



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:34 AM UTC

PDB ID : 6Y9T / pdb_00006y9t
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

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

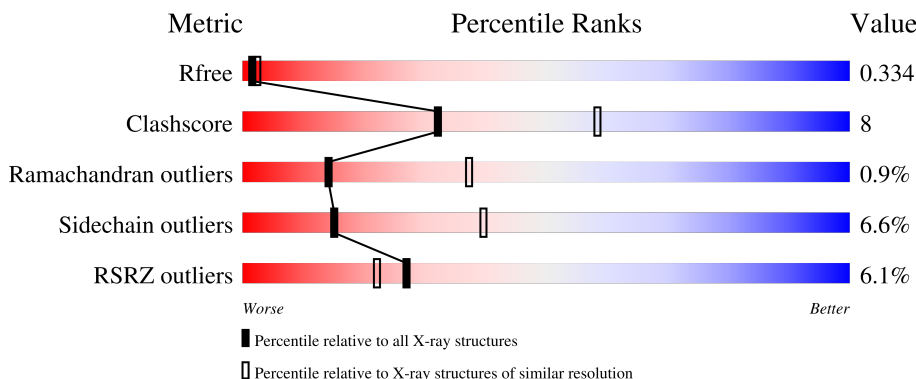
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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}	180053	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (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 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	571	4% 73% 18% 6%
1	B	571	7% 71% 20% 6%

2 Entry composition

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
1	A	536	Total	C	N	O	S	0	0	0
			4328	2769	725	813	21			
1	B	535	Total	C	N	O	S	0	1	0
			4329	2769	725	815	20			

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

Continued on next page...

Continued from previous page...

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 (CCD ID: CA) (formula: Ca).

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

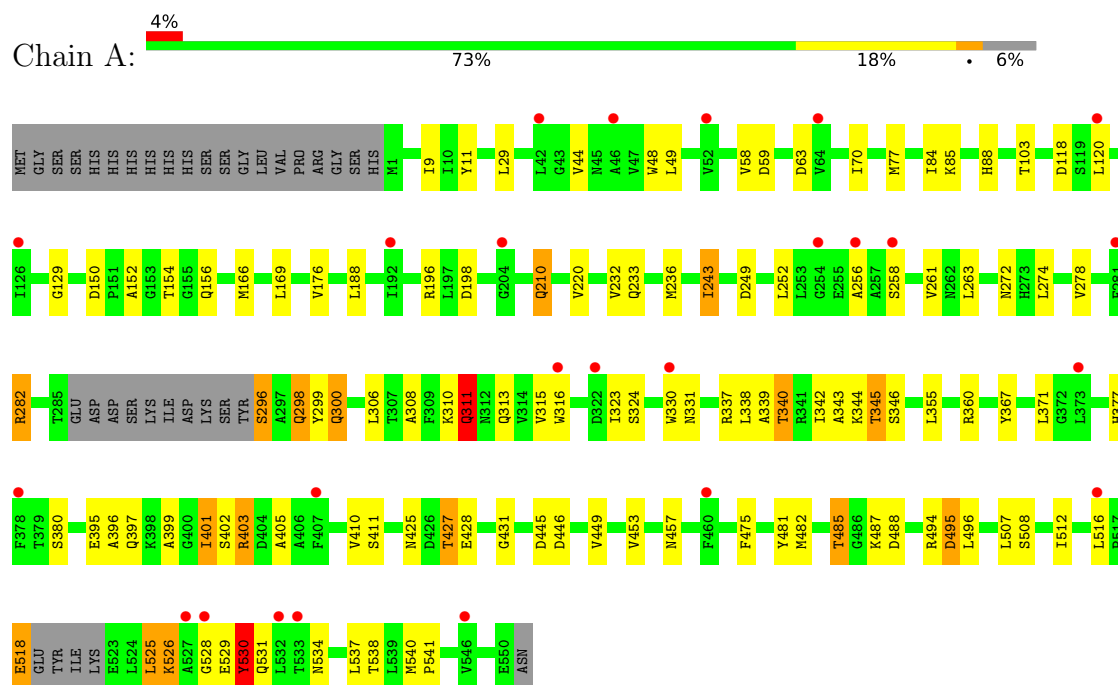
- Molecule 3 is water.

