



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 08:23 PM EDT

PDB ID : 6HR5 / pdb_00006hr5
Title : Structure of the S1_25 family sulfatase module of the rhamnosidase FA22250 from *Formosa agariphila*
Authors : Roret, T.; Prechoux, A.; Czjzek, M.; Michel, G.
Deposited on : 2018-09-26
Resolution : 2.91 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

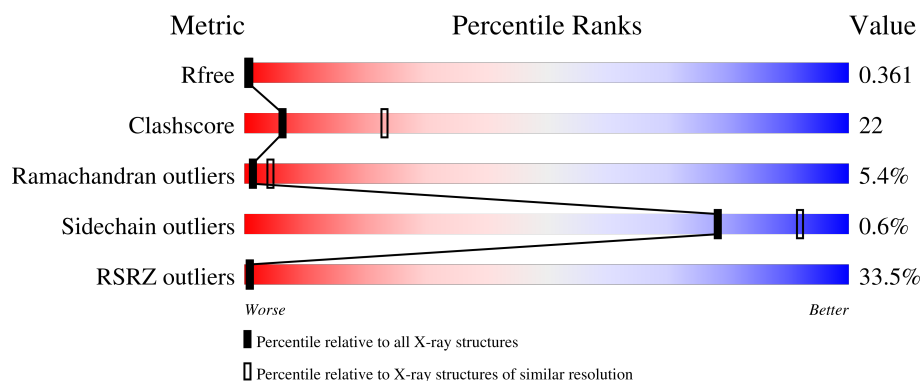
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	467	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3077 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 Alpha-L-rhamnosidase/sulfatase (GH78).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	0	0	0
			3076	1963	522	583	8			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP T2KM26
A	-19	GLY	-	expression tag	UNP T2KM26
A	-18	SER	-	expression tag	UNP T2KM26
A	-17	SER	-	expression tag	UNP T2KM26
A	-16	HIS	-	expression tag	UNP T2KM26
A	-15	HIS	-	expression tag	UNP T2KM26
A	-14	HIS	-	expression tag	UNP T2KM26
A	-13	HIS	-	expression tag	UNP T2KM26
A	-12	HIS	-	expression tag	UNP T2KM26
A	-11	HIS	-	expression tag	UNP T2KM26
A	-10	SER	-	expression tag	UNP T2KM26
A	-9	SER	-	expression tag	UNP T2KM26
A	-8	GLY	-	expression tag	UNP T2KM26
A	-7	LEU	-	expression tag	UNP T2KM26
A	-6	VAL	-	expression tag	UNP T2KM26
A	-5	PRO	-	expression tag	UNP T2KM26
A	-4	ARG	-	expression tag	UNP T2KM26
A	-3	GLY	-	expression tag	UNP T2KM26
A	-2	SER	-	expression tag	UNP T2KM26
A	-1	HIS	-	expression tag	UNP T2KM26
A	0	MET	-	expression tag	UNP T2KM26
A	1	ALA	-	expression tag	UNP T2KM26

