



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 05:28 AM EDT

PDB ID : 7NPD / pdb_00007npd
Title : Vibrio cholerae ParA2
Authors : Parker, A.V.; Bergeron, J.R.C.
Deposited on : 2021-02-26
Resolution : 2.60 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

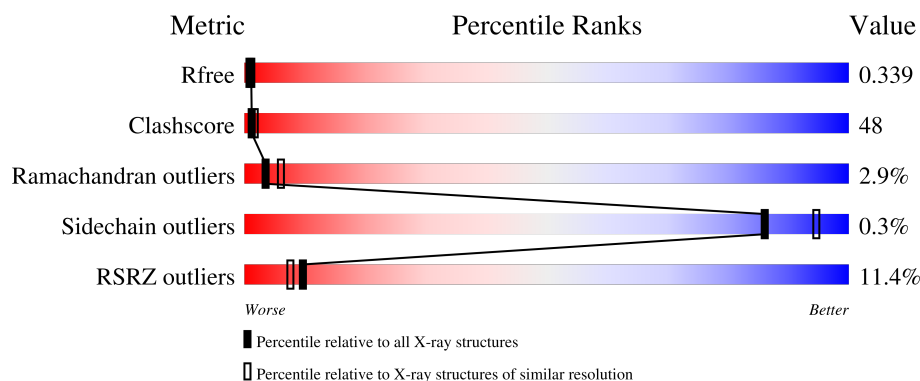
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	A	407	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2946 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 Walker A-type ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	1	0
			2899	1833	494	553	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A085S0Z4
A	2	ALA	-	expression tag	UNP A0A085S0Z4

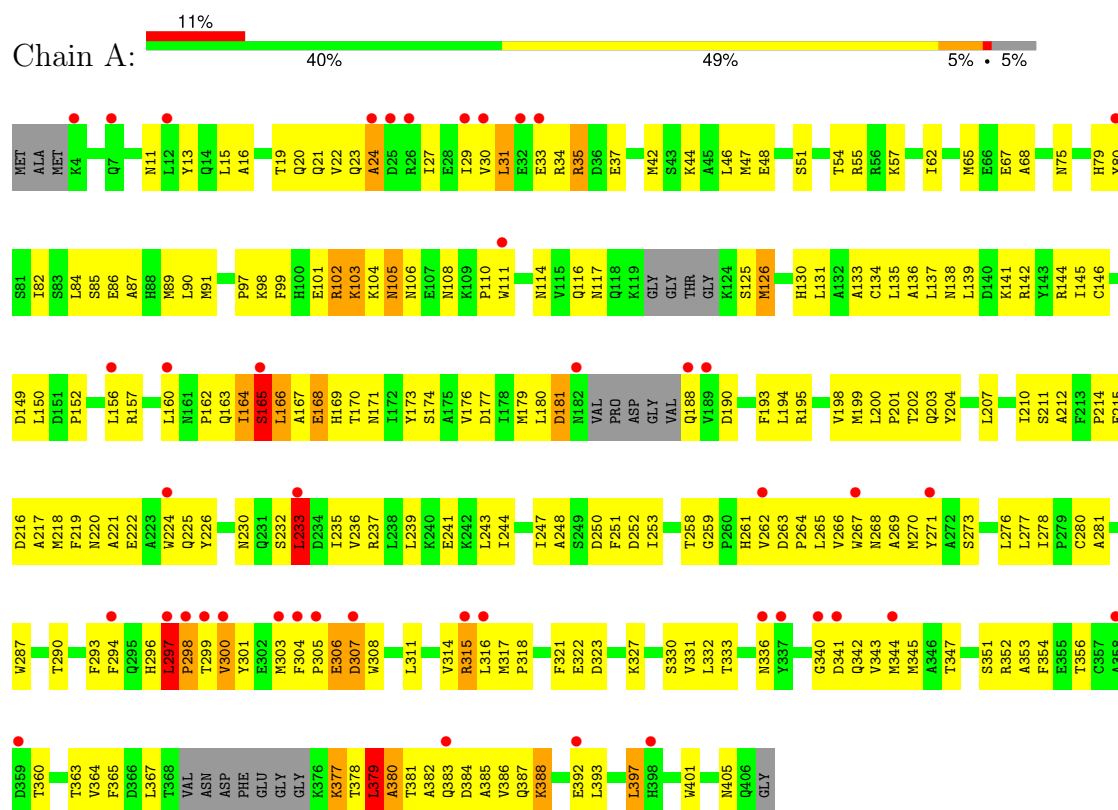
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	47	Total	O	0	0
			47	47		

