



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:37 AM UTC

PDB ID : 1EUT / pdb_00001eut
Title : SIALIDASE, LARGE 68KD FORM, COMPLEXED WITH GALACTOSE
Authors : Gaskell, A.; Crennell, S.J.; Taylor, G.L.
Deposited on : 1996-06-21
Resolution : 2.50 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

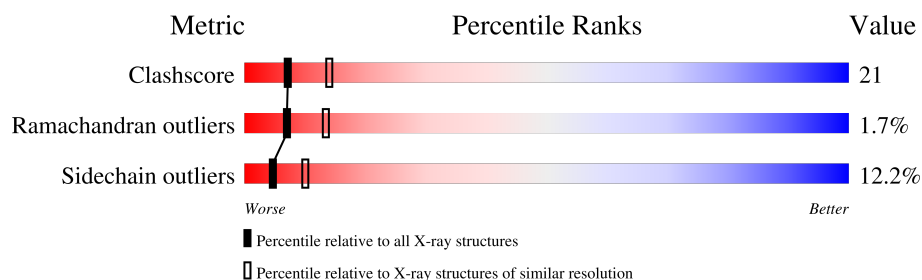
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	605	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4536 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 SIALIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	0	0	0
			4535	2809	819	900	7			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

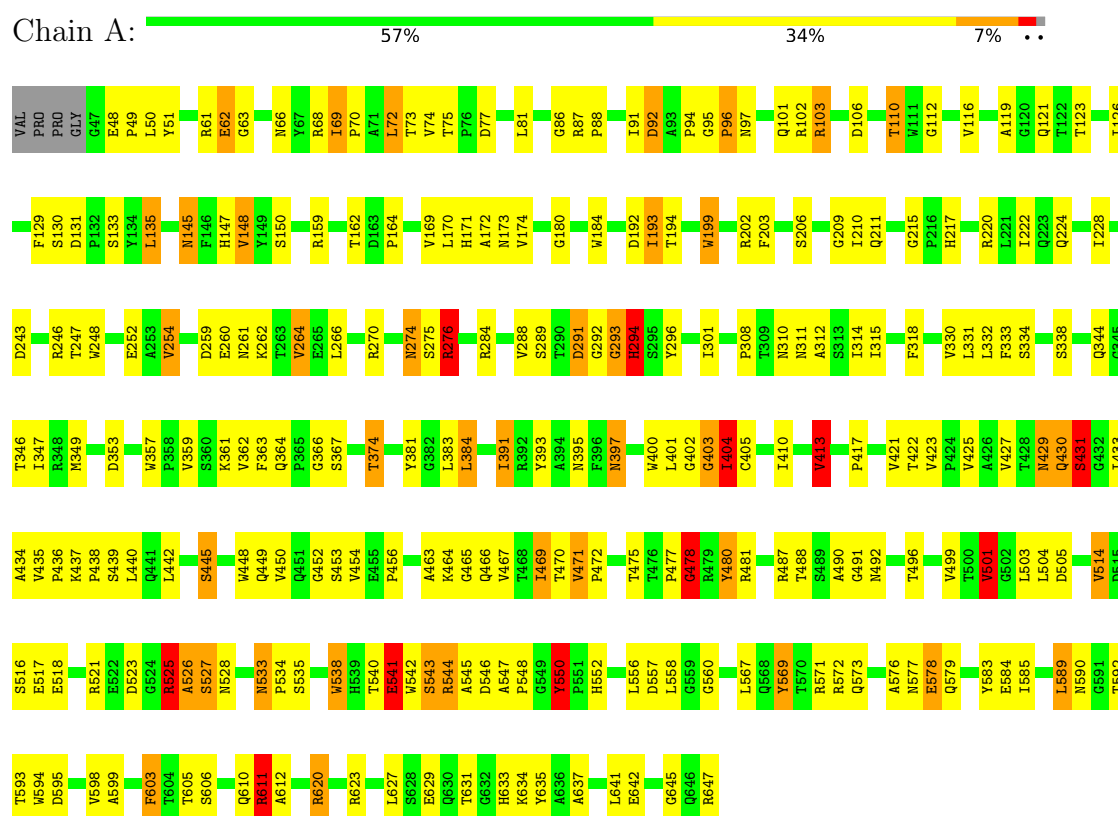
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

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. 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. 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.

