Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 06:55 AM EDT

PDB ID	:	6HR5
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 (i) 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 (1)) were used in the production of this report:

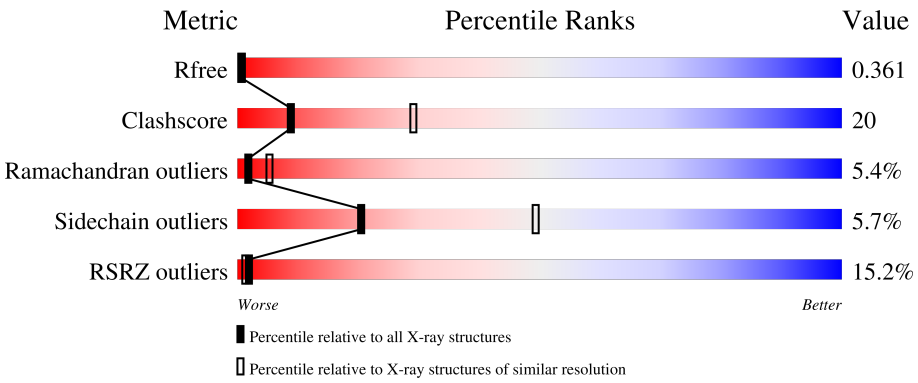
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

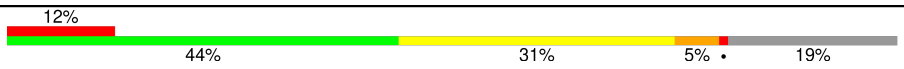
The reported resolution of this entry is 2.91 Å.

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}	130704	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (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 <=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 (i)

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
			Total	C	N	O	S			
1	A	376	3076	1963	522	583	8	0	0	0

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 (three-letter code: CA) (formula: Ca).

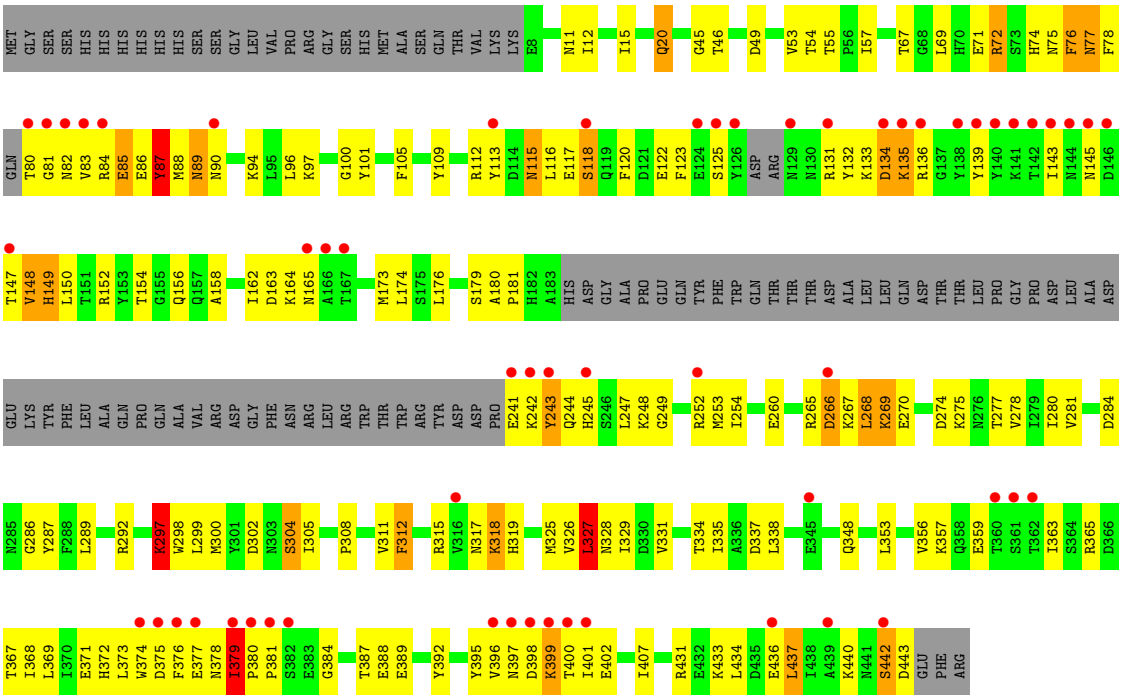
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	1	1	1	0	0

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: Alpha-L-rhamnosidase/sulfatase (GH78)

Chain A:



4 Data and refinement statistics (i)

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) 99.6 (44.61-2.91)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.24%)	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)	0.32 , 64.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.30	0/3143	0.57	1/4243 (0.0%)

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.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	268	LEU	CB-CG-CD2	-5.61	101.47	111.00

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	124	0
2	A	1	0	0	0	0
All	All	3077	0	3014	124	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 20.

