



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:30 PM UTC

PDB ID : 1EWZ / pdb_00001ewz
Title : CRYSTAL STRUCTURE OF THE OXA-10 BETA-LACTAMASE FROM PSEUDOMONAS AERUGINOSA
Authors : Golemi, D.; Maveyraud, L.; Vakulenko, S.; Tranier, S.; Ishiwata, A.; Kotra, L.P.; Samama, J.P.; Mobashery, S.
Deposited on : 2000-04-28
Resolution : 2.40 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

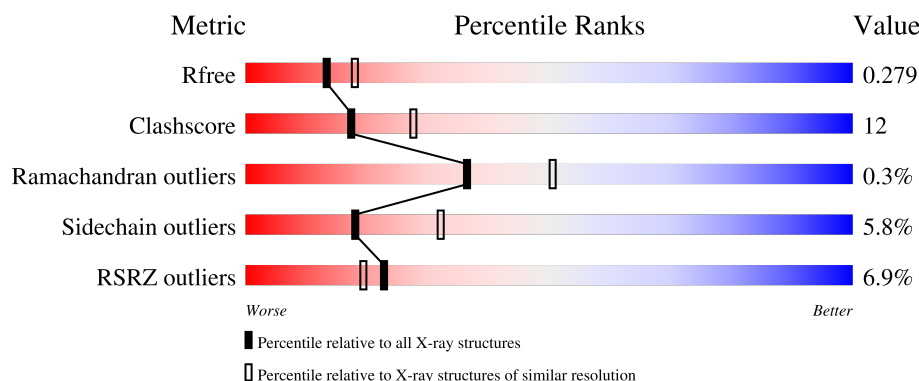
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	246	8% 69% 26% ..
1	B	246	5% 70% 26% ..
1	C	246	7% 71% 23% 5% .
1	D	246	8% 70% 24% ...

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8030 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 BETA LACTAMASE OXA-10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			1905	1221	321	357	6			
1	B	243	Total	C	N	O	S	0	0	0
			1906	1218	319	363	6			
1	C	243	Total	C	N	O	S	0	0	0
			1883	1206	313	358	6			
1	D	242	Total	C	N	O	S	0	0	0
			1875	1202	310	357	6			

- Molecule 2 is water.

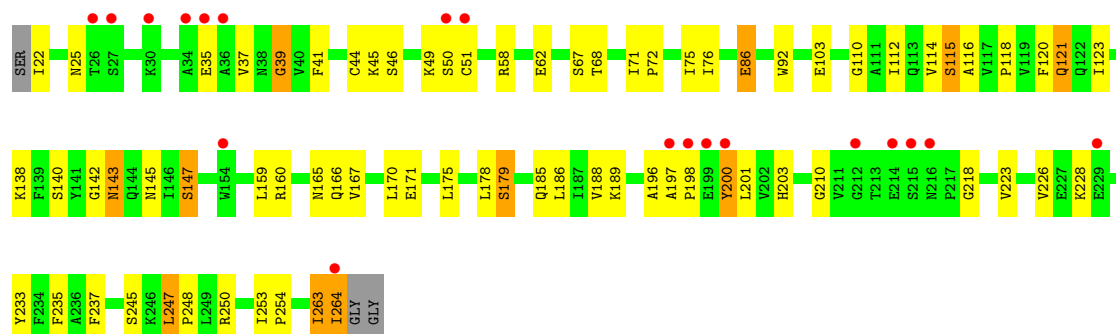
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	97	Total	O	0	0
			97	97		
2	B	135	Total	O	0	0
			135	135		
2	C	116	Total	O	0	0
			116	116		
2	D	113	Total	O	0	0
			113	113		

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.

