



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 12:08 PM BST

PDB ID : 6Y9T  
Title : Family GH13\_31 enzyme  
Authors : Andersen, S.; Poulsen, J.C.N.; Moeller, M.S.; Abou Hachem, M.; Lo Leggio, L.  
Deposited on : 2020-03-10  
Resolution : 2.78 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

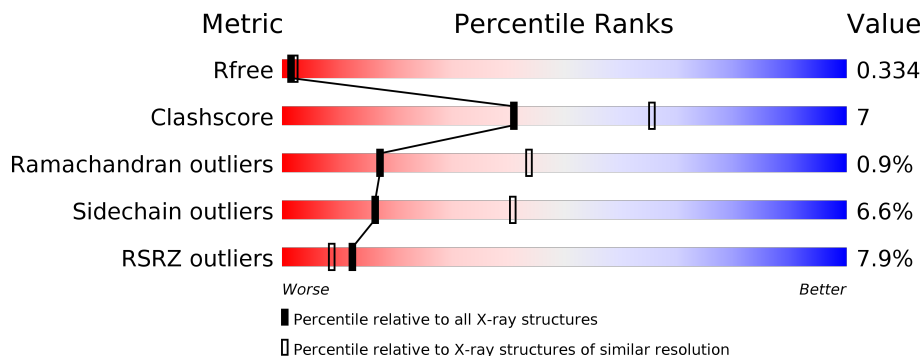
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.78 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	571	 5% 75% 16% • 6%
1	B	571	 10% 72% 20% • 6%

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 8777 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-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	536	4328	2769	725	813	21	0	0	0
1	B	535	4329	2769	725	815	20	0	1	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A3A9XV51
A	-18	GLY	-	expression tag	UNP A0A3A9XV51
A	-17	SER	-	expression tag	UNP A0A3A9XV51
A	-16	SER	-	expression tag	UNP A0A3A9XV51
A	-15	HIS	-	expression tag	UNP A0A3A9XV51
A	-14	HIS	-	expression tag	UNP A0A3A9XV51
A	-13	HIS	-	expression tag	UNP A0A3A9XV51
A	-12	HIS	-	expression tag	UNP A0A3A9XV51
A	-11	HIS	-	expression tag	UNP A0A3A9XV51
A	-10	HIS	-	expression tag	UNP A0A3A9XV51
A	-9	SER	-	expression tag	UNP A0A3A9XV51
A	-8	SER	-	expression tag	UNP A0A3A9XV51
A	-7	GLY	-	expression tag	UNP A0A3A9XV51
A	-6	LEU	-	expression tag	UNP A0A3A9XV51
A	-5	VAL	-	expression tag	UNP A0A3A9XV51
A	-4	PRO	-	expression tag	UNP A0A3A9XV51
A	-3	ARG	-	expression tag	UNP A0A3A9XV51
A	-2	GLY	-	expression tag	UNP A0A3A9XV51
A	-1	SER	-	expression tag	UNP A0A3A9XV51
A	0	HIS	-	expression tag	UNP A0A3A9XV51
B	-19	MET	-	initiating methionine	UNP A0A3A9XV51
B	-18	GLY	-	expression tag	UNP A0A3A9XV51
B	-17	SER	-	expression tag	UNP A0A3A9XV51
B	-16	SER	-	expression tag	UNP A0A3A9XV51
B	-15	HIS	-	expression tag	UNP A0A3A9XV51

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP A0A3A9XV51
B	-13	HIS	-	expression tag	UNP A0A3A9XV51
B	-12	HIS	-	expression tag	UNP A0A3A9XV51
B	-11	HIS	-	expression tag	UNP A0A3A9XV51
B	-10	HIS	-	expression tag	UNP A0A3A9XV51
B	-9	SER	-	expression tag	UNP A0A3A9XV51
B	-8	SER	-	expression tag	UNP A0A3A9XV51
B	-7	GLY	-	expression tag	UNP A0A3A9XV51
B	-6	LEU	-	expression tag	UNP A0A3A9XV51
B	-5	VAL	-	expression tag	UNP A0A3A9XV51
B	-4	PRO	-	expression tag	UNP A0A3A9XV51
B	-3	ARG	-	expression tag	UNP A0A3A9XV51
B	-2	GLY	-	expression tag	UNP A0A3A9XV51
B	-1	SER	-	expression tag	UNP A0A3A9XV51
B	0	HIS	-	expression tag	UNP A0A3A9XV51

