



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 12:49 AM UTC

PDB ID : 6H2F / pdb_00006h2f
Title : Structure of the pre-pore AhlB of the tripartite alpha-pore forming toxin, AHL, from *Aeromonas hydrophila*.
Authors : Churchill-Angus, A.M.; Wilson, J.S.; Baker, P.J.
Deposited on : 2018-07-13
Resolution : 2.55 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

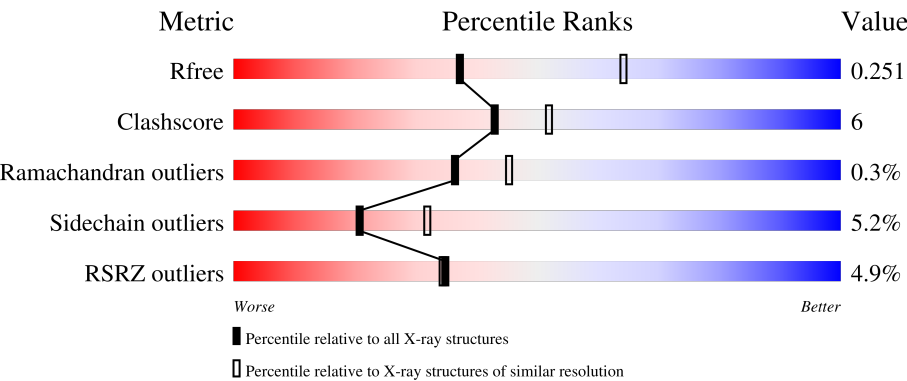
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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.



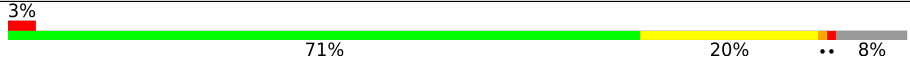
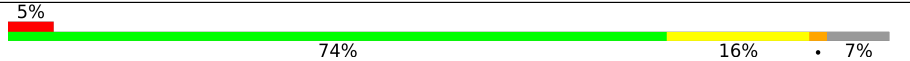
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	367	3% 75% 13% • 10%
1	B	367	6% 78% 14% • 6%
1	C	367	3% 75% 14% • 8%
1	D	367	6% 71% 19% • 8%
1	E	367	2% 70% 17% • 10%

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Mol	Chain	Length	Quality of chain
1	F	367	
1	G	367	
1	H	367	
1	I	367	
1	J	367	

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 2 unique types of molecules in this entry. The entry contains 24766 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 AhlB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2436	1515	424	489	8			
1	B	344	Total	C	N	O	S	0	0	0
			2533	1584	439	504	6			
1	C	338	Total	C	N	O	S	0	0	0
			2485	1546	431	500	8			
1	D	338	Total	C	N	O	S	0	0	0
			2493	1558	433	496	6			
1	E	329	Total	C	N	O	S	0	0	0
			2424	1507	422	487	8			
1	F	326	Total	C	N	O	S	0	0	0
			2398	1498	415	479	6			
1	G	328	Total	C	N	O	S	0	0	0
			2417	1503	421	485	8			
1	H	345	Total	C	N	O	S	0	0	0
			2550	1594	444	506	6			
1	I	338	Total	C	N	O	S	0	0	0
			2485	1546	431	500	8			
1	J	343	Total	C	N	O	S	0	0	0
			2525	1578	438	503	6			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	360	LEU	-	expression tag	UNP A0A081US78
A	361	GLU	-	expression tag	UNP A0A081US78
A	362	HIS	-	expression tag	UNP A0A081US78
A	363	HIS	-	expression tag	UNP A0A081US78
A	364	HIS	-	expression tag	UNP A0A081US78
A	365	HIS	-	expression tag	UNP A0A081US78
A	366	HIS	-	expression tag	UNP A0A081US78
A	367	HIS	-	expression tag	UNP A0A081US78
B	360	LEU	-	expression tag	UNP A0A081US78

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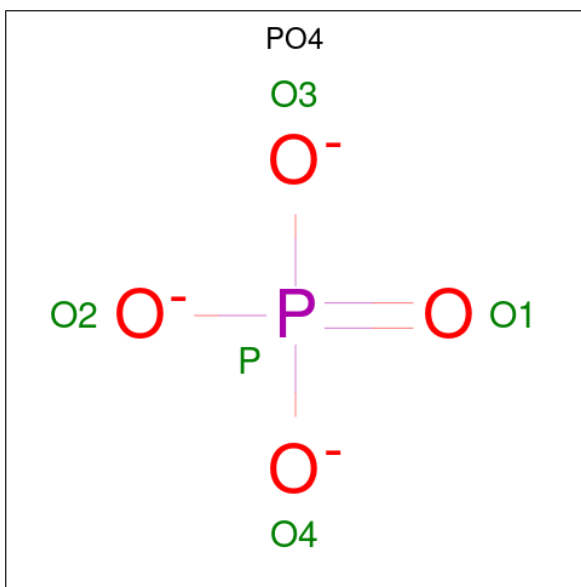
Chain	Residue	Modelled	Actual	Comment	Reference
B	361	GLU	-	expression tag	UNP A0A081US78
B	362	HIS	-	expression tag	UNP A0A081US78
B	363	HIS	-	expression tag	UNP A0A081US78
B	364	HIS	-	expression tag	UNP A0A081US78
B	365	HIS	-	expression tag	UNP A0A081US78
B	366	HIS	-	expression tag	UNP A0A081US78
B	367	HIS	-	expression tag	UNP A0A081US78
C	360	LEU	-	expression tag	UNP A0A081US78
C	361	GLU	-	expression tag	UNP A0A081US78
C	362	HIS	-	expression tag	UNP A0A081US78
C	363	HIS	-	expression tag	UNP A0A081US78
C	364	HIS	-	expression tag	UNP A0A081US78
C	365	HIS	-	expression tag	UNP A0A081US78
C	366	HIS	-	expression tag	UNP A0A081US78
C	367	HIS	-	expression tag	UNP A0A081US78
D	360	LEU	-	expression tag	UNP A0A081US78
D	361	GLU	-	expression tag	UNP A0A081US78
D	362	HIS	-	expression tag	UNP A0A081US78
D	363	HIS	-	expression tag	UNP A0A081US78
D	364	HIS	-	expression tag	UNP A0A081US78
D	365	HIS	-	expression tag	UNP A0A081US78
D	366	HIS	-	expression tag	UNP A0A081US78
D	367	HIS	-	expression tag	UNP A0A081US78
E	360	LEU	-	expression tag	UNP A0A081US78
E	361	GLU	-	expression tag	UNP A0A081US78
E	362	HIS	-	expression tag	UNP A0A081US78
E	363	HIS	-	expression tag	UNP A0A081US78
E	364	HIS	-	expression tag	UNP A0A081US78
E	365	HIS	-	expression tag	UNP A0A081US78
E	366	HIS	-	expression tag	UNP A0A081US78
E	367	HIS	-	expression tag	UNP A0A081US78
F	360	LEU	-	expression tag	UNP A0A081US78
F	361	GLU	-	expression tag	UNP A0A081US78
F	362	HIS	-	expression tag	UNP A0A081US78
F	363	HIS	-	expression tag	UNP A0A081US78
F	364	HIS	-	expression tag	UNP A0A081US78
F	365	HIS	-	expression tag	UNP A0A081US78
F	366	HIS	-	expression tag	UNP A0A081US78
F	367	HIS	-	expression tag	UNP A0A081US78
G	360	LEU	-	expression tag	UNP A0A081US78
G	361	GLU	-	expression tag	UNP A0A081US78
G	362	HIS	-	expression tag	UNP A0A081US78

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Chain	Residue	Modelled	Actual	Comment	Reference
G	363	HIS	-	expression tag	UNP A0A081US78
G	364	HIS	-	expression tag	UNP A0A081US78
G	365	HIS	-	expression tag	UNP A0A081US78
G	366	HIS	-	expression tag	UNP A0A081US78
G	367	HIS	-	expression tag	UNP A0A081US78
H	360	LEU	-	expression tag	UNP A0A081US78
H	361	GLU	-	expression tag	UNP A0A081US78
H	362	HIS	-	expression tag	UNP A0A081US78
H	363	HIS	-	expression tag	UNP A0A081US78
H	364	HIS	-	expression tag	UNP A0A081US78
H	365	HIS	-	expression tag	UNP A0A081US78
H	366	HIS	-	expression tag	UNP A0A081US78
H	367	HIS	-	expression tag	UNP A0A081US78
I	360	LEU	-	expression tag	UNP A0A081US78
I	361	GLU	-	expression tag	UNP A0A081US78
I	362	HIS	-	expression tag	UNP A0A081US78
I	363	HIS	-	expression tag	UNP A0A081US78
I	364	HIS	-	expression tag	UNP A0A081US78
I	365	HIS	-	expression tag	UNP A0A081US78
I	366	HIS	-	expression tag	UNP A0A081US78
I	367	HIS	-	expression tag	UNP A0A081US78
J	360	LEU	-	expression tag	UNP A0A081US78
J	361	GLU	-	expression tag	UNP A0A081US78
J	362	HIS	-	expression tag	UNP A0A081US78
J	363	HIS	-	expression tag	UNP A0A081US78
J	364	HIS	-	expression tag	UNP A0A081US78
J	365	HIS	-	expression tag	UNP A0A081US78
J	366	HIS	-	expression tag	UNP A0A081US78
J	367	HIS	-	expression tag	UNP A0A081US78