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: Walker A-type ATPase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α , β , γ	63.25Å 63.25Å 214.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.31 – 2.60 38.31 – 2.60	Depositor EDS
% Data completeness (in resolution range)	75.2 (38.31-2.60) 91.0 (38.31-2.60)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.274 , 0.337 0.275 , 0.339	Depositor DCC
R_{free} test set	1469 reflections (9.17%)	wwPDB-VP
Wilson B-factor (Å ²)	70.1	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 85.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2946	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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	0.79	3/2957 (0.1%)	1.30	24/4040 (0.6%)

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	8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	300	VAL	CB-CG1	-8.51	1.24	1.52
1	A	165	SER	CB-OG	5.72	1.53	1.42
1	A	300	VAL	CB-CG2	-5.41	1.34	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	GLU	CA-CB-CG	-10.80	92.49	114.10
1	A	164	ILE	CA-C-N	8.12	137.05	121.54
1	A	164	ILE	C-N-CA	8.12	137.05	121.54
1	A	35	ARG	N-CA-C	-7.30	104.32	112.57
1	A	379	LEU	CA-C-N	7.10	135.10	121.54
1	A	379	LEU	C-N-CA	7.10	135.10	121.54
1	A	297	LEU	CA-CB-CG	6.80	140.09	116.30
1	A	300	VAL	CA-C-N	6.70	135.39	122.53
1	A	300	VAL	C-N-CA	6.70	135.39	122.53
1	A	22	VAL	N-CA-C	6.68	116.70	110.42
1	A	31	LEU	CA-CB-CG	-6.67	92.96	116.30
1	A	397	LEU	CA-CB-CG	6.14	137.81	116.30
1	A	164	ILE	O-C-N	6.13	127.82	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	THR	CA-C-N	6.07	128.77	120.46
1	A	299	THR	C-N-CA	6.07	128.77	120.46
1	A	233	LEU	CB-CG-CD1	-5.59	93.94	110.70
1	A	388	LYS	CG-CD-CE	-5.42	98.83	111.30
1	A	24	ALA	N-CA-C	5.35	122.20	110.80
1	A	31	LEU	CD1-CG-CD2	5.35	122.57	110.80
1	A	126	MET	CA-C-N	-5.34	112.28	122.53
1	A	126	MET	C-N-CA	-5.34	112.28	122.53
1	A	315	ARG	CA-CB-CG	5.26	124.62	114.10
1	A	23	GLN	CA-C-N	5.10	131.28	121.54
1	A	23	GLN	C-N-CA	5.10	131.28	121.54

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ARG	Peptide
1	A	165	SER	Peptide
1	A	181	ASP	Mainchain
1	A	188	GLN	Peptide
1	A	297	LEU	Peptide
1	A	377	LYS	Peptide
1	A	379	LEU	Peptide
1	A	380	ALA	Mainchain

5.2 Too-close contacts [i](#)

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	2899	0	2658	265	1
2	A	47	0	0	10	0
All	All	2946	0	2658	265	1

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 48.

