



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:53 AM UTC

PDB ID : 6H2D / pdb_00006h2d
Title : Structure of the soluble AhlC 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 : 2.62 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
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

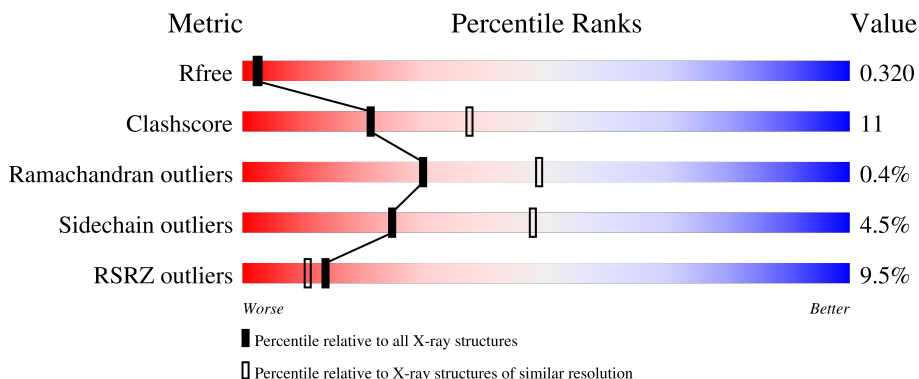
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	P	274	
1	Q	274	
1	R	274	
1	S	274	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6152 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 AhlC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	215	Total	C	N	O	S	0	0	0
			1642	1022	292	326	2			
1	Q	197	Total	C	N	O	S	0	0	0
			1483	914	265	302	2			
1	R	177	Total	C	N	O	S	0	0	0
			1336	821	240	273	2			
1	S	224	Total	C	N	O	S	0	0	0
			1691	1051	300	338	2			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	267	LEU	-	expression tag	UNP A0A1N6TH80
P	268	GLU	-	expression tag	UNP A0A1N6TH80
P	269	HIS	-	expression tag	UNP A0A1N6TH80
P	270	HIS	-	expression tag	UNP A0A1N6TH80
P	271	HIS	-	expression tag	UNP A0A1N6TH80
P	272	HIS	-	expression tag	UNP A0A1N6TH80
P	273	HIS	-	expression tag	UNP A0A1N6TH80
P	274	HIS	-	expression tag	UNP A0A1N6TH80
Q	267	LEU	-	expression tag	UNP A0A1N6TH80
Q	268	GLU	-	expression tag	UNP A0A1N6TH80
Q	269	HIS	-	expression tag	UNP A0A1N6TH80
Q	270	HIS	-	expression tag	UNP A0A1N6TH80
Q	271	HIS	-	expression tag	UNP A0A1N6TH80
Q	272	HIS	-	expression tag	UNP A0A1N6TH80
Q	273	HIS	-	expression tag	UNP A0A1N6TH80
Q	274	HIS	-	expression tag	UNP A0A1N6TH80
R	267	LEU	-	expression tag	UNP A0A1N6TH80
R	268	GLU	-	expression tag	UNP A0A1N6TH80
R	269	HIS	-	expression tag	UNP A0A1N6TH80
R	270	HIS	-	expression tag	UNP A0A1N6TH80
R	271	HIS	-	expression tag	UNP A0A1N6TH80