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

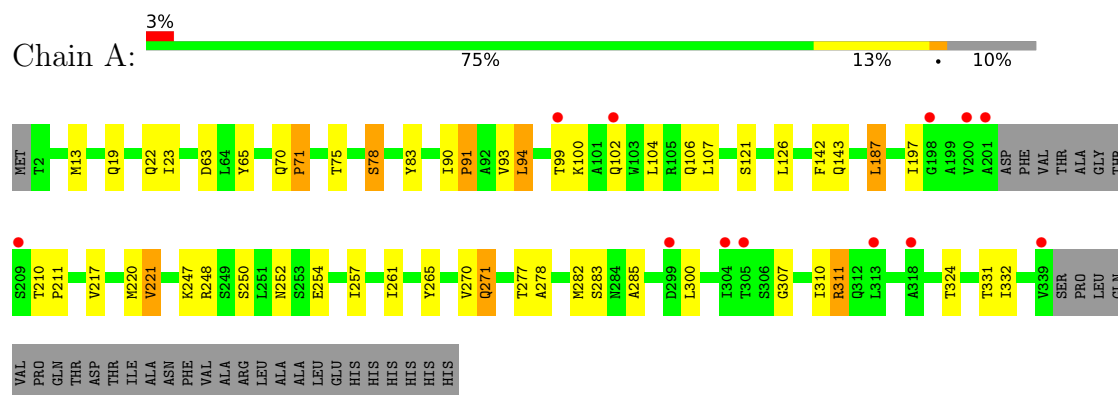


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	I	1	Total	O	P	0	0
			5	4	1		

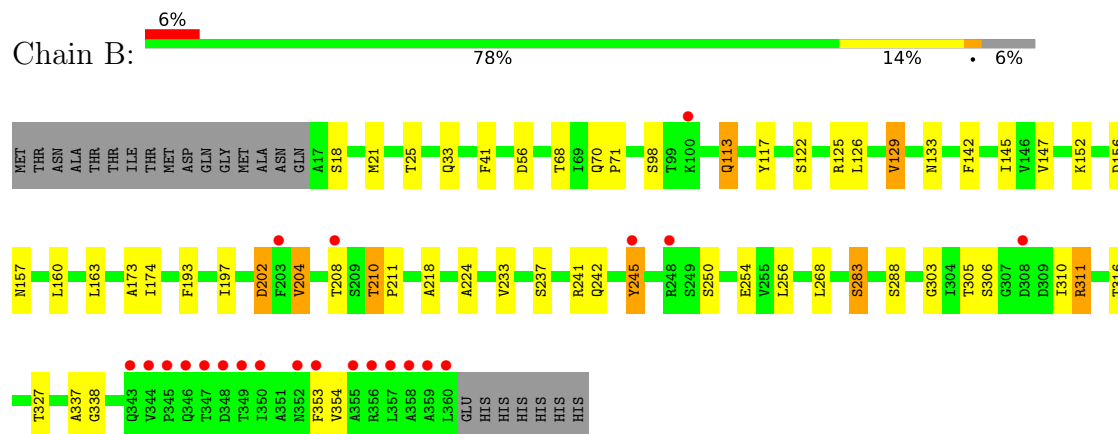
3 Residue-property plots [i](#)

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.

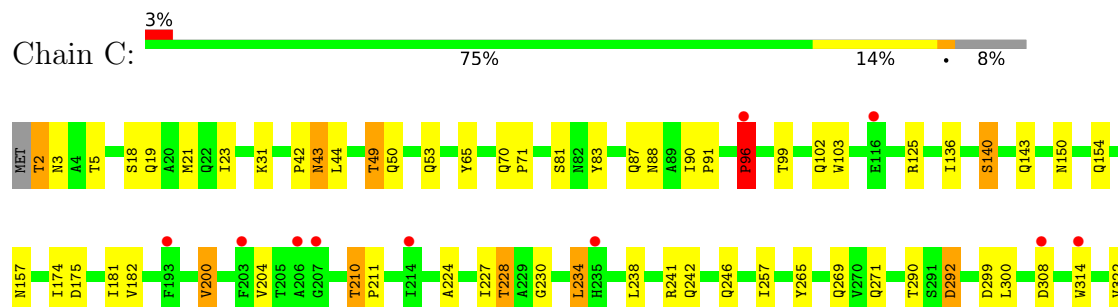
• Molecule 1: AhlB

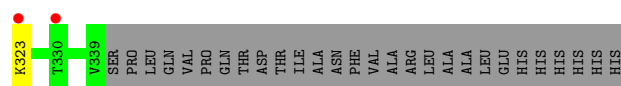


• Molecule 1: AhlB

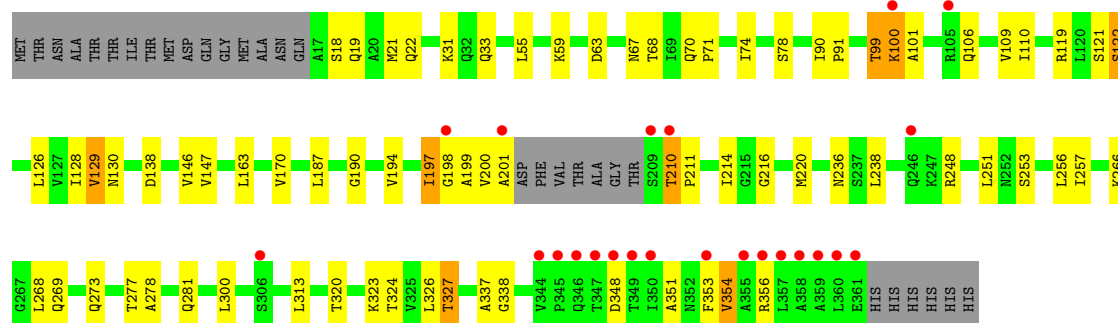


• Molecule 1: AhlB

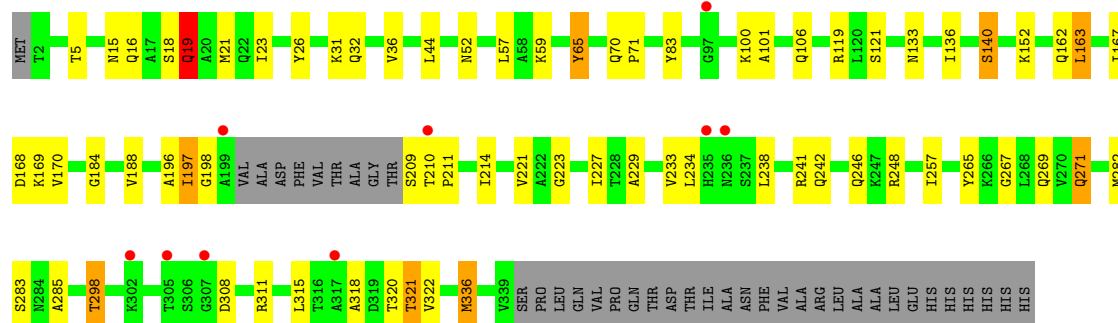




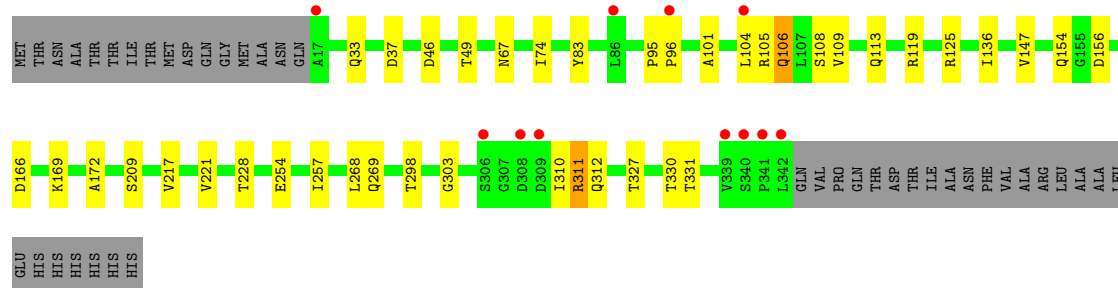
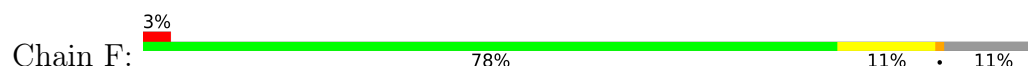
• Molecule 1: AhlB



