



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:51 AM UTC

PDB ID : 3HL6 / pdb_00003hl6
Title : Staphylococcus aureus pathogenicity island 3 ORF9 protein
Authors : Kruse, A.C.; Huseby, M.; Shi, K.; Digre, J.; Schlievert, P.M.; Ohlendorf, D.H.; Earhart, C.A.
Deposited on : 2009-05-26
Resolution : 2.50 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

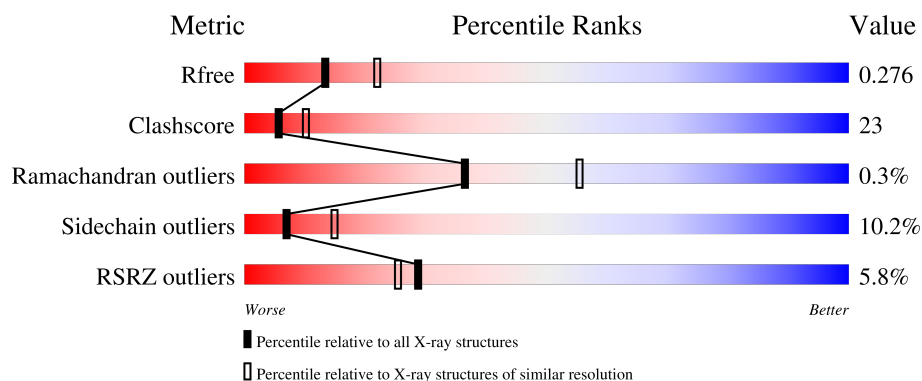
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	225	5% 57% 20% 6% 16%
1	B	225	5% 55% 26% • 15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3143 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 Pathogenicity island protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	0	0
			1536	980	244	302	10			
1	B	192	Total	C	N	O	S	0	0	0
			1547	989	246	302	10			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ASP	ASN	conflict	UNP Q5HHI6
A	214	LEU	-	expression tag	UNP Q5HHI6
A	215	ALA	-	expression tag	UNP Q5HHI6
A	216	ALA	-	expression tag	UNP Q5HHI6
A	217	ALA	-	expression tag	UNP Q5HHI6
A	218	LEU	-	expression tag	UNP Q5HHI6
A	219	GLU	-	expression tag	UNP Q5HHI6
A	220	HIS	-	expression tag	UNP Q5HHI6
A	221	HIS	-	expression tag	UNP Q5HHI6
A	222	HIS	-	expression tag	UNP Q5HHI6
A	223	HIS	-	expression tag	UNP Q5HHI6
A	224	HIS	-	expression tag	UNP Q5HHI6
A	225	HIS	-	expression tag	UNP Q5HHI6
B	2	ASP	ASN	conflict	UNP Q5HHI6
B	214	LEU	-	expression tag	UNP Q5HHI6
B	215	ALA	-	expression tag	UNP Q5HHI6
B	216	ALA	-	expression tag	UNP Q5HHI6
B	217	ALA	-	expression tag	UNP Q5HHI6
B	218	LEU	-	expression tag	UNP Q5HHI6
B	219	GLU	-	expression tag	UNP Q5HHI6
B	220	HIS	-	expression tag	UNP Q5HHI6
B	221	HIS	-	expression tag	UNP Q5HHI6
B	222	HIS	-	expression tag	UNP Q5HHI6
B	223	HIS	-	expression tag	UNP Q5HHI6
B	224	HIS	-	expression tag	UNP Q5HHI6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	225	HIS	-	expression tag	UNP Q5HHI6