Note EDS was not executed.

• Molecule 1: SIALIDASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.28Å 117.30Å 60.24Å 90.00° 96.17° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.50)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.214 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4536	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.81	1/4642 (0.0%)	1.31	58/6339 (0.9%)

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	471	VAL	CA-CB	8.13	1.60	1.54

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	550	TYR	N-CA-C	14.36	133.38	113.57
1	A	291	ASP	N-CA-C	12.13	124.23	108.34
1	A	544	ARG	N-CA-C	-11.82	96.07	111.92
1	A	403	GLY	N-CA-C	11.57	125.10	110.29
1	A	550	TYR	CA-C-N	-11.22	105.82	119.84
1	A	550	TYR	C-N-CA	-11.22	105.82	119.84
1	A	95	GLY	CA-C-N	10.74	133.26	119.84
1	A	95	GLY	C-N-CA	10.74	133.26	119.84
1	A	526	ALA	N-CA-C	-10.63	92.99	109.25
1	A	634	LYS	N-CA-C	10.31	125.95	113.16
1	A	573	GLN	N-CA-C	9.86	122.10	111.36
1	A	478	GLY	N-CA-C	8.69	133.77	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	GLY	N-CA-C	8.03	125.36	114.92
1	A	275	SER	N-CA-C	7.91	122.52	109.95
1	A	533	ASN	CA-C-N	7.26	126.97	119.56
1	A	533	ASN	C-N-CA	7.26	126.97	119.56
1	A	276	ARG	N-CA-C	-7.06	100.54	110.50
1	A	193	ILE	N-CA-C	6.93	118.81	112.29
1	A	477	PRO	N-CA-C	6.84	121.96	111.15
1	A	429	ASN	N-CA-C	6.83	121.19	110.32
1	A	86	GLY	N-CA-C	-6.81	97.04	113.18
1	A	294	HIS	N-CA-C	6.77	125.23	110.80
1	A	501	VAL	N-CA-C	6.62	117.44	108.17
1	A	69	ILE	CA-C-N	6.62	126.60	119.78
1	A	69	ILE	C-N-CA	6.62	126.60	119.78
1	A	318	PHE	CA-C-N	6.40	126.61	119.32
1	A	318	PHE	C-N-CA	6.40	126.61	119.32
1	A	431	SER	N-CA-C	6.27	124.16	110.80
1	A	215	GLY	CA-C-N	6.23	127.03	120.12
1	A	215	GLY	C-N-CA	6.23	127.03	120.12
1	A	293	GLY	CA-C-N	6.07	133.14	121.54
1	A	293	GLY	C-N-CA	6.07	133.14	121.54
1	A	228	ILE	N-CA-C	-6.07	97.64	107.28
1	A	77	ASP	N-CA-C	6.04	119.96	112.59
1	A	293	GLY	N-CA-C	-5.75	99.55	113.18
1	A	590	ASN	N-CA-C	-5.71	106.48	113.50
1	A	611	ARG	N-CA-C	5.69	119.51	109.96
1	A	413	VAL	N-CA-C	5.67	116.75	108.53
1	A	557	ASP	N-CA-C	-5.64	98.56	108.20
1	A	130	SER	N-CA-C	5.63	117.64	109.07
1	A	525	ARG	N-CA-C	5.63	118.40	109.96
1	A	330	VAL	N-CA-C	5.61	116.81	108.23
1	A	538	TRP	N-CA-C	-5.56	100.62	109.96
1	A	210	ILE	N-CA-C	5.50	116.62	108.65
1	A	528	ASN	N-CA-C	-5.48	106.55	113.18
1	A	572	ARG	N-CA-C	-5.35	101.26	109.76
1	A	576	ALA	N-CA-C	5.32	119.74	112.88
1	A	480	TYR	N-CA-C	5.25	116.96	108.41
1	A	437	LYS	N-CA-C	5.22	119.35	108.39
1	A	577	ASN	N-CA-C	5.21	119.74	113.17
1	A	598	VAL	N-CA-C	-5.19	105.95	113.07
1	A	434	ALA	N-CA-C	-5.19	96.92	107.41
1	A	471	VAL	CA-C-N	5.18	125.46	119.92
1	A	471	VAL	C-N-CA	5.18	125.46	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	GLU	N-CA-C	5.04	118.70	112.24
1	A	402	GLY	N-CA-C	-5.04	101.24	113.18
1	A	357	TRP	CA-C-N	5.03	124.52	119.19
1	A	357	TRP	C-N-CA	5.03	124.52	119.19