• Molecule 1: AhlB

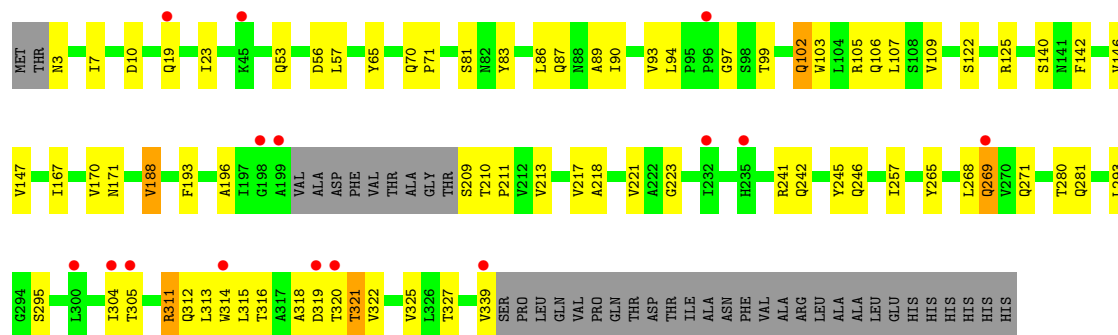


• Molecule 1: AhlB

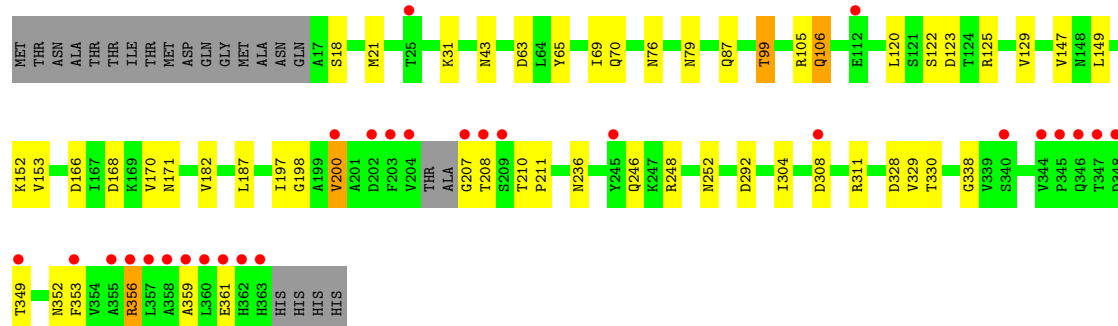
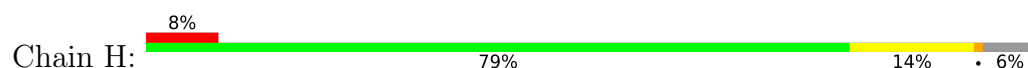


• Molecule 1: AhlB

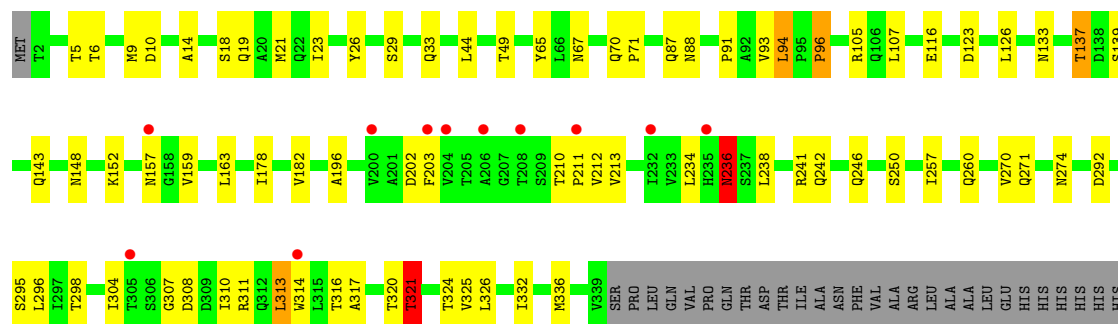




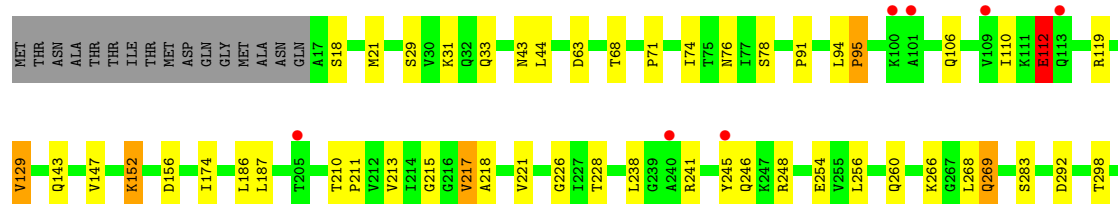
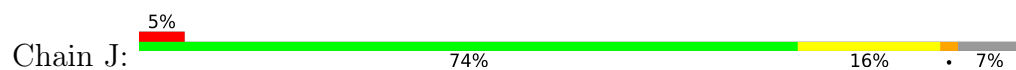
• Molecule 1: AhlB



• Molecule 1: AhlB



• Molecule 1: AhlB





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	117.66Å 178.18Å 485.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.55 – 2.55 39.55 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.55-2.55) 99.8 (39.55-2.55)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.191 , 0.278 (Not available) , 0.251	Depositor DCC
R_{free} test set	8387 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24766	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.93	1/2460 (0.0%)	1.39	10/3350 (0.3%)
1	B	0.96	1/2562 (0.0%)	1.33	9/3495 (0.3%)
1	C	0.96	1/2511 (0.0%)	1.36	7/3422 (0.2%)
1	D	0.94	2/2520 (0.1%)	1.36	8/3435 (0.2%)
1	E	0.94	0/2448	1.37	10/3333 (0.3%)
1	F	0.93	0/2425	1.37	6/3306 (0.2%)
1	G	0.95	3/2441 (0.1%)	1.37	8/3323 (0.2%)
1	H	0.93	0/2580	1.36	8/3517 (0.2%)
1	I	0.95	1/2511 (0.0%)	1.35	7/3422 (0.2%)
1	J	0.95	1/2554 (0.0%)	1.39	15/3484 (0.4%)
All	All	0.94	10/25012 (0.0%)	1.36	88/34087 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	2
1	E	0	2
1	F	0	3
1	G	0	2
1	H	0	5
1	I	0	1
1	J	0	3
All	All	0	21

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	269	GLN	N-CA	7.12	1.55	1.46
1	C	50	GLN	N-CA	6.72	1.54	1.46
1	G	97	GLY	N-CA	6.68	1.55	1.45
1	D	122	SER	N-CA	6.61	1.54	1.46
1	J	29	SER	N-CA	-5.87	1.39	1.46
1	D	128	ILE	C-O	5.61	1.31	1.24
1	B	305	THR	C-O	-5.31	1.17	1.24
1	I	44	LEU	N-CA	5.27	1.52	1.46
1	G	3	ASN	N-CA	5.22	1.56	1.46
1	A	187	LEU	N-CA	5.19	1.52	1.46