All (265) 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:A:27:ILE:O	1:A:31:LEU:HD12	1.29	1.25
1:A:31:LEU:CD2	1:A:164:ILE:HG21	1.75	1.15
1:A:31:LEU:HD21	1:A:164:ILE:CG2	1.82	1.08
1:A:27:ILE:O	1:A:31:LEU:CD1	2.08	1.00
1:A:377:LYS:O	1:A:378:THR:HG23	1.60	0.99
1:A:31:LEU:HD21	1:A:164:ILE:HG21	0.94	0.94
1:A:27:ILE:HG22	1:A:31:LEU:HD13	1.49	0.91
1:A:11:ASN:ND2	2:A:505:HOH:O	2.03	0.91
1:A:321:PHE:CE2	1:A:323:ASP:OD1	2.23	0.91
1:A:297:LEU:HA	1:A:300:VAL:HG11	1.50	0.89
1:A:277:LEU:C	1:A:278:ILE:HD12	1.98	0.89
1:A:224:TRP:CZ2	1:A:264:PRO:HD3	2.09	0.88
1:A:163:GLN:NE2	2:A:503:HOH:O	1.98	0.85
1:A:321:PHE:HE2	1:A:323:ASP:OD1	1.60	0.83
1:A:163:GLN:OE1	2:A:502:HOH:O	1.96	0.82
1:A:15:LEU:O	1:A:19:THR:OG1	1.97	0.81
1:A:220:ASN:HB3	1:A:224:TRP:CZ3	2.15	0.80
1:A:136:ALA:O	2:A:504:HOH:O	2.00	0.79
1:A:111:TRP:NE1	1:A:397:LEU:HB3	1.98	0.79
1:A:97:PRO:HB2	1:A:101:GLU:HB3	1.62	0.79
1:A:202:THR:O	1:A:204:TYR:N	2.14	0.78
1:A:125:SER:O	1:A:156:LEU:HD21	1.83	0.78
1:A:297:LEU:HA	1:A:300:VAL:CG1	2.12	0.78
1:A:165:SER:OG	1:A:169:HIS:HE1	1.67	0.77
1:A:264:PRO:O	1:A:268:ASN:HB2	1.84	0.77
1:A:27:ILE:CG2	1:A:31:LEU:HD13	2.13	0.77
1:A:65:MET:HE1	1:A:90:LEU:HA	1.66	0.76
1:A:27:ILE:CG2	1:A:31:LEU:CD1	2.64	0.76
1:A:135:LEU:O	2:A:506:HOH:O	2.03	0.76
1:A:353:ALA:HB2	1:A:378:THR:OG1	1.86	0.76
1:A:345:MET:HE2	1:A:388:LYS:NZ	2.01	0.74
1:A:177:ASP:O	1:A:181:ASP:HA	1.85	0.74
1:A:105:ASN:O	1:A:105:ASN:ND2	2.21	0.73
1:A:377:LYS:O	1:A:378:THR:CG2	2.37	0.73
1:A:297:LEU:HD22	1:A:300:VAL:HG21	1.70	0.73
1:A:331:VAL:O	2:A:507:HOH:O	2.06	0.73
1:A:224:TRP:HZ2	1:A:264:PRO:HD3	1.51	0.72
1:A:258:THR:HB	1:A:266:VAL:HG12	1.71	0.72
1:A:179:MET:HE3	1:A:239:LEU:HB2	1.72	0.71
1:A:270:MET:HB3	1:A:301:TYR:CE1	2.26	0.70
1:A:237:ARG:HA	1:A:271:TYR:CE1	2.27	0.70
1:A:27:ILE:HG23	1:A:31:LEU:CD1	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:VAL:O	1:A:315:ARG:HD3	1.92	0.69
1:A:145:ILE:HG23	1:A:253:ILE:HB	1.75	0.69
1:A:264:PRO:HA	1:A:267:TRP:HB2	1.74	0.69
1:A:164:ILE:H	1:A:164:ILE:HD12	1.57	0.68
1:A:336:ASN:O	1:A:340:GLY:N	2.25	0.67
1:A:194:LEU:HD12	1:A:247:ILE:HG23	1.74	0.67
1:A:51:SER:HB2	1:A:91:MET:HE1	1.76	0.67
1:A:102:ARG:O	1:A:104:LYS:N	2.27	0.67
1:A:230:ASN:CB	1:A:232:SER:HB2	2.25	0.66
1:A:134:CYS:SG	1:A:365:PHE:CZ	2.89	0.66
