



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 06:45 PM GMT

PDB ID : 2JKP
Title : STRUCTURE OF A FAMILY 97 ALPHA-GLUCOSIDASE FROM
BACTEROIDES THETA IOTAOMICRON IN COMPLEX WITH CAS-
TANOSPERMINE
Authors : Gloster, T.M.; Turkenburg, J.P.; Potts, J.R.; Henrissat, B.; Davies, G.J.
Deposited on : 2008-08-29
Resolution : 1.99 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

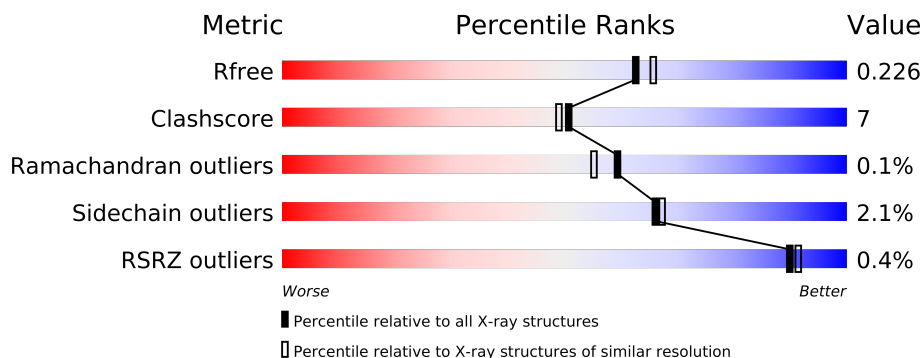
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance



The reported resolution of this entry is 1.99 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}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	727	
1	B	727	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	EDO	A	1729	-	X

2 Entry composition i

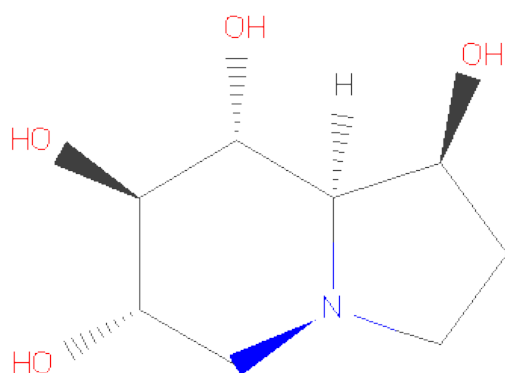
There are 5 unique types of molecules in this entry. The entry contains 12478 atoms, of which 0 are hydrogen and 0 are deuterium.

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 (ALPHA-GLUCOSIDASE SUSB).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	687	Total	C	N	O	S	0	21	0
			5634	3593	937	1075	29			
1	B	687	Total	C	N	O	S	0	8	0
			5545	3530	921	1064	30			

- Molecule 2 is CASTANOSPERMINE (three-letter code: CTS) (formula: $C_8H_{15}NO_4$).

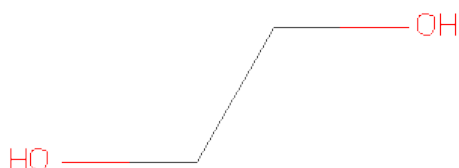


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	8	1	4		
2	B	1	Total	C	N	O	0	0
			13	8	1	4		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	656	Total O 656 656	0	0
5	B	599	Total O 599 599	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

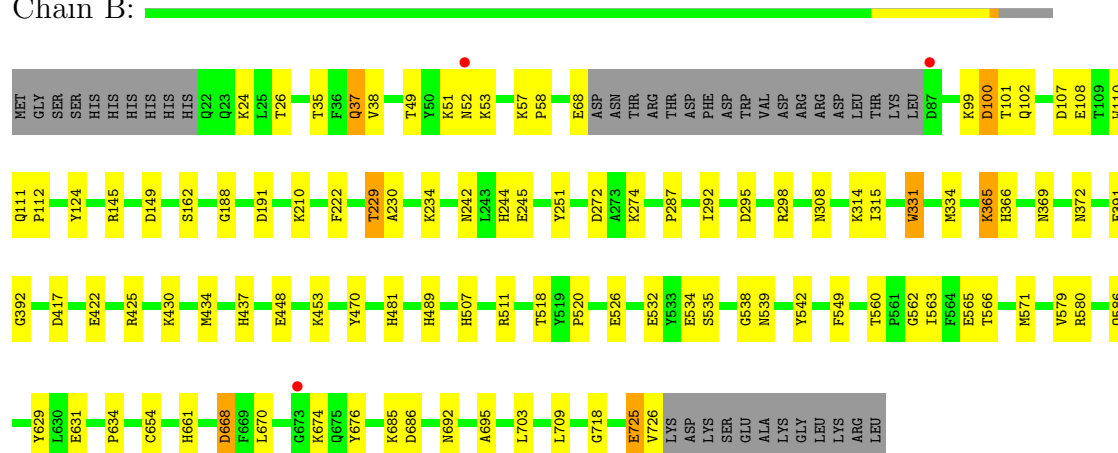
• Molecule 1: ALPHA-GLUCOSIDASE (ALPHA-GLUCOSIDASE SUSB)