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	THR	CA-CB-OG1	-7.78	97.94	109.60
1	H	308	ASP	CB-CA-C	-7.38	108.07	116.63
1	J	91	PRO	CB-CA-C	7.12	117.85	111.87
1	D	327	THR	CA-CB-OG1	-7.02	99.07	109.60
1	I	203	PHE	CA-CB-CG	6.93	120.73	113.80
1	H	99	THR	CB-CA-C	-6.83	97.61	110.51
1	C	49	THR	CA-CB-OG1	-6.52	99.83	109.60
1	B	202	ASP	CA-CB-CG	6.31	118.91	112.60
1	E	133	ASN	CA-CB-CG	6.19	118.79	112.60
1	E	298	THR	CA-CB-OG1	-6.16	100.37	109.60
1	G	269	GLN	N-CA-CB	6.08	119.17	110.16
1	B	25	THR	CA-CB-OG1	-6.08	100.48	109.60
1	J	76	ASN	CB-CA-C	5.91	120.27	110.81
1	B	224	ALA	CA-C-N	5.89	126.48	119.94
1	B	224	ALA	C-N-CA	5.89	126.48	119.94
1	F	166	ASP	CA-CB-CG	5.88	118.48	112.60
1	G	293	LEU	CA-C-N	5.87	126.45	119.94
1	G	293	LEU	C-N-CA	5.87	126.45	119.94
1	A	277	THR	CA-CB-OG1	-5.84	100.84	109.60
1	E	308	ASP	CA-CB-CG	5.78	118.38	112.60
1	B	327	THR	CA-CB-OG1	-5.74	100.99	109.60
1	E	101	ALA	CA-C-N	5.71	128.19	120.65
1	E	101	ALA	C-N-CA	5.71	128.19	120.65
1	A	247	LYS	N-CA-C	-5.69	105.00	111.14
1	J	112	GLU	CA-C-N	5.66	128.12	120.65
1	J	112	GLU	C-N-CA	5.66	128.12	120.65
1	J	320	THR	CA-C-N	5.64	127.84	120.28
1	J	320	THR	C-N-CA	5.64	127.84	120.28
1	J	316	THR	CA-C-N	5.62	128.12	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	316	THR	C-N-CA	5.62	128.12	120.54
1	H	353	PHE	CA-CB-CG	5.60	119.40	113.80
1	A	278	ALA	CA-C-N	5.59	128.23	120.29
1	A	278	ALA	C-N-CA	5.59	128.23	120.29
1	B	129	VAL	N-CA-CB	5.59	119.89	110.56
1	G	171	ASN	CA-C-N	5.54	127.98	120.44
1	G	171	ASN	C-N-CA	5.54	127.98	120.44
1	I	49	THR	CB-CA-C	5.50	120.81	110.63
1	A	75	THR	CA-CB-OG1	-5.45	101.42	109.60
1	J	91	PRO	N-CA-C	-5.43	101.72	110.74
1	J	95	PRO	N-CA-C	5.38	116.34	110.58
1	E	16	GLN	CA-C-N	5.37	127.74	120.65
1	E	16	GLN	C-N-CA	5.37	127.74	120.65
1	C	175	ASP	CA-C-N	5.37	125.91	120.00
1	C	175	ASP	C-N-CA	5.37	125.91	120.00
1	B	316	THR	CA-CB-OG1	-5.37	101.55	109.60
1	D	99	THR	CA-CB-OG1	-5.34	101.59	109.60
1	C	96	PRO	N-CA-C	5.31	123.41	112.47
1	F	106	GLN	CA-C-N	5.30	127.69	120.54
1	F	106	GLN	C-N-CA	5.30	127.69	120.54
1	E	271	GLN	CB-CA-C	5.27	120.79	110.67
1	F	330	THR	CB-CA-C	5.25	119.78	110.85
1	H	308	ASP	CA-C-N	5.25	128.29	120.31
1	H	308	ASP	C-N-CA	5.25	128.29	120.31
1	I	67	ASN	CB-CA-C	5.24	118.36	109.55
1	I	321	THR	CB-CA-C	5.23	120.28	110.70
1	E	65	TYR	N-CA-CB	5.23	117.59	110.01
1	A	271	GLN	CB-CA-C	5.22	119.46	110.79
1	G	245	TYR	CA-C-N	5.22	127.70	120.29
1	G	245	TYR	C-N-CA	5.22	127.70	120.29
1	D	238	LEU	CA-C-N	5.22	125.73	119.94
1	D	238	LEU	C-N-CA	5.22	125.73	119.94
1	J	228	THR	CA-CB-OG1	-5.22	101.78	109.60
1	B	56	ASP	CA-CB-CG	-5.21	107.39	112.60
1	B	208	THR	CA-CB-OG1	-5.21	101.78	109.60
1	I	236	ASN	CB-CA-C	-5.21	104.81	111.22
1	C	292	ASP	CB-CA-C	5.20	118.97	110.96
1	H	123	ASP	CA-CB-CG	5.20	117.80	112.60
1	J	302	LYS	CA-C-N	5.19	125.70	119.94
1	J	302	LYS	C-N-CA	5.19	125.70	119.94
1	F	298	THR	CA-CB-OG1	-5.19	101.82	109.60
1	F	331	THR	CA-CB-OG1	-5.18	101.83	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	326	LEU	CA-C-N	5.17	127.16	120.44
1	I	326	LEU	C-N-CA	5.17	127.16	120.44
1	J	324	THR	CA-CB-OG1	-5.15	101.87	109.60
1	C	299	ASP	CA-C-N	5.13	127.47	120.54
1	C	299	ASP	C-N-CA	5.13	127.47	120.54
1	D	138	ASP	N-CA-C	-5.12	105.59	111.07
1	A	252	ASN	CA-CB-CG	5.12	117.72	112.60
1	G	268	LEU	CA-C-O	-5.09	114.11	119.97
1	D	326	LEU	CA-C-N	5.08	127.04	120.44
1	D	326	LEU	C-N-CA	5.08	127.04	120.44
1	J	129	VAL	N-CA-CB	5.08	117.45	110.54
1	H	330	THR	CB-CA-C	5.07	120.41	110.67
1	H	330	THR	N-CA-C	-5.07	105.94	111.82
1	D	100	LYS	N-CA-C	-5.06	105.45	110.97
1	A	78	SER	O-C-N	5.06	127.35	122.09
1	A	91	PRO	CB-CA-C	-5.04	104.69	111.85
1	E	19	GLN	CB-CG-CD	5.01	121.12	112.60

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	248	ARG	Sidechain
1	B	311	ARG	Sidechain
1	C	125	ARG	Sidechain
1	D	119	ARG	Sidechain
1	D	248	ARG	Sidechain
1	E	119	ARG	Sidechain
1	E	248	ARG	Sidechain
1	F	119	ARG	Sidechain
1	F	125	ARG	Sidechain
1	F	311	ARG	Sidechain
1	G	241	ARG	Sidechain
1	G	311	ARG	Sidechain
1	H	105	ARG	Sidechain
1	H	125	ARG	Sidechain
1	H	207	GLY	Peptide
1	H	248	ARG	Sidechain
1	H	356	ARG	Sidechain
1	I	241	ARG	Sidechain
1	J	119	ARG	Sidechain
1	J	241	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	J	248	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2436	0	2465	25	0
1	B	2533	0	2571	29	0
1	C	2485	0	2510	36	0
1	D	2493	0	2532	44	0
1	E	2424	0	2451	36	0
1	F	2398	0	2431	20	0
1	G	2417	0	2444	44	0
1	H	2550	0	2578	26	0
1	I	2485	0	2510	44	0
1	J	2525	0	2560	41	0
2	A	5	0	0	0	0
2	C	5	0	0	2	0
2	G	5	0	0	0	0
2	I	5	0	0	0	0
All	All	24766	0	25052	309	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 6.

