O	1:D:245:PRO:C	2.55	0.47
1:F:219:ALA:HA	1:F:223:GLY:HA3	1.95	0.47
1:H:88:THR:HG21	1:H:102:ASP:O	2.15	0.47
1:B:235[B]:ILE:HD11	1:B:334:VAL:HG23	1.95	0.47
1:H:112:TYR:HB3	1:H:149:GLN:O	2.14	0.47
1:B:1:ASN:CB	3:B:506:HOH:O	2.56	0.47
1:A:208:GLN:OE1	1:F:51:LYS:HA	2.15	0.47
1:C:85:PHE:HB3	1:C:107:LEU:HB2	1.97	0.47
1:F:255:THR:HA	1:F:269:LEU:HB2	1.96	0.47
1:A:235[B]:ILE:CD1	1:A:334:VAL:CG2	2.92	0.46
2:C:401:PO4:O4	3:C:521:HOH:O	2.20	0.46
1:E:17:LYS:O	1:E:20:LEU:HD12	2.15	0.46
1:D:80:LYS:HB3	1:D:82:LYS:HG3	1.98	0.46
1:F:79:ASN:OD1	1:F:250:ARG:HD3	2.16	0.46
1:G:100:PRO:HD2	3:G:594:HOH:O	2.15	0.46
1:C:294:LYS:HB2	1:C:295:PRO:HD2	1.98	0.46
1:C:59:ILE:CG2	1:C:225:LYS:HB3	2.45	0.46
1:H:77:ALA:HB1	1:H:82:LYS:HB2	1.97	0.46
1:D:48[A]:VAL:HG22	1:D:203:TYR:CZ	2.50	0.46
1:G:88:THR:HB	1:G:89:PRO:HD2	1.97	0.46
1:D:80:LYS:NZ	1:D:247:ASP:HB3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:HIS:CD2	1:A:311:HIS:C	2.94	0.45
1:B:311:HIS:CD2	1:B:311:HIS:C	2.95	0.45
1:A:276:TYR:HB3	1:A:307[B]:VAL:HG12	1.99	0.45
1:G:17:LYS:N	1:G:18:PRO:HD2	2.32	0.45
1:G:71:ALA:HB1	1:G:269:LEU:HB3	1.99	0.45
1:G:95[B]:GLU:CD	1:G:95[B]:GLU:H	2.25	0.45
1:B:85:PHE:HB3	1:B:107:LEU:HB2	1.98	0.45
1:H:240:ASN:HB3	1:H:243:LYS:HG3	1.98	0.45
1:B:331:ILE:HG12	1:B:354:LEU:HD22	1.99	0.45
1:B:235[B]:ILE:CD1	1:B:334:VAL:CG2	2.95	0.45
1:D:311:HIS:CD2	1:D:311:HIS:C	2.95	0.45
1:D:100:PRO:C	1:D:102:ASP:H	2.24	0.45
1:B:84:SER:OG	1:B:86[B]:ASP:OD1	2.34	0.44
1:F:311:HIS:C	1:F:311:HIS:CD2	2.95	0.44
1:A:307[A]:VAL:CG1	3:A:507:HOH:O	2.66	0.44
1:D:239:LEU:O	1:D:240[B]:ASN:ND2	2.47	0.44
1:F:169:PRO:HB2	1:F:171:ASP:OD1	2.18	0.44
1:A:93:TRP:CZ3	1:A:160:LYS:HD3	2.53	0.44
1:B:1:ASN:CG	3:B:506:HOH:O	2.60	0.44
1:C:99:THR:HB	1:C:100:PRO:CD	2.48	0.44
1:F:74:GLY:HA2	1:F:162:VAL:HG21	2.00	0.44
1:B:71:ALA:HB1	1:B:269:LEU:HB3	2.00	0.43
1:A:59:ILE:HB	1:A:199:TYR:HA	2.00	0.43
1:A:323:VAL:HG12	1:A:334:VAL:HG22	2.00	0.43
1:E:22[A]:LYS:NZ	3:E:630:HOH:O	2.39	0.43
1:G:225:LYS:CD	1:G:225:LYS:N	2.81	0.43
1:B:276:TYR:HA	1:B:277:PRO:C	2.42	0.43
1:E:87:ASP:CG	1:E:91:LYS:HE3	2.43	0.43
1:G:219:ALA:N	1:G:220:PRO:HD2	2.34	0.43
1:C:311:HIS:C	1:C:311:HIS:CD2	2.96	0.43
1:D:263:ASN:OD1	1:G:49[A]:GLN:CD	2.61	0.43
1:D:80:LYS:HZ2	1:D:247:ASP:HB3	1.83	0.43
1:D:291:ILE:CG1	1:G:49[A]:GLN:NE2	2.81	0.43
1:D:241:PRO:HB2	1:D:249:GLN:HG2	1.99	0.43