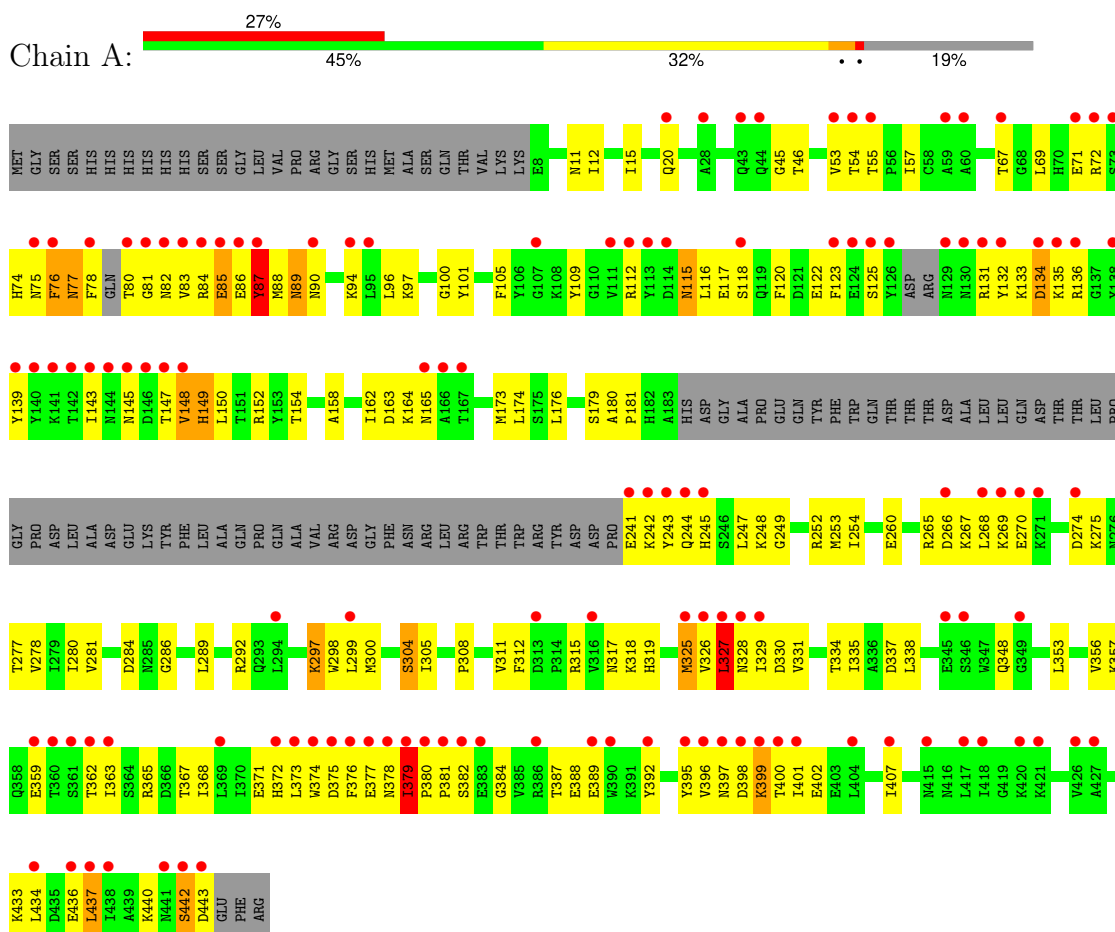
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Ca 1	0	0

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: Alpha-L-rhamnosidase/sulfatase (GH78)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.88Å 48.87Å 92.65Å 90.00° 105.64° 90.00°	Depositor
Resolution (Å)	44.61 – 2.91 44.61 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.61-2.91) 99.8 (44.61-2.91)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.13-2998	Depositor
R, R_{free}	0.322 , 0.361 0.324 , 0.361	Depositor DCC
R_{free} test set	535 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.903	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	3077	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.24	0/3143	0.59	0/4243

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	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	THR	Peptide
1	A	165	ASN	Peptide
1	A	325	MET	Peptide
1	A	326	VAL	Peptide
1	A	379	ILE	Peptide
1	A	86	GLU	Peptide
1	A	87	TYR	Peptide

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	3076	0	3014	135	0
2	A	1	0	0	0	0
All	All	3077	0	3014	135	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 22.