All (309) 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:I:242:GLN:O	1:I:246:GLN:HG2	1.66	0.93
1:J:302:LYS:O	1:J:306:SER:OG	1.95	0.83
1:A:307:GLY:O	1:A:310:ILE:HG22	1.80	0.80
1:I:139:SER:O	1:I:143:GLN:HG2	1.84	0.77
1:G:94:LEU:O	1:G:311:ARG:NH1	2.18	0.76
1:H:252:ASN:ND2	1:H:361:GLU:HG2	2.03	0.74
1:J:21:MET:HE2	1:J:338:GLY:HA3	1.70	0.74
1:I:316:THR:O	1:I:320:THR:HG22	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:LEU:HD21	1:E:242:GLN:HE22	1.53	0.72
1:G:210:THR:N	1:G:211:PRO:HD2	2.05	0.72
1:B:197:ILE:HG21	1:E:214:ILE:HD13	1.71	0.71
1:C:96:PRO:O	1:C:308:ASP:OD1	2.09	0.70
1:I:96:PRO:O	1:I:308:ASP:OD1	2.11	0.68
1:I:210:THR:HA	1:I:213:VAL:HG12	1.74	0.68
1:J:215:GLY:O	1:J:218:ALA:HB3	1.94	0.68
1:J:112:GLU:OE2	1:J:112:GLU:HA	1.94	0.68
1:H:43:ASN:O	1:H:152:LYS:HE2	1.95	0.66
1:D:31:LYS:HE2	1:D:63:ASP:OD1	1.95	0.66
1:G:70:GLN:HB3	1:G:71:PRO:HD3	1.77	0.66
1:D:210:THR:H	1:D:211:PRO:HD2	1.61	0.65
1:H:252:ASN:HD22	1:H:361:GLU:HG2	1.60	0.65
1:I:87:GLN:HG3	1:I:314:TRP:CZ3	2.32	0.64
1:B:113:GLN:NE2	1:B:117:TYR:CE2	2.65	0.64
1:H:87:GLN:HE22	1:H:106:GLN:NE2	1.97	0.63
1:C:204:VAL:HG12	1:C:204:VAL:O	1.99	0.62
1:I:94:LEU:O	1:I:311:ARG:NH1	2.31	0.62
1:J:292:ASP:OD2	1:J:328:ASP:OD2	2.18	0.62
1:J:210:THR:N	1:J:211:PRO:HD2	2.14	0.62
1:D:21:MET:HE2	1:D:338:GLY:HA3	1.82	0.62
1:F:147:VAL:HG11	1:I:257:ILE:HD11	1.82	0.62
1:H:252:ASN:ND2	1:H:361:GLU:CG	2.62	0.62
1:H:252:ASN:HD22	1:H:361:GLU:CG	2.11	0.62
1:A:257:ILE:HD11	1:H:147:VAL:HG11	1.82	0.61
1:A:307:GLY:O	1:A:310:ILE:CG2	2.49	0.61
1:D:200:VAL:O	1:D:201:ALA:CB	2.48	0.61
1:H:31:LYS:HE3	1:H:63:ASP:OD1	2.00	0.61
1:D:348:ASP:OD1	1:D:356:ARG:NH1	2.35	0.60
1:A:93:VAL:HG12	1:A:94:LEU:HD13	1.83	0.60
1:F:67:ASN:ND2	1:G:281:GLN:OE1	2.34	0.60
1:G:109:VAL:HG21	1:J:310:ILE:HD13	1.84	0.60
1:I:133:ASN:O	1:I:137:THR:HG22	2.02	0.60
1:C:224:ALA:O	1:C:228:THR:HG23	2.02	0.59
1:H:87:GLN:HE22	1:H:106:GLN:HE21	1.49	0.59
1:D:273:GLN:HG2	1:E:32:GLN:OE1	2.02	0.59
1:E:184:GLY:O	1:E:188:VAL:HG23	2.02	0.59
1:A:311:ARG:NH2	1:A:311:ARG:HG3	2.17	0.58
1:G:23:ILE:HB	1:G:271:GLN:HG3	1.84	0.58
1:D:198:GLY:C	1:D:200:VAL:H	2.11	0.58
1:E:318:ALA:HA	1:E:322:VAL:HB	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:99:THR:OG1	1:G:102:GLN:HG2	2.04	0.57
1:G:304:ILE:O	1:G:305:THR:HG23	2.05	0.57
1:I:5:THR:OG1	1:I:292:ASP:OD2	2.17	0.57
1:G:320:THR:HG23	1:G:321:THR:H	1.69	0.57
1:D:163:LEU:HD12	1:E:241:ARG:NH2	2.19	0.56
1:D:210:THR:H	1:D:211:PRO:CD	2.17	0.56
1:A:23:ILE:HB	1:A:271:GLN:HG3	1.87	0.56
1:C:242:GLN:O	1:C:246:GLN:HG2	2.05	0.56
1:F:101:ALA:O	1:F:105:ARG:HG3	2.06	0.56
1:A:99:THR:O	1:A:102:GLN:HG2	2.05	0.56
1:I:320:THR:HG23	1:I:321:THR:H	1.70	0.56
1:C:136:ILE:O	1:C:140:SER:OG	2.24	0.56
1:E:196:ALA:C	1:E:198:GLY:H	2.14	0.55
1:H:349:THR:OG1	1:H:352:ASN:OD1	2.19	0.55
1:B:218:ALA:HB1	1:C:200:VAL:HG21	1.88	0.55
1:C:290:THR:CB	2:C:401:PO4:O2	2.54	0.55
1:E:18:SER:HA	1:E:21:MET:HE3	1.87	0.55
1:G:10:ASP:HB2	1:G:325:VAL:HG22	1.88	0.55
1:A:187:LEU:HD11	1:J:186:LEU:HD13	1.89	0.55
1:I:23:ILE:HB	1:I:271:GLN:HG3	1.89	0.55
1:B:41:PHE:CD1	1:B:254:GLU:HG3	2.41	0.55
1:D:19:GLN:N	1:D:19:GLN:OE1	2.39	0.55
1:E:242:GLN:O	1:E:246:GLN:HG2	2.06	0.55
1:B:173:ALA:HB2	1:C:182:VAL:HG22	1.88	0.55
1:D:277:THR:O	1:D:281:GLN:HG3	2.06	0.55
1:G:167:ILE:O	1:G:170:VAL:HG12	2.06	0.55
1:J:74:ILE:O	1:J:78:SER:OG	2.23	0.55
1:G:209:SER:C	1:G:211:PRO:HD2	2.31	0.54
1:F:310:ILE:HD11	1:I:105:ARG:HG2	1.89	0.54
1:C:290:THR:OG1	2:C:401:PO4:O2	2.20	0.54
1:I:6:THR:HG21	1:I:321:THR:HG23	1.88	0.54
1:B:174:ILE:HG13	1:B:237:SER:HB3	1.88	0.54
1:J:143:GLN:HA	1:J:143:GLN:NE2	2.23	0.54
1:B:156:ASP:OD2	1:B:254:GLU:OE2	2.26	0.54
1:D:190:GLY:O	1:D:194:VAL:HG23	2.08	0.54
1:E:311:ARG:O	1:E:315:LEU:HG	2.08	0.54
1:B:33:GLN:HG3	1:B:268:LEU:HD11	1.89	0.53
1:F:46:ASP:HA	1:F:49:THR:HG22	1.91	0.53
1:A:217:VAL:O	1:A:221:VAL:HG13	2.09	0.53
1:G:316:THR:O	1:G:320:THR:HG22	2.09	0.53
1:H:18:SER:H	1:H:21:MET:HE3	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:218:ALA:HA	1:G:221:VAL:HG22	1.91	0.53
1:C:210:THR:N	1:C:211:PRO:HD2	2.24	0.53
1:F:104:LEU:HD21	1:F:311:ARG:NH1	2.24	0.53
1:B:113:GLN:NE2	1:B:117:TYR:CZ	2.78	0.53
1:E:234:LEU:O	1:E:238:LEU:HG	2.09	0.53
1:G:320:THR:HG23	1:G:321:THR:N	2.24	0.53
1:A:70:GLN:HB3	1:A:71:PRO:HD3	1.91	0.52
1:F:83:TYR:CZ	1:F:113:GLN:HG3	2.44	0.52
1:F:83:TYR:CE1	1:F:113:GLN:HG3	2.44	0.52
1:C:103:TRP:HB3	1:C:300:LEU:HD21	1.91	0.52
1:D:147:VAL:HG11	1:E:257:ILE:HD11	1.91	0.52
1:H:208:THR:HG23	1:H:208:THR:O	2.10	0.52
1:I:10:ASP:HB2	1:I:325:VAL:HG22	1.92	0.52
1:F:106:GLN:O	1:F:109:VAL:HB	2.11	0.51
1:G:142:PHE:O	1:G:146:VAL:HG23	2.10	0.51
1:E:167:ILE:O	1:E:170:VAL:HG12	2.10	0.51
1:B:256:LEU:HD23	1:B:353:PHE:CZ	2.45	0.51
1:C:210:THR:N	1:C:211:PRO:CD	2.74	0.51
1:J:33:GLN:HG3	1:J:268:LEU:HD11	1.91	0.51
1:A:90:ILE:HG23	1:A:106:GLN:HE21	1.75	0.51
1:D:256:LEU:HD23	1:D:353:PHE:CE1	2.45	0.51
1:A:311:ARG:HG3	1:A:311:ARG:HH21	1.74	0.51
1:D:33:GLN:HG3	1:D:268:LEU:HD11	1.93	0.51
1:G:105:ARG:HH12	1:J:309:ASP:CG	2.19	0.51
1:H:304:ILE:HA	1:H:311:ARG:HH12	1.76	0.50
1:D:31:LYS:HA	1:D:59:LYS:HG2	1.93	0.50
1:G:93:VAL:HG22	1:J:312:GLN:HG2	1.94	0.50
1:D:236:ASN:ND2	1:E:227:ILE:HG23	2.27	0.50
1:E:23:ILE:HB	1:E:271:GLN:HG3	1.94	0.50
1:F:33:GLN:HG3	1:F:268:LEU:HD11	1.94	0.50
1:I:321:THR:O	1:I:324:THR:HB	2.12	0.50
1:G:242:GLN:HE21	1:J:43:ASN:ND2	2.10	0.50
1:I:87:GLN:HG3	1:I:314:TRP:CH2	2.46	0.50
1:A:23:ILE:HA	1:A:271:GLN:HG2	1.94	0.49
1:D:100:LYS:O	1:D:101:ALA:C	2.54	0.49
1:G:213:VAL:O	1:G:217:VAL:HG23	2.12	0.49
1:I:236:ASN:N	1:I:236:ASN:OD1	2.45	0.49
1:B:233:VAL:O	1:B:237:SER:HB2	2.13	0.49
1:G:83:TYR:CD2	1:G:83:TYR:C	2.91	0.49
1:F:169:LYS:O	1:F:172:ALA:HB3	2.13	0.49
1:D:253:SER:O	1:D:257:ILE:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:ARG:NH1	1:B:283:SER:HB3	2.28	0.49
1:J:210:THR:N	1:J:211:PRO:CD	2.76	0.49
1:J:213:VAL:O	1:J:217:VAL:HG13	2.13	0.49
1:B:21:MET:HE2	1:B:338:GLY:HA3	1.94	0.49
1:C:181:ILE:HG13	1:C:230:GLY:HA3	1.95	0.49
1:G:210:THR:N	1:G:211:PRO:CD	2.75	0.49
1:C:204:VAL:O	1:C:204:VAL:CG1	2.62	0.48
1:B:303:GLY:O	1:B:311:ARG:HD3	2.13	0.48
1:F:303:GLY:O	1:F:311:ARG:HG3	2.13	0.48
1:C:87:GLN:HG3	1:C:314:TRP:CZ3	2.49	0.48
1:G:318:ALA:HA	1:G:322:VAL:HB	1.94	0.48
1:B:21:MET:HE2	1:B:337:ALA:O	2.13	0.48
1:B:147:VAL:HG11	1:C:257:ILE:HD11	1.95	0.48
1:C:23:ILE:HG23	1:C:65:TYR:CZ	2.48	0.48
1:G:188:VAL:HG12	1:G:223:GLY:HA3	1.94	0.48
1:A:282:MET:HE3	1:A:285:ALA:HB3	1.95	0.48
1:B:133:ASN:OD1	1:C:31:LYS:NZ	2.44	0.48
1:E:70:GLN:HE22	1:E:336:MET:HE2	1.77	0.48
1:J:143:GLN:CD	1:J:269:GLN:HE22	2.22	0.48
1:C:87:GLN:HG3	1:C:314:TRP:CH2	2.49	0.48
1:G:23:ILE:HA	1:G:271:GLN:HG2	1.94	0.48
1:G:257:ILE:HD11	1:J:147:VAL:HG11	1.94	0.48
1:A:104:LEU:HD23	1:A:300:LEU:HD23	1.96	0.48
1:B:70:GLN:HB3	1:B:71:PRO:HD3	1.96	0.48
1:C:83:TYR:C	1:C:83:TYR:CD2	2.91	0.48
1:C:18:SER:HA	1:C:21:MET:HE3	1.95	0.48
1:J:18:SER:H	1:J:21:MET:HE3	1.79	0.48
1:E:136:ILE:O	1:E:140:SER:OG	2.31	0.48
1:J:260:GLN:HE21	1:J:356:ARG:HH11	1.62	0.48