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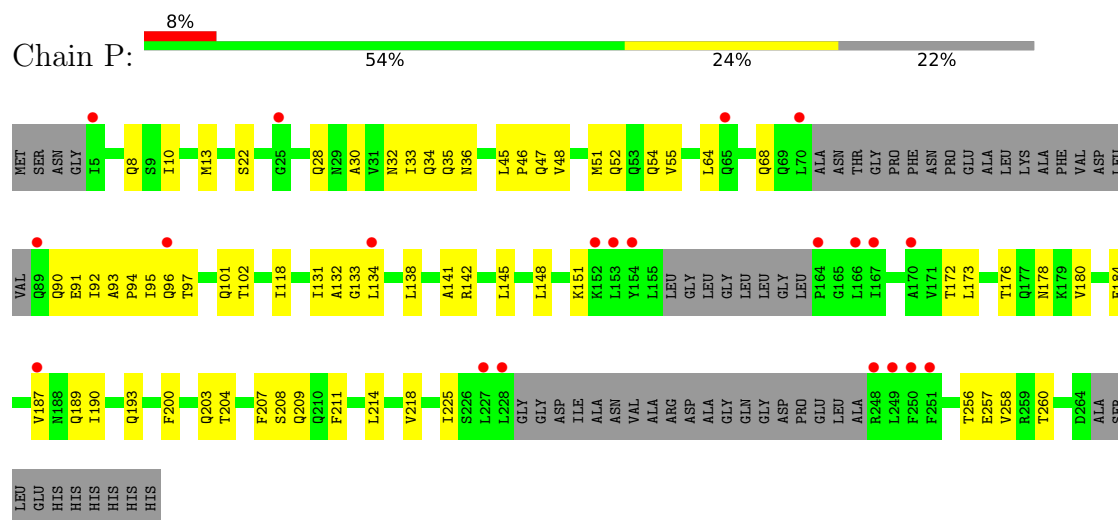
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Chain	Residue	Modelled	Actual	Comment	Reference
R	272	HIS	-	expression tag	UNP A0A1N6TH80
R	273	HIS	-	expression tag	UNP A0A1N6TH80
R	274	HIS	-	expression tag	UNP A0A1N6TH80
S	267	LEU	-	expression tag	UNP A0A1N6TH80
S	268	GLU	-	expression tag	UNP A0A1N6TH80
S	269	HIS	-	expression tag	UNP A0A1N6TH80
S	270	HIS	-	expression tag	UNP A0A1N6TH80
S	271	HIS	-	expression tag	UNP A0A1N6TH80
S	272	HIS	-	expression tag	UNP A0A1N6TH80
S	273	HIS	-	expression tag	UNP A0A1N6TH80
S	274	HIS	-	expression tag	UNP A0A1N6TH80