All (124) 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:300:MET:HE3	1:A:371:GLU:HG2	1.71	0.72
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:94:LYS:HZ2	1:A:117:GLU:HB2	1.67	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
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:375:ASP:CG	1:A:376:PHE:H	2.11	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: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: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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:LYS:O	1:A:299:LEU:HD12	2.14	0.48
1:A:265:ARG:HA	1:A:268:LEU:HD13	1.96	0.47
1:A:269:LYS:HD2	1:A:270:GLU:N	2.28	0.47
1:A:20:GLN:OE1	1:A:308:PRO:HG2	2.15	0.47
1:A:132:TYR:HD2	1:A:133:LYS:H	1.58	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:69:LEU:C	1:A:329:ILE:HD11	2.37	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:328:ASN:OD1	1:A:328:ASN:C	2.55	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:399:LYS:CG	1:A:400:THR:H	2.30	0.44
1:A:327:LEU:HD23	1:A:327:LEU:HA	1.82	0.44
1:A:278:VAL:HG11	1:A:338:LEU:HD21	1.99	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: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:380:PRO:HA	1:A:381:PRO:HD3	1.89	0.42
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:139:TYR:HE1	1:A:143:ILE:C	2.23	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:84:ARG:O	1:A:85:GLU:C	2.58	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: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:375:ASP:CG	1:A:376:PHE:N	2.73	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

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%)	2 5

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 (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	A	333/414 (80%)	314 (94%)	19 (6%)	20 49

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	49	ASP
1	A	72	ARG
1	A	113	TYR
1	A	118	SER
1	A	135	LYS
1	A	156	GLN
1	A	243	TYR
1	A	266	ASP
1	A	269	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	287	TYR
1	A	297	LYS
1	A	302	ASP
1	A	304	SER
1	A	312	PHE
1	A	318	LYS
1	A	327	LEU
1	A	369	LEU
1	A	431	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	244	GLN
1	A	378	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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.85	57 (15%) 2 1	13, 36, 72, 112	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	TYR	10.3
1	A	144	ASN	7.7
1	A	80	THR	7.4
1	A	316	VAL	7.0
1	A	138	TYR	6.8
1	A	360	THR	6.3
1	A	136	ARG	5.5
1	A	140	TYR	5.1
1	A	379	ILE	5.0
1	A	243	TYR	5.0
1	A	398	ASP	4.9
1	A	397	ASN	4.6
1	A	125	SER	4.5
1	A	143	ILE	4.2
1	A	377	GLU	4.1
1	A	146	ASP	4.0
1	A	135	LYS	3.8
1	A	396	VAL	3.8
1	A	142	THR	3.7
1	A	361	SER	3.6
1	A	374	TRP	3.3
1	A	83	VAL	3.2
1	A	266	ASP	3.2
1	A	166	ALA	3.1
1	A	375	ASP	3.1
1	A	124	GLU	3.1
1	A	126	TYR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	245	HIS	2.9
1	A	82	ASN	2.8
1	A	380	PRO	2.7
1	A	90	ASN	2.7
1	A	145	ASN	2.6
1	A	129	ASN	2.6
1	A	401	ILE	2.5
1	A	242	LYS	2.5
1	A	252	ARG	2.5
1	A	134	ASP	2.5
1	A	345	GLU	2.4
1	A	118	SER	2.4
1	A	84	ARG	2.4
1	A	113	TYR	2.4
1	A	241	GLU	2.3
1	A	147	THR	2.3
1	A	165	ASN	2.3
1	A	362	THR	2.3
1	A	436	GLU	2.3
1	A	167	THR	2.2
1	A	141	LYS	2.2
1	A	439	ALA	2.2
1	A	381	PRO	2.1
1	A	382	SER	2.1
1	A	400	THR	2.1
1	A	442	SER	2.0
1	A	81	GLY	2.0
1	A	376	PHE	2.0
1	A	131	ARG	2.0
1	A	399	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 monosaccharides 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(Å^2)	Q<0.9
2	CA	A	500	1/1	0.77	0.09	35,35,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.