1:C:227:ILE:O	1:C:228:THR:C	2.57	0.47
1:G:90:ILE:HD12	1:G:314:TRP:CZ3	2.49	0.47
1:J:326:LEU:O	1:J:330:THR:HG23	2.14	0.47
1:H:65:TYR:CZ	1:H:70:GLN:HB2	2.50	0.47
1:F:74:ILE:HG22	1:G:7:ILE:HD12	1.96	0.47
1:E:320:THR:OG1	1:E:321:THR:N	2.48	0.47
1:G:94:LEU:HD21	1:G:106:GLN:HG3	1.97	0.47
1:I:210:THR:N	1:I:211:PRO:CD	2.78	0.47
1:B:68:THR:C	1:B:71:PRO:HD2	2.39	0.47
1:D:313:LEU:HD22	1:E:106:GLN:OE1	2.15	0.47
1:I:178:ILE:O	1:I:182:VAL:HG23	2.15	0.47
1:G:105:ARG:NH1	1:J:309:ASP:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:THR:N	1:B:211:PRO:CD	2.78	0.47
1:F:312:GLN:HG2	1:I:93:VAL:HG22	1.97	0.47
1:G:339:VAL:HG12	1:G:339:VAL:O	2.15	0.47
1:I:23:ILE:HG23	1:I:65:TYR:CZ	2.50	0.47
1:J:68:THR:C	1:J:71:PRO:HD2	2.40	0.47
1:D:320:THR:O	1:D:323:LYS:HB2	2.15	0.46
1:H:43:ASN:O	1:H:152:LYS:CE	2.63	0.46
1:H:166:ASP:O	1:H:170:VAL:HG23	2.15	0.46
1:C:70:GLN:HB3	1:C:71:PRO:HD3	1.98	0.46
1:D:210:THR:N	1:D:211:PRO:CD	2.79	0.46
1:B:204:VAL:HG23	1:B:204:VAL:O	2.16	0.46
1:J:31:LYS:HE3	1:J:63:ASP:OD1	2.16	0.46
1:A:83:TYR:CD2	1:A:83:TYR:C	2.94	0.46
1:E:229:ALA:O	1:E:233:VAL:HG23	2.16	0.46
1:J:345:PRO:O	1:J:347:THR:HG23	2.16	0.45
1:B:193:PHE:HB2	1:E:221:VAL:HG21	1.98	0.45
1:F:221:VAL:HG12	1:I:196:ALA:HB1	1.98	0.45
1:D:210:THR:N	1:D:211:PRO:HD2	2.28	0.45
1:F:37:ASP:OD1	1:F:37:ASP:C	2.58	0.45
1:I:33:GLN:NE2	1:I:260:GLN:OE1	2.45	0.45
1:H:168:ASP:O	1:H:171:ASN:HB2	2.17	0.45
1:I:88:ASN:O	1:I:91:PRO:HD2	2.16	0.45
1:B:18:SER:HB3	1:B:21:MET:HE3	1.98	0.45
1:C:234:LEU:O	1:C:238:LEU:HG	2.17	0.45
1:A:210:THR:N	1:A:211:PRO:CD	2.80	0.45
1:E:70:GLN:HB3	1:E:71:PRO:HD3	1.98	0.45
1:I:123:ASP:O	1:I:126:LEU:HB2	2.17	0.45
1:H:210:THR:N	1:H:211:PRO:CD	2.80	0.45
1:E:26:TYR:OH	1:E:267:GLY:HA3	2.17	0.45
1:G:312:GLN:O	1:G:313:LEU:C	2.59	0.45
1:I:14:ALA:HA	1:I:332:ILE:HD11	1.99	0.44
1:D:18:SER:H	1:D:21:MET:HE3	1.82	0.44
1:I:70:GLN:N	1:I:71:PRO:CD	2.81	0.44
1:I:234:LEU:O	1:I:238:LEU:HG	2.17	0.44
1:G:65:TYR:CD2	1:G:65:TYR:C	2.96	0.44
1:D:70:GLN:HB3	1:D:71:PRO:HD3	1.99	0.44
1:I:19:GLN:NE2	1:I:274:ASN:HB2	2.33	0.44
1:E:184:GLY:HA2	1:E:223:GLY:HA2	1.98	0.44
1:A:19:GLN:O	1:A:22:GLN:HB2	2.17	0.44
1:E:15:ASN:O	1:E:19:GLN:HB3	2.18	0.44
1:G:193:PHE:CZ	1:J:226:GLY:HA3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:THR:HG22	1:C:5:THR:H	1.83	0.44
1:C:42:PRO:C	1:C:44:LEU:H	2.26	0.44
1:J:43:ASN:ND2	1:J:254:GLU:OE2	2.44	0.43
1:D:33:GLN:HB2	1:D:55:LEU:HD11	2.00	0.43
1:G:87:GLN:HG3	1:G:314:TRP:CZ3	2.52	0.43
1:I:5:THR:CB	1:I:292:ASP:OD2	2.66	0.43
1:D:19:GLN:HB3	1:D:278:ALA:HB1	2.01	0.43
1:F:95:PRO:O	1:F:96:PRO:C	2.62	0.43
1:I:70:GLN:HB3	1:I:71:PRO:HD3	2.00	0.43
1:A:90:ILE:HB	1:A:91:PRO:HD3	2.00	0.43
1:A:142:PHE:CZ	1:A:261:ILE:HG22	2.53	0.43
1:C:88:ASN:HD21	1:C:322:VAL:HG11	1.83	0.43
1:H:292:ASP:OD2	1:H:328:ASP:OD2	2.37	0.43
1:C:49:THR:O	1:C:53:GLN:HG3	2.18	0.43
1:H:21:MET:HE2	1:H:338:GLY:HA3	1.99	0.43
1:I:320:THR:HG23	1:I:321:THR:N	2.34	0.43
1:I:316:THR:O	1:I:317:ALA:C	2.62	0.43
1:G:86:LEU:O	1:G:89:ALA:HB3	2.19	0.42
1:B:152:LYS:HA	1:B:152:LYS:HD2	1.82	0.42
1:G:246:GLN:NE2	1:J:156:ASP:OD1	2.52	0.42
1:B:142:PHE:HA	1:B:145:ILE:HD12	2.02	0.42
1:G:53:GLN:O	1:G:56:ASP:HB2	2.19	0.42
1:I:18:SER:HA	1:I:21:MET:HE3	2.02	0.42
1:C:99:THR:OG1	1:C:102:GLN:HG2	2.18	0.42
1:D:163:LEU:CD1	1:E:241:ARG:NH2	2.82	0.42
1:J:174:ILE:HD13	1:J:238:LEU:HD23	2.00	0.42
1:C:150:ASN:O	1:C:154:GLN:HB2	2.19	0.42
1:H:76:ASN:ND2	1:H:120:LEU:HD11	2.35	0.42
1:J:44:LEU:HD23	1:J:152:LYS:HG3	2.02	0.42
1:J:260:GLN:NE2	1:J:356:ARG:HH11	2.18	0.42
1:D:197:ILE:HD13	1:D:197:ILE:HA	1.92	0.42
1:E:282:MET:HE3	1:E:285:ALA:HB3	2.02	0.42
1:E:163:LEU:O	1:E:167:ILE:HG13	2.19	0.42
1:E:83:TYR:CD2	1:E:83:TYR:C	2.97	0.42
1:G:125:ARG:HD2	1:G:280:THR:HA	2.02	0.42
1:D:146:VAL:CG1	1:D:266:LYS:HE2	2.49	0.42
1:E:36:VAL:HG22	1:E:52:ASN:OD1	2.20	0.42
1:H:356:ARG:O	1:H:359:ALA:HB3	2.19	0.42
1:D:91:PRO:HG3	1:D:106:GLN:NE2	2.34	0.41
1:D:324:THR:O	1:D:327:THR:HB	2.20	0.41
1:J:31:LYS:HD2	1:J:63:ASP:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:303:GLY:O	1:J:311:ARG:HG3	2.20	0.41
1:D:216:GLY:O	1:D:220:MET:HG3	2.20	0.41
1:E:44:LEU:HD23	1:E:152:LYS:HE2	2.02	0.41
1:E:196:ALA:C	1:E:198:GLY:N	2.77	0.41
1:H:65:TYR:HA	1:H:69:ILE:HB	2.02	0.41
1:J:152:LYS:HD2	1:J:152:LYS:HA	1.96	0.41
1:G:196:ALA:HB1	1:J:221:VAL:HG12	2.02	0.41
1:I:152:LYS:O	1:I:159:VAL:HG23	2.19	0.41
1:B:306:SER:HB3	1:B:310:ILE:HG22	2.02	0.41
1:I:26:TYR:O	1:I:29:SER:HB2	2.20	0.41
1:I:65:TYR:CD2	1:I:65:TYR:C	2.98	0.41
1:B:157:ASN:HA	1:B:160:LEU:HD12	2.01	0.41
1:C:3:ASN:ND2	1:H:79:ASN:OD1	2.49	0.41
1:C:90:ILE:N	1:C:91:PRO:HD2	2.35	0.41
1:D:74:ILE:O	1:D:78:SER:OG	2.25	0.41
1:D:126:LEU:HA	1:D:129:VAL:HG13	2.01	0.41
1:J:106:GLN:O	1:J:110:ILE:HG13	2.20	0.41
1:D:146:VAL:HG13	1:D:266:LYS:HE2	2.03	0.41
1:G:103:TRP:O	1:G:107:LEU:HG	2.20	0.41
1:G:242:GLN:O	1:G:246:GLN:HG2	2.20	0.41
1:J:324:THR:O	1:J:327:THR:HB	2.20	0.41
1:C:2:THR:HB	1:C:292:ASP:OD2	2.20	0.41
1:H:198:GLY:C	1:H:200:VAL:H	2.29	0.41
1:I:6:THR:O	1:I:9:MET:HB2	2.20	0.41
1:D:106:GLN:O	1:D:110:ILE:HG13	2.21	0.41
1:F:74:ILE:CG2	1:G:7:ILE:HD12	2.50	0.41
1:J:94:LEU:HA	1:J:95:PRO:HD3	1.94	0.41
1:A:250:SER:O	1:A:254:GLU:HG2	2.20	0.41
1:B:18:SER:H	1:B:21:MET:HE3	1.85	0.41
1:D:21:MET:HE2	1:D:337:ALA:O	2.21	0.41
1:D:67:ASN:OD1	1:D:67:ASN:C	2.64	0.41
1:D:68:THR:C	1:D:71:PRO:HD2	2.46	0.41
1:D:90:ILE:HD12	1:D:300:LEU:HD21	2.02	0.41
1:D:354:VAL:CG1	1:F:154:GLN:HG3	2.51	0.41
1:G:70:GLN:N	1:G:71:PRO:CD	2.84	0.41
1:A:187:LEU:CD1	1:J:186:LEU:HD13	2.50	0.41
1:C:174:ILE:HD13	1:C:241:ARG:CZ	2.51	0.41
1:F:156:ASP:OD2	1:F:254:GLU:OE2	2.39	0.41
1:A:13:MET:HE3	1:A:332:ILE:HD12	2.03	0.40
1:C:23:ILE:HA	1:C:271:GLN:CG	2.52	0.40
1:A:220:MET:HE2	1:A:220:MET:HB3	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:PRO:C	1:C:44:LEU:N	2.78	0.40
1:E:65:TYR:CD2	1:E:65:TYR:C	2.98	0.40
1:A:65:TYR:CD2	1:A:65:TYR:C	2.99	0.40
1:I:19:GLN:NE2	1:I:274:ASN:CB	2.84	0.40
1:I:296:LEU:HA	1:I:296:LEU:HD23	1.84	0.40
1:I:313:LEU:HA	1:I:313:LEU:HD12	1.88	0.40
1:E:31:LYS:HA	1:E:59:LYS:HD3	2.02	0.40
1:H:149:LEU:O	1:H:153:VAL:HG23	2.22	0.40
1:I:307:GLY:O	1:I:310:ILE:HG22	2.22	0.40
1:B:241:ARG:HH21	1:E:168:ASP:CG	2.30	0.40
1:D:251:LEU:HD21	1:E:242:GLN:NE2	2.30	0.40
1:I:87:GLN:O	1:I:314:TRP:HZ3	2.04	0.40
1:J:256:LEU:HD11	1:J:356:ARG:HB3	2.03	0.40
1:J:266:LYS:HA	1:J:266:LYS:HD2	1.93	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	327/367 (89%)	316 (97%)	10 (3%)	1 (0%)	36	45
1	B	342/367 (93%)	337 (98%)	4 (1%)	1 (0%)	36	45
1	C	336/367 (92%)	320 (95%)	15 (4%)	1 (0%)	36	45
1	D	334/367 (91%)	322 (96%)	8 (2%)	4 (1%)	10	13
1	E	325/367 (89%)	313 (96%)	11 (3%)	1 (0%)	36	45
1	F	324/367 (88%)	305 (94%)	19 (6%)	0	100	100
1	G	324/367 (88%)	315 (97%)	9 (3%)	0	100	100
1	H	341/367 (93%)	326 (96%)	15 (4%)	0	100	100
1	I	336/367 (92%)	321 (96%)	14 (4%)	1 (0%)	36	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	341/367 (93%)	325 (95%)	16 (5%)	0	100	100
All	All	3330/3670 (91%)	3200 (96%)	121 (4%)	9 (0%)	36	45