1:A:202:THR:C	1:A:204:TYR:H	2.03	0.66
1:A:111:TRP:HE1	1:A:397:LEU:HB3	1.61	0.66
1:A:315:ARG:HH21	1:A:342:GLN:HG3	1.61	0.66
1:A:215:GLU:OE1	1:A:215:GLU:N	2.26	0.65
1:A:27:ILE:C	1:A:31:LEU:HD12	2.19	0.65
1:A:235:ILE:O	1:A:268:ASN:ND2	2.29	0.65
1:A:165:SER:OG	1:A:169:HIS:CE1	2.50	0.64
1:A:42:MET:HG2	1:A:46:LEU:HG	1.79	0.64
1:A:387:GLN:NE2	2:A:508:HOH:O	2.20	0.63
1:A:401:TRP:O	1:A:405:ASN:ND2	2.27	0.63
1:A:97:PRO:HB2	1:A:101:GLU:CB	2.29	0.62
1:A:278:ILE:HD12	1:A:278:ILE:N	2.14	0.62
1:A:144:ARG:NE	1:A:252:ASP:OD2	2.32	0.62
1:A:202:THR:O	1:A:202:THR:OG1	2.13	0.62
1:A:224:TRP:CZ2	1:A:264:PRO:CD	2.83	0.62
1:A:298:PRO:C	1:A:300:VAL:H	2.07	0.62
1:A:133:ALA:O	1:A:137:LEU:HB2	1.99	0.62
1:A:162:PRO:HB3	1:A:200:LEU:HB2	1.82	0.62
1:A:75:ASN:HB2	1:A:79:HIS:H	1.63	0.62
1:A:75:ASN:CB	1:A:79:HIS:H	2.13	0.61
1:A:305:PRO:O	1:A:307:ASP:N	2.33	0.61
1:A:65:MET:HE1	1:A:90:LEU:CA	2.30	0.61
1:A:236:VAL:HG11	1:A:304:PHE:CE1	2.36	0.61
1:A:114:ASN:HB3	1:A:276:LEU:HD12	1.82	0.61
1:A:301:TYR:CD1	1:A:304:PHE:HE2	2.18	0.61
1:A:380:ALA:O	1:A:384:ASP:N	2.25	0.61
1:A:378:THR:O	1:A:381:THR:N	2.34	0.60
1:A:297:LEU:CD2	1:A:300:VAL:HG21	2.30	0.60
1:A:15:LEU:HD22	1:A:19:THR:HG23	1.84	0.59
1:A:160:LEU:HD11	1:A:204:TYR:HE2	1.66	0.59
1:A:277:LEU:HD11	1:A:317:MET:SD	2.43	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ASP:O	1:A:267:TRP:CG	2.56	0.58
1:A:180:LEU:HD11	1:A:219:PHE:HD1	1.69	0.58
1:A:15:LEU:CD2	1:A:19:THR:HG23	2.33	0.58
1:A:27:ILE:HD11	1:A:170:THR:O	2.03	0.58
1:A:301:TYR:C	1:A:303:MET:H	2.12	0.58
1:A:176:VAL:HG22	1:A:216:ASP:CG	2.28	0.57
1:A:287:TRP:HA	1:A:287:TRP:CE3	2.38	0.57
1:A:167:ALA:C	1:A:169:HIS:H	2.11	0.57
1:A:180:LEU:HD11	1:A:219:PHE:CD1	2.39	0.57
1:A:106:ASN:ND2	1:A:106:ASN:O	2.37	0.57
1:A:290:THR:O	1:A:293:PHE:HB3	2.04	0.57
1:A:308:TRP:CZ2	1:A:311:LEU:CD1	2.87	0.57
1:A:152:PRO:O	1:A:214:PRO:HD3	2.05	0.57
1:A:308:TRP:CZ2	1:A:311:LEU:HD12	2.40	0.57
1:A:33:GLU:O	1:A:34:ARG:C	2.48	0.56
1:A:65:MET:CE	1:A:90:LEU:HA	2.34	0.56
1:A:280:CYS:SG	1:A:281:ALA:N	2.79	0.56
1:A:308:TRP:HZ2	1:A:311:LEU:CD1	2.19	0.56
1:A:287:TRP:HA	1:A:287:TRP:HE3	1.71	0.56
1:A:194:LEU:HD13	1:A:243:LEU:HD12	1.86	0.56
1:A:379:LEU:HD12	1:A:383:GLN:OE1	2.05	0.56
1:A:27:ILE:HG23	1:A:31:LEU:HD11	1.87	0.56
1:A:333:THR:HA	1:A:336:ASN:HB2	1.88	0.56