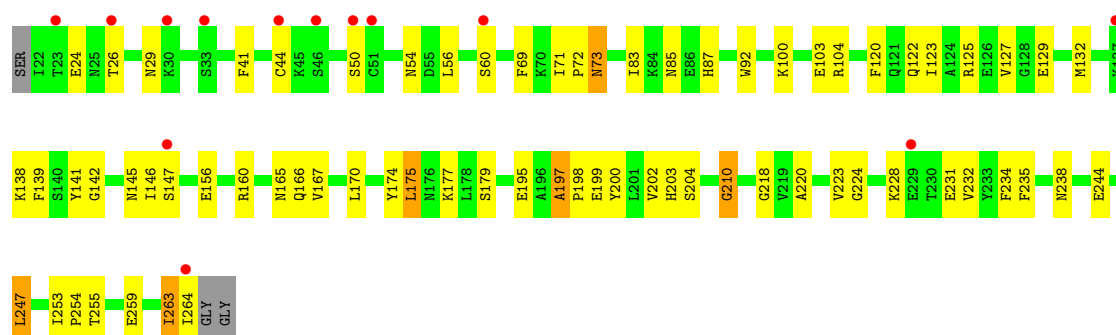
• Molecule 1: BETA LACTAMASE OXA-10

Chain A: 



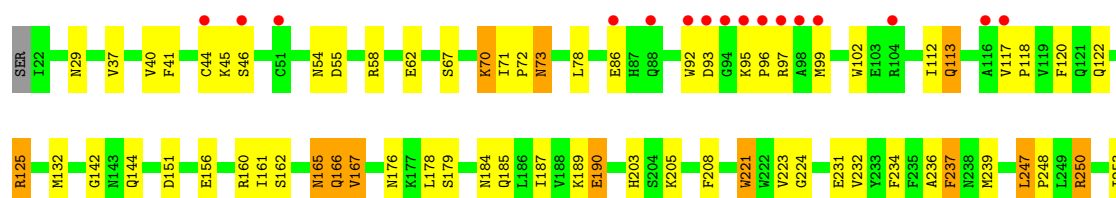
• Molecule 1: BETA LACTAMASE OXA-10

Chain B: 



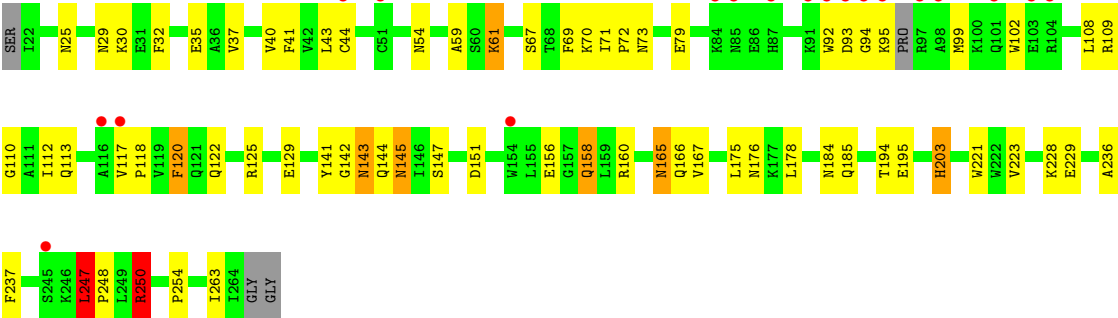
• Molecule 1: BETA LACTAMASE OXA-10

Chain C: 





● Molecule 1: BETA LACTAMASE OXA-10



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.42Å 82.39Å 101.49Å 90.00° 95.40° 90.00°	Depositor
Resolution (Å)	31.22 – 2.40 31.22 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.3 (31.22-2.40) 97.4 (31.22-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.23 (at 2.42Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.187 , 0.254 0.235 , 0.279	Depositor DCC
R_{free} test set	2101 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	1.6	Xtriage
Anisotropy	1.744	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 49.4	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	0.86	EDS
Total number of atoms	8030	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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)

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	0.55	0/1946	1.40	12/2634 (0.5%)
1	B	0.55	0/1947	1.45	9/2637 (0.3%)
1	C	0.58	0/1924	1.50	11/2611 (0.4%)
1	D	0.59	0/1914	1.57	20/2594 (0.8%)
All	All	0.57	0/7731	1.48	52/10476 (0.5%)