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	43	ASN
1	D	199	ALA
1	E	197	ILE
1	A	100	LYS
1	D	351	ALA
1	I	304	ILE
1	B	245	TYR
1	D	210	THR
1	D	197	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	265/295 (90%)	250 (94%)	15 (6%)	18	28
1	B	275/295 (93%)	260 (94%)	15 (6%)	19	29
1	C	270/295 (92%)	255 (94%)	15 (6%)	19	29
1	D	271/295 (92%)	259 (96%)	12 (4%)	25	38
1	E	264/295 (90%)	245 (93%)	19 (7%)	13	18
1	F	261/295 (88%)	253 (97%)	8 (3%)	35	53
1	G	263/295 (89%)	248 (94%)	15 (6%)	18	28
1	H	277/295 (94%)	266 (96%)	11 (4%)	28	42
1	I	270/295 (92%)	252 (93%)	18 (7%)	15	21
1	J	274/295 (93%)	261 (95%)	13 (5%)	23	36
All	All	2690/2950 (91%)	2549 (95%)	141 (5%)	21	32

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ASP
1	A	71	PRO
1	A	78	SER
1	A	94	LEU
1	A	107	LEU
1	A	121	SER
1	A	126	LEU
1	A	143	GLN
1	A	197	ILE
1	A	221	VAL
1	A	265	TYR
1	A	270	VAL
1	A	283	SER
1	A	311	ARG
1	A	331	THR
1	B	98	SER
1	B	113	GLN
1	B	122	SER
1	B	126	LEU
1	B	129	VAL
1	B	163	LEU
1	B	202	ASP
1	B	204	VAL
1	B	210	THR
1	B	242	GLN
1	B	245	TYR
1	B	250	SER
1	B	283	SER
1	B	288	SER
1	B	354	VAL
1	C	2	THR
1	C	19	GLN
1	C	43	ASN
1	C	81	SER
1	C	96	PRO
1	C	140	SER
1	C	143	GLN
1	C	157	ASN
1	C	200	VAL
1	C	210	THR
1	C	228	THR
1	C	234	LEU

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Mol	Chain	Res	Type
1	C	265	TYR
1	C	269	GLN
1	C	323	LYS
1	D	22	GLN
1	D	99	THR
1	D	109	VAL
1	D	121	SER
1	D	122	SER
1	D	129	VAL
1	D	130	ASN
1	D	170	VAL
1	D	187	LEU
1	D	214	ILE
1	D	269	GLN
1	D	354	VAL
1	E	5	THR
1	E	19	GLN
1	E	57	LEU
1	E	100	LYS
1	E	121	SER
1	E	140	SER
1	E	162	GLN
1	E	163	LEU
1	E	169	LYS
1	E	197	ILE
1	E	209	SER
1	E	210	THR
1	E	211	PRO
1	E	265	TYR
1	E	269	GLN
1	E	283	SER
1	E	298	THR
1	E	321	THR
1	E	336	MET
1	F	108	SER
1	F	136	ILE
1	F	209	SER
1	F	217	VAL
1	F	228	THR
1	F	257	ILE
1	F	269	GLN
1	F	327	THR

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Mol	Chain	Res	Type
1	G	19	GLN
1	G	57	LEU
1	G	81	SER
1	G	102	GLN
1	G	122	SER
1	G	140	SER
1	G	147	VAL
1	G	188	VAL
1	G	265	TYR
1	G	269	GLN
1	G	295	SER
1	G	315	LEU
1	G	319	ASP
1	G	321	THR
1	G	327	THR
1	H	99	THR
1	H	106	GLN
1	H	122	SER
1	H	129	VAL
1	H	182	VAL
1	H	187	LEU
1	H	197	ILE
1	H	200	VAL
1	H	236	ASN
1	H	246	GLN
1	H	329	VAL
1	I	94	LEU
1	I	96	PRO
1	I	107	LEU
1	I	116	GLU
1	I	137	THR
1	I	148	ASN
1	I	157	ASN
1	I	163	LEU
1	I	202	ASP
1	I	212	VAL
1	I	236	ASN
1	I	250	SER
1	I	270	VAL
1	I	295	SER
1	I	298	THR
1	I	313	LEU