All (135) 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:241:GLU:HB3	1:A:242:LYS:HA	1.59	0.83
1:A:75:ASN:O	1:A:84:ARG:NH2	2.20	0.74
1:A:83:VAL:HG13	1:A:84:ARG:HB2	1.68	0.74
1:A:125:SER:HB2	1:A:136:ARG:H	1.52	0.73
1:A:399:LYS:HG3	1:A:401:ILE:HG13	1.71	0.72
1:A:372:HIS:HE2	1:A:374:TRP:HB2	1.54	0.72
1:A:150:LEU:HD13	1:A:179:SER:HB2	1.71	0.72
1:A:84:ARG:HD2	1:A:87:TYR:HD2	1.54	0.72
1:A:74:HIS:O	1:A:84:ARG:NH2	2.24	0.71
1:A:55:THR:HG22	1:A:57:ILE:HG22	1.74	0.69
1:A:389:GLU:HA	1:A:407:ILE:HB	1.75	0.68
1:A:89:ASN:H	1:A:90:ASN:HB2	1.58	0.68
1:A:12:ILE:HB	1:A:173:MET:HG2	1.76	0.67
1:A:381:PRO:HG2	1:A:396:VAL:HG23	1.75	0.67
1:A:53:VAL:HG23	1:A:328:ASN:HD22	1.59	0.67
1:A:67:THR:HG22	1:A:69:LEU:HD12	1.79	0.64
1:A:317:ASN:ND2	1:A:319:HIS:O	2.31	0.64
1:A:331:VAL:O	1:A:335:ILE:HG12	1.98	0.64
1:A:67:THR:HG22	1:A:69:LEU:CD1	2.28	0.64
1:A:94:LYS:NZ	1:A:117:GLU:HB2	2.13	0.63
1:A:357:LYS:NZ	1:A:359:GLU:OE1	2.33	0.62
1:A:378:ASN:HA	1:A:379:ILE:HG13	1.81	0.61
1:A:249:GLY:HA2	1:A:252:ARG:HD2	1.82	0.61
1:A:97:LYS:HE3	1:A:117:GLU:HB3	1.82	0.61
1:A:375:ASP:CG	1:A:376:PHE:H	2.11	0.59
1:A:81:GLY:H	1:A:112:ARG:HE	1.51	0.58
1:A:84:ARG:O	1:A:87:TYR:N	2.36	0.58
1:A:174:LEU:HG	1:A:176:LEU:HD13	1.85	0.57
1:A:280:ILE:HG23	1:A:311:VAL:HG22	1.85	0.57
1:A:163:ASP:HB2	1:A:267:LYS:HD2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:LEU:HD22	1:A:328:ASN:H	1.70	0.55
1:A:46:THR:HG21	1:A:356:VAL:HA	1.88	0.55
1:A:133:LYS:HD3	1:A:148:VAL:O	2.06	0.55
1:A:53:VAL:HG23	1:A:328:ASN:ND2	2.22	0.55
1:A:337:ASP:HB3	1:A:353:LEU:HD13	1.88	0.54
1:A:372:HIS:NE2	1:A:374:TRP:HB2	2.21	0.54
1:A:433:LYS:O	1:A:437:LEU:HB2	2.08	0.54
1:A:109:TYR:HB2	1:A:122:GLU:HG3	1.89	0.53
1:A:84:ARG:HD2	1:A:87:TYR:CD2	2.39	0.53
1:A:275:LYS:O	1:A:315:ARG:HG2	2.09	0.53
1:A:247:LEU:HG	1:A:289:LEU:HD22	1.90	0.53
1:A:387:THR:HG22	1:A:388:GLU:H	1.74	0.53
1:A:363:ILE:O	1:A:365:ARG:N	2.39	0.52
1:A:381:PRO:HD2	1:A:397:ASN:H	1.72	0.52
1:A:372:HIS:CG	1:A:373:LEU:N	2.76	0.52