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	381	TYR	Sidechain
1	A	393	TYR	Sidechain

5.2 Too-close contacts ⓘ

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	4535	0	4353	185	0
2	A	1	0	0	0	0
All	All	4536	0	4353	185	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 21.

All (185) 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:488:THR:HG22	1:A:490:ALA:H	1.26	0.99
1:A:481:ARG:H	1:A:481:ARG:HD3	1.29	0.98
1:A:430:GLN:HG3	1:A:433:ILE:HG13	1.45	0.97
1:A:547:ALA:HB1	1:A:548:PRO:HD2	1.44	0.95
1:A:585:ILE:HD12	1:A:599:ALA:HB3	1.56	0.87
1:A:69:ILE:HG21	1:A:131:ASP:HA	1.60	0.84
1:A:73:THR:HG22	1:A:81:LEU:HB2	1.62	0.80
1:A:194:THR:HG23	1:A:199:TRP:HB2	1.64	0.78
1:A:547:ALA:HB1	1:A:548:PRO:CD	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:ILE:HD11	1:A:612:ALA:HB1	1.68	0.75
1:A:148:VAL:HG13	1:A:170:LEU:HD11	1.70	0.73
1:A:540:THR:HG21	1:A:552:HIS:CE1	2.25	0.71
1:A:472:PRO:HG2	1:A:475:THR:OG1	1.90	0.70
1:A:145:ASN:HD22	1:A:147:HIS:HD2	1.41	0.69
1:A:435:VAL:HG11	1:A:488:THR:HG23	1.74	0.69
1:A:220:ARG:HH12	1:A:292:GLY:HA2	1.59	0.68
1:A:217:HIS:CE1	1:A:292:GLY:HA3	2.29	0.67
1:A:349:MET:HB3	1:A:359:VAL:HB	1.76	0.67
1:A:571:ARG:NH1	1:A:603:PHE:CE2	2.64	0.66
1:A:192:ASP:HB3	1:A:248:TRP:O	1.95	0.65
1:A:410:ILE:HG12	1:A:425:VAL:HG22	1.77	0.65
1:A:526:ALA:O	1:A:527:SER:HB3	1.94	0.65
1:A:346:THR:HG22	1:A:362:VAL:HG22	1.77	0.64
1:A:384:LEU:HD21	1:A:391:ILE:HD12	1.79	0.64
1:A:550:TYR:CE2	1:A:629:GLU:HB2	2.32	0.64
1:A:603:PHE:H	1:A:603:PHE:HD1	1.46	0.64
1:A:413:VAL:HG22	1:A:423:VAL:HG11	1.79	0.63
1:A:571:ARG:HH12	1:A:603:PHE:HE2	1.46	0.63
1:A:430:GLN:HE21	1:A:431:SER:N	1.97	0.63
1:A:478:GLY:HA2	1:A:501:VAL:H	1.63	0.63
1:A:50:LEU:H	1:A:397:ASN:HD21	1.44	0.63
1:A:50:LEU:H	1:A:397:ASN:ND2	1.97	0.62
1:A:516:SER:OG	1:A:540:THR:HG23	2.00	0.62
1:A:259:ASP:HB3	1:A:276:ARG:HD2	1.82	0.62
1:A:413:VAL:HG11	1:A:421:VAL:HG21	1.82	0.61
1:A:116:VAL:HG11	1:A:119:ALA:HB2	1.83	0.61
1:A:291:ASP:OD1	1:A:294:HIS:HA	2.01	0.60
1:A:523:ASP:OD1	1:A:525:ARG:HD3	2.01	0.60
1:A:243:ASP:OD2	1:A:246:ARG:HB2	2.01	0.60
1:A:464:LYS:HG2	1:A:465:GLY:N	2.17	0.60