Chain A:



• Molecule 1: ALPHA-GLUCOSIDASE (ALPHA-GLUCOSIDASE SUSB)

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.57Å 111.99Å 104.13Å 90.00° 100.89° 90.00°	Depositor
Resolution (Å)	102.06 – 1.99 19.69 – 1.99	Depositor EDS
% Data completeness (in resolution range)	94.7 (102.06-1.99) 94.8 (19.69-1.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.173 , 0.227 0.173 , 0.226	Depositor DCC
R_{free} test set	5452 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 108851 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12478	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, EDO, CTS

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	0.72	0/5847	0.73	2/7932 (0.0%)
1	B	0.72	0/5716	0.73	2/7763 (0.0%)
All	All	0.72	0/11563	0.73	4/15695 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	703	LEU	CA-CB-CG	5.73	128.47	115.30
1	A	63[A]	LEU	CA-CB-CG	5.47	127.89	115.30
1	A	63[B]	LEU	CA-CB-CG	5.47	127.89	115.30
1	B	272	ASP	CB-CG-OD1	5.41	123.17	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5634	0	5447	82	0
1	B	5545	0	5280	80	0
2	A	13	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	13	0	14	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	8	0	12	0	0
4	B	8	0	12	1	0
5	A	656	0	0	10	1
5	B	599	0	0	6	1
All	All	12478	0	10779	162	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (162) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:608[B]:GLU:OE2	5:A:2574:HOH:O	1.72	1.05
1:A:648:ASP:HB2	5:A:2626:HOH:O	1.57	1.05
1:A:109[A]:THR:CG2	1:A:119:GLU:HG2	1.97	0.93
1:B:229[A]:THR:CG2	1:B:244:HIS:ND1	2.32	0.92
1:A:211:GLU:HG3	5:A:2199:HOH:O	1.68	0.92
1:B:229[A]:THR:HG23	1:B:244:HIS:ND1	1.85	0.91
1:B:37[B]:GLN:NE2	5:B:2010:HOH:O	1.91	0.89
1:A:585:ARG:O	1:A:585:ARG:HG3	1.73	0.86
1:B:366:HIS:HD2	1:B:417:ASP:OD2	1.58	0.85
1:A:501[B]:LYS:NZ	5:A:2506:HOH:O	1.98	0.84
1:A:109[A]:THR:HG21	1:A:119:GLU:HG2	1.61	0.83
1:A:662[B]:THR:HG22	1:A:712:HIS:HD2	1.45	0.81
1:A:315:ILE:HD12	1:A:520:PRO:HD2	1.63	0.81
1:B:37[B]:GLN:NE2	1:B:37[B]:GLN:HA	1.96	0.80
1:A:181:HIS:HD2	1:A:233[B]:MET:HE2	1.49	0.77
1:B:470:TYR:O	1:B:481:HIS:HE1	1.72	0.73
1:A:667:PHE:O	1:A:705:ASN:HA	1.88	0.72
1:B:37[B]:GLN:HE21	1:B:37[B]:GLN:HA	1.54	0.72
1:A:45:THR:HG21	5:A:2017:HOH:O	1.89	0.71
1:B:562:GLY:H	1:B:586:GLN:NE2	1.90	0.69
1:B:315:ILE:HD12	1:B:520:PRO:HD2	1.74	0.69
1:A:674:LYS:HD3	1:A:725:GLU:CD	2.13	0.69
1:B:470:TYR:OH	1:B:489:HIS:HE1	1.75	0.68
1:A:366:HIS:HD2	1:A:417:ASP:OD2	1.76	0.68
1:A:110:TRP:HE1	1:A:308:ASN:ND2	1.92	0.67
1:A:623:ASP:OD2	1:A:645[A]:LYS:HE3	1.95	0.66
1:B:562:GLY:H	1:B:586:GLN:HE21	1.44	0.65
1:A:162:SER:HB2	5:A:2119:HOH:O	1.97	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:191:ASP:OD1	1:A:481:HIS:HD2	1.80	0.65
1:A:37:GLN:HG3	5:A:2015:HOH:O	1.97	0.65
1:A:109[A]:THR:HG22	1:A:119:GLU:HG2	1.78	0.64
1:B:110:TRP:HE1	1:B:308:ASN:ND2	1.94	0.64