1:A:81:GLY:HA2	1:A:112:ARG:HH21	1.74	0.52
1:A:158:ALA:O	1:A:162:ILE:HG12	2.11	0.51
1:A:150:LEU:O	1:A:154:THR:HG22	2.11	0.51
1:A:268:LEU:HD23	1:A:274:ASP:HA	1.92	0.50
1:A:69:LEU:C	1:A:329:ILE:HD11	2.37	0.50
1:A:398:ASP:O	1:A:399:LYS:HB2	2.11	0.50
1:A:399:LYS:CG	1:A:401:ILE:HG13	2.39	0.50
1:A:328:ASN:OD1	1:A:328:ASN:C	2.55	0.49
1:A:53:VAL:HG12	1:A:305:ILE:HA	1.95	0.49
1:A:392:TYR:HE2	1:A:434:LEU:HD22	1.77	0.49
1:A:105:PHE:O	1:A:120:PHE:HA	2.11	0.49
1:A:300:MET:HE1	1:A:372:HIS:HA	1.95	0.49
1:A:373:LEU:CD1	1:A:375:ASP:HB2	2.43	0.49
1:A:245:HIS:ND1	1:A:248:LYS:HB2	2.28	0.49
1:A:334:THR:O	1:A:338:LEU:HB2	2.13	0.49
1:A:11:ASN:O	1:A:277:THR:HA	2.12	0.49
1:A:266:ASP:O	1:A:269:LYS:HG3	2.13	0.49
1:A:368:ILE:HD12	1:A:433:LYS:HG2	1.95	0.49
1:A:436:GLU:O	1:A:440:LYS:HD2	2.13	0.48
1:A:94:LYS:HZ2	1:A:117:GLU:HB2	1.78	0.48
1:A:327:LEU:HD13	1:A:329:ILE:HG22	1.95	0.48
1:A:373:LEU:HD13	1:A:375:ASP:HB2	1.94	0.48
1:A:15:ILE:HB	1:A:281:VAL:HG13	1.95	0.48
1:A:297:LYS:O	1:A:299:LEU:HD12	2.14	0.48
1:A:94:LYS:HZ1	1:A:117:GLU:HB2	1.78	0.48
1:A:265:ARG:HA	1:A:268:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LYS:HD2	1:A:270:GLU:N	2.28	0.47
1:A:300:MET:HE1	1:A:372:HIS:CA	2.45	0.47
1:A:20:GLN:OE1	1:A:308:PRO:HG2	2.15	0.47
1:A:84:ARG:O	1:A:85:GLU:C	2.58	0.47
1:A:375:ASP:CG	1:A:376:PHE:N	2.73	0.47
1:A:132:TYR:HD2	1:A:133:LYS:H	1.58	0.47
1:A:139:TYR:HE1	1:A:143:ILE:C	2.23	0.47
1:A:442:SER:OG	1:A:443:ASP:N	2.46	0.47
1:A:96:LEU:HB3	1:A:101:TYR:HB2	1.96	0.46
1:A:378:ASN:CA	1:A:379:ILE:HG13	2.44	0.46
1:A:69:LEU:HD23	1:A:348:GLN:NE2	2.31	0.46
1:A:78:PHE:CD2	1:A:80:THR:HB	2.50	0.46
1:A:242:LYS:HG3	1:A:243:TYR:N	2.31	0.46
1:A:148:VAL:HG13	1:A:149:HIS:N	2.30	0.46
1:A:134:ASP:OD1	1:A:135:LYS:N	2.48	0.45
1:A:123:PHE:CE2	1:A:154:THR:HB	2.50	0.45
1:A:397:ASN:HA	1:A:398:ASP:HA	1.53	0.45
1:A:54:THR:O	1:A:371:GLU:HB2	2.16	0.45
1:A:83:VAL:HA	1:A:84:ARG:HA	1.80	0.45
1:A:181:PRO:HB3	1:A:253:MET:HB2	1.98	0.45