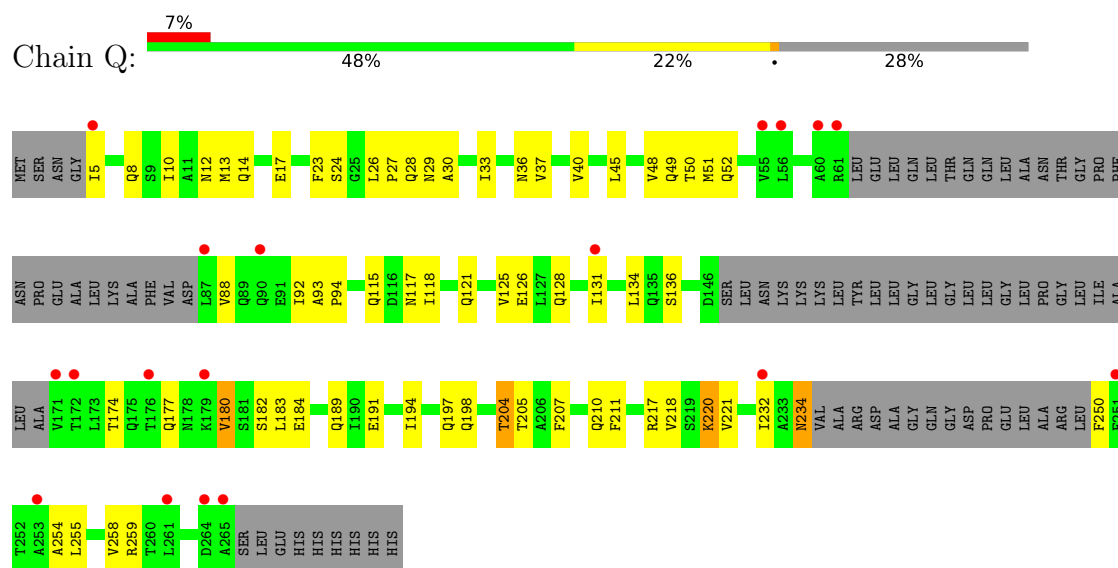
3 Residue-property plots

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: AhlC

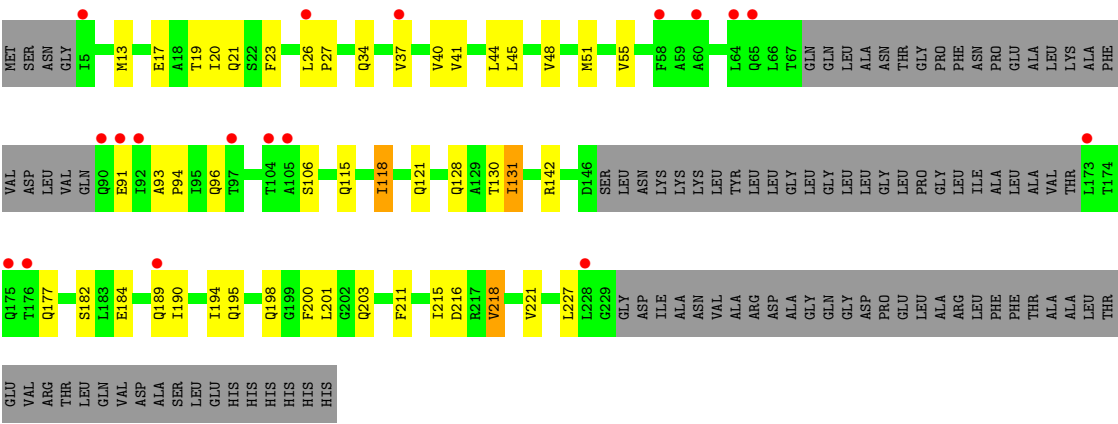


• Molecule 1: AhlC

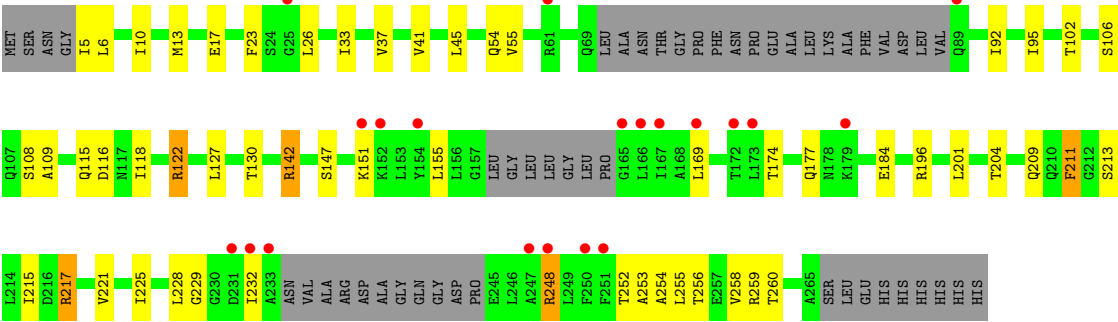


• Molecule 1: AhlC





● Molecule 1: AhIC



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.07 Å 61.66 Å 129.77 Å 90.00° 92.01° 90.00°	Depositor
Resolution (Å)	46.74 – 2.62 46.74 – 2.62	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.74-2.62) 99.6 (46.74-2.62)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.61 Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.269 , 0.334 0.264 , 0.320	Depositor DCC
R_{free} test set	1448 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	50.0	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 31.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.076 for h,-k,-l	Xtriage
Reported twinning fraction	0.888 for H, K, L 0.112 for -h,-k,l	Depositor
Outliers	2 of 31139 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6152	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.41% 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