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
All	All	0	2

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	25	ASN	CA-CB-CG	8.95	121.55	112.60
1	D	221	TRP	CA-CB-CG	8.75	130.23	113.60
1	D	92	TRP	CA-C-O	8.55	130.50	120.58
1	D	143	ASN	OD1-CG-ND2	-8.47	114.13	122.60
1	D	165	ASN	CA-CB-CG	8.20	120.80	112.60
1	B	210	GLY	CA-C-O	-8.03	115.58	122.16
1	A	233	TYR	CA-C-O	-7.80	111.93	120.36
1	C	55	ASP	CA-CB-CG	7.45	120.05	112.60
1	D	195	GLU	CA-CB-CG	6.91	127.92	114.10
1	A	116	ALA	CA-C-N	6.83	126.99	120.43
1	A	116	ALA	C-N-CA	6.83	126.99	120.43
1	B	210	GLY	N-CA-C	-6.47	104.19	111.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	120	PHE	CA-CB-CG	-6.42	107.38	113.80
1	C	70	LYS	CB-CG-CD	6.40	126.03	111.30
1	B	160	ARG	NE-CZ-NH2	6.40	124.96	119.20
1	D	160	ARG	CD-NE-CZ	6.21	133.10	124.40
1	C	237	PHE	CA-CB-CG	6.19	119.99	113.80
1	A	86	GLU	CB-CG-CD	6.18	123.11	112.60
1	B	69	PHE	CA-CB-CG	-6.16	107.64	113.80
1	D	92	TRP	CA-C-N	6.13	133.25	121.54
1	D	92	TRP	C-N-CA	6.13	133.25	121.54
1	D	108	LEU	CA-C-O	-6.06	113.99	120.42
1	C	234	PHE	CA-CB-CG	-6.04	107.76	113.80
1	B	120	PHE	CA-CB-CG	-5.91	107.89	113.80
1	B	234	PHE	CA-CB-CG	-5.90	107.90	113.80
1	B	197	ALA	CA-C-O	-5.83	114.72	120.26
1	C	208	PHE	CA-CB-CG	5.83	119.62	113.80
1	B	139	PHE	CA-CB-CG	5.59	119.39	113.80
1	D	203	HIS	CA-C-O	-5.56	114.37	120.43
1	D	151	ASP	CA-CB-CG	5.50	118.10	112.60
1	C	125	ARG	NE-CZ-NH2	-5.49	114.26	119.20
1	D	61	LYS	N-CA-CB	5.48	118.10	110.04
1	A	51	CYS	CA-C-O	5.47	126.51	120.71
1	D	32	PHE	CA-CB-CG	-5.40	108.40	113.80
1	A	39	GLY	CA-C-N	-5.39	114.74	121.96
1	A	39	GLY	C-N-CA	-5.39	114.74	121.96
1	C	125	ARG	CA-C-O	-5.38	114.84	120.55
1	C	224	GLY	CA-C-O	5.38	125.29	121.04
1	C	221	TRP	O-C-N	5.35	129.82	123.24
1	D	250	ARG	CD-NE-CZ	5.34	131.88	124.40
1	A	171	GLU	O-C-N	5.30	128.19	122.15
1	D	247	LEU	CA-C-O	5.29	123.47	118.34
1	C	165	ASN	CA-CB-CG	5.27	117.87	112.60
1	A	200	TYR	CA-CB-CG	5.20	123.25	113.90
1	D	250	ARG	NE-CZ-NH1	5.14	126.64	121.50
1	A	121	GLN	CA-C-O	-5.13	114.98	120.42
1	D	160	ARG	NE-CZ-NH1	-5.11	116.39	121.50
1	A	68	THR	CA-C-N	5.06	128.70	120.60
1	A	68	THR	C-N-CA	5.06	128.70	120.60
1	D	195	GLU	CB-CG-CD	5.05	121.19	112.60
1	C	190	GLU	O-C-N	-5.05	116.84	122.09
1	B	199	GLU	CB-CG-CD	-5.04	104.04	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	263	ILE	Peptide
1	B	263	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	1905	0	1888	47	0
1	B	1906	0	1869	55	0
1	C	1883	0	1831	48	0
1	D	1875	0	1825	42	0
2	A	97	0	0	1	0
2	B	135	0	0	1	0
2	C	116	0	0	3	0
2	D	113	0	0	4	0
All	All	8030	0	7413	187	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 12.

