



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 25, 2025 – 12:16 pm GMT

PDB ID : 9EU2
Title : GH29A alpha-L-fucosidase
Authors : Yang, Y.Y.; Zeuner, B.; Morth, J.P.
Deposited on : 2024-03-27
Resolution : 1.84 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

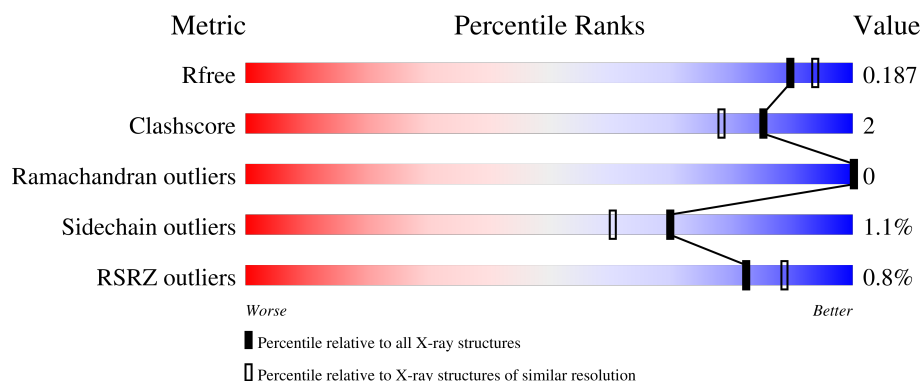
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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}	164625	1150 (1.84-1.84)
Clashscore	180529	1248 (1.84-1.84)
Ramachandran outliers	177936	1240 (1.84-1.84)
Sidechain outliers	177891	1240 (1.84-1.84)
RSRZ outliers	164620	1149 (1.84-1.84)

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	435	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> % 92% 5% . </div> </div>
1	B	435	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 99%, yellow 1%, orange 1%, red 1%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> 90% 6% . </div> </div>
1	C	435	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> % 92% 5% . </div> </div>
1	D	435	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 99%, yellow 1%, orange 1%, red 1%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> 91% 5% . </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28870 atoms, of which 13349 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-L-fucosidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	422	Total	C	H	N	O	S	0	2	0
			6739	2182	3323	586	633	15			
1	B	420	Total	C	H	N	O	S	0	1	0
			6688	2170	3292	582	629	15			
1	C	425	Total	C	H	N	O	S	0	2	0
			6782	2196	3346	589	636	15			
1	D	421	Total	C	H	N	O	S	0	3	0
			6741	2184	3322	586	633	16			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP G8UMQ6
A	447	LEU	-	expression tag	UNP G8UMQ6
A	448	GLU	-	expression tag	UNP G8UMQ6
A	449	HIS	-	expression tag	UNP G8UMQ6
A	450	HIS	-	expression tag	UNP G8UMQ6
A	451	HIS	-	expression tag	UNP G8UMQ6
A	452	HIS	-	expression tag	UNP G8UMQ6
A	453	HIS	-	expression tag	UNP G8UMQ6
A	454	HIS	-	expression tag	UNP G8UMQ6
B	20	MET	-	initiating methionine	UNP G8UMQ6
B	447	LEU	-	expression tag	UNP G8UMQ6
B	448	GLU	-	expression tag	UNP G8UMQ6
B	449	HIS	-	expression tag	UNP G8UMQ6
B	450	HIS	-	expression tag	UNP G8UMQ6
B	451	HIS	-	expression tag	UNP G8UMQ6
B	452	HIS	-	expression tag	UNP G8UMQ6
B	453	HIS	-	expression tag	UNP G8UMQ6
B	454	HIS	-	expression tag	UNP G8UMQ6
C	20	MET	-	initiating methionine	UNP G8UMQ6
C	447	LEU	-	expression tag	UNP G8UMQ6
C	448	GLU	-	expression tag	UNP G8UMQ6

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