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0

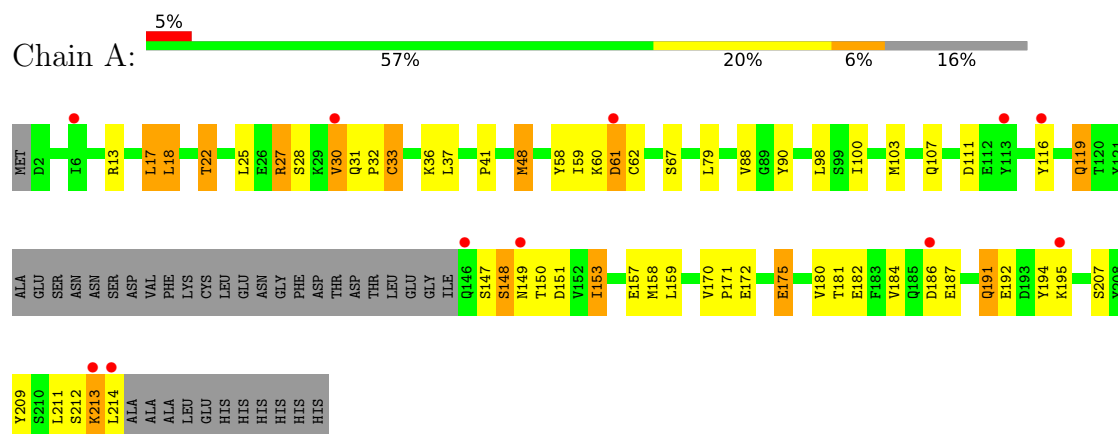
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	22	Total O 22 22	0	0
3	B	36	Total O 36 36	0	0

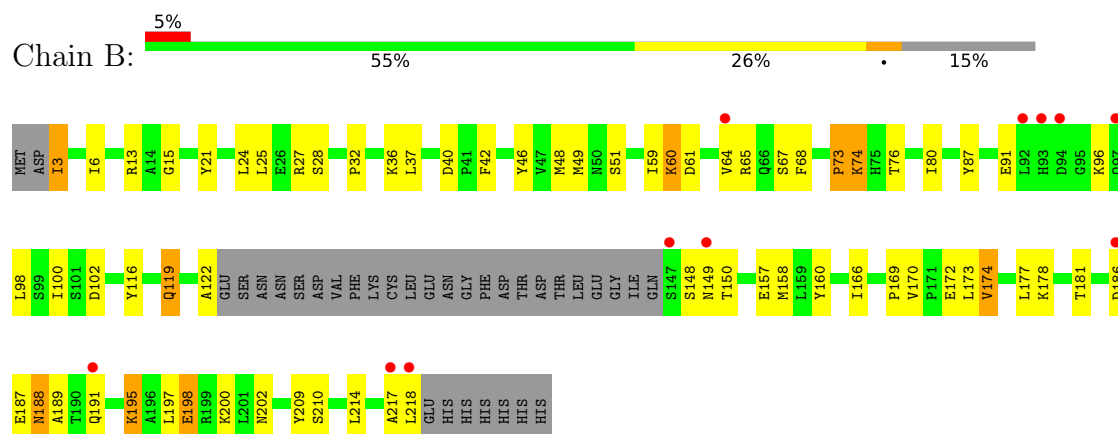
3 Residue-property plots [i](#)

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: Pathogenicity island protein



• Molecule 1: Pathogenicity island protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	82.74Å 78.58Å 83.54Å 90.00° 107.41° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 30.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.6 (30.00-2.50) 96.6 (30.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.228 , 0.276 0.226 , 0.276	Depositor DCC
R_{free} test set	889 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	55.5	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3143	wwPDB-VP
Average B, all atoms (Å ²)	61.0	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 20.17 % 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 9.2106e-03. 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.75	1/1565 (0.1%)	0.97	2/2111 (0.1%)
1	B	0.81	2/1576 (0.1%)	0.95	4/2127 (0.2%)
All	All	0.78	3/3141 (0.1%)	0.96	6/4238 (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	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	PRO	N-CD	8.78	1.60	1.47
1	B	3	ILE	CG1-CD1	7.48	1.80	1.51
1	A	148	SER	CB-OG	5.08	1.52	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ASP	N-CA-C	-12.48	97.75	111.36
1	B	174	VAL	N-CA-C	5.39	115.84	110.23
1	A	213	LYS	CB-CA-C	-5.33	108.88	116.34
1	B	15	GLY	N-CA-C	5.15	118.47	112.50
1	B	40	ASP	CA-C-N	-5.08	114.58	119.87
1	B	40	ASP	C-N-CA	-5.08	114.58	119.87