All (187) 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:29:ASN:HD21	1:B:54:ASN:HD22	1.07	1.01
1:B:85:ASN:HD22	1:B:87:HIS:H	1.07	0.98
1:B:85:ASN:ND2	1:B:87:HIS:H	1.64	0.96
1:B:29:ASN:ND2	1:B:54:ASN:HD22	1.67	0.93
1:D:147:SER:HB2	1:D:158:GLN:HG3	1.61	0.82
1:A:253:ILE:HB	1:A:254:PRO:HD3	1.62	0.79
1:A:35:GLU:HB2	1:A:37:VAL:HG23	1.67	0.76
1:B:197:ALA:O	1:D:109:ARG:NH2	2.21	0.72
1:C:239:MET:HE2	2:C:374:HOH:O	1.90	0.71
1:B:85:ASN:HD22	1:B:87:HIS:N	1.86	0.69
1:B:85:ASN:ND2	1:B:87:HIS:N	2.40	0.68
1:B:228:LYS:NZ	1:B:264:ILE:HG22	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:ASN:C	1:D:145:ASN:HD22	2.07	0.62
1:C:44:CYS:SG	1:C:167:VAL:HG11	2.39	0.62
1:A:75:ILE:HG13	1:A:188:VAL:HG21	1.82	0.62
1:C:29:ASN:ND2	1:C:54:ASN:HD22	1.97	0.62
1:A:44:CYS:SG	1:A:167:VAL:HG11	2.41	0.61
1:B:122:GLN:NE2	1:B:125:ARG:HH11	1.98	0.61
1:D:69:PHE:HA	1:D:72:PRO:HG2	1.82	0.61
1:A:142:GLY:H	1:A:165:ASN:HD21	1.48	0.61
1:D:71:ILE:HB	1:D:72:PRO:CD	2.32	0.60
1:A:247:LEU:HD22	1:A:250:ARG:HD3	1.83	0.59
1:B:29:ASN:HD21	1:B:54:ASN:ND2	1.90	0.59
1:A:143:ASN:HD21	1:A:159:LEU:HA	1.66	0.59
1:D:44:CYS:SG	1:D:167:VAL:HG11	2.42	0.59
1:B:145:ASN:HD22	1:B:145:ASN:C	2.11	0.58
1:C:86:GLU:HB3	1:C:187:ILE:HG12	1.86	0.58
1:C:253:ILE:HB	1:C:254:PRO:HD3	1.85	0.58
1:A:145:ASN:HD22	1:A:147:SER:H	1.51	0.58
1:C:41:PHE:HD2	1:C:237:PHE:HB2	1.69	0.58
1:B:210:GLY:O	1:B:218:GLY:HA3	2.03	0.58
1:C:112:ILE:HG22	1:C:113:GLN:NE2	2.19	0.58
1:B:255:THR:O	1:B:259:GLU:HG3	2.05	0.57
1:B:129:GLU:HG3	1:B:146:ILE:HD11	1.86	0.57
1:D:142:GLY:HA2	1:D:165:ASN:ND2	2.20	0.56
1:A:200:TYR:CZ	1:A:264:ILE:HG12	2.40	0.56
1:D:122:GLN:OE1	1:D:125:ARG:NH1	2.39	0.56
1:B:145:ASN:ND2	1:B:147:SER:H	2.04	0.56
1:D:72:PRO:HG3	1:D:141:TYR:CE1	2.41	0.55
1:B:145:ASN:HD22	1:B:147:SER:H	1.53	0.55
1:A:145:ASN:HD22	1:A:145:ASN:C	2.15	0.55
1:A:142:GLY:H	1:A:165:ASN:ND2	2.04	0.55
1:B:220:ALA:O	1:B:238:ASN:HA	2.07	0.54
1:B:195:GLU:HB3	1:B:202:VAL:HB	1.89	0.54
1:A:253:ILE:CB	1:A:254:PRO:HD3	2.36	0.54
1:C:71:ILE:HB	1:C:72:PRO:CD	2.38	0.54
1:D:145:ASN:ND2	1:D:147:SER:H	2.05	0.54
1:B:203:HIS:O	1:B:224:GLY:HA3	2.08	0.54
1:B:123:ILE:O	1:B:127:VAL:HG23	2.07	0.54
1:D:70:LYS:HE3	1:D:120:PHE:CE1	2.43	0.54
1:A:145:ASN:ND2	1:A:147:SER:H	2.06	0.53
1:C:37:VAL:HG11	1:C:239:MET:HE1	1.90	0.53
1:D:41:PHE:CE2	1:D:254:PRO:HB3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:LEU:O	1:C:250:ARG:HD2	2.08	0.53
1:C:223:VAL:HG12	1:C:236:ALA:CB	2.39	0.53
1:B:72:PRO:HG3	1:B:141:TYR:CE1	2.44	0.53
1:C:93:ASP:OD2	1:C:95:LYS:N	2.42	0.52
1:A:247:LEU:HB3	1:A:248:PRO:HD3	1.91	0.52
1:D:145:ASN:HD22	1:D:147:SER:H	1.55	0.52
1:D:247:LEU:HB3	1:D:248:PRO:HD3	1.92	0.52
1:C:113:GLN:HE21	1:C:113:GLN:N	2.08	0.52
1:B:228:LYS:HZ2	1:B:264:ILE:CG2	2.22	0.52
1:A:186:LEU:HD21	1:C:86:GLU:OE2	2.10	0.51
1:A:145:ASN:HD21	1:A:147:SER:HB3	1.74	0.51