1:A:392:TYR:CE1	1:A:402:GLU:HG2	2.51	0.45
1:A:57:ILE:HD12	1:A:298:TRP:HE1	1.81	0.44
1:A:292:ARG:HH11	1:A:292:ARG:HG2	1.82	0.44
1:A:82:ASN:O	1:A:83:VAL:HG23	2.17	0.44
1:A:136:ARG:HD3	1:A:145:ASN:ND2	2.33	0.44
1:A:325:MET:HE1	1:A:362:THR:O	2.17	0.44
1:A:399:LYS:CG	1:A:400:THR:H	2.30	0.44
1:A:300:MET:HE2	1:A:382:SER:C	2.43	0.44
1:A:327:LEU:HD23	1:A:327:LEU:HA	1.82	0.44
1:A:363:ILE:C	1:A:365:ARG:H	2.26	0.44
1:A:278:VAL:HG11	1:A:338:LEU:HD21	1.99	0.44
1:A:77:ASN:O	1:A:78:PHE:C	2.61	0.44
1:A:84:ARG:HB3	1:A:87:TYR:HB2	2.00	0.43
1:A:72:ARG:HE	1:A:72:ARG:HB3	1.58	0.43
1:A:181:PRO:HA	1:A:253:MET:HE2	2.00	0.43
1:A:87:TYR:HD1	1:A:88:MET:H	1.65	0.43
1:A:123:PHE:HE2	1:A:154:THR:HB	1.83	0.43
1:A:53:VAL:HG21	1:A:284:ASP:O	2.19	0.43
1:A:286:GLY:HA3	1:A:304:SER:HA	2.00	0.43
1:A:328:ASN:C	1:A:330:ASP:H	2.26	0.43
1:A:380:PRO:HA	1:A:381:PRO:HD3	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:PHE:HB2	1:A:377:GLU:H	1.62	0.42
1:A:84:ARG:HB2	1:A:84:ARG:CZ	2.48	0.42
1:A:125:SER:HB2	1:A:136:ARG:N	2.29	0.42
1:A:115:ASN:HB3	1:A:116:LEU:H	1.62	0.42
1:A:433:LYS:HA	1:A:436:GLU:HB2	2.01	0.42
1:A:76:PHE:O	1:A:77:ASN:HB2	2.19	0.42
1:A:384:GLY:HA2	1:A:434:LEU:HD13	2.01	0.42
1:A:328:ASN:C	1:A:330:ASP:N	2.78	0.42
1:A:71:GLU:HA	1:A:74:HIS:CE1	2.55	0.42
1:A:318:LYS:HB3	1:A:318:LYS:HE3	1.83	0.42
1:A:378:ASN:HA	1:A:379:ILE:HA	1.79	0.42
1:A:20:GLN:HE21	1:A:254:ILE:HG23	1.84	0.41
1:A:45:GLY:HA3	1:A:312:PHE:HA	2.01	0.41
1:A:367:THR:O	1:A:387:THR:HG23	2.20	0.41
1:A:375:ASP:OD2	1:A:376:PHE:N	2.53	0.41
1:A:69:LEU:HD23	1:A:348:GLN:CD	2.46	0.41
1:A:152:ARG:HD3	1:A:260:GLU:OE1	2.20	0.41
1:A:180:ALA:HB1	1:A:253:MET:HB3	2.03	0.41
1:A:392:TYR:HE1	1:A:402:GLU:HG2	1.86	0.40
1:A:395:TYR:O	1:A:400:THR:HA	2.21	0.40
1:A:268:LEU:HD21	1:A:277:THR:HB	2.03	0.40
1:A:55:THR:HG23	1:A:372:HIS:O	2.21	0.40
1:A:300:MET:HE2	1:A:382:SER:HB2	2.03	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	368/467 (79%)	300 (82%)	48 (13%)	20 (5%)	1 4