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	187	GLU	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	1536	0	1499	74	0
1	B	1547	0	1518	70	0
2	A	1	0	0	1	0
2	B	1	0	0	0	0
3	A	22	0	0	2	0
3	B	36	0	0	2	0
All	All	3143	0	3017	143	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 23.

All (143) 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:B:3:ILE:CD1	1:B:3:ILE:CG1	1.80	1.57
1:B:122:ALA:HB1	1:B:189:ALA:O	1.15	1.22
1:A:58:TYR:CE1	1:A:60:LYS:HG2	1.75	1.21
1:B:60:LYS:H	1:B:60:LYS:HD3	0.98	1.15
1:A:191:GLN:NE2	1:A:191:GLN:HA	1.63	1.11
1:A:170:VAL:HG11	3:A:235:HOH:O	1.48	1.10
1:B:122:ALA:CB	1:B:189:ALA:O	2.00	1.10
1:B:160:TYR:OH	1:B:181:THR:HG21	1.58	1.03
1:B:209:TYR:HB3	1:B:214:LEU:HD11	1.41	1.01
1:A:58:TYR:HE1	1:A:60:LYS:HG2	1.25	0.99
1:B:209:TYR:CB	1:B:214:LEU:HD11	1.93	0.99
1:A:170:VAL:CG1	3:A:235:HOH:O	2.07	0.96
1:B:60:LYS:HD3	1:B:60:LYS:N	1.83	0.93
1:A:153:ILE:O	1:A:157:GLU:HG3	1.69	0.93
1:A:58:TYR:CE1	1:A:60:LYS:CG	2.53	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:TYR:HB2	1:A:211:LEU:HD13	1.54	0.87
1:A:170:VAL:HG13	1:A:171:PRO:HD2	1.57	0.86
1:B:13:ARG:NH1	1:B:166:ILE:O	2.10	0.83
1:A:186:ASP:O	1:A:187:GLU:HG2	1.78	0.83
1:B:188:ASN:N	1:B:188:ASN:HD22	1.77	0.81
1:A:191:GLN:HA	1:A:191:GLN:HE21	1.42	0.80
1:B:209:TYR:HB3	1:B:214:LEU:CD1	2.12	0.79
1:B:60:LYS:H	1:B:60:LYS:CD	1.85	0.79
1:B:170:VAL:HG12	1:B:172:GLU:OE1	1.84	0.77
1:A:61:ASP:OD1	1:A:62:CYS:N	2.18	0.77
1:A:107:GLN:NE2	1:A:158:MET:HE2	2.00	0.76
1:A:209:TYR:CB	1:A:211:LEU:CD1	2.64	0.76
1:A:209:TYR:HB2	1:A:211:LEU:CD1	2.14	0.76
1:A:172:GLU:OE2	1:A:207:SER:OG	2.02	0.76
1:A:61:ASP:OD1	1:A:61:ASP:C	2.30	0.75
1:A:107:GLN:HB2	1:A:159:LEU:HD21	1.71	0.72
1:B:25:LEU:HD11	1:B:51:SER:HB2	1.72	0.72
1:B:3:ILE:CD1	1:B:3:ILE:CB	2.67	0.71
1:A:170:VAL:CG1	1:A:171:PRO:HD2	2.20	0.71
1:B:170:VAL:CG1	1:B:172:GLU:OE1	2.39	0.71
1:B:91:GLU:HG3	1:B:96:LYS:O	1.92	0.70
1:A:170:VAL:HG12	1:A:172:GLU:OE1	1.92	0.70
1:B:3:ILE:CD1	1:B:3:ILE:CG2	2.70	0.69
1:B:198:GLU:O	1:B:202:ASN:ND2	2.24	0.69
1:B:209:TYR:HB2	1:B:214:LEU:HD11	1.72	0.69
1:B:188:ASN:HD22	1:B:188:ASN:H	1.40	0.69
1:B:3:ILE:CD1	1:B:3:ILE:HG21	2.23	0.68
1:B:217:ALA:O	1:B:218:LEU:HB2	1.95	0.67
1:A:209:TYR:HB3	1:A:211:LEU:CD1	2.27	0.65