1:A:186:LEU:HD23	1:A:189:LYS:HE3	1.93	0.51
1:B:122:GLN:HE21	1:B:125:ARG:HH11	1.58	0.51
1:A:203:HIS:HD2	2:A:312:HOH:O	1.94	0.51
1:D:203:HIS:HD2	2:D:278:HOH:O	1.93	0.51
1:B:41:PHE:CE2	1:B:235:PHE:HB2	2.46	0.51
1:B:200:TYR:CZ	1:B:264:ILE:HG12	2.46	0.50
1:B:73:ASN:ND2	1:B:132:MET:HE1	2.25	0.50
1:D:70:LYS:HE2	1:D:112:ILE:HA	1.92	0.50
1:A:72:PRO:O	1:A:76:ILE:HG13	2.11	0.50
1:C:62:GLU:HB3	1:C:160:ARG:HB3	1.92	0.50
1:B:71:ILE:HB	1:B:72:PRO:CD	2.41	0.50
1:C:142:GLY:HA2	2:C:268:HOH:O	2.11	0.50
1:A:197:ALA:HB1	1:A:198:PRO:CD	2.41	0.50
1:B:228:LYS:HZ3	1:B:264:ILE:HG22	1.75	0.50
1:C:99:MET:HG3	1:C:102:TRP:CZ2	2.46	0.50
1:D:237:PHE:CE1	1:D:250:ARG:HA	2.47	0.50
1:D:40:VAL:HG21	1:D:59:ALA:CA	2.41	0.49
1:B:83:ILE:HD11	1:B:123:ILE:HD13	1.94	0.49
1:D:29:ASN:ND2	1:D:54:ASN:HD22	2.11	0.49
1:A:170:LEU:HD11	1:A:223:VAL:HB	1.94	0.49
1:A:198:PRO:HB3	1:C:113:GLN:HB3	1.93	0.49
1:D:178:LEU:H	1:D:185:GLN:HE22	1.61	0.49
1:D:142:GLY:H	1:D:165:ASN:HD21	1.61	0.49
1:B:231:GLU:HG3	1:B:232:VAL:N	2.28	0.49
1:C:92:TRP:NE1	1:C:95:LYS:N	2.61	0.49
1:C:247:LEU:HB3	1:C:248:PRO:HD3	1.95	0.48
1:B:228:LYS:HZ2	1:B:264:ILE:HG22	1.78	0.48
1:D:40:VAL:HG21	1:D:59:ALA:HA	1.95	0.48
1:A:178:LEU:H	1:A:185:GLN:HE22	1.61	0.47
1:D:99:MET:HG3	1:D:102:TRP:CZ2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:GLY:HA3	2:D:279:HOH:O	2.14	0.47
1:B:29:ASN:ND2	1:B:54:ASN:HB2	2.30	0.47
1:B:85:ASN:ND2	1:B:85:ASN:C	2.73	0.47
1:C:92:TRP:HE1	1:C:95:LYS:CB	2.28	0.47
1:A:45:LYS:O	1:A:46:SER:HB2	2.14	0.47
1:A:263:ILE:O	1:A:264:ILE:C	2.57	0.47
1:C:203:HIS:HD2	2:C:279:HOH:O	1.96	0.47
1:B:244:GLU:O	1:B:247:LEU:HB2	2.15	0.46
1:C:223:VAL:HG12	1:C:236:ALA:HB1	1.97	0.46
1:B:92:TRP:CZ2	1:B:103:GLU:HB3	2.50	0.46
1:C:40:VAL:HB	1:C:58:ARG:HB3	1.97	0.46
1:D:247:LEU:N	1:D:248:PRO:HD2	2.30	0.46
1:A:67:SER:OG	1:A:115:SER:HB3	2.15	0.46
1:A:228:LYS:NZ	1:A:264:ILE:HG22	2.31	0.46
1:B:200:TYR:CE2	1:B:264:ILE:HG23	2.50	0.46
1:A:92:TRP:CZ2	1:A:103:GLU:HB3	2.50	0.46
1:B:253:ILE:HB	1:B:254:PRO:HD3	1.97	0.46
1:D:35:GLU:HB2	1:D:37:VAL:HG22	1.97	0.46
1:D:40:VAL:HG21	1:D:59:ALA:N	2.31	0.46
1:A:25:ASN:C	1:A:25:ASN:HD22	2.24	0.45
1:C:142:GLY:HA2	1:C:165:ASN:ND2	2.31	0.45
1:C:73:ASN:ND2	1:C:132:MET:HE1	2.31	0.45
1:B:253:ILE:N	1:B:254:PRO:HD2	2.31	0.45
1:B:104:ARG:NH1	1:D:229:GLU:OE2	2.50	0.45
1:D:71:ILE:HB	1:D:72:PRO:HD2	1.99	0.45
1:D:228:LYS:HD3	2:D:370:HOH:O	2.17	0.45
1:A:86:GLU:OE2	1:C:176:ASN:ND2	2.44	0.45
1:C:37:VAL:HG11	1:C:239:MET:CE	2.47	0.45
1:B:44:CYS:SG	1:B:167:VAL:HG11	2.57	0.45
1:B:71:ILE:HB	1:B:72:PRO:HD3	1.99	0.45
1:C:45:LYS:O	1:C:46:SER:HB2	2.17	0.45
1:C:117:VAL:HB	1:C:118:PRO:HD3	1.97	0.44
1:C:231:GLU:HG3	1:C:232:VAL:N	2.32	0.44
1:A:138:LYS:HB3	1:A:179:SER:OG	2.17	0.44
1:A:39:GLY:O	1:A:58:ARG:HD3	2.18	0.44
1:A:71:ILE:HB	1:A:72:PRO:HD3	2.00	0.44