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

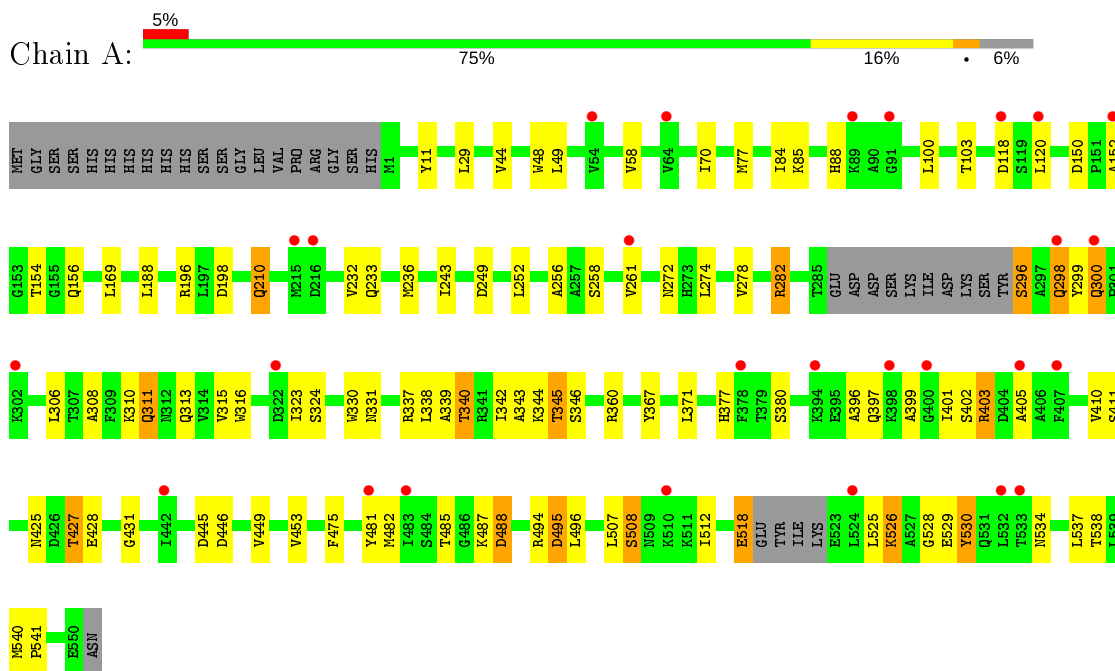
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	59	Total O 59 59	0	0
3	B	59	Total O 59 59	0	0

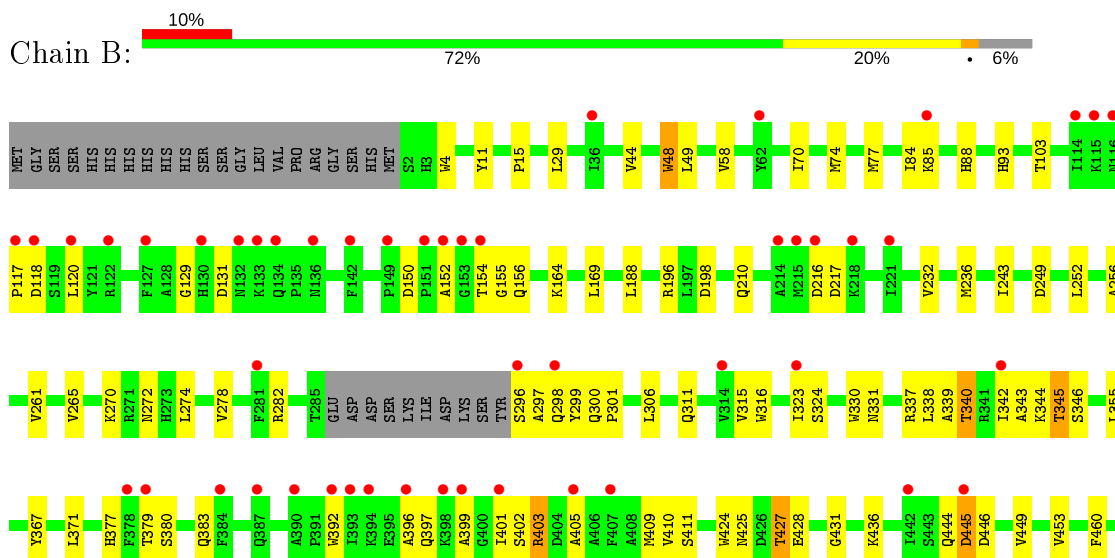
### 3 Residue-property plots [i](#)