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Mol	Chain	Res	Type
1	I	321	THR
1	I	336	MET
1	J	112	GLU
1	J	129	VAL
1	J	152	LYS
1	J	187	LEU
1	J	217	VAL
1	J	245	TYR
1	J	246	GLN
1	J	269	GLN
1	J	283	SER
1	J	298	THR
1	J	310	ILE
1	J	327	THR
1	J	344	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	19	GLN
1	A	40	GLN
1	A	72	GLN
1	A	82	ASN
1	A	106	GLN
1	B	32	GLN
1	B	130	ASN
1	B	352	ASN
1	C	40	GLN
1	C	70	GLN
1	C	72	GLN
1	C	87	GLN
1	C	269	GLN
1	D	113	GLN
1	D	171	ASN
1	D	236	ASN
1	E	16	GLN
1	E	82	ASN
1	E	113	GLN
1	E	132	ASN
1	E	242	GLN
1	E	246	GLN

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Mol	Chain	Res	Type
1	E	273	GLN
1	F	22	GLN
1	F	50	GLN
1	F	150	ASN
1	G	16	GLN
1	G	40	GLN
1	G	82	ASN
1	G	132	ASN
1	G	150	ASN
1	H	22	GLN
1	H	106	GLN
1	H	113	GLN
1	H	148	ASN
1	H	236	ASN
1	H	252	ASN
1	H	269	GLN
1	H	363	HIS
1	I	19	GLN
1	I	82	ASN
1	I	88	ASN
1	I	102	GLN
1	I	118	GLN
1	I	271	GLN
1	I	312	GLN
1	J	22	GLN
1	J	32	GLN
1	J	43	ASN
1	J	72	GLN
1	J	102	GLN
1	J	236	ASN
1	J	260	GLN
1	J	269	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](#)

4 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	C	401	-	4,4,4	1.28	0	6,6,6	0.97	0
2	PO4	I	401	-	4,4,4	0.98	0	6,6,6	1.71	2 (33%)
2	PO4	G	401	-	4,4,4	1.04	0	6,6,6	0.72	0
2	PO4	A	401	-	4,4,4	1.02	0	6,6,6	1.52	1 (16%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	401	PO4	O3-P-O1	-2.89	100.72	110.95
2	I	401	PO4	O4-P-O2	2.37	115.29	107.91
2	I	401	PO4	O3-P-O2	-2.30	100.76	107.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	PO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	331/367 (90%)	-0.20	12 (3%)	46	47	12, 34, 79, 230	0
1	B	344/367 (93%)	-0.20	22 (6%)	25	24	9, 31, 90, 296	0
1	C	338/367 (92%)	-0.22	12 (3%)	46	47	13, 33, 88, 153	0
1	D	338/367 (92%)	-0.05	23 (6%)	23	22	15, 36, 110, 244	0
1	E	329/367 (89%)	-0.16	9 (2%)	56	57	16, 35, 72, 155	0
1	F	326/367 (88%)	-0.15	11 (3%)	48	49	14, 35, 79, 206	0
1	G	328/367 (89%)	-0.09	15 (4%)	37	38	18, 35, 76, 159	0
1	H	345/367 (94%)	-0.04	28 (8%)	18	17	16, 33, 127, 259	0
1	I	338/367 (92%)	-0.12	11 (3%)	49	50	15, 35, 82, 177	0
1	J	343/367 (93%)	-0.07	20 (5%)	29	28	15, 35, 99, 244	0
All	All	3360/3670 (91%)	-0.13	163 (4%)	35	34	9, 34, 89, 296	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	349	THR	6.1
1	J	358	ALA	6.0
1	D	201	ALA	5.9
1	H	347	THR	5.8
1	D	359	ALA	5.6
1	I	203	PHE	5.5
1	A	198	GLY	5.5
1	H	345	PRO	5.5
1	B	347	THR	5.4
1	H	203	PHE	5.4
1	H	344	VAL	5.3
1	A	200	VAL	5.3
1	D	347	THR	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	209	SER	5.1
1	B	344	VAL	5.1
1	B	345	PRO	5.1
1	F	339	VAL	4.9
1	J	100	LYS	4.6
1	J	344	VAL	4.6
1	B	358	ALA	4.6
1	B	353	PHE	4.5
1	F	342	LEU	4.4
1	B	245	TYR	4.3
1	G	199	ALA	4.3
1	E	305	THR	4.2
1	E	235	HIS	4.2
1	H	363	HIS	4.2
1	I	235	HIS	4.2
1	D	357	LEU	4.1
1	B	359	ALA	4.1
1	F	340	SER	4.1
1	D	358	ALA	4.1
1	H	207	GLY	4.1
1	H	362	HIS	4.1
1	D	345	PRO	4.0
1	D	198	GLY	4.0
1	H	340	SER	4.0
1	H	349	THR	3.9
1	G	269	GLN	3.9
1	H	360	LEU	3.9
1	E	317	ALA	3.9
1	J	347	THR	3.9
1	D	306	SER	3.8
1	B	208	THR	3.8
1	I	204	VAL	3.8
1	H	359	ALA	3.8
1	E	199	ALA	3.8
1	D	348	ASP	3.8
1	C	330	THR	3.8
1	D	360	LEU	3.7
1	D	353	PHE	3.7
1	B	352	ASN	3.7
1	D	246	GLN	3.7
1	C	235	HIS	3.6
1	F	308	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	349	THR	3.6
1	A	318	ALA	3.6
1	A	305	THR	3.5
1	G	304	ILE	3.5
1	J	356	ARG	3.5
1	G	19	GLN	3.5
1	J	351	ALA	3.5
1	B	343	GLN	3.5
1	J	205	THR	3.5
1	B	348	ASP	3.4
1	D	100	LYS	3.4
1	H	353	PHE	3.4
1	F	309	ASP	3.4
1	B	346	GLN	3.4
1	G	314	TRP	3.3
1	J	101	ALA	3.3
1	E	236	ASN	3.3
1	I	211	PRO	3.3
1	J	240	ALA	3.3
1	G	235	HIS	3.2
1	H	348	ASP	3.2
1	G	339	VAL	3.2
1	I	232	ILE	3.2
1	J	350	ILE	3.2
1	A	304	ILE	3.1
1	D	350	ILE	3.1
1	D	346	GLN	3.1
1	B	360	LEU	3.1
1	J	357	LEU	3.1
1	G	320	THR	3.1
1	F	96	PRO	3.1
1	F	341	PRO	3.1
1	C	308	ASP	3.1
1	H	356	ARG	3.1
1	B	308	ASP	3.0
1	C	203	PHE	3.0
1	C	96	PRO	3.0
1	B	100	LYS	2.9
1	B	203	PHE	2.9
1	H	209	SER	2.9
1	H	245	TYR	2.9
1	H	204	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	308	ASP	2.9
1	G	96	PRO	2.9
1	J	345	PRO	2.9
1	G	198	GLY	2.9
1	H	25	THR	2.8
1	H	208	THR	2.8
1	I	305	THR	2.8
1	B	357	LEU	2.8
1	H	358	ALA	2.8
1	G	45	LYS	2.8
1	F	17	ALA	2.8
1	B	356	ARG	2.8
1	J	109	VAL	2.7
1	A	102	GLN	2.7
1	A	313	LEU	2.7
1	I	206	ALA	2.7
1	J	346	GLN	2.7
1	J	308	ASP	2.7
1	B	350	ILE	2.7
1	F	104	LEU	2.7
1	J	353	PHE	2.7
1	F	306	SER	2.7
1	D	355	ALA	2.7
1	H	200	VAL	2.6
1	A	209	SER	2.6
1	H	357	LEU	2.6
1	D	210	THR	2.6
1	I	157	ASN	2.5
1	A	201	ALA	2.5
1	J	359	ALA	2.5
1	H	112	GLU	2.5
1	D	361	GLU	2.4
1	C	323	LYS	2.4
1	D	344	VAL	2.4
1	G	300	LEU	2.4
1	C	193	PHE	2.4
1	J	113	GLN	2.4
1	A	339	VAL	2.4
1	I	200	VAL	2.4
1	B	355	ALA	2.4
1	I	314	TRP	2.3
1	E	97	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	352	ASN	2.3
1	E	210	THR	2.3
1	C	214	ILE	2.2
1	I	208	THR	2.2
1	E	307	GLY	2.2
1	F	86	LEU	2.2
1	H	346	GLN	2.2
1	D	356	ARG	2.2
1	C	314	TRP	2.2
1	A	99	THR	2.1
1	G	319	ASP	2.1
1	E	302	LYS	2.1
1	C	206	ALA	2.1
1	G	232	ILE	2.1
1	C	116	GLU	2.1
1	H	361	GLU	2.1
1	J	245	TYR	2.1
1	H	202	ASP	2.1
1	B	248	ARG	2.1
1	D	105	ARG	2.1
1	G	305	THR	2.1
1	H	355	ALA	2.0
1	C	207	GLY	2.0
1	A	299	ASP	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 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	0.88	0.19	18,27,28,602	0
2	PO4	C	401	5/5	0.89	0.14	45,49,95,157	0
2	PO4	G	401	5/5	0.95	0.10	39,41,102,204	0
2	PO4	I	401	5/5	0.97	0.08	16,20,24,183	0

6.5 Other polymers [i](#)

There are no such residues in this entry.