5.1 Standard geometry

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	P	0.99	1/1650 (0.1%)	1.31	4/2232 (0.2%)
1	Q	0.94	2/1489 (0.1%)	1.26	2/2017 (0.1%)
1	R	0.88	0/1341	1.30	1/1815 (0.1%)
1	S	0.93	1/1698 (0.1%)	1.25	2/2297 (0.1%)
All	All	0.94	4/6178 (0.1%)	1.28	9/8361 (0.1%)

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	S	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	36	ASN	N-CA	5.43	1.52	1.46
1	S	213	SER	C-O	5.39	1.30	1.24
1	Q	121	GLN	C-O	5.11	1.30	1.24
1	Q	204	THR	C-O	-5.04	1.18	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	205	THR	CA-CB-OG1	-6.95	99.17	109.60
1	S	92	ILE	N-CA-C	-6.16	106.91	111.90
1	S	211	PHE	CA-CB-CG	5.42	119.22	113.80
1	P	35	GLN	CA-C-N	5.26	127.28	120.44
1	P	35	GLN	C-N-CA	5.26	127.28	120.44
1	Q	191	GLU	CB-CA-C	-5.17	102.54	110.81
1	R	130	THR	CB-CA-C	5.10	119.36	110.79
1	P	218	VAL	N-CA-CB	5.04	116.45	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	211	PHE	CA-CB-CG	5.04	118.84	113.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	S	122	ARG	Sidechain
1	S	196	ARG	Sidechain
1	S	217	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	P	1642	0	1687	43	0
1	Q	1483	0	1493	40	0
1	R	1336	0	1350	26	0
1	S	1691	0	1729	38	0
All	All	6152	0	6259	137	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 11.