1:A:170:THR:OG1	1:A:171:ASN:N	2.38	0.56
1:A:225:GLN:O	1:A:225:GLN:HG2	2.05	0.55
1:A:144:ARG:NH2	1:A:252:ASP:OD2	2.38	0.55
1:A:62:ILE:O	1:A:65:MET:N	2.39	0.55
1:A:277:LEU:HA	1:A:315:ARG:O	2.07	0.55
1:A:401:TRP:CD1	1:A:405:ASN:HD21	2.25	0.55
1:A:19:THR:C	1:A:21:GLN:H	2.14	0.54
1:A:276:LEU:HB2	1:A:314:VAL:HG22	1.88	0.54
1:A:215:GLU:C	1:A:217:ALA:H	2.15	0.54
1:A:263:ASP:HB3	1:A:265:LEU:H	1.73	0.54
1:A:222:GLU:O	1:A:226:TYR:CB	2.54	0.54
1:A:99:PHE:C	1:A:99:PHE:CD2	2.86	0.54
1:A:294:PHE:HA	1:A:297:LEU:HB3	1.89	0.54
1:A:139:LEU:O	1:A:142:ARG:HG3	2.08	0.53
1:A:401:TRP:HD1	1:A:405:ASN:ND2	2.06	0.53
1:A:293:PHE:CZ	1:A:297:LEU:HG	2.44	0.53
1:A:152:PRO:HB3	1:A:214:PRO:HA	1.90	0.53
1:A:219:PHE:HZ	1:A:268:ASN:ND2	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ASP:HB3	1:A:265:LEU:N	2.24	0.53
1:A:364:VAL:HA	1:A:367:LEU:HD21	1.91	0.53
1:A:27:ILE:HG22	1:A:31:LEU:CD1	2.24	0.52
1:A:308:TRP:HZ2	1:A:311:LEU:HD12	1.75	0.52
1:A:29:ILE:O	1:A:33:GLU:HG3	2.10	0.52
1:A:301:TYR:HD1	1:A:304:PHE:HE2	1.56	0.52
1:A:237:ARG:O	1:A:241:GLU:OE1	2.29	0.51
1:A:215:GLU:C	1:A:217:ALA:N	2.69	0.51
1:A:116:GLN:OE1	1:A:270:MET:HE3	2.11	0.51
1:A:316:LEU:HD23	1:A:317:MET:N	2.25	0.51
1:A:301:TYR:C	1:A:303:MET:N	2.66	0.51
1:A:13:TYR:HA	1:A:16:ALA:HB3	1.91	0.51
1:A:162:PRO:HB3	1:A:200:LEU:CB	2.40	0.51
1:A:176:VAL:HG11	1:A:265:LEU:HD11	1.93	0.51
1:A:232:SER:O	1:A:233:LEU:HB2	2.11	0.51
1:A:343:VAL:O	1:A:344:MET:HE3	2.11	0.50
1:A:80:TYR:HE1	2:A:537:HOH:O	1.94	0.50
1:A:194:LEU:HA	1:A:198:VAL:HG12	1.93	0.50
1:A:364:VAL:HG12	1:A:379:LEU:CD1	2.41	0.50
1:A:301:TYR:O	1:A:303:MET:N	2.44	0.50
1:A:311:LEU:HD23	1:A:314:VAL:CG2	2.42	0.50
1:A:173:TYR:CD2	1:A:173:TYR:N	2.79	0.50
1:A:316:LEU:HD23	1:A:317:MET:C	2.37	0.50
1:A:318:PRO:HG2	1:A:347:THR:HA	1.94	0.49
1:A:98:LYS:O	1:A:101:GLU:HB2	2.12	0.49
1:A:306:GLU:C	1:A:308:TRP:H	2.19	0.49
1:A:44:LYS:HA	1:A:47:MET:HB3	1.93	0.49
1:A:401:TRP:HD1	1:A:405:ASN:HD21	1.59	0.49
1:A:48:GLU:OE2	1:A:55:ARG:NE	2.44	0.49
1:A:277:LEU:CA	1:A:278:ILE:HD12	2.43	0.48
1:A:166:LEU:C	1:A:168:GLU:H	2.22	0.48
1:A:163:GLN:HB2	1:A:201:PRO:HG2	1.95	0.48
1:A:252:ASP:O	1:A:253:ILE:HD13	2.14	0.48
1:A:341:ASP:O	1:A:342:GLN:HB2	2.14	0.48
1:A:82:ILE:HG23	1:A:86:GLU:HB3	1.96	0.48
1:A:219:PHE:CD2	1:A:265:LEU:HG	2.49	0.48