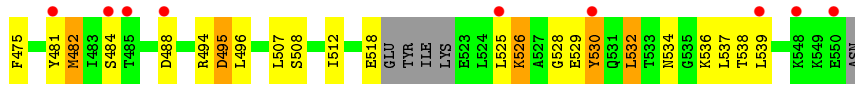
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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-glucosidase



- Molecule 1: Alpha-glucosidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.21Å 105.30Å 92.23Å 90.00° 96.95° 90.00°	Depositor
Resolution (Å)	50.01 – 2.78 47.93 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.01-2.78) 99.1 (47.93-2.78)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 2.77Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.258 , 0.337 0.271 , 0.334	Depositor DCC
$R_{free}$ test set	1787 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.8	Xtrriage
Anisotropy	0.258	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 78.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8777	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.59	0/4444	0.77	2/6032 (0.0%)
1	B	0.58	0/4445	0.78	0/6034
All	All	0.58	0/8889	0.78	2/12066 (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	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	100	LEU	CA-CB-CG	5.98	129.05	115.30
1	A	360	ARG	NE-CZ-NH1	5.32	122.96	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	484	SER	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	4328	0	4172	53	0
1	B	4329	0	4165	69	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	59	0	0	2	0
3	B	59	0	0	2	0
All	All	8777	0	8337	120	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 7.