All (137) 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:P:28:GLN:NE2	1:P:32:ASN:OD1	2.18	0.77
1:R:23:PHE:HB3	1:R:26:LEU:HD11	1.68	0.75
1:R:21:GLN:NE2	1:R:34:GLN:O	2.22	0.71
1:S:248:ARG:O	1:S:252:THR:HG23	1.93	0.68
1:S:256:THR:O	1:S:260:THR:HG23	1.95	0.66
1:P:256:THR:O	1:P:260:THR:HG23	1.97	0.66
1:Q:17:GLU:HG3	1:Q:37:VAL:HG12	1.77	0.65
1:S:254:ALA:O	1:S:258:VAL:HG23	1.96	0.65
1:R:23:PHE:CB	1:R:26:LEU:HD11	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:225:ILE:O	1:P:225:ILE:HG22	1.97	0.64
1:P:51:MET:HG3	1:P:52:GLN:N	2.11	0.64
1:Q:10:ILE:O	1:Q:14:GLN:HG3	1.98	0.63
1:Q:37:VAL:HG13	1:Q:207:PHE:CZ	2.34	0.62
1:Q:27:PRO:O	1:Q:30:ALA:HB3	1.99	0.62
1:R:106:SER:HB3	1:R:215:ILE:HD11	1.82	0.62
1:P:96:GLN:HG3	1:P:225:ILE:HG22	1.82	0.61
1:P:131:ILE:HD12	1:P:131:ILE:C	2.26	0.60
1:P:134:LEU:HB3	1:P:187:VAL:HG12	1.82	0.60
1:S:55:VAL:HG23	1:S:95:ILE:HD11	1.83	0.59
1:P:189:GLN:OE1	1:Q:8:GLN:NE2	2.36	0.59
1:S:115:GLN:O	1:S:118:ILE:HG13	2.02	0.59
1:S:106:SER:HB3	1:S:215:ILE:HD11	1.84	0.58
1:S:255:LEU:HD21	1:S:259:ARG:NH2	2.19	0.58
1:P:141:ALA:HB1	1:P:180:VAL:HG12	1.86	0.58
1:S:106:SER:HB3	1:S:215:ILE:CD1	2.33	0.58
1:S:142:ARG:NH1	1:S:184:GLU:OE2	2.37	0.58
1:Q:37:VAL:HG13	1:Q:207:PHE:CE2	2.39	0.58
1:Q:115:GLN:HA	1:Q:118:ILE:HG12	1.85	0.58
1:P:48:VAL:HG22	1:P:102:THR:CG2	2.34	0.58
1:P:145:LEU:HB2	1:P:176:THR:HG22	1.86	0.58
1:S:33:ILE:HG21	1:S:204:THR:HG21	1.86	0.57
1:S:228:LEU:HD22	1:S:232:ILE:HD11	1.86	0.57
1:R:121:GLN:HG2	1:R:201:LEU:HD11	1.86	0.57
1:R:177:GLN:OE1	1:S:260:THR:HG22	2.05	0.56
1:S:174:THR:HA	1:S:177:GLN:HB2	1.87	0.56
1:P:13:MET:HE3	1:P:207:PHE:CE1	2.41	0.56
1:R:106:SER:CB	1:R:215:ILE:HD11	2.35	0.56
1:P:33:ILE:HG21	1:P:204:THR:HG21	1.86	0.55
1:Q:33:ILE:HG21	1:Q:204:THR:CG2	2.37	0.54
1:R:218:VAL:O	1:R:221:VAL:HG22	2.07	0.54
1:S:54:GLN:HB3	1:S:95:ILE:HD13	1.89	0.54
1:P:97:THR:O	1:P:101:GLN:HG3	2.07	0.54
1:Q:254:ALA:O	1:Q:258:VAL:HG13	2.07	0.54
1:Q:88:VAL:CG2	1:Q:232:ILE:HG21	2.38	0.54
1:Q:17:GLU:CG	1:Q:37:VAL:HG12	2.39	0.53
1:P:97:THR:HG22	1:P:101:GLN:HE21	1.73	0.53
1:P:91:GLU:O	1:P:94:PRO:HD2	2.09	0.52