1:A:237:ARG:HA	1:A:271:TYR:CD1	2.49	0.48
1:A:293:PHE:O	1:A:297:LEU:N	2.47	0.48
1:A:296:HIS:O	1:A:300:VAL:HG13	2.14	0.47
1:A:332:LEU:HD12	1:A:332:LEU:O	2.14	0.47
1:A:16:ALA:O	1:A:20:GLN:CB	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:LEU:HD21	1:A:137:LEU:HD11	1.97	0.47
1:A:278:ILE:N	1:A:278:ILE:CD1	2.78	0.47
1:A:108:ASN:HA	1:A:405:ASN:OD1	2.14	0.47
1:A:98:LYS:O	1:A:99:PHE:C	2.57	0.47
1:A:190:ASP:H	1:A:193:PHE:HB3	1.79	0.47
1:A:381:THR:O	1:A:385:ALA:HB2	2.15	0.47
1:A:215:GLU:O	1:A:217:ALA:N	2.48	0.46
1:A:322:GLU:OE2	1:A:322:GLU:N	2.43	0.46
1:A:180:LEU:CD1	1:A:219:PHE:HD1	2.27	0.46
1:A:204:TYR:HB2	1:A:207:LEU:HB3	1.97	0.46
1:A:99:PHE:HD1	1:A:141:LYS:HD2	1.80	0.46
1:A:110:PRO:HG3	1:A:248:ALA:HB1	1.96	0.46
1:A:116:GLN:HG2	1:A:258:THR:OG1	2.16	0.46
1:A:126:MET:HE1	1:A:354:PHE:O	2.15	0.46
1:A:298:PRO:C	1:A:300:VAL:N	2.68	0.46
1:A:166:LEU:CA	1:A:168:GLU:HG2	2.46	0.46
1:A:327:LYS:O	1:A:330:SER:OG	2.21	0.46
1:A:195:ARG:HA	1:A:199:MET:HE3	1.97	0.46
1:A:130:HIS:HB3	1:A:386:VAL:HG11	1.98	0.46
1:A:166:LEU:CB	1:A:168:GLU:HG2	2.46	0.46
1:A:215:GLU:H	1:A:215:GLU:CD	2.22	0.46
1:A:265:LEU:HA	1:A:265:LEU:HD23	1.48	0.46
1:A:149:ASP:OD1	1:A:150:LEU:N	2.49	0.45
1:A:166:LEU:C	1:A:168:GLU:N	2.74	0.45
1:A:345:MET:HE2	1:A:388:LYS:HZ3	1.80	0.45
1:A:383:GLN:O	1:A:387:GLN:HB2	2.17	0.45
1:A:114:ASN:HB2	1:A:273:SER:OG	2.17	0.45
1:A:247:ILE:O	1:A:251:PHE:HD1	2.00	0.45
1:A:15:LEU:HA	1:A:15:LEU:HD23	1.43	0.45
1:A:131:LEU:O	1:A:135:LEU:HG	2.17	0.45
1:A:150:LEU:HD12	1:A:150:LEU:HA	1.50	0.45
1:A:356:THR:O	1:A:360:THR:HG22	2.16	0.45
1:A:30:VAL:HG13	1:A:31:LEU:HD12	1.98	0.45
1:A:111:TRP:HA	1:A:111:TRP:CE3	2.52	0.45
1:A:179:MET:CE	1:A:239:LEU:HB2	2.42	0.45
1:A:270:MET:HB3	1:A:301:TYR:HE1	1.77	0.45
1:A:306:GLU:C	1:A:308:TRP:N	2.72	0.45
1:A:35:ARG:O	1:A:37:GLU:N	2.50	0.44
1:A:321:PHE:CE1	1:A:332:LEU:CD2	3.00	0.44
1:A:174:SER:HB2	1:A:211:SER:O	2.17	0.44
1:A:276:LEU:CB	1:A:314:VAL:HG22	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:TRP:CD1	1:A:397:LEU:HD13	2.53	0.44
1:A:138:ASN:OD1	1:A:141:LYS:HB2	2.17	0.44
1:A:294:PHE:C	1:A:297:LEU:H	2.26	0.44
1:A:315:ARG:NH1	2:A:515:HOH:O	2.50	0.44
1:A:378:THR:OG1	1:A:379:LEU:N	2.51	0.44
1:A:145:ILE:HG22	1:A:146:CYS:H	1.83	0.44
1:A:261:HIS:HB3	1:A:262:VAL:O	2.18	0.44