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	PHE
1	A	87	TYR
1	A	131	ARG
1	A	148	VAL
1	A	379	ILE
1	A	77	ASN
1	A	89	ASN
1	A	134	ASP
1	A	244	GLN
1	A	327	LEU
1	A	100	GLY
1	A	115	ASN
1	A	118	SER
1	A	164	LYS
1	A	399	LYS
1	A	149	HIS
1	A	297	LYS
1	A	437	LEU
1	A	442	SER
1	A	85	GLU

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	333/414 (80%)	331 (99%)	2 (1%)	78	92

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	304	SER
1	A	327	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	77	ASN
1	A	98	ASN
1	A	99	ASN
1	A	165	ASN
1	A	170	GLN
1	A	397	ASN

5.3.3 RNA [i](#)

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](#)

Of 1 ligands modelled in this entry, 1 is 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 [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	376/467 (80%)	1.71	126 (33%) 1 1	13, 36, 72, 112	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	TYR	7.7
1	A	374	TRP	6.2
1	A	316	VAL	5.8
1	A	83	VAL	5.8
1	A	138	TYR	5.7
1	A	135	LYS	5.6
1	A	398	ASP	5.2
1	A	379	ILE	5.2
1	A	147	THR	5.1
1	A	401	ILE	5.1
1	A	380	PRO	5.0
1	A	377	GLU	5.0
1	A	84	ARG	4.9
1	A	140	TYR	4.8
1	A	166	ALA	4.7
1	A	80	THR	4.6
1	A	136	ARG	4.4
1	A	144	ASN	4.4
1	A	243	TYR	4.3
1	A	396	VAL	4.3
1	A	125	SER	4.3
1	A	360	THR	4.3
1	A	242	LYS	4.2
1	A	90	ASN	4.1
1	A	361	SER	4.1
1	A	82	ASN	4.1
1	A	375	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	376	PHE	4.0
1	A	113	TYR	3.9
1	A	362	THR	3.8
1	A	145	ASN	3.8
1	A	397	ASN	3.7
1	A	346	SER	3.7
1	A	118	SER	3.6
1	A	407	ILE	3.6
1	A	124	GLU	3.6
1	A	131	ARG	3.5
1	A	143	ILE	3.5
1	A	372	HIS	3.4
1	A	142	THR	3.4
1	A	328	ASN	3.3
1	A	274	ASP	3.3
1	A	81	GLY	3.3
1	A	141	LYS	3.3
1	A	241	GLU	3.2
1	A	132	TYR	3.1
1	A	271	LYS	3.1
1	A	443	ASP	3.1
1	A	95	LEU	3.1
1	A	244	GLN	3.1
1	A	85	GLU	3.1
1	A	126	TYR	3.0
1	A	442	SER	3.0
1	A	167	THR	2.9
1	A	129	ASN	2.9
1	A	437	LEU	2.9
1	A	78	PHE	2.9
1	A	381	PRO	2.9
1	A	266	ASP	2.9
1	A	55	THR	2.8
1	A	53	VAL	2.8
1	A	146	ASP	2.8
1	A	345	GLU	2.8
1	A	76	PHE	2.8
1	A	87	TYR	2.8
1	A	382	SER	2.8
1	A	54	THR	2.7
1	A	134	ASP	2.7
1	A	72	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	326	VAL	2.6
1	A	404	LEU	2.6
1	A	373	LEU	2.6
1	A	43	GLN	2.6
1	A	383	GLU	2.6
1	A	389	GLU	2.6
1	A	418	ILE	2.6
1	A	123	PHE	2.6
1	A	420	LYS	2.6
1	A	438	ILE	2.6
1	A	434	LEU	2.6
1	A	400	THR	2.6
1	A	313	ASP	2.6
1	A	94	LYS	2.5
1	A	73	SER	2.5
1	A	269	LYS	2.5
1	A	112	ARG	2.5
1	A	378	ASN	2.5
1	A	107	GLY	2.5
1	A	86	GLU	2.5
1	A	399	LYS	2.5
1	A	421	LYS	2.5
1	A	415	ASN	2.5
1	A	395	TYR	2.4
1	A	427	ALA	2.4
1	A	436	GLU	2.4
1	A	268	LEU	2.4
1	A	148	VAL	2.3
1	A	114	ASP	2.3
1	A	20	GLN	2.3
1	A	392	TYR	2.3
1	A	329	ILE	2.3
1	A	130	ASN	2.3
1	A	325	MET	2.3
1	A	270	GLU	2.2
1	A	426	VAL	2.2
1	A	369	LEU	2.2
1	A	44	GLN	2.2
1	A	28	ALA	2.2
1	A	59	ALA	2.2
1	A	71	GLU	2.2
1	A	165	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	441	ASN	2.2
1	A	245	HIS	2.2
1	A	417	LEU	2.2
1	A	60	ALA	2.2
1	A	363	ILE	2.2
1	A	390	TRP	2.2
1	A	327	LEU	2.2
1	A	299	LEU	2.1
1	A	111	VAL	2.1
1	A	386	ARG	2.0
1	A	294	LEU	2.0
1	A	75	ASN	2.0
1	A	349	GLY	2.0
1	A	67	THR	2.0
1	A	359	GLU	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	CA	A	500	1/1	0.90	0.07	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.