1:Q:33:ILE:HG21	1:Q:204:THR:HG21	1.91	0.52
1:R:115:GLN:O	1:R:118:ILE:HG12	2.09	0.52
1:R:195:GLN:NE2	1:S:209:GLN:OE1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:13:MET:HE1	1:S:211:PHE:CD1	2.45	0.52
1:Q:126:GLU:CD	1:S:122:ARG:HH11	2.17	0.52
1:Q:13:MET:HE3	1:Q:207:PHE:CE1	2.45	0.51
1:S:5:ILE:HG22	1:S:217:ARG:NH2	2.25	0.51
1:P:33:ILE:HG21	1:P:204:THR:CG2	2.40	0.50
1:R:93:ALA:N	1:R:94:PRO:HD2	2.27	0.50
1:R:194:ILE:O	1:R:198:GLN:HG3	2.11	0.50
1:P:96:GLN:CG	1:P:225:ILE:HG22	2.43	0.49
1:P:208:SER:O	1:P:209:GLN:C	2.55	0.49
1:P:151:LYS:HA	1:R:227:LEU:CD1	2.42	0.49
1:P:184:GLU:HB3	1:Q:5:ILE:HD11	1.95	0.49
1:Q:10:ILE:HG23	1:Q:45:LEU:HD13	1.95	0.48
1:P:148:LEU:HD13	1:P:173:LEU:HA	1.96	0.48
1:P:134:LEU:HB3	1:P:187:VAL:CG1	2.43	0.48
1:S:225:ILE:O	1:S:225:ILE:HG22	2.14	0.48
1:P:138:LEU:HD21	1:P:142:ARG:HH21	1.79	0.47
1:P:225:ILE:O	1:P:225:ILE:CG2	2.62	0.47
1:R:17:GLU:HB2	1:R:41:VAL:HG21	1.94	0.47
1:P:200:PHE:O	1:P:203:GLN:HB2	2.14	0.47
1:Q:126:GLU:OE1	1:S:122:ARG:NH1	2.47	0.47
1:Q:180:VAL:O	1:Q:184:GLU:HB2	2.15	0.47
1:Q:218:VAL:HA	1:Q:221:VAL:HG22	1.96	0.47
1:P:55:VAL:HG23	1:P:95:ILE:HD11	1.96	0.47
1:P:214:LEU:O	1:P:214:LEU:HD23	2.15	0.47
1:P:10:ILE:HG23	1:P:45:LEU:HD13	1.97	0.47
1:Q:36:ASN:O	1:Q:40:VAL:HG23	2.14	0.47
1:Q:128:GLN:O	1:Q:131:ILE:HG12	2.15	0.46
1:R:128:GLN:O	1:R:131:ILE:HG13	2.15	0.46
1:P:214:LEU:HD23	1:P:214:LEU:C	2.40	0.46
1:Q:255:LEU:O	1:Q:259:ARG:HG3	2.15	0.46
1:Q:125:VAL:HG11	1:S:122:ARG:HG2	1.98	0.46
1:Q:51:MET:HG3	1:Q:52:GLN:N	2.31	0.46
1:P:131:ILE:HG23	1:P:190:ILE:HG21	1.98	0.46
1:Q:13:MET:HE1	1:Q:211:PHE:CD1	2.51	0.46
1:S:217:ARG:HD3	1:S:217:ARG:HA	1.65	0.46
1:P:257:GLU:HA	1:P:257:GLU:OE1	2.15	0.46
1:R:19:THR:HG21	1:R:203:GLN:OE1	2.16	0.46
1:P:30:ALA:O	1:P:34:GLN:HG3	2.16	0.45
1:P:55:VAL:CG2	1:P:95:ILE:HD11	2.46	0.45
1:Q:12:ASN:ND2	1:Q:210:GLN:OE1	2.38	0.45
1:R:51:MET:O	1:R:55:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:108:SER:O	1:S:109:ALA:C	2.59	0.45
1:S:118:ILE:HD13	1:S:122:ARG:NH2	2.32	0.45
1:S:17:GLU:HG3	1:S:41:VAL:HG21	1.98	0.45
1:Q:88:VAL:HG23	1:Q:232:ILE:HG21	1.98	0.45
1:S:33:ILE:HG21	1:S:204:THR:CG2	2.47	0.45