1:A:445:SER:O	1:A:448:TRP:HB2	2.01	0.59
1:A:518:GLU:HG2	1:A:542:TRP:CD1	2.37	0.59
1:A:384:LEU:CD2	1:A:391:ILE:HD12	2.33	0.59
1:A:88:PRO:HG2	1:A:96:PRO:HG2	1.85	0.58
1:A:436:PRO:HA	1:A:456:PRO:HB3	1.84	0.58
1:A:220:ARG:HH11	1:A:294:HIS:HD2	1.49	0.58
1:A:430:GLN:CG	1:A:433:ILE:HG13	2.29	0.58
1:A:503:LEU:HD22	1:A:642:GLU:HG3	1.85	0.58
1:A:364:GLN:HE21	1:A:366:GLY:H	1.52	0.58
1:A:478:GLY:HA3	1:A:503:LEU:HD11	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:GLY:C	1:A:620:ARG:HG2	2.30	0.57
1:A:145:ASN:ND2	1:A:147:HIS:HD2	2.02	0.56
1:A:538:TRP:O	1:A:637:ALA:HA	2.05	0.56
1:A:569:TYR:HB3	1:A:641:LEU:HD23	1.86	0.56
1:A:589:LEU:HD12	1:A:589:LEU:H	1.69	0.56
1:A:220:ARG:HH11	1:A:294:HIS:CD2	2.23	0.56
1:A:361:LYS:HE3	1:A:400:TRP:O	2.07	0.55
1:A:550:TYR:O	1:A:552:HIS:N	2.40	0.55
1:A:404:ILE:HD12	1:A:488:THR:HG21	1.88	0.54
1:A:585:ILE:CD1	1:A:612:ALA:HB1	2.38	0.54
1:A:413:VAL:CG2	1:A:423:VAL:HG11	2.37	0.53
1:A:543:SER:O	1:A:544:ARG:HB2	2.08	0.53
1:A:220:ARG:NH1	1:A:292:GLY:HA2	2.24	0.53
1:A:592:THR:HG23	1:A:593:THR:HG23	1.91	0.53
1:A:266:LEU:CD1	1:A:270:ARG:NH1	2.72	0.52
1:A:405:CYS:HB2	1:A:430:GLN:HB3	1.91	0.52
1:A:453:SER:O	1:A:465:GLY:HA3	2.10	0.52
1:A:521:ARG:CZ	1:A:544:ARG:HB3	2.40	0.52
1:A:66:ASN:HB3	1:A:87:ARG:HB2	1.92	0.51
1:A:217:HIS:NE2	1:A:292:GLY:HA3	2.23	0.51
1:A:438:PRO:HG2	1:A:454:VAL:HG13	1.93	0.51
1:A:569:TYR:N	1:A:569:TYR:CD1	2.78	0.51
1:A:259:ASP:O	1:A:260:GLU:C	2.53	0.51
1:A:264:VAL:HG22	1:A:314:ILE:HG23	1.91	0.51
1:A:361:LYS:HB3	1:A:401:LEU:HD23	1.93	0.51
1:A:361:LYS:HG2	1:A:400:TRP:CH2	2.46	0.51
1:A:344:GLN:O	1:A:346:THR:HG23	2.10	0.50
1:A:404:ILE:HG13	1:A:433:ILE:HD12	1.94	0.50
1:A:135:LEU:HD22	1:A:209:GLY:HA3	1.94	0.50
1:A:274:ASN:ND2	1:A:284:ARG:HE	2.10	0.50
1:A:429:ASN:HD21	1:A:433:ILE:HB	1.76	0.50
1:A:504:LEU:HD12	1:A:504:LEU:N	2.27	0.50
1:A:550:TYR:O	1:A:550:TYR:CD1	2.64	0.50
1:A:403:GLY:HA3	1:A:491:GLY:HA3	1.94	0.49
1:A:514:VAL:HG21	1:A:526:ALA:CB	2.41	0.49
1:A:349:MET:HE2	1:A:359:VAL:HG21	1.95	0.49
1:A:331:LEU:HD21	1:A:353:ASP:HA	1.93	0.49
1:A:603:PHE:N	1:A:603:PHE:CD1	2.79	0.49
1:A:478:GLY:HA3	1:A:503:LEU:CD1	2.43	0.49