1:A:534:GLU:HA	1:A:538:GLY:HA2	1.79	0.64
1:A:448:GLU:OE2	1:A:489:HIS:HD2	1.81	0.64
1:A:109[A]:THR:HG23	1:A:120:ILE:O	1.98	0.63
1:B:37[B]:GLN:HE21	1:B:37[B]:GLN:CA	2.13	0.62
1:B:107:ASP:O	1:B:108:GLU:OE2	2.18	0.61
1:B:99:LYS:O	1:B:100:ASP:HB3	2.00	0.61
1:B:37[B]:GLN:HE21	1:B:38:VAL:H	1.48	0.60
1:B:507:HIS:HD2	2:B:1727:CTS:O2	1.84	0.60
1:B:229[A]:THR:HG23	1:B:244:HIS:HA	1.83	0.60
1:B:366:HIS:HE1	1:B:392:GLY:O	1.84	0.59
1:A:643:LYS:HE3	1:A:648:ASP:OD1	2.03	0.59
1:A:470:TYR:OH	1:A:489:HIS:HE1	1.86	0.59
1:B:448:GLU:OE2	1:B:489:HIS:HD2	1.86	0.59
1:B:674:LYS:CD	1:B:725:GLU:OE1	2.50	0.58
1:A:470:TYR:O	1:A:481:HIS:HE1	1.87	0.58
1:B:37[B]:GLN:HE21	1:B:38:VAL:N	2.01	0.58
1:A:662[B]:THR:HG22	1:A:712:HIS:CD2	2.33	0.58
1:A:38:VAL:CG1	1:A:42:GLY:HA2	2.34	0.58
1:B:366:HIS:CD2	1:B:417:ASP:OD2	2.49	0.57
1:A:491:LEU:HG	1:A:495:LYS:HD2	1.87	0.57
1:A:662[B]:THR:CG2	1:A:712:HIS:HD2	2.16	0.57
1:A:331:TRP:CE2	1:A:335:ILE:HG13	2.40	0.56
1:A:507:HIS:HD2	2:A:1727:CTS:O2	1.88	0.56
1:A:181:HIS:CE1	1:A:235:THR:HG22	2.40	0.56
1:A:169:LYS:O	1:A:170[A]:GLU:HG2	2.06	0.56
1:B:391:GLU:HG2	1:B:437:HIS:CD2	2.41	0.56
1:B:51:LYS:NZ	1:B:295:ASP:OD2	2.31	0.56
1:B:562:GLY:N	1:B:586:GLN:HE21	2.03	0.56
1:B:37[B]:GLN:NE2	1:B:37[B]:GLN:CA	2.66	0.55
1:A:181:HIS:HD2	1:A:233[B]:MET:CE	2.18	0.55
1:B:229[A]:THR:CG2	1:B:244:HIS:HA	2.37	0.54
1:A:534:GLU:HB3	1:A:579:VAL:HG22	1.90	0.54
1:B:230:ALA:HB2	1:B:244:HIS:CG	2.42	0.54
1:B:101:THR:O	1:B:102:GLN:HG3	2.07	0.54
1:A:101:THR:C	1:A:102:GLN:HG3	2.29	0.53
1:A:105:THR:HG23	1:A:125:ASN:OD1	2.09	0.52
1:A:232:MET:HE3	1:A:240:TYR:HB3	1.92	0.52
1:A:539:ASN:O	1:A:580[B]:ARG:HG3	2.10	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:631:GLU:OE2	1:B:661:HIS:NE2	2.31	0.51
1:B:685:LYS:O	1:B:686:ASP:HB2	2.09	0.51
1:A:331:TRP:CZ2	1:A:335:ILE:HG13	2.44	0.51
1:A:89:LYS:HD3	5:A:2118:HOH:O	2.08	0.51
1:B:191:ASP:OD1	1:B:481:HIS:HD2	1.93	0.51
1:B:534:GLU:HA	1:B:538:GLY:HA2	1.91	0.51
1:B:49:THR:HA	1:B:53:LYS:O	2.11	0.51
1:A:45:THR:HG22	1:A:60:THR:HG22	1.92	0.51
1:B:298:ARG:HD2	1:B:629:TYR:O	2.10	0.50
1:B:242:ASN:HB3	1:B:292:ILE:HB	1.92	0.50
1:A:548:PRO:HA	1:A:552[A]:LEU:HB2	1.94	0.50
1:A:311:GLU:HA	1:A:311:GLU:OE1	2.11	0.49
1:B:229[A]:THR:HG22	1:B:244:HIS:ND1	2.26	0.49
1:B:437:HIS:HD2	5:B:2326:HOH:O	1.95	0.49
1:A:177:MET:SD	1:A:233[B]:MET:HE2	2.53	0.49
1:A:101:THR:O	1:A:102:GLN:HG3	2.13	0.49
1:A:678:ALA:HA	1:A:722:SER:O	2.12	0.49
1:B:229[B]:THR:HB	1:B:230:ALA:HA	1.94	0.48
1:B:563:ILE:H	1:B:586:GLN:HE21	1.61	0.48
1:A:109[A]:THR:CG2	1:A:119:GLU:CG	2.82	0.48
1:B:692:ASN:HD21	1:B:695:ALA:HB2	1.78	0.48
1:A:244:HIS:HE1	1:A:553:VAL:O	1.97	0.48
1:A:109[A]:THR:HG22	1:A:119:GLU:CG	2.45	0.47
1:B:369:ASN:ND2	1:B:372:ASN:H	2.13	0.47
1:B:229[A]:THR:HG23	1:B:230:ALA:HA	1.97	0.47
1:A:110:TRP:HE1	1:A:308:ASN:HD21	1.63	0.47
1:B:391:GLU:HG2	1:B:437:HIS:CG	2.50	0.46