1:S:151:LYS:O	1:S:155:LEU:HG	2.16	0.45
1:P:260:THR:HG22	1:Q:177:GLN:OE1	2.17	0.45
1:Q:234:ASN:HB3	1:Q:250:PHE:CE2	2.52	0.44
1:P:132:ALA:O	1:P:133:GLY:C	2.61	0.44
1:S:118:ILE:CD1	1:S:122:ARG:NH2	2.80	0.44
1:R:13:MET:HE1	1:R:211:PHE:CD1	2.52	0.44
1:Q:23:PHE:HB3	1:Q:26:LEU:CD1	2.48	0.44
1:Q:197:GLN:O	1:Q:198:GLN:C	2.57	0.44
1:S:17:GLU:HG2	1:S:37:VAL:HG12	1.99	0.44
1:S:54:GLN:CB	1:S:95:ILE:HD13	2.48	0.44
1:Q:49:GLN:O	1:Q:50:THR:C	2.61	0.43
1:Q:93:ALA:N	1:Q:94:PRO:HD2	2.33	0.43
1:S:253:ALA:O	1:S:256:THR:HB	2.18	0.43
1:Q:40:VAL:O	1:Q:45:LEU:HG	2.18	0.43
1:R:131:ILE:HG23	1:R:190:ILE:HB	2.01	0.43
1:S:127:LEU:O	1:S:130:THR:OG1	2.33	0.43
1:S:201:LEU:HD23	1:S:201:LEU:HA	1.82	0.43
1:P:141:ALA:CB	1:P:180:VAL:HG12	2.47	0.42
1:P:54:GLN:HB3	1:P:95:ILE:HD12	2.02	0.42
1:Q:217:ARG:O	1:Q:220:LYS:N	2.52	0.42
1:Q:51:MET:HE1	1:Q:221:VAL:HG21	2.01	0.42
1:R:45:LEU:O	1:R:48:VAL:N	2.48	0.42
1:P:64:LEU:O	1:P:68:GLN:HG2	2.20	0.42
1:R:20:ILE:HG23	1:R:200:PHE:CE1	2.54	0.42
1:Q:182:SER:O	1:Q:183:LEU:C	2.62	0.42
1:P:8:GLN:NE2	1:Q:189:GLN:HB2	2.34	0.42
1:R:93:ALA:HA	1:R:96:GLN:HE21	1.85	0.42
1:S:225:ILE:O	1:S:225:ILE:CG2	2.68	0.42
1:R:91:GLU:O	1:R:94:PRO:HG2	2.20	0.41
1:Q:28:GLN:O	1:Q:29:ASN:C	2.63	0.41
1:S:23:PHE:HB3	1:S:26:LEU:HD11	2.01	0.41
1:P:96:GLN:HG3	1:P:225:ILE:CG2	2.49	0.41
1:S:33:ILE:HD11	1:S:116:ASP:HB3	2.03	0.41
1:S:228:LEU:O	1:S:229:GLY:C	2.64	0.41
1:S:10:ILE:HG23	1:S:45:LEU:HD13	2.03	0.41
1:P:45:LEU:N	1:P:46:PRO:HD2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:106:SER:CB	1:R:215:ILE:CD1	2.99	0.40
1:P:92:ILE:O	1:P:93:ALA:C	2.64	0.40
1:Q:92:ILE:C	1:Q:94:PRO:HD2	2.46	0.40
1:R:40:VAL:HA	1:R:44:LEU:HB3	2.03	0.40
1:R:142:ARG:HH12	1:R:184:GLU:HG2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	207/274 (76%)	194 (94%)	12 (6%)	1 (0%)	24	44
1	Q	189/274 (69%)	176 (93%)	12 (6%)	1 (0%)	24	44
1	R	171/274 (62%)	163 (95%)	7 (4%)	1 (1%)	21	39
1	S	216/274 (79%)	201 (93%)	15 (7%)	0	100	100
All	All	783/1096 (71%)	734 (94%)	46 (6%)	3 (0%)	30	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	90	GLN
1	Q	134	LEU
1	R	27	PRO