1:A:85:SER:O	1:A:89:MET:HG3	2.18	0.43
1:A:269:ALA:O	1:A:273:SER:HB2	2.17	0.43
1:A:276:LEU:HD12	1:A:276:LEU:HA	1.62	0.43
1:A:306:GLU:H	1:A:306:GLU:HG3	1.57	0.43
1:A:218:MET:O	1:A:219:PHE:C	2.60	0.43
1:A:87:ALA:HA	1:A:90:LEU:HD12	2.00	0.43
1:A:114:ASN:HB3	1:A:276:LEU:CD1	2.47	0.43
1:A:134:CYS:SG	1:A:387:GLN:HG3	2.58	0.43
1:A:117:ASN:HB2	1:A:259:GLY:HA2	1.99	0.43
1:A:233:LEU:HD11	1:A:303:MET:HG2	1.99	0.43
1:A:130:HIS:CD2	1:A:363:THR:HB	2.53	0.43
1:A:174:SER:HB2	1:A:212:ALA:HA	2.01	0.43
1:A:176:VAL:CG2	1:A:216:ASP:CG	2.91	0.43
1:A:219:PHE:CZ	1:A:268:ASN:ND2	2.86	0.43
1:A:31:LEU:HD23	1:A:31:LEU:HA	1.94	0.43
1:A:236:VAL:HG11	1:A:304:PHE:CD1	2.53	0.43
1:A:392:GLU:O	1:A:393:LEU:C	2.62	0.43
1:A:55:ARG:HE	1:A:55:ARG:HB2	1.57	0.42
1:A:103:LYS:HA	1:A:106:ASN:HB2	2.01	0.42
1:A:380:ALA:O	1:A:384:ASP:CG	2.63	0.42
1:A:301:TYR:HD1	1:A:304:PHE:CE2	2.36	0.42
1:A:199:MET:HG2	1:A:210:ILE:HD11	2.02	0.42
1:A:233:LEU:CD1	1:A:303:MET:HG2	2.48	0.42
1:A:278:ILE:O	1:A:316:LEU:HG	2.19	0.42
1:A:15:LEU:HD22	1:A:19:THR:CG2	2.50	0.42
1:A:136:ALA:HB2	1:A:145:ILE:HD12	2.00	0.42
1:A:167:ALA:C	1:A:169:HIS:N	2.78	0.42
1:A:237:ARG:HA	1:A:271:TYR:HE1	1.81	0.42
1:A:353:ALA:CB	1:A:378:THR:OG1	2.64	0.42
1:A:68:ALA:N	2:A:516:HOH:O	2.53	0.42
1:A:233:LEU:HA	1:A:233:LEU:HD13	1.78	0.42
1:A:263:ASP:O	1:A:267:TRP:CD1	2.73	0.42
1:A:157:ARG:HE	1:A:211:SER:HB3	1.84	0.41
1:A:301:TYR:HA	1:A:304:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:VAL:CG1	1:A:344:MET:N	2.83	0.41
1:A:380:ALA:C	1:A:384:ASP:OD2	2.64	0.41
1:A:103:LYS:HA	1:A:106:ASN:CB	2.51	0.41
1:A:166:LEU:N	1:A:168:GLU:HG2	2.35	0.41
1:A:239:LEU:HG	1:A:244:ILE:HD13	2.02	0.41
1:A:315:ARG:HD2	1:A:342:GLN:HA	2.03	0.41
1:A:316:LEU:O	1:A:344:MET:SD	2.78	0.41
1:A:218:MET:O	1:A:221:ALA:N	2.54	0.41
1:A:343:VAL:HG12	1:A:344:MET:N	2.35	0.41
1:A:381:THR:O	1:A:385:ALA:CB	2.69	0.41
1:A:217:ALA:O	1:A:218:MET:C	2.63	0.41
1:A:134:CYS:SG	1:A:365:PHE:HZ	2.43	0.41
1:A:54:THR:HG1	1:A:57:LYS:H	1.65	0.40
1:A:401:TRP:CD1	1:A:405:ASN:ND2	2.86	0.40
1:A:250:ASP:OD1	1:A:250:ASP:N	2.54	0.40
1:A:277:LEU:N	1:A:278:ILE:HD12	2.36	0.40
1:A:364:VAL:HG11	1:A:382:ALA:CB	2.51	0.40
1:A:321:PHE:CE1	1:A:332:LEU:HD22	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:GLU:OE2	1:A:98:LYS:NZ[6_565]	2.11	0.09