1:A:518:GLU:HG2	1:A:542:TRP:NE1	2.28	0.49
1:A:148:VAL:HG23	1:A:203:PHE:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:THR:CG2	1:A:81:LEU:HG	2.43	0.49
1:A:603:PHE:HB2	1:A:610:GLN:NE2	2.28	0.48
1:A:133:SER:HB2	1:A:206:SER:HA	1.96	0.48
1:A:631:THR:HG23	1:A:633:HIS:ND1	2.28	0.48
1:A:314:ILE:HB	1:A:333:PHE:HD1	1.77	0.48
1:A:452:GLY:HA2	1:A:466:GLN:O	2.13	0.48
1:A:148:VAL:CG1	1:A:170:LEU:HD11	2.42	0.48
1:A:542:TRP:O	1:A:543:SER:O	2.32	0.48
1:A:129:PHE:HA	1:A:148:VAL:O	2.12	0.48
1:A:347:ILE:HG12	1:A:363:PHE:HD2	1.79	0.48
1:A:92:ASP:HA	1:A:97:ASN:HD21	1.79	0.48
1:A:571:ARG:HD3	1:A:579:GLN:OE1	2.14	0.48
1:A:578:GLU:HA	1:A:635:TYR:O	2.14	0.48
1:A:480:TYR:HB2	1:A:499:VAL:O	2.14	0.47
1:A:164:PRO:HA	1:A:171:HIS:CE1	2.49	0.47
1:A:259:ASP:CB	1:A:276:ARG:HD2	2.44	0.47
1:A:514:VAL:HG11	1:A:526:ALA:HB2	1.96	0.47
1:A:359:VAL:HG22	1:A:403:GLY:O	2.15	0.47
1:A:421:VAL:HG13	1:A:469:ILE:CD1	2.45	0.47
1:A:172:ALA:CB	1:A:193:ILE:HD11	2.45	0.46
1:A:206:SER:O	1:A:262:LYS:HE2	2.14	0.46
1:A:308:PRO:HG2	1:A:310:ASN:HB2	1.96	0.46
1:A:364:GLN:HE21	1:A:366:GLY:N	2.13	0.46
1:A:558:LEU:HB2	1:A:620:ARG:O	2.15	0.46
1:A:51:TYR:HA	1:A:395:ASN:O	2.16	0.46
1:A:315:ILE:HD11	1:A:332:LEU:HD12	1.98	0.45
1:A:578:GLU:N	1:A:578:GLU:CD	2.75	0.45
1:A:433:ILE:HG23	1:A:435:VAL:HG23	1.99	0.45
1:A:611:ARG:NE	1:A:611:ARG:H	2.14	0.45
1:A:87:ARG:NH1	1:A:92:ASP:OD1	2.50	0.45
1:A:429:ASN:OD1	1:A:430:GLN:N	2.50	0.45
1:A:611:ARG:H	1:A:611:ARG:CD	2.30	0.45
1:A:421:VAL:HG13	1:A:469:ILE:HD12	1.99	0.45
1:A:594:TRP:CZ3	1:A:623:ARG:HB3	2.52	0.45
1:A:430:GLN:NE2	1:A:431:SER:HB2	2.32	0.44
1:A:504:LEU:HD11	1:A:645:GLY:HA3	2.00	0.44
1:A:405:CYS:HB2	1:A:430:GLN:CB	2.47	0.44
1:A:439:SER:HB2	1:A:487:ARG:HB2	2.00	0.44
1:A:361:LYS:HG3	1:A:362:VAL:N	2.32	0.44
1:A:569:TYR:CE2	1:A:603:PHE:CZ	3.06	0.44
1:A:222:ILE:HG22	1:A:224:GLN:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ARG:NE	1:A:246:ARG:HA	2.32	0.43
1:A:514:VAL:HG21	1:A:526:ALA:HB3	1.99	0.43
1:A:431:SER:O	1:A:433:ILE:N	2.51	0.43
1:A:61:ARG:HD2	1:A:61:ARG:N	2.32	0.43
1:A:430:GLN:HE21	1:A:431:SER:H	1.65	0.43
1:A:516:SER:HB2	1:A:541:GLU:HB2	2.00	0.43