1:B:434[A]:MET:HE2	1:B:434[A]:MET:HA	1.97	0.46
1:B:314:LYS:HE2	1:B:518:THR:CG2	2.45	0.46
1:B:51:LYS:O	1:B:52:ASN:HB2	2.15	0.46
1:A:683:ASP:HB3	1:A:687:ALA:HB3	1.97	0.46
1:B:110:TRP:HE1	1:B:308:ASN:HD21	1.62	0.45
1:B:725:GLU:HG3	1:B:726:VAL:N	2.32	0.45
1:A:229:THR:OG1	1:A:244:HIS:HD2	1.99	0.45
1:A:244:HIS:CE1	1:A:553:VAL:O	2.69	0.45
1:B:365:LYS:HE2	5:B:2301:HOH:O	2.16	0.45
1:A:581:SER:HB2	5:A:2563:HOH:O	2.16	0.45
1:A:565:GLU:OE1	1:A:609[B]:ARG:NH2	2.50	0.45
1:B:670:LEU:HB3	1:B:676:TYR:CE2	2.51	0.45
1:B:654:CYS:O	1:B:718:GLY:HA3	2.18	0.44
1:A:62:GLY:C	1:A:63[A]:LEU:HD23	2.37	0.44
1:B:366:HIS:CE1	1:B:392:GLY:O	2.66	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:563:ILE:O	1:B:586:GLN:HG3	2.18	0.44
1:A:366:HIS:HE1	1:A:392:GLY:O	2.01	0.44
1:A:43:ALA:O	1:A:45:THR:HG23	2.18	0.44
1:A:703:LEU:HD22	1:A:707:SER:CB	2.48	0.43
1:B:571:MET:HG2	5:B:2487:HOH:O	2.18	0.43
1:B:566:THR:HB	1:B:579:VAL:HB	2.00	0.43
1:B:668:ASP:OD1	1:B:668:ASP:N	2.52	0.43
1:B:57:LYS:O	1:B:58:PRO:C	2.57	0.43
1:B:562:GLY:N	1:B:586:GLN:NE2	2.61	0.42
1:B:331:TRP:HA	1:B:334:MET:HE2	2.00	0.42
1:B:532:GLU:O	1:B:535[B]:SER:OG	2.36	0.42
1:B:549:PHE:CZ	1:B:634:PRO:HD3	2.53	0.42
1:B:188:GLY:HA3	1:B:222:PHE:CE2	2.55	0.42
1:A:109[A]:THR:HG21	1:A:119:GLU:CG	2.40	0.42
1:B:24:LYS:CG	1:B:35:THR:HG22	2.50	0.42
1:A:537:GLY:O	1:A:580[B]:ARG:NH2	2.53	0.42
1:B:434[A]:MET:CE	1:B:434[A]:MET:HA	2.50	0.42
1:B:539:ASN:O	1:B:580:ARG:HG2	2.20	0.42
1:A:188:GLY:HA3	1:A:222:PHE:CE2	2.54	0.42
1:B:274:LYS:HD3	5:B:2230:HOH:O	2.18	0.42
1:B:149:ASP:OD1	1:B:149:ASP:N	2.53	0.42
1:B:520:PRO:HB3	4:B:1729:EDO:H11	2.01	0.42
1:B:111:GLN:HA	1:B:112:PRO:HD2	1.93	0.42
1:B:244:HIS:CG	1:B:245:GLU:H	2.37	0.41
1:A:68:GLU:OE1	1:A:89:LYS:NZ	2.51	0.41
1:A:91:ASN:OD1	1:A:91:ASN:C	2.58	0.41
1:A:211:GLU:CG	5:A:2199:HOH:O	2.44	0.41
1:B:453:LYS:HB3	1:B:453:LYS:HE2	1.52	0.41
1:A:612:ASP:OD1	1:A:613:ALA:N	2.53	0.41
1:B:507:HIS:CG	1:B:526:GLU:HB2	2.56	0.41
1:A:244:HIS:CD2	1:A:245:GLU:H	2.38	0.41
1:B:234:LYS:NZ	5:B:2191:HOH:O	2.35	0.41
1:B:470:TYR:OH	1:B:489:HIS:CE1	2.64	0.41
1:A:671:THR:HG21	1:A:674:LYS:HE3	2.03	0.41
1:B:692:ASN:ND2	1:B:695:ALA:HB2	2.36	0.41
1:A:563:ILE:O	1:A:586:GLN:HG3	2.20	0.41
1:B:251:TYR:CG	1:B:287:PRO:HD3	2.56	0.41
1:A:654:CYS:HB2	1:A:719:TYR:CZ	2.56	0.41
1:A:569:ASN:HA	1:A:572:ASN:O	2.21	0.41
1:A:170[C]:GLU:HG3	1:A:171:GLU:O	2.21	0.41
1:B:124:TYR:CE1	1:B:145:ARG:HD3	2.56	0.41
1:B:422:GLU:OE1	1:B:425:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:43:ALA:HA	1:A:44:PRO:HD3	1.95	0.40
1:A:298:ARG:HD2	1:A:629:TYR:O	2.21	0.40
1:A:181:HIS:CD2	1:A:233[B]:MET:CE	3.03	0.40
1:A:170[B]:GLU:CD	1:A:277:LYS:HZ2	2.25	0.40
1:A:623:ASP:OD2	1:A:645[A]:LYS:CE	2.68	0.40
1:A:62:GLY:C	1:A:63[A]:LEU:CD2	2.90	0.40
1:A:327:TYR:CZ	1:A:599:MET:HB2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:A:2051:HOH:O	5:B:2363:HOH:O[2_556]	2.07	0.13