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	380/407 (93%)	315 (83%)	54 (14%)	11 (3%)	3 6

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	LYS
1	A	298	PRO
1	A	24	ALA
1	A	166	LEU
1	A	203	GLN
1	A	233	LEU
1	A	306	GLU
1	A	297	LEU
1	A	307	ASP
1	A	352	ARG
1	A	351	SER

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	288/358 (80%)	287 (100%)	1 (0%)	86	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ASN

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	169	HIS
1	A	261	HIS
1	A	292	ASN
1	A	296	HIS
1	A	336	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	A	387/407 (95%)	0.78	44 (11%) 10 7	35, 78, 128, 167	1 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	224	TRP	5.1
1	A	304	PHE	4.4
1	A	337	TYR	4.1
1	A	299	THR	3.9
1	A	344	MET	3.7
1	A	300	VAL	3.4
1	A	303	MET	3.3
1	A	29	ILE	3.3
1	A	4	LYS	3.3
1	A	182	ASN	3.1
1	A	297	LEU	3.1
1	A	111	TRP	2.9
1	A	189	VAL	2.9
1	A	160	LEU	2.9
1	A	336	ASN	2.8
1	A	80	TYR	2.7
1	A	341	ASP	2.7
1	A	307	ASP	2.7
1	A	7	GLN	2.6
1	A	262	VAL	2.6
1	A	156	LEU	2.6
1	A	358	ALA	2.5
1	A	24	ALA	2.5
1	A	25	ASP	2.5
1	A	267	TRP	2.5
1	A	305	PRO	2.4
1	A	315	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	316	LEU	2.3
1	A	32	GLU	2.3
1	A	30	VAL	2.3
1	A	26	ARG	2.3
1	A	165	SER	2.2
1	A	12	LEU	2.2
1	A	392	GLU	2.2
1	A	188	GLN	2.2
1	A	359	ASP	2.1
1	A	298	PRO	2.1
1	A	340	GLY	2.1
1	A	33	GLU	2.1
1	A	398	HIS	2.1
1	A	383	GLN	2.0
1	A	294	PHE	2.0
1	A	233	LEU	2.0
1	A	271	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.