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

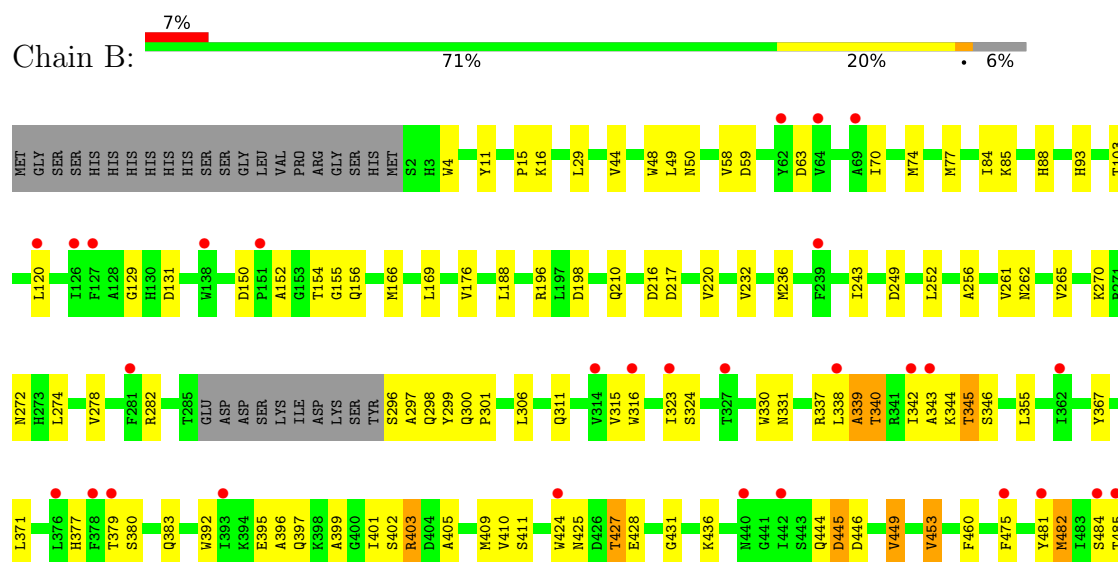
3 Residue-property plots [i](#)

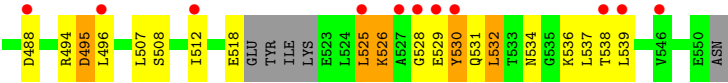
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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, α , β , γ	73.21Å 105.30Å 92.23Å 90.00° 96.95° 90.00°	Depositor
Resolution (Å)	50.01 – 2.78 50.01 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.01-2.78) 99.1 (50.01-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.77Å)	Xtriage
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 (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	65.8	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 79.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8777	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage'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.*

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

5.1 Standard geometry

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	0.80	1/4444 (0.0%)	1.00	9/6032 (0.1%)
1	B	0.78	0/4445	1.00	5/6034 (0.1%)
All	All	0.79	1/8889 (0.0%)	1.00	14/12066 (0.1%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	530	TYR	CA-C	6.13	1.60	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	339	ALA	N-CA-C	-6.74	101.48	110.24
1	B	534	ASN	N-CA-C	6.46	118.40	111.36
1	A	401	ILE	N-CA-C	-6.16	100.83	109.21
1	B	485	THR	N-CA-C	6.13	118.28	108.41
1	A	531	GLN	N-CA-C	6.08	116.58	108.38
1	B	531	GLN	N-CA-C	5.92	116.37	108.38
1	A	129	GLY	N-CA-C	5.87	117.95	110.96
1	A	243	ILE	CB-CA-C	-5.85	104.48	111.97
1	A	311	GLN	N-CA-CB	5.83	118.46	110.01
1	A	534	ASN	N-CA-C	5.82	117.70	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	485	THR	N-CA-C	5.40	117.53	108.73
1	A	446	ASP	N-CA-C	5.23	116.67	109.15
1	A	516	LEU	N-CA-C	5.20	112.90	108.22
1	B	446	ASP	N-CA-C	5.16	116.58	109.15

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	62	0
1	B	4329	0	4165	77	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	136	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 8.