1:A:116:TYR:O	1:A:119:GLN:HB2	1.97	0.64
1:A:58:TYR:CZ	1:A:60:LYS:HB2	2.34	0.63
1:B:37:LEU:HD23	1:B:46:TYR:CE1	2.34	0.62
1:A:18:LEU:HD11	1:A:79:LEU:HB3	1.82	0.61
1:A:18:LEU:O	1:A:22:THR:HG23	1.99	0.61
1:B:51:SER:O	1:B:73:PRO:HD3	2.00	0.61
1:B:60:LYS:HE3	1:B:178:LYS:NZ	2.15	0.61
1:A:194:TYR:C	1:A:194:TYR:CD2	2.79	0.60
1:A:175:GLU:HA	1:A:175:GLU:OE2	2.01	0.60
1:B:214:LEU:CD1	1:B:214:LEU:H	2.15	0.60
1:A:58:TYR:CD1	1:A:60:LYS:HG2	2.35	0.60
1:A:213:LYS:HB2	1:A:214:LEU:CD1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLN:HG3	1:A:32:PRO:O	2.02	0.59
1:B:160:TYR:CZ	1:B:181:THR:HG21	2.35	0.59
1:A:58:TYR:CE1	1:A:60:LYS:CB	2.85	0.59
1:B:3:ILE:HG21	1:B:3:ILE:HD13	1.85	0.59
1:B:214:LEU:H	1:B:214:LEU:HD12	1.68	0.59
1:A:170:VAL:HG13	1:A:171:PRO:CD	2.32	0.58
1:A:28:SER:HA	1:A:31:GLN:O	2.04	0.58
1:A:60:LYS:N	1:A:60:LYS:HD2	2.18	0.57
1:B:198:GLU:O	1:B:198:GLU:HG3	2.05	0.57
1:A:191:GLN:HE21	1:A:191:GLN:CA	2.16	0.57
1:A:119:GLN:HG2	1:A:194:TYR:CE1	2.40	0.57
1:A:17:LEU:CD2	1:A:37:LEU:HD11	2.35	0.56
1:A:209:TYR:HB3	1:A:211:LEU:HD12	1.88	0.56
1:B:177:LEU:O	1:B:181:THR:HG23	2.05	0.56
1:B:21:TYR:OH	1:B:73:PRO:HD3	2.05	0.56
1:B:188:ASN:N	1:B:188:ASN:ND2	2.47	0.56
1:A:30:VAL:O	1:A:30:VAL:CG1	2.54	0.56
1:B:210:SER:O	1:B:214:LEU:HD13	2.07	0.55
1:A:214:LEU:HD12	1:A:214:LEU:N	2.21	0.55
1:B:25:LEU:HD11	1:B:51:SER:CB	2.36	0.55
1:B:3:ILE:CG2	1:B:3:ILE:HD13	2.37	0.54
1:A:170:VAL:CG1	1:A:171:PRO:CD	2.86	0.54
1:A:213:LYS:HB2	1:A:214:LEU:HD12	1.89	0.54
1:B:214:LEU:HD12	1:B:214:LEU:N	2.22	0.54
1:A:58:TYR:CD1	1:A:60:LYS:HD3	2.43	0.53
1:A:107:GLN:HB2	1:A:159:LEU:CD2	2.39	0.53
1:A:58:TYR:CE1	1:A:60:LYS:HB2	2.45	0.52
1:A:107:GLN:HE21	1:A:158:MET:HE2	1.73	0.52
1:A:181:THR:O	1:A:184:VAL:HG22	2.10	0.51
1:A:59:ILE:HD13	1:A:182:GLU:HB2	1.92	0.51
1:B:217:ALA:O	1:B:218:LEU:CB	2.58	0.51
1:B:191:GLN:O	1:B:195:LYS:HG2	2.09	0.51
1:B:198:GLU:HG2	3:B:238:HOH:O	2.10	0.50
1:B:200:LYS:NZ	3:B:245:HOH:O	2.15	0.50
1:A:17:LEU:HD22	1:A:37:LEU:HD11	1.93	0.48
1:A:59:ILE:O	1:A:60:LYS:HB2	2.13	0.48
1:B:149:ASN:O	1:B:149:ASN:OD1	2.31	0.48
1:A:27:ARG:HH21	1:A:31:GLN:HG2	1.78	0.48
1:A:41:PRO:HG3	2:A:226:CL:CL	2.50	0.48
1:B:60:LYS:HG2	1:B:61:ASP:H	1.79	0.48