1:A:103:ARG:NH2	1:A:180:GLY:O	2.45	0.43
1:A:533:ASN:HA	1:A:534:PRO:HD3	1.80	0.43
1:A:102:ARG:NH1	1:A:112:GLY:O	2.52	0.43
1:A:397:ASN:C	1:A:397:ASN:HD22	2.27	0.43
1:A:92:ASP:HA	1:A:97:ASN:ND2	2.33	0.42
1:A:224:GLN:HB3	1:A:261:ASN:OD1	2.19	0.42
1:A:72:LEU:HG	1:A:384:LEU:HB2	2.00	0.42
1:A:404:ILE:HD11	1:A:433:ILE:CG2	2.49	0.42
1:A:413:VAL:O	1:A:499:VAL:HA	2.19	0.42
1:A:449:GLN:HB2	1:A:470:THR:HB	2.01	0.42
1:A:583:TYR:CD1	1:A:603:PHE:CD1	3.07	0.42
1:A:589:LEU:HD12	1:A:589:LEU:N	2.31	0.42
1:A:101:GLN:HE22	1:A:184:TRP:HZ2	1.66	0.42
1:A:542:TRP:HA	1:A:635:TYR:CE1	2.54	0.42
1:A:69:ILE:HA	1:A:70:PRO:HD2	1.90	0.42
1:A:211:GLN:HA	1:A:220:ARG:O	2.19	0.42
1:A:106:ASP:OD2	1:A:110:THR:HB	2.19	0.42
1:A:603:PHE:HB2	1:A:610:GLN:HE21	1.84	0.42
1:A:571:ARG:HG2	1:A:571:ARG:HH11	1.84	0.42
1:A:571:ARG:HG3	1:A:606:SER:O	2.19	0.42
1:A:585:ILE:HD11	1:A:612:ALA:CB	2.44	0.42
1:A:405:CYS:HB2	1:A:430:GLN:CG	2.50	0.41
1:A:66:ASN:ND2	1:A:68:ARG:HG3	2.35	0.41
1:A:413:VAL:CG1	1:A:421:VAL:HG21	2.48	0.41
1:A:422:THR:HA	1:A:467:VAL:O	2.20	0.41
1:A:220:ARG:NH1	1:A:294:HIS:CD2	2.87	0.41
1:A:254:VAL:HG11	1:A:296:TYR:HB2	2.01	0.41
1:A:417:PRO:HG3	1:A:501:VAL:HG23	2.02	0.41
1:A:427:VAL:HB	1:A:463:ALA:HB3	2.03	0.41
1:A:521:ARG:NH2	1:A:544:ARG:HB3	2.36	0.41
1:A:505:ASP:HB2	1:A:647:ARG:NH1	2.36	0.41
1:A:584:GLU:HG3	1:A:627:LEU:HD11	2.03	0.41
1:A:94:PRO:HA	1:A:150:SER:OG	2.21	0.40
1:A:121:GLN:HG2	1:A:123:THR:O	2.21	0.40
1:A:266:LEU:CD1	1:A:270:ARG:HH12	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:PRO:HD3	1:A:338:SER:O	2.20	0.40
1:A:311:ASN:HD22	1:A:312:ALA:H	1.69	0.40
1:A:543:SER:O	1:A:544:ARG:CB	2.68	0.40
1:A:73:THR:CG2	1:A:81:LEU:HB2	2.42	0.40
1:A:569:TYR:HB3	1:A:641:LEU:CD2	2.49	0.40
1:A:72:LEU:HD13	1:A:374:THR:CG2	2.52	0.40
1:A:266:LEU:HD22	1:A:353:ASP:HB3	2.03	0.40
1:A:334:SER:HB3	1:A:347:ILE:HD13	2.04	0.40
1:A:48:GLU:HA	1:A:49:PRO:HD3	1.91	0.40
1:A:162:THR:O	1:A:164:PRO:HD3	2.22	0.40
1:A:517:GLU:HG2	1:A:526:ALA:H	1.86	0.40
1:A:288:VAL:HG22	1:A:289:SER:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	599/605 (99%)	542 (90%)	47 (8%)	10 (2%)	7	13