1:B:186[B]:HIS:CE1	3:B:501:HOH:O	2.70	0.43
1:C:255:THR:HA	1:C:269:LEU:HB2	2.00	0.43
1:G:132:LEU:HD21	1:G:136:LYS:HE3	2.00	0.43
1:F:113:THR:HA	1:F:147:TYR:O	2.19	0.43
1:G:276:TYR:HA	1:G:277:PRO:C	2.44	0.43
1:H:333:LEU:HD23	1:H:334:VAL:N	2.33	0.43
1:D:34:GLN:HG3	1:D:331:ILE:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:ILE:CD1	3:F:534:HOH:O	2.67	0.42
1:F:179:PHE:HB2	1:F:180:PRO:HD3	2.01	0.42
1:B:30:VAL:O	1:B:41:MET:HE3	2.19	0.42
1:D:115:GLY:C	1:D:142:ASN:HB2	2.45	0.42
1:E:33:ILE:O	1:E:331:ILE:HA	2.20	0.42
1:H:39:TYR:HB3	1:H:41:MET:HE1	2.02	0.42
1:F:117:LEU:O	1:F:149:GLN:HG2	2.19	0.42
1:E:311:HIS:C	1:E:311:HIS:CD2	2.97	0.42
1:F:276:TYR:O	1:F:307:VAL:HG13	2.19	0.42
1:G:26:PRO:HG2	1:G:203:TYR:CD2	2.54	0.42
1:G:101:ILE:HD13	1:G:138:TRP:CD2	2.55	0.42
1:C:158:PHE:O	1:C:162:VAL:HG23	2.20	0.42
1:F:217:LEU:O	1:F:220:PRO:HD2	2.20	0.42
1:C:150:TYR:N	3:C:608:HOH:O	2.31	0.41
1:E:67:LYS:HE3	1:E:155:ILE:HG21	2.03	0.41
1:D:108:GLN:HA	3:D:503:HOH:O	2.19	0.41
1:H:88:THR:HB	1:H:89:PRO:HD2	2.03	0.41
1:H:179:PHE:HB2	1:H:180:PRO:HD3	2.02	0.41
1:G:57:ASN:O	1:G:198:ASN:HB3	2.21	0.41
1:H:39:TYR:CB	1:H:41:MET:HE1	2.51	0.41
1:B:17:LYS:N	1:B:18:PRO:CD	2.84	0.41
1:E:266:TYR:HB2	1:E:273:GLU:HB3	2.02	0.41
1:E:26:PRO:HG2	1:E:203:TYR:CD1	2.56	0.41
1:H:112:TYR:OH	3:H:636:HOH:O	2.22	0.41
1:A:276:TYR:HA	1:A:277:PRO:C	2.46	0.41
1:C:88:THR:HB	1:C:89:PRO:HD2	2.03	0.41
1:D:202:GLY:O	1:D:209:PRO:HA	2.21	0.41
1:F:93:TRP:CZ2	1:F:160:LYS:HE2	2.56	0.41
1:G:219:ALA:HB3	1:G:220:PRO:HD3	2.03	0.41
1:H:41:MET:HE3	1:H:41:MET:N	2.35	0.41
1:C:179:PHE:HB2	1:C:180:PRO:HD3	2.03	0.40
1:E:113:THR:HA	1:E:147:TYR:O	2.21	0.40
1:F:281:GLN:NE2	1:F:285:ASP:OD1	2.53	0.40
1:D:246:THR:HG23	1:D:247:ASP:N	2.36	0.40
1:B:125:VAL:O	1:B:216:PRO:HG3	2.21	0.40
1:D:225:LYS:HD2	1:D:225:LYS:N	2.36	0.40
1:A:52:LYS:HD2	1:A:52:LYS:HA	1.92	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	362/360 (101%)	350 (97%)	12 (3%)	0	100	100
1	B	364/360 (101%)	354 (97%)	10 (3%)	0	100	100
1	C	352/360 (98%)	338 (96%)	14 (4%)	0	100	100
1	D	345/360 (96%)	336 (97%)	8 (2%)	1 (0%)	36	23
1	E	356/360 (99%)	348 (98%)	8 (2%)	0	100	100
1	F	352/360 (98%)	341 (97%)	11 (3%)	0	100	100
1	G	348/360 (97%)	341 (98%)	7 (2%)	0	100	100
1	H	346/360 (96%)	334 (96%)	12 (4%)	0	100	100
All	All	2825/2880 (98%)	2742 (97%)	82 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	116	ASN