1:A:187:GLU:HG3	1:A:187:GLU:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:THR:O	1:B:80:ILE:HG13	2.13	0.47
1:B:64:VAL:HG23	1:B:64:VAL:O	2.13	0.47
1:B:116:TYR:O	1:B:119:GLN:HB2	2.14	0.47
1:B:149:ASN:OD1	1:B:149:ASN:C	2.58	0.47
1:B:42:PHE:CE2	1:B:169:PRO:HG3	2.49	0.47
1:B:25:LEU:C	1:B:25:LEU:HD12	2.39	0.47
1:B:100:ILE:HG23	1:B:166:ILE:HG12	1.97	0.46
1:A:88:VAL:HG21	1:B:87:TYR:CE1	2.51	0.46
1:B:150:THR:O	1:B:150:THR:HG22	2.15	0.46
1:B:214:LEU:CD1	1:B:214:LEU:N	2.80	0.45
1:A:60:LYS:HA	1:A:62:CYS:O	2.17	0.45
1:B:21:TYR:HH	1:B:73:PRO:HD3	1.82	0.45
1:A:33:CYS:HB3	1:A:48:MET:HB2	1.99	0.44
1:A:48:MET:HB3	1:A:48:MET:HE2	1.67	0.44
1:B:150:THR:O	1:B:150:THR:CG2	2.66	0.44
1:A:90:TYR:HE2	1:A:100:ILE:HA	1.83	0.44
1:A:13:ARG:O	1:A:17:LEU:HD23	2.17	0.43
1:A:149:ASN:OD1	1:A:150:THR:N	2.48	0.43
1:B:21:TYR:HD2	1:B:48:MET:SD	2.41	0.43
1:A:170:VAL:CG1	1:A:172:GLU:OE1	2.65	0.43
1:B:160:TYR:CE2	1:B:181:THR:HG21	2.54	0.43
1:A:213:LYS:O	1:A:214:LEU:C	2.61	0.43
1:A:107:GLN:CB	1:A:159:LEU:HD21	2.45	0.42
1:A:103:MET:O	1:A:107:GLN:HG2	2.19	0.42
1:B:37:LEU:HD22	1:B:37:LEU:N	2.34	0.42
1:B:74:LYS:HE2	1:B:74:LYS:HB3	1.45	0.42
1:A:214:LEU:HD12	1:A:214:LEU:H	1.85	0.42
1:B:32:PRO:HB3	1:B:49:MET:HE2	2.02	0.42
1:A:25:LEU:HA	1:A:25:LEU:HD23	1.69	0.42
1:A:212:SER:O	1:A:212:SER:OG	2.31	0.42
1:B:37:LEU:HD13	1:B:37:LEU:HA	1.82	0.42
1:A:59:ILE:HD11	1:A:181:THR:HG22	2.01	0.42
1:A:18:LEU:HD11	1:A:79:LEU:CB	2.49	0.41
1:B:24:LEU:O	1:B:28:SER:HB3	2.20	0.41
1:A:17:LEU:HA	1:A:17:LEU:HD13	1.83	0.41
1:A:30:VAL:O	1:A:30:VAL:HG12	2.20	0.41
1:B:160:TYR:CE2	1:B:177:LEU:HD11	2.55	0.41
1:B:48:MET:HE3	1:B:48:MET:HB3	1.72	0.41
1:B:98:LEU:HD22	1:B:102:ASP:HB3	2.02	0.41
1:B:60:LYS:HG2	1:B:61:ASP:N	2.35	0.41
1:A:90:TYR:N	1:A:98:LEU:O	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ILE:CG2	1:B:36:LYS:HG3	2.51	0.41
1:B:68:PHE:HB3	1:B:157:GLU:HG2	2.02	0.41
1:B:25:LEU:HD12	1:B:25:LEU:O	2.22	0.40
1:A:214:LEU:CD1	1:A:214:LEU:N	2.83	0.40
1:A:111:ASP:OD1	1:A:111:ASP:C	2.65	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	A	185/225 (82%)	170 (92%)	15 (8%)	0	100	100
1	B	188/225 (84%)	180 (96%)	7 (4%)	1 (0%)	24	43
All	All	373/450 (83%)	350 (94%)	22 (6%)	1 (0%)	36	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	27	ARG