All (120) 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:425:ASN:HD21	1:A:431:GLY:HA3	1.49	0.76
1:B:532:LEU:HD12	1:B:538:THR:H	1.51	0.74
1:B:397:GLN:HE22	1:B:403:ARG:HA	1.51	0.74
1:B:532:LEU:HD12	1:B:538:THR:N	2.09	0.67
1:B:539:LEU:O	3:B:701:HOH:O	2.12	0.67
1:A:313:GLN:NE2	3:A:702:HOH:O	2.27	0.66
1:B:475:PHE:O	1:B:494:ARG:NH2	2.31	0.63
1:A:397:GLN:HE22	1:A:403:ARG:HG3	1.63	0.63
1:B:306:LEU:HD21	1:B:507:LEU:HD13	1.79	0.62
1:A:306:LEU:HD21	1:A:507:LEU:HD13	1.80	0.61
1:A:299:TYR:CD2	1:A:410:VAL:HG13	2.36	0.61
1:B:299:TYR:CD2	1:B:410:VAL:HG13	2.36	0.61
1:B:532:LEU:HD13	1:B:532:LEU:C	2.21	0.60
1:A:339:ALA:HA	1:A:343:ALA:HB3	1.84	0.59
1:A:475:PHE:O	1:A:494:ARG:NH2	2.37	0.58
1:A:330:TRP:HB3	1:A:338:LEU:HD13	1.85	0.57
1:B:337:ARG:NH2	1:B:367:TYR:O	2.35	0.57
1:B:532:LEU:HD12	1:B:537:LEU:HA	1.85	0.57
1:B:425:ASN:HD21	1:B:431:GLY:HA3	1.70	0.57
1:B:330:TRP:HB3	1:B:338:LEU:HD13	1.87	0.56
1:A:103:THR:HG23	1:A:169:LEU:HD21	1.86	0.56
1:B:196:ARG:NH1	1:B:198:ASP:OD2	2.39	0.56
1:B:103:THR:HG23	1:B:169:LEU:HD21	1.87	0.56
1:B:339:ALA:HA	1:B:343:ALA:HB3	1.88	0.56
1:A:310:LYS:NZ	1:A:485:THR:OG1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:LYS:HE3	1:B:216:ASP:CG	2.26	0.55
1:A:196:ARG:NH1	1:A:198:ASP:OD2	2.38	0.55
1:A:296:SER:HB2	1:A:300:GLN:OE1	2.07	0.55
1:A:306:LEU:HD21	1:A:507:LEU:CD1	2.38	0.54
1:B:532:LEU:CD1	1:B:537:LEU:HA	2.38	0.54
1:B:306:LEU:HD21	1:B:507:LEU:CD1	2.38	0.53
1:B:528:GLY:C	1:B:529:GLU:OE2	2.46	0.53
1:B:311:GLN:O	1:B:315:VAL:HG23	2.08	0.53
1:A:311:GLN:O	1:A:315:VAL:HG23	2.09	0.52
1:A:11:TYR:HB2	1:A:44:VAL:HG11	1.89	0.52
1:A:396:ALA:O	1:A:399:ALA:HB3	2.09	0.52
1:B:131:ASP:O	1:B:155:GLY:O	2.28	0.52
1:B:427:THR:HG22	1:B:428:GLU:H	1.74	0.52
1:A:331:ASN:HD22	1:A:337:ARG:HA	1.75	0.52
1:B:488:ASP:OD2	1:B:512:ILE:HG21	2.10	0.52
1:A:233:GLN:HB2	3:A:730:HOH:O	2.09	0.52
1:B:377:HIS:HA	1:B:411:SER:HB3	1.93	0.51
1:A:377:HIS:HA	1:A:411:SER:HB3	1.93	0.51
1:A:427:THR:HG22	1:A:428:GLU:H	1.75	0.51
1:B:11:TYR:HB2	1:B:44:VAL:HG11	1.93	0.51
1:B:396:ALA:O	1:B:399:ALA:HB3	2.10	0.51
1:A:339:ALA:O	1:A:340:THR:HB	2.12	0.50
1:A:337:ARG:NH2	1:A:367:TYR:O	2.36	0.50
1:B:74:MET:HE2	3:B:723:HOH:O	2.12	0.50
1:A:243:ILE:HG21	1:A:252:LEU:HD21	1.94	0.49
1:B:532:LEU:HD11	1:B:536:LYS:O	2.12	0.49
1:A:272:ASN:O	1:A:274:LEU:HD13	2.13	0.49
1:B:339:ALA:O	1:B:340:THR:HB	2.13	0.49
1:A:396:ALA:HB1	1:A:401:ILE:HD12	1.95	0.48
1:A:150:ASP:OD2	1:A:152:ALA:HB3	2.14	0.48
1:B:272:ASN:O	1:B:274:LEU:HD13	2.14	0.47
1:B:150:ASP:OD2	1:B:152:ALA:HB3	2.14	0.47
1:B:396:ALA:HB1	1:B:401:ILE:HD12	1.95	0.47
1:A:537:LEU:HD12	1:A:538:THR:N	2.29	0.47
1:B:532:LEU:HD13	1:B:532:LEU:O	2.14	0.47
1:B:243:ILE:HG21	1:B:252:LEU:HD21	1.96	0.47
1:B:4:TRP:CG	1:B:93:HIS:CE1	3.03	0.46
1:A:70:ILE:HG21	1:A:77:MET:N	2.31	0.46
1:A:344:LYS:O	1:A:345:THR:HG23	2.15	0.46
1:B:261:VAL:HG22	1:B:316:TRP:NE1	2.30	0.46
1:B:270:LYS:NZ	1:B:324:SER:OG	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ILE:HG21	1:B:77:MET:N	2.31	0.46
1:B:232:VAL:O	1:B:236:MET:HG2	2.16	0.46
1:B:529:GLU:O	1:B:530:TYR:HB2	2.15	0.46
1:A:84:ILE:O	1:A:88:HIS:ND1	2.49	0.46
1:A:529:GLU:O	1:A:530:TYR:HB2	2.16	0.45
1:B:344:LYS:O	1:B:345:THR:HG23	2.15	0.45
1:B:537:LEU:HD12	1:B:538:THR:N	2.31	0.45
1:A:232:VAL:O	1:A:236:MET:HG2	2.16	0.45
1:B:331:ASN:HD22	1:B:337:ARG:HA	1.82	0.45
1:B:29:LEU:CD1	1:B:70:ILE:HD11	2.47	0.45
1:B:379:THR:O	1:B:383:GLN:OE1	2.35	0.45
1:B:154:THR:HG23	1:B:156:GLN:HG3	1.99	0.45
1:B:453:VAL:HG22	1:B:460:PHE:CE2	2.52	0.45
1:A:495:ASP:N	1:A:495:ASP:OD1	2.50	0.45
1:A:261:VAL:HG22	1:A:316:TRP:NE1	2.31	0.44
1:A:29:LEU:CD1	1:A:70:ILE:HD11	2.47	0.44
1:B:84:ILE:O	1:B:88:HIS:ND1	2.51	0.44
1:A:449:VAL:O	1:A:453:VAL:HG22	2.17	0.43
1:B:495:ASP:OD1	1:B:495:ASP:N	2.52	0.43
1:B:401:ILE:HG22	1:B:405:ALA:HB3	2.01	0.43
1:A:401:ILE:HG22	1:A:405:ALA:HB3	2.00	0.43
1:B:265:VAL:HG22	1:B:323:ILE:HD11	2.01	0.43
1:A:308:ALA:HA	1:A:311:GLN:HG2	2.01	0.42
1:A:526:LYS:CD	1:A:526:LYS:N	2.82	0.42
1:B:216:ASP:HA	1:B:217:ASP:HA	1.85	0.42
1:B:526:LYS:CD	1:B:526:LYS:N	2.82	0.42
1:B:355:LEU:C	1:B:355:LEU:HD23	2.39	0.42
1:A:528:GLY:C	1:A:529:GLU:OE2	2.58	0.42
1:A:256:ALA:HB3	1:A:278:VAL:HG11	2.02	0.42
1:B:256:ALA:HB3	1:B:278:VAL:HG11	2.02	0.42
1:A:154:THR:HG23	1:A:156:GLN:HG3	2.01	0.42
1:B:129:GLY:O	1:B:156:GLN:HG2	2.20	0.42
1:A:188:LEU:CD1	1:A:243:ILE:HG23	2.49	0.42
1:A:488:ASP:OD1	1:A:508:SER:HB2	2.20	0.42
1:B:301:PRO:HD3	1:B:409:MET:HG2	2.00	0.42
1:B:48:TRP:C	1:B:48:TRP:CD1	2.92	0.41
1:B:339:ALA:O	1:B:340:THR:CB	2.68	0.41
1:A:339:ALA:O	1:A:340:THR:CB	2.68	0.41
1:A:210:GLN:HE22	1:B:482:MET:HB3	1.85	0.41
1:B:444:GLN:HA	1:B:445:ASP:HA	1.88	0.41
1:B:188:LEU:CD1	1:B:243:ILE:HG23	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ILE:O	1:A:324:SER:HB3	2.21	0.41
1:B:371:LEU:HD11	1:B:449:VAL:HG12	2.03	0.41
1:B:529:GLU:N	1:B:529:GLU:OE2	2.54	0.40
1:A:518:GLU:N	1:A:518:GLU:OE1	2.54	0.40
1:B:338:LEU:C	1:B:339:ALA:O	2.58	0.40
1:B:424:TRP:O	1:B:449:VAL:HG22	2.22	0.40
1:A:371:LEU:HD11	1:A:449:VAL:HG12	2.03	0.40
1:A:488:ASP:HB3	1:A:512:ILE:HD13	2.03	0.40
1:A:540:MET:HB3	1:A:541:PRO:HD2	2.04	0.40
1:B:15:PRO:HG2	1:B:74:MET:CE	2.51	0.40
1:A:258:SER:HA	1:A:282:ARG:HG2	2.03	0.40
1:B:297:ALA:O	1:B:392:TRP:NE1	2.54	0.40
1:B:530:TYR:N	1:B:530:TYR:CD1	2.90	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	530/571 (93%)	487 (92%)	38 (7%)	5 (1%)	17	44
1	B	530/571 (93%)	486 (92%)	39 (7%)	5 (1%)	17	44
All	All	1060/1142 (93%)	973 (92%)	77 (7%)	10 (1%)	17	44