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	705/727 (97%)	676 (96%)	29 (4%)	0	100	100
1	B	691/727 (95%)	661 (96%)	29 (4%)	1 (0%)	59	55
All	All	1396/1454 (96%)	1337 (96%)	58 (4%)	1 (0%)	59	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	331	TRP

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	608/627 (97%)	597 (98%)	11 (2%)	71	73
1	B	589/627 (94%)	571 (97%)	18 (3%)	52	49
All	All	1197/1254 (96%)	1168 (98%)	29 (2%)	66	61

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57[A]	LYS
1	A	57[B]	LYS
1	A	63[A]	LEU
1	A	63[B]	LEU
1	A	87	ASP
1	A	210	LYS
1	A	262	ASN
1	A	511	ARG
1	A	542	TYR
1	A	585	ARG
1	A	686	ASP
1	B	26	THR
1	B	37[A]	GLN
1	B	37[B]	GLN
1	B	68	GLU
1	B	100	ASP
1	B	162	SER
1	B	210	LYS
1	B	229[A]	THR
1	B	229[B]	THR
1	B	365	LYS
1	B	430	LYS
1	B	511	ARG
1	B	542	TYR
1	B	560	THR
1	B	565	GLU
1	B	668	ASP
1	B	709	LEU
1	B	725	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN