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	172/202 (85%)	153 (89%)	19 (11%)	6	13
1	B	171/202 (85%)	155 (91%)	16 (9%)	8	18
All	All	343/404 (85%)	308 (90%)	35 (10%)	7	15

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	18	LEU
1	A	22	THR
1	A	27	ARG
1	A	30	VAL
1	A	33	CYS
1	A	36	LYS
1	A	48	MET
1	A	67	SER
1	A	119	GLN
1	A	147	SER
1	A	148	SER
1	A	151	ASP
1	A	153	ILE
1	A	175	GLU
1	A	180	VAL
1	A	191	GLN
1	A	192	GLU
1	A	195	LYS
1	B	6	ILE
1	B	59	ILE
1	B	60	LYS
1	B	65	ARG
1	B	67	SER
1	B	74	LYS
1	B	119	GLN
1	B	148	SER
1	B	158	MET
1	B	173	LEU
1	B	174	VAL
1	B	186	ASP
1	B	188	ASN

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Mol	Chain	Res	Type
1	B	195	LYS
1	B	197	LEU
1	B	198	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	A	191	GLN
1	B	119	GLN
1	B	188	ASN
1	B	202	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	189/225 (84%)	0.46	11 (5%) 29 25	40, 60, 91, 100	0
1	B	192/225 (85%)	0.33	11 (5%) 29 26	37, 56, 79, 89	0
All	All	381/450 (84%)	0.39	22 (5%) 29 25	37, 58, 85, 100	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	186	ASP	4.4
1	A	214	LEU	4.4
1	B	93	HIS	3.5
1	A	213	LYS	3.0
1	B	94	ASP	2.9
1	A	195	LYS	2.6
1	A	61	ASP	2.5
1	A	6	ILE	2.4
1	B	191	GLN	2.3
1	B	64	VAL	2.3
1	B	92	LEU	2.2
1	A	146	GLN	2.2
1	B	147	SER	2.2
1	B	218	LEU	2.2
1	B	186	ASP	2.1
1	B	97	GLN	2.1
1	A	149	ASN	2.1
1	B	149	ASN	2.1
1	A	113	TYR	2.1
1	A	30	VAL	2.0
1	B	217	ALA	2.0
1	A	116	TYR	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	CL	A	226	1/1	0.92	0.12	69,69,69,69	0
2	CL	B	226	1/1	0.96	0.07	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.