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	298	GLN
1	A	298	GLN
1	A	380	SER
1	B	380	SER
1	A	340	THR

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Mol	Chain	Res	Type
1	A	530	TYR
1	B	340	THR
1	B	530	TYR
1	B	342	ILE
1	A	342	ILE

### 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	466/498 (94%)	436 (94%)	30 (6%)	17	42
1	B	466/498 (94%)	435 (93%)	31 (7%)	16	40
All	All	932/996 (94%)	871 (94%)	61 (6%)	16	41

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	TRP
1	A	49	LEU
1	A	58	VAL
1	A	85	LYS
1	A	118	ASP
1	A	120	LEU
1	A	210	GLN
1	A	249	ASP
1	A	282	ARG
1	A	296	SER
1	A	298	GLN
1	A	300	GLN
1	A	311	GLN
1	A	345	THR
1	A	346	SER
1	A	402	SER
1	A	403	ARG
1	A	427	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	445	ASP
1	A	446	ASP
1	A	481	TYR
1	A	482	MET
1	A	488	ASP
1	A	495	ASP
1	A	496	LEU
1	A	508	SER
1	A	518	GLU
1	A	525	LEU
1	A	526	LYS
1	A	534	ASN
1	B	48	TRP
1	B	49	LEU
1	B	58	VAL
1	B	85	LYS
1	B	117	PRO
1	B	118	ASP
1	B	120	LEU
1	B	164	LYS
1	B	210	GLN
1	B	249	ASP
1	B	282	ARG
1	B	296	SER
1	B	300	GLN
1	B	345	THR
1	B	346	SER
1	B	402	SER
1	B	403	ARG
1	B	427	THR
1	B	436	LYS
1	B	445	ASP
1	B	446	ASP
1	B	481	TYR
1	B	482	MET
1	B	495	ASP
1	B	496	LEU
1	B	508	SER
1	B	518	GLU
1	B	525	LEU
1	B	526	LYS
1	B	532	LEU