1:A:110:GLY:O	1:A:114:VAL:HG22	2.18	0.44
1:D:223:VAL:HG12	1:D:236:ALA:HA	1.99	0.44
1:A:210:GLY:O	1:A:218:GLY:HA3	2.17	0.44
1:B:204:SER:HA	1:B:223:VAL:O	2.18	0.44
1:C:71:ILE:HB	1:C:72:PRO:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:PHE:HD2	1:D:237:PHE:HB2	1.82	0.44
1:D:129:GLU:HG2	2:D:369:HOH:O	2.17	0.44
1:D:142:GLY:H	1:D:165:ASN:ND2	2.15	0.44
1:A:71:ILE:HB	1:A:72:PRO:CD	2.48	0.44
1:C:117:VAL:N	1:C:118:PRO:CD	2.81	0.44
1:C:253:ILE:HB	1:C:254:PRO:CD	2.48	0.44
1:D:79:GLU:OE2	1:D:184:ASN:ND2	2.38	0.44
1:A:62:GLU:HB3	1:A:160:ARG:HB3	1.99	0.43
1:B:170:LEU:HD13	1:B:224:GLY:HA2	1.99	0.43
1:C:161:ILE:HG12	1:C:162:SER:N	2.33	0.43
1:A:237:PHE:CD2	1:A:254:PRO:HG3	2.52	0.43
1:A:200:TYR:CE2	1:A:264:ILE:HG12	2.53	0.43
1:B:138:LYS:HD3	1:B:179:SER:HB2	1.99	0.43
1:C:178:LEU:H	1:C:185:GLN:HE22	1.66	0.43
1:B:253:ILE:HB	1:B:254:PRO:CD	2.48	0.43
1:B:263:ILE:O	1:B:264:ILE:C	2.62	0.43
1:B:203:HIS:NE2	2:B:381:HOH:O	2.37	0.43
1:A:120:PHE:HA	1:A:123:ILE:HD12	2.01	0.43
1:C:205:LYS:HD2	1:C:205:LYS:HA	1.81	0.43
1:D:247:LEU:HB3	1:D:248:PRO:CD	2.48	0.43
1:D:143:ASN:O	1:D:144:GLN:HB2	2.18	0.43
1:D:176:ASN:HA	1:D:185:GLN:NE2	2.34	0.43
1:C:142:GLY:O	1:C:144:GLN:HG3	2.19	0.42
1:A:118:PRO:HA	1:A:121:GLN:HE21	1.84	0.42
1:C:166:GLN:HG3	1:C:221:TRP:CZ3	2.54	0.42
1:B:142:GLY:H	1:B:165:ASN:ND2	2.18	0.42
1:B:129:GLU:HG3	1:B:146:ILE:CD1	2.49	0.42
1:B:142:GLY:H	1:B:165:ASN:HD21	1.67	0.42
1:B:175:LEU:HB3	1:B:177:LYS:HG3	2.00	0.42
1:D:117:VAL:HB	1:D:118:PRO:HD3	2.01	0.42
1:C:41:PHE:CE2	1:C:254:PRO:HB3	2.54	0.42
1:D:70:LYS:HG2	1:D:120:PHE:CE2	2.54	0.42
1:B:24:GLU:HB2	1:B:56:LEU:CD1	2.50	0.42
1:B:174:TYR:HD2	1:B:175:LEU:HD13	1.84	0.42
1:C:122:GLN:OE1	1:C:125:ARG:NH1	2.53	0.42
1:C:142:GLY:H	1:C:165:ASN:ND2	2.18	0.42
1:A:35:GLU:HB2	1:A:37:VAL:CG2	2.45	0.41
1:B:29:ASN:ND2	1:B:54:ASN:ND2	2.49	0.41
1:B:85:ASN:HD22	1:B:85:ASN:C	2.27	0.41
1:A:143:ASN:ND2	1:A:160:ARG:H	2.19	0.41
1:C:78:LEU:HB3	1:C:184:ASN:CG	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:PHE:CE2	1:A:235:PHE:HB2	2.56	0.41
1:C:189:LYS:O	1:C:190:GLU:C	2.64	0.41
1:A:247:LEU:CB	1:A:248:PRO:HD3	2.50	0.40
1:C:178:LEU:HB2	1:C:185:GLN:NE2	2.36	0.40
1:C:247:LEU:N	1:C:248:PRO:CD	2.84	0.40
1:A:196:ALA:HA	1:A:201:LEU:HD12	2.03	0.40
1:A:228:LYS:HZ2	1:A:264:ILE:CG2	2.33	0.40
1:C:70:LYS:HD2	1:C:120:PHE:CD1	2.56	0.40
1:D:43:LEU:HD21	1:D:263:ILE:HD11	2.03	0.40
1:D:94:GLY:O	1:D:95:LYS:C	2.64	0.40
1:C:125:ARG:NH2	1:C:151:ASP:OD2	2.53	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	241/246 (98%)	225 (93%)	16 (7%)	0	100	100
1	B	241/246 (98%)	230 (95%)	11 (5%)	0	100	100
1	C	241/246 (98%)	229 (95%)	10 (4%)	2 (1%)	16	25
1	D	238/246 (97%)	228 (96%)	9 (4%)	1 (0%)	30	43
All	All	961/984 (98%)	912 (95%)	46 (5%)	3 (0%)	36	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	93	ASP
1	C	96	PRO
1	C	97	ARG