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	315/318 (99%)	312 (99%)	3 (1%)	68	54
1	B	316/318 (99%)	312 (99%)	4 (1%)	61	43
1	C	295/318 (93%)	285 (97%)	10 (3%)	32	10
1	D	287/318 (90%)	274 (96%)	13 (4%)	24	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	304/318 (96%)	297 (98%)	7 (2%)	44	20
1	F	298/318 (94%)	284 (95%)	14 (5%)	23	5
1	G	292/318 (92%)	283 (97%)	9 (3%)	35	12
1	H	288/318 (91%)	283 (98%)	5 (2%)	53	32
All	All	2395/2544 (94%)	2330 (97%)	65 (3%)	39	16

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	52	LYS
1	A	311	HIS
1	B	197	GLN
1	B	269	LEU
1	B	289	GLU
1	B	330	ASN
1	C	9	LYS
1	C	84	SER
1	C	136	LYS
1	C	144	ILE
1	C	149	GLN
1	C	225	LYS
1	C	307	VAL
1	C	308	LYS
1	C	311	HIS
1	C	344	GLU
1	D	8	ILE
1	D	79	ASN
1	D	124	GLU
1	D	127	THR
1	D	142	ASN
1	D	197	GLN
1	D	247	ASP
1	D	249	GLN
1	D	269	LEU
1	D	307	VAL
1	D	311	HIS
1	D	330	ASN
1	D	334	VAL
1	E	83	ILE
1	E	149	GLN

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Mol	Chain	Res	Type
1	E	167	ASN
1	E	297	LYS
1	E	308	LYS
1	E	311	HIS
1	E	344	GLU
1	F	20	LEU
1	F	84	SER
1	F	99	THR
1	F	105	ASN
1	F	107	LEU
1	F	149	GLN
1	F	206	GLU
1	F	243	LYS
1	F	294	LYS
1	F	302	SER
1	F	306	SER
1	F	308	LYS
1	F	311	HIS
1	F	358	LYS
1	G	21	GLU
1	G	33	ILE
1	G	97	LYS
1	G	103	GLN
1	G	132	LEU
1	G	261	GLN
1	G	294	LYS
1	G	307	VAL
1	G	311	HIS
1	H	41	MET
1	H	84	SER
1	H	225	LYS
1	H	311	HIS
1	H	354	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	205	GLN
1	A	343	ASN
1	B	35	ASN
1	B	142	ASN