All (136) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ASP:HB2	1:A:166:MET:HE1	1.77	0.65
1:B:532:LEU:HD13	1:B:532:LEU:C	2.21	0.65
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:59:ASP:HB2	1:B:166:MET:HE1	1.81	0.62
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:A:487:LYS:HE3	1:B:216:ASP:CG	2.26	0.60
1:A:339:ALA:HA	1:A:343:ALA:HB3	1.84	0.59
1:B:528:GLY:C	1:B:529:GLU:OE2	2.46	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
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:B:63:ASP:HB3	1:B:166:MET:HE2	1.88	0.54
1:A:306:LEU:HD21	1:A:507:LEU:CD1	2.38	0.54
1:B:74:MET:HE2	3:B:723:HOH:O	2.06	0.54
1:B:532:LEU:CD1	1:B:537:LEU:HA	2.38	0.54
1:A:63:ASP:HB3	1:A:166:MET:HE2	1.90	0.53
1:B:306:LEU:HD21	1:B:507:LEU:CD1	2.38	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:59:ASP:CB	1:A:166:MET:HE1	2.39	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:337:ARG:NH2	1:A:367:TYR:O	2.36	0.50
1:A:339:ALA:O	1:A:340:THR:HB	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:B:16:LYS:HG3	1:B:74:MET:HE1	1.95	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:59:ASP:CB	1:B:166:MET:HE1	2.43	0.47
1:B:355:LEU:C	1:B:355:LEU:HD23	2.39	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:A:528:GLY:C	1:A:529:GLU:OE2	2.58	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:B:48:TRP:CD1	1:B:48:TRP:C	2.92	0.46
1:A:344:LYS:O	1:A:345:THR:HG23	2.15	0.46
1:B:70:ILE:HG21	1:B:77:MET:N	2.31	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
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: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:338:LEU:C	1:B:339:ALA:O	2.58	0.45
1:A:529:GLU:O	1:A:530:TYR:HB2	2.16	0.45
1:B:379:THR:O	1:B:383:GLN:OE1	2.35	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OD1	1:A:495:ASP:N	2.50	0.45
1:A:48:TRP:CD1	1:A:48:TRP:C	2.96	0.44
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:525:LEU:C	1:A:525:LEU:HD12	2.43	0.44
1:A:355:LEU:C	1:A:355:LEU:HD23	2.43	0.44
1:B:15:PRO:HG2	1:B:74:MET:HE3	1.99	0.44
1:A:449:VAL:O	1:A:453:VAL:HG22	2.17	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:B:495:ASP:OD1	1:B:495:ASP:N	2.52	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:N	1:B:526:LYS:CD	2.82	0.42
1:B:525:LEU:HD12	1:B:525:LEU:C	2.44	0.42
1:A:256:ALA:HB3	1:A:278:VAL:HG11	2.02	0.42
1:A:457:ASN:OD1	1:A:457:ASN:C	2.62	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: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:263:LEU:HD11	1:B:262:ASN:CG	2.46	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:A:323:ILE:O	1:A:324:SER:HB3	2.21	0.41
1:A:338:LEU:C	1:A:339:ALA:O	2.61	0.41
1:B:188:LEU:CD1	1:B:243:ILE:HG23	2.50	0.41
1:B:371:LEU:HD11	1:B:449:VAL:HG12	2.03	0.41
1:B:529:GLU:OE2	1:B:529:GLU:N	2.54	0.40
1:A:518:GLU:N	1:A:518:GLU:OE1	2.54	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:532:LEU:C	1:B:532:LEU:CD1	2.93	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%)	14	37
1	B	530/571 (93%)	486 (92%)	39 (7%)	5 (1%)	14	37
All	All	1060/1142 (93%)	973 (92%)	77 (7%)	10 (1%)	14	37

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
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 ⓘ

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%)	16	41
1	B	466/498 (94%)	435 (93%)	31 (7%)	15	39
All	All	932/996 (94%)	871 (94%)	61 (6%)	15	40