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Mol	Chain	Res	Type
1	A	159	GLN
1	A	181	HIS
1	A	219	GLN
1	A	244	HIS
1	A	262	ASN
1	A	308	ASN
1	A	366	HIS
1	A	369	ASN
1	A	473	ASN
1	A	481	HIS
1	A	489	HIS
1	A	507	HIS
1	A	525	ASN
1	A	712	HIS
1	B	31	ASN
1	B	111	GLN
1	B	123	HIS
1	B	133	GLN
1	B	136	ASN
1	B	159	GLN
1	B	164	ASN
1	B	219	GLN
1	B	255	HIS
1	B	281	GLN
1	B	308	ASN
1	B	366	HIS
1	B	369	ASN
1	B	437	HIS
1	B	461	ASN
1	B	473	ASN
1	B	481	HIS
1	B	489	HIS
1	B	507	HIS
1	B	525	ASN
1	B	586	GLN
1	B	692	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	CTS	A	1727	3	14,14,14	1.03	1 (7%)	21,21,21	2.03	7 (33%)
4	EDO	A	1729	-	3,3,3	0.44	0	2,2,2	0.52	0
4	EDO	A	1730	-	3,3,3	0.60	0	2,2,2	0.17	0
2	CTS	B	1727	3	14,14,14	0.55	0	21,21,21	2.22	7 (33%)
4	EDO	B	1729	-	3,3,3	0.67	0	2,2,2	0.56	0
4	EDO	B	1730	-	3,3,3	0.58	0	2,2,2	0.53	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CTS	A	1727	3	-	0/0/29/29	0/0/2/2
4	EDO	A	1729	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1730	-	-	0/1/1/1	0/0/0/0
2	CTS	B	1727	3	-	0/0/29/29	0/0/2/2
4	EDO	B	1729	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1730	-	-	0/1/1/1	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1727	CTS	C6-C5	-2.42	1.51	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1727	CTS	C7-C6-C5	-5.54	97.49	102.63
2	B	1727	CTS	C1-N-C5	5.19	124.53	112.05
2	A	1727	CTS	C1-N-C5	4.43	122.71	112.05
2	A	1727	CTS	C8-N-C1	3.23	124.58	113.17
2	B	1727	CTS	C8-N-C1	3.10	124.14	113.17
2	B	1727	CTS	C2-C3-C4	-3.01	105.56	110.89
2	A	1727	CTS	C6-C5-N	-2.91	101.08	104.67
2	A	1727	CTS	O2-C2-C1	-2.63	104.29	109.41
2	A	1727	CTS	O2-C2-C3	2.49	115.07	110.23
2	B	1727	CTS	C6-C5-N	-2.43	101.67	104.67
2	A	1727	CTS	C2-C3-C4	-2.38	106.67	110.89
2	B	1727	CTS	C1-C2-C3	-2.27	107.53	110.14
2	A	1727	CTS	C2-C1-N	2.13	114.27	110.63
2	B	1727	CTS	O3-C3-C2	-2.07	106.28	110.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	687/727 (94%)	-0.30	2 (0%) 91 93	18, 30, 43, 52	0
1	B	687/727 (94%)	-0.26	3 (0%) 90 91	19, 31, 48, 58	0
All	All	1374/1454 (94%)	-0.28	5 (0%) 90 91	18, 30, 45, 58	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	87	ASP	2.6
1	B	673	GLY	2.2
1	A	40	SER	2.1
1	A	726	VAL	2.0
1	B	52	ASN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	EDO	A	1729	4/4	0.15	2.77	26,33,33,34	0
4	EDO	B	1729	4/4	0.10	0.27	31,32,33,36	0
2	CTS	A	1727	13/13	0.08	-0.03	28,31,33,34	0
4	EDO	A	1730	4/4	0.10	-0.04	32,33,34,35	0
2	CTS	B	1727	13/13	0.06	-0.75	25,28,31,31	0
3	CA	A	1728	1/1	0.07	-0.99	26,26,26,26	0
4	EDO	B	1730	4/4	0.05	-1.80	30,30,32,32	0
3	CA	B	1728	1/1	0.05	-2.64	24,24,24,24	0

6.5 Other polymers

There are no such residues in this entry.