Full wwPDB X-ray Structure Validation Report (i)

Oct 12, 2024 – 04:49 PM EDT

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

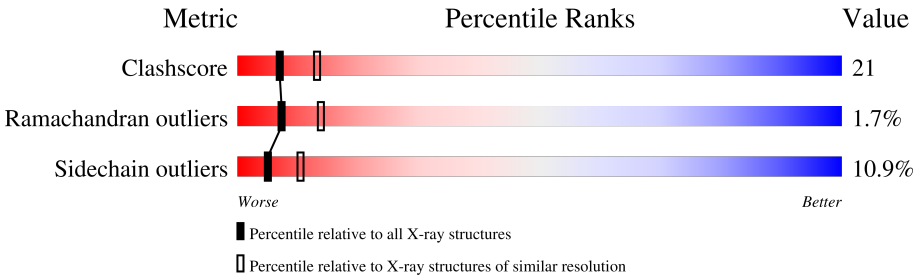
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.50 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	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	605	61% 31% 7% ••

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	601	4535	2809	819	900	7	0	0	0

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

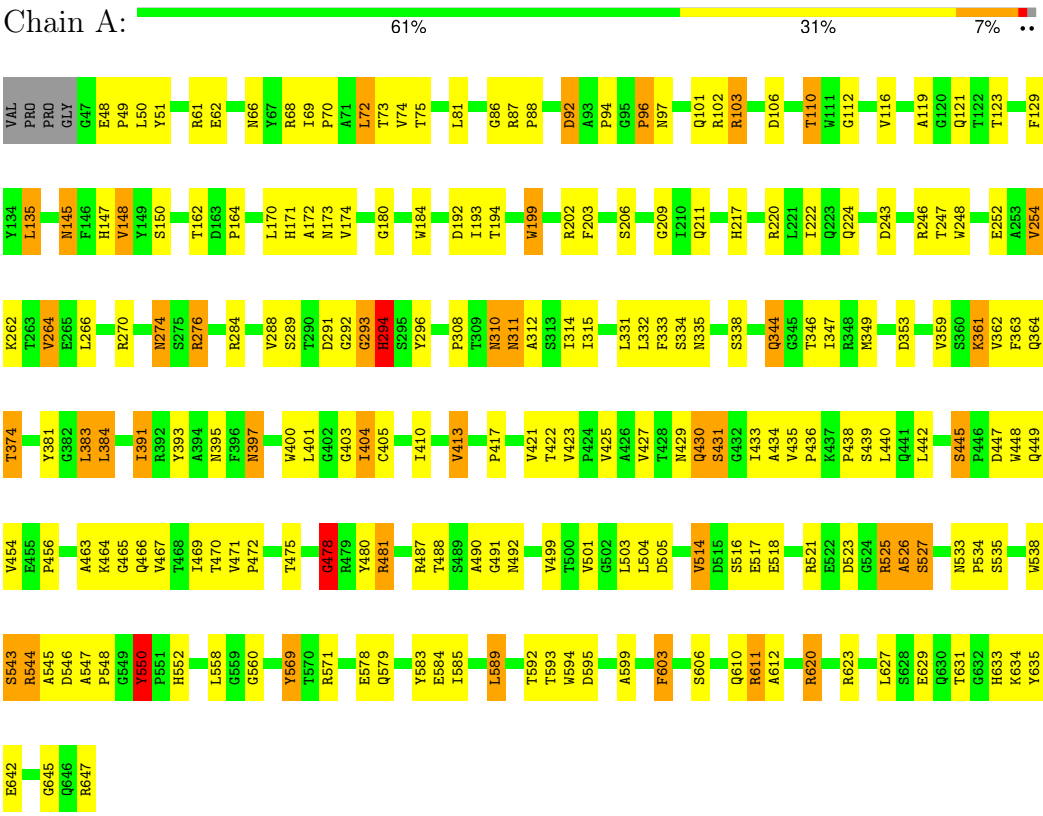
3 Residue-property plots (i)

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. 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

Chain A:



4 Data and refinement statistics (i)

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	0.63	0/4642	0.94	11/6339 (0.2%)

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

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	550	TYR	N-CA-C	8.29	133.38	111.00
1	A	478	GLY	N-CA-C	8.27	133.77	113.10
1	A	526	ALA	N-CA-C	-6.67	92.99	111.00
1	A	86	GLY	N-CA-C	-6.42	97.04	113.10
1	A	383	LEU	CA-CB-CG	5.82	128.68	115.30
1	A	634	LYS	N-CA-C	5.54	125.95	111.00
1	A	544	ARG	N-CA-C	-5.53	96.07	111.00
1	A	293	GLY	N-CA-C	-5.42	99.55	113.10
1	A	294	HIS	N-CA-C	5.27	125.23	111.00
1	A	434	ALA	N-CA-C	-5.21	96.92	111.00
1	A	550	TYR	C-N-CD	5.04	138.98	128.40

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 (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	4535	0	4353	184	0
2	A	1	0	0	0	0
All	All	4536	0	4353	184	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 (184) 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
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:526:ALA:O	1:A:527:SER:HB3	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:472:PRO:HG2	1:A:475:THR:HG1	1.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:560:GLY:C	1:A:620:ARG:HG2	2.30	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:259:ASP:O	1:A:260:GLU:C	2.53	0.46
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:578:GLU:CD	1:A:578:GLU:N	2.75	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 (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	599/605 (99%)	542 (90%)	47 (8%)	10 (2%)	7 14

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
1	A	96	PRO

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	477/480 (99%)	425 (89%)	52 (11%)	5 10

All (52) 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	92	ASP
1	A	103	ARG
1	A	110	THR
1	A	135	LEU
1	A	145	ASN
1	A	148	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	310	ASN
1	A	311	ASN
1	A	335	ASN
1	A	344	GLN
1	A	361	LYS
1	A	367	SER
1	A	374	THR
1	A	383	LEU
1	A	384	LEU
1	A	391	ILE
1	A	397	ASN
1	A	413	VAL
1	A	430	GLN
1	A	440	LEU
1	A	442	LEU
1	A	445	SER
1	A	447	ASP
1	A	450	VAL
1	A	471	VAL
1	A	481	ARG
1	A	492	ASN
1	A	514	VAL
1	A	525	ARG
1	A	535	SER

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Mol	Chain	Res	Type
1	A	541	GLU
1	A	546	ASP
1	A	550	TYR
1	A	569	TYR
1	A	589	LEU
1	A	595	ASP
1	A	603	PHE
1	A	611	ARG
1	A	620	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	101	GLN
1	A	115	GLN
1	A	145	ASN
1	A	147	HIS
1	A	171	HIS
1	A	173	ASN
1	A	186	HIS
1	A	217	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	364	GLN
1	A	395	ASN
1	A	397	ASN
1	A	419	GLN
1	A	430	GLN
1	A	466	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.