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Mol	Chain	Res	Type
1	B	197	GLN
1	B	198	ASN
1	B	281	GLN
1	B	343	ASN
1	C	14	GLN
1	C	35	ASN
1	C	167	ASN
1	C	186	HIS
1	C	205	GLN
1	C	249	GLN
1	D	35	ASN
1	D	116	ASN
1	D	195	GLN
1	D	198	ASN
1	D	249	GLN
1	D	261	GLN
1	D	281	GLN
1	D	287	ASN
1	D	343	ASN
1	E	34	GLN
1	E	142	ASN
1	E	290	GLN
1	F	36	ASN
1	F	98	ASN
1	F	186	HIS
1	F	195	GLN
1	F	197	GLN
1	F	198	ASN
1	F	263	ASN
1	F	281	GLN
1	G	281	GLN
1	H	35	ASN
1	H	186	HIS
1	H	205	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	D	401	-	4,4,4	1.38	1 (25%)	6,6,6	1.36	2 (33%)
2	PO4	B	401	-	4,4,4	1.66	1 (25%)	6,6,6	2.70	2 (33%)
2	PO4	F	401	-	4,4,4	0.59	0	6,6,6	1.69	2 (33%)
2	PO4	H	401	-	4,4,4	0.62	0	6,6,6	1.99	3 (50%)
2	PO4	C	401	-	4,4,4	1.08	0	6,6,6	3.14	4 (66%)
2	PO4	E	401	-	4,4,4	0.82	0	6,6,6	1.53	1 (16%)
2	PO4	G	401	-	4,4,4	0.65	0	6,6,6	2.02	3 (50%)
2	PO4	A	401	-	4,4,4	0.74	0	6,6,6	1.71	2 (33%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	PO4	P-O1	3.01	1.57	1.50
2	D	401	PO4	P-O4	-2.58	1.47	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	PO4	O4-P-O3	5.56	125.20	107.91
2	C	401	PO4	O4-P-O1	4.72	127.63	110.95
2	C	401	PO4	O2-P-O1	-3.82	97.44	110.95
2	C	401	PO4	O3-P-O1	-3.29	99.31	110.95
2	G	401	PO4	O4-P-O2	3.29	118.15	107.91
2	C	401	PO4	O4-P-O3	3.21	117.88	107.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	PO4	O2-P-O1	2.92	121.29	110.95
2	B	401	PO4	O2-P-O1	-2.81	101.03	110.95
2	H	401	PO4	O4-P-O3	-2.79	99.25	107.91
2	A	401	PO4	O3-P-O1	-2.52	102.04	110.95
2	G	401	PO4	O2-P-O1	-2.50	102.12	110.95
2	E	401	PO4	O4-P-O2	2.45	115.53	107.91
2	H	401	PO4	O3-P-O1	2.45	119.61	110.95
2	H	401	PO4	O4-P-O2	2.43	115.46	107.91
2	F	401	PO4	O4-P-O2	2.38	115.33	107.91
2	D	401	PO4	O4-P-O1	2.34	119.23	110.95
2	G	401	PO4	O4-P-O3	-2.15	101.23	107.91
2	D	401	PO4	O4-P-O3	-2.08	101.42	107.91
2	F	401	PO4	O4-P-O1	-2.00	103.87	110.95

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	401	PO4	1	0
2	C	401	PO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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, 95th 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 ²)	Q<0.9
1	A	357/360 (99%)	-1.24	0 100 100	9, 21, 36, 45	7 (1%)
1	B	358/360 (99%)	-1.26	0 100 100	9, 21, 35, 51	8 (2%)
1	C	352/360 (97%)	-0.92	0 100 100	14, 33, 63, 73	2 (0%)
1	D	346/360 (96%)	-0.89	0 100 100	11, 32, 60, 75	3 (0%)
1	E	354/360 (98%)	-1.06	0 100 100	14, 34, 56, 70	4 (1%)
1	F	355/360 (98%)	-0.93	0 100 100	16, 38, 63, 80	1 (0%)
1	G	348/360 (96%)	-0.96	0 100 100	15, 38, 56, 69	4 (1%)
1	H	349/360 (96%)	-0.88	0 100 100	18, 38, 55, 71	1 (0%)
All	All	2819/2880 (97%)	-1.02	0 100 100	9, 31, 58, 80	30 (1%)

There are no RSRZ outliers to report.

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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
2	PO4	A	401	5/5	0.99	0.05	23,24,25,26	0
2	PO4	B	401	5/5	0.99	0.05	23,23,25,26	0
2	PO4	C	401	5/5	0.99	0.06	35,36,38,39	0
2	PO4	D	401	5/5	0.99	0.04	34,34,35,36	0
2	PO4	E	401	5/5	0.99	0.03	39,41,42,46	0
2	PO4	F	401	5/5	0.99	0.03	41,42,45,49	0
2	PO4	H	401	5/5	0.99	0.04	31,32,34,34	0
2	PO4	G	401	5/5	1.00	0.02	34,34,35,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.