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Mol	Chain	Res	Type
1	B	534	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	210	GLN
1	A	211	ASN
1	A	233	GLN
1	A	397	GLN
1	B	12	GLN
1	B	50	ASN
1	B	82	ASN
1	B	93	HIS
1	B	170	ASN
1	B	211	ASN
1	B	333	HIS
1	B	397	GLN
1	B	534	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	536/571 (93%)	0.56	27 (5%) 28 23	38, 82, 123, 186	0
1	B	535/571 (93%)	0.80	58 (10%) 5 4	38, 84, 140, 173	0
All	All	1071/1142 (93%)	0.68	85 (7%) 12 9	38, 83, 133, 186	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	378	PHE	9.8
1	B	215	MET	8.7
1	B	151	PRO	6.5
1	B	401	ILE	6.4
1	A	407	PHE	5.7
1	B	392	TRP	5.1
1	B	153	GLY	4.9
1	B	117	PRO	4.9
1	A	533	THR	4.6
1	B	379	THR	4.6
1	A	215	MET	4.3
1	B	399	ALA	4.2
1	B	152	ALA	4.1
1	B	393	ILE	3.9
1	B	118	ASP	3.7
1	B	132	ASN	3.7
1	B	214	ALA	3.5
1	B	394	LYS	3.3
1	B	481	TYR	3.3
1	B	154	THR	3.3
1	B	384	PHE	3.3
1	A	378	PHE	3.2
1	B	485	THR	3.2
1	B	136	ASN	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	302	LYS	3.2
1	A	524	LEU	3.1
1	B	134	GLN	3.0
1	B	484	SER	3.0
1	A	89	LYS	2.9
1	A	442	ILE	2.9
1	A	152	ALA	2.8
1	B	130	HIS	2.8
1	A	400	GLY	2.7
1	B	530	TYR	2.7
1	A	118	ASP	2.7
1	B	116	ASN	2.7
1	B	323	ILE	2.7
1	B	120	LEU	2.7
1	B	281	PHE	2.6
1	A	405	ALA	2.6
1	B	218	LYS	2.6
1	B	115	LYS	2.6
1	A	300	GLN	2.6
1	B	62	TYR	2.6
1	B	548	LYS	2.6
1	B	396	ALA	2.5
1	A	91	GLY	2.5
1	B	127	PHE	2.5
1	B	405	ALA	2.5
1	B	216	ASP	2.5
1	A	298	GLN	2.5
1	A	64	VAL	2.5
1	B	398	LYS	2.4
1	A	510	LYS	2.4
1	B	342	ILE	2.4
1	A	120	LEU	2.4
1	A	394	LYS	2.4
1	A	481	TYR	2.3
1	B	488	ASP	2.3
1	A	54	VAL	2.3
1	B	114	ILE	2.3
1	A	398	LYS	2.3
1	B	296	SER	2.3
1	B	390	ALA	2.2
1	A	483	ILE	2.2
1	B	407	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	322	ASP	2.2
1	B	445	ASP	2.2
1	B	525	LEU	2.2
1	B	149	PRO	2.2
1	B	314	VAL	2.1
1	B	550	GLU	2.1
1	B	133	LYS	2.1
1	B	387	GLN	2.1
1	B	539	LEU	2.1
1	B	221	ILE	2.1
1	B	442	ILE	2.1
1	B	85	LYS	2.0
1	B	122	ARG	2.0
1	B	142	PHE	2.0
1	B	298	GLN	2.0
1	A	532	LEU	2.0
1	B	36	ILE	2.0
1	A	261	VAL	2.0
1	A	216	ASP	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	CA	B	601	1/1	0.97	0.09	59,59,59,59	0
2	CA	A	601	1/1	0.98	0.06	52,52,52,52	0

## 6.5 Other polymers

There are no such residues in this entry.