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	HIS
1	A	404	ILE
1	A	431	SER
1	A	478	GLY
1	A	527	SER
1	A	543	SER
1	A	545	ALA
1	A	293	GLY
1	A	541	GLU

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Mol	Chain	Res	Type
1	A	96	PRO

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	477/480 (99%)	419 (88%)	58 (12%)	5 10

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	GLU
1	A	72	LEU
1	A	74	VAL
1	A	91	ILE
1	A	92	ASP
1	A	103	ARG
1	A	110	THR
1	A	126	ILE
1	A	135	LEU
1	A	145	ASN
1	A	148	VAL
1	A	159	ARG
1	A	169	VAL
1	A	173	ASN
1	A	174	VAL
1	A	199	TRP
1	A	202	ARG
1	A	247	THR
1	A	252	GLU
1	A	254	VAL
1	A	264	VAL
1	A	274	ASN
1	A	276	ARG
1	A	301	ILE
1	A	367	SER

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Mol	Chain	Res	Type
1	A	374	THR
1	A	383	LEU
1	A	384	LEU
1	A	391	ILE
1	A	397	ASN
1	A	404	ILE
1	A	413	VAL
1	A	430	GLN
1	A	440	LEU
1	A	442	LEU
1	A	445	SER
1	A	450	VAL
1	A	469	ILE
1	A	471	VAL
1	A	492	ASN
1	A	496	THR
1	A	501	VAL
1	A	514	VAL
1	A	525	ARG
1	A	535	SER
1	A	541	GLU
1	A	546	ASP
1	A	550	TYR
1	A	556	LEU
1	A	567	LEU
1	A	569	TYR
1	A	578	GLU
1	A	589	LEU
1	A	595	ASP
1	A	603	PHE
1	A	605	THR
1	A	611	ARG
1	A	620	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	101	GLN
1	A	115	GLN
1	A	145	ASN
1	A	147	HIS

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Mol	Chain	Res	Type
1	A	168	ASN
1	A	186	HIS
1	A	223	GLN
1	A	224	GLN
1	A	244	HIS
1	A	274	ASN
1	A	294	HIS
1	A	310	ASN
1	A	311	ASN
1	A	355	GLN
1	A	364	GLN
1	A	397	ASN
1	A	419	GLN
1	A	420	GLN
1	A	430	GLN
1	A	466	GLN
1	A	492	ASN
1	A	573	GLN
1	A	577	ASN
1	A	610	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 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

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.