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

Mol	Chain	Res	Type
1	A	9	ILE
1	A	49	LEU
1	A	58	VAL
1	A	85	LYS
1	A	118	ASP
1	A	120	LEU
1	A	176	VAL
1	A	210	GLN
1	A	220	VAL
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	360	ARG
1	A	395	GLU
1	A	402	SER
1	A	403	ARG
1	A	427	THR
1	A	445	ASP
1	A	481	TYR
1	A	482	MET
1	A	495	ASP
1	A	496	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	518	GLU
1	A	525	LEU
1	A	526	LYS
1	B	49	LEU
1	B	50	ASN
1	B	58	VAL
1	B	85	LYS
1	B	120	LEU
1	B	176	VAL
1	B	210	GLN
1	B	220	VAL
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	395	GLU
1	B	402	SER
1	B	403	ARG
1	B	427	THR
1	B	436	LYS
1	B	445	ASP
1	B	449	VAL
1	B	453	VAL
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	50	ASN
1	A	57	GLN
1	A	82	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	107	HIS
1	A	242	GLN
1	A	325	GLN
1	A	397	GLN
1	A	425	ASN
1	A	444	GLN
1	B	12	GLN
1	B	50	ASN
1	B	82	ASN
1	B	93	HIS
1	B	170	ASN
1	B	242	GLN
1	B	333	HIS
1	B	383	GLN
1	B	397	GLN
1	B	444	GLN

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 ⓘ

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 [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	536/571 (93%)	0.69	25 (4%)	36 31	38, 82, 123, 186	0
1	B	535/571 (93%)	0.79	40 (7%)	20 16	32, 84, 140, 173	1 (0%)
All	All	1071/1142 (93%)	0.74	65 (6%)	27 22	32, 83, 133, 186	1 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	378	PHE	5.2
1	A	532	LEU	3.6
1	B	362	ILE	3.6
1	A	527	ALA	3.5
1	A	378	PHE	3.3
1	B	484	SER	3.2
1	B	525	LEU	3.0
1	B	485	THR	3.0
1	B	530	TYR	2.9
1	B	323	ILE	2.9
1	A	407	PHE	2.8
1	A	120	LEU	2.8
1	B	338	LEU	2.8
1	B	69	ALA	2.8
1	B	127	PHE	2.8
1	A	533	THR	2.7
1	B	539	LEU	2.7
1	B	528	GLY	2.7
1	B	316	TRP	2.7
1	B	481	TYR	2.6
1	B	120	LEU	2.6
1	B	314	VAL	2.6
1	B	376	LEU	2.5
1	B	529	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	151	PRO	2.5
1	B	281	PHE	2.5
1	B	62	TYR	2.5
1	A	52	VAL	2.5
1	A	64	VAL	2.5
1	A	254	GLY	2.5
1	A	528	GLY	2.5
1	B	64	VAL	2.4
1	A	281	PHE	2.4
1	B	379	THR	2.4
1	A	316	TRP	2.4
1	B	138	TRP	2.3
1	B	424	TRP	2.3
1	A	516	LEU	2.3
1	A	46	ALA	2.3
1	A	256	ALA	2.2
1	A	258	SER	2.2
1	B	546	VAL	2.2
1	A	192	ILE	2.2
1	A	204	GLY	2.2
1	A	322	ASP	2.2
1	B	488	ASP	2.2
1	B	342	ILE	2.2
1	B	527	ALA	2.2
1	A	126	ILE	2.2
1	B	475	PHE	2.2
1	A	546	VAL	2.1
1	B	442	ILE	2.1
1	B	512	ILE	2.1
1	A	460	PHE	2.1
1	B	327	THR	2.1
1	B	126	ILE	2.1
1	B	343	ALA	2.1
1	A	42	LEU	2.1
1	B	393	ILE	2.1
1	A	330	TRP	2.0
1	A	373	LEU	2.0
1	B	440	ASN	2.0
1	B	239	PHE	2.0
1	B	538	THR	2.0
1	B	496	LEU	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	B	601	1/1	0.99	0.02	59,59,59,59	0
2	CA	A	601	1/1	1.00	0.04	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.