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	204/210 (97%)	189 (93%)	15 (7%)	13	22
1	B	204/210 (97%)	194 (95%)	10 (5%)	22	39
1	C	199/210 (95%)	190 (96%)	9 (4%)	24	42
1	D	198/210 (94%)	185 (93%)	13 (7%)	15	26
All	All	805/840 (96%)	758 (94%)	47 (6%)	18	32

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ILE
1	A	49	LYS
1	A	50	SER
1	A	112	ILE
1	A	115	SER
1	A	140	SER
1	A	143	ASN
1	A	147	SER
1	A	166	GLN
1	A	175	LEU
1	A	179	SER
1	A	226	VAL
1	A	245	SER
1	A	247	LEU
1	A	264	ILE
1	B	26	THR
1	B	50	SER
1	B	60	SER
1	B	73	ASN
1	B	100	LYS
1	B	156	GLU
1	B	166	GLN
1	B	175	LEU
1	B	198	PRO

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Mol	Chain	Res	Type
1	B	247	LEU
1	C	67	SER
1	C	73	ASN
1	C	113	GLN
1	C	156	GLU
1	C	166	GLN
1	C	167	VAL
1	C	179	SER
1	C	247	LEU
1	C	250	ARG
1	D	30	LYS
1	D	61	LYS
1	D	67	SER
1	D	73	ASN
1	D	113	GLN
1	D	145	ASN
1	D	156	GLU
1	D	158	GLN
1	D	166	GLN
1	D	175	LEU
1	D	194	THR
1	D	247	LEU
1	D	250	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	73	ASN
1	A	121	GLN
1	A	122	GLN
1	A	143	ASN
1	A	145	ASN
1	A	158	GLN
1	A	165	ASN
1	A	166	GLN
1	A	185	GLN
1	A	203	HIS
1	B	29	ASN
1	B	73	ASN
1	B	85	ASN
1	B	122	GLN