5.3.2 Protein sidechains [i](#)

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	P	181/223 (81%)	174 (96%)	7 (4%)	28	53
1	Q	162/223 (73%)	153 (94%)	9 (6%)	19	39
1	R	147/223 (66%)	140 (95%)	7 (5%)	23	45
1	S	183/223 (82%)	176 (96%)	7 (4%)	29	54
All	All	673/892 (75%)	643 (96%)	30 (4%)	24	48

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	22	SER
1	P	47	GLN
1	P	118	ILE
1	P	172	THR
1	P	178	ASN
1	P	193	GLN
1	P	258	VAL
1	Q	24	SER
1	Q	48	VAL
1	Q	117	ASN
1	Q	136	SER
1	Q	174	THR
1	Q	180	VAL
1	Q	194	ILE
1	Q	220	LYS
1	Q	234	ASN
1	R	37	VAL
1	R	118	ILE
1	R	131	ILE
1	R	182	SER
1	R	189	GLN
1	R	216	ASP
1	R	218	VAL
1	S	6	LEU
1	S	102	THR
1	S	142	ARG
1	S	147	SER
1	S	169	LEU
1	S	221	VAL
1	S	248	ARG

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

Mol	Chain	Res	Type
1	P	15	GLN
1	P	53	GLN
1	P	101	GLN
1	P	110	ASN
1	P	175	GLN
1	P	189	GLN
1	P	193	GLN
1	P	197	GLN
1	P	203	GLN
1	Q	8	GLN
1	Q	52	GLN
1	Q	89	GLN
1	R	8	GLN
1	R	29	ASN
1	R	32	ASN
1	R	47	GLN
1	R	52	GLN
1	R	53	GLN
1	R	65	GLN
1	R	96	GLN
1	S	28	GLN
1	S	101	GLN
1	S	115	GLN
1	S	128	GLN
1	S	135	GLN
1	S	188	ASN
1	S	189	GLN
1	S	203	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](#)

There are no ligands in this entry.

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	P	215/274 (78%)	0.52	21 (9%)	13 10	28, 49, 82, 165	0
1	Q	197/274 (71%)	0.74	18 (9%)	15 11	31, 60, 88, 101	0
1	R	177/274 (64%)	0.75	18 (10%)	12 9	35, 59, 89, 104	0
1	S	224/274 (81%)	0.63	20 (8%)	15 12	30, 52, 95, 131	0
All	All	813/1096 (74%)	0.65	77 (9%)	14 11	28, 55, 90, 165	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	250	PHE	7.8
1	Q	87	LEU	5.9
1	R	176	THR	5.5
1	Q	251	PHE	5.4
1	P	154	TYR	5.3
1	Q	5	ILE	4.9
1	S	232	ILE	4.5
1	P	70	LEU	4.5
1	R	104	THR	4.4
1	R	173	LEU	4.4
1	R	92	ILE	4.1
1	S	165	GLY	4.1
1	Q	172	THR	3.7
1	Q	171	VAL	3.6
1	Q	56	LEU	3.6
1	R	189	GLN	3.5
1	P	248	ARG	3.5
1	Q	261	LEU	3.5
1	R	58	PHE	3.5
1	R	5	ILE	3.4
1	S	172	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	R	97	THR	3.3
1	S	233	ALA	3.3
1	P	153	LEU	3.1
1	S	231	ASP	3.0
1	S	169	LEU	3.0
1	S	248	ARG	3.0
1	P	96	GLN	3.0
1	Q	60	ALA	2.9
1	P	134	LEU	2.9
1	P	228	LEU	2.9
1	S	89	GLN	2.9
1	Q	264	ASP	2.9
1	P	166	LEU	2.8
1	Q	265	ALA	2.8
1	S	152	LYS	2.8
1	Q	55	VAL	2.8
1	P	164	PRO	2.8
1	P	5	ILE	2.8
1	Q	61	ARG	2.8
1	R	105	ALA	2.7
1	R	64	LEU	2.7
1	P	249	LEU	2.7
1	Q	131	ILE	2.7
1	R	26	LEU	2.7
1	S	251	PHE	2.7
1	P	167	ILE	2.6
1	P	227	LEU	2.6
1	Q	90	GLN	2.6
1	P	170	ALA	2.6
1	Q	253	ALA	2.5
1	P	251	PHE	2.5
1	S	61	ARG	2.4
1	R	228	LEU	2.4
1	R	175	GLN	2.4
1	S	154	TYR	2.4
1	Q	176	THR	2.4
1	S	250	PHE	2.3
1	S	173	LEU	2.3
1	P	152	LYS	2.3
1	S	25	GLY	2.3
1	P	25	GLY	2.3
1	R	60	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	S	167	ILE	2.2
1	S	179	LYS	2.2
1	R	90	GLN	2.2
1	S	166	LEU	2.2
1	R	91	GLU	2.1
1	R	65	GLN	2.1
1	P	187	VAL	2.1
1	Q	232	ILE	2.1
1	R	37	VAL	2.1
1	S	247	ALA	2.0
1	Q	179	LYS	2.0
1	S	151	LYS	2.0
1	P	65	GLN	2.0
1	P	89	GLN	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.