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Mol	Chain	Res	Type
1	B	145	ASN
1	B	185	GLN
1	C	29	ASN
1	C	73	ASN
1	C	113	GLN
1	C	121	GLN
1	C	145	ASN
1	C	165	ASN
1	C	166	GLN
1	C	185	GLN
1	C	203	HIS
1	D	29	ASN
1	D	73	ASN
1	D	113	GLN
1	D	121	GLN
1	D	145	ASN
1	D	165	ASN
1	D	166	GLN
1	D	185	GLN
1	D	203	HIS

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 ⓘ

There are no ligands in this entry.

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	243/246 (98%)	0.42	19 (7%) 19 15	5, 14, 33, 40	0
1	B	243/246 (98%)	0.46	13 (5%) 32 28	5, 15, 30, 38	0
1	C	243/246 (98%)	0.45	16 (6%) 24 20	5, 14, 33, 52	0
1	D	242/246 (98%)	0.56	19 (7%) 18 15	5, 13, 32, 52	0
All	All	971/984 (98%)	0.47	67 (6%) 23 19	5, 14, 32, 52	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	93	ASP	9.0
1	D	94	GLY	8.8
1	C	94	GLY	7.9
1	C	95	LYS	5.1
1	D	85	ASN	5.0
1	D	92	TRP	4.5
1	A	264	ILE	4.3
1	A	212	GLY	4.3
1	C	96	PRO	4.2
1	D	95	LYS	4.2
1	D	103	GLU	3.7
1	C	92	TRP	3.7
1	B	264	ILE	3.6
1	B	26	THR	3.6
1	A	215	SER	3.6
1	A	50	SER	3.5
1	C	117	VAL	3.5
1	A	214	GLU	3.2
1	C	98	ALA	3.1
1	B	44	CYS	3.1
1	A	199	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	97	ARG	3.0
1	A	27	SER	3.0
1	D	97	ARG	2.9
1	B	51	CYS	2.9
1	D	117	VAL	2.9
1	A	198	PRO	2.8
1	A	51	CYS	2.8
1	C	51	CYS	2.8
1	D	245	SER	2.7
1	D	98	ALA	2.7
1	A	30	LYS	2.7
1	A	197	ALA	2.7
1	B	23	THR	2.6
1	D	51	CYS	2.6
1	C	116	ALA	2.5
1	C	88	GLN	2.5
1	A	26	THR	2.5
1	A	200	TYR	2.4
1	B	137	LYS	2.4
1	A	229	GLU	2.4
1	A	34	ALA	2.4
1	B	33	SER	2.4
1	B	60	SER	2.4
1	D	87	HIS	2.4
1	D	44	CYS	2.4
1	C	104	ARG	2.3
1	C	86	GLU	2.3
1	D	116	ALA	2.2
1	D	101	GLN	2.2
1	B	50	SER	2.2
1	B	147	SER	2.2
1	C	93	ASP	2.2
1	A	216	ASN	2.2
1	B	46	SER	2.2
1	C	46	SER	2.2
1	D	104	ARG	2.2
1	B	229	GLU	2.1
1	D	154	TRP	2.1
1	A	35	GLU	2.1
1	C	44	CYS	2.1
1	A	154	TRP	2.1
1	D	91	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	99	MET	2.1
1	A	36	ALA	2.0
1	B	30	LYS	2.0
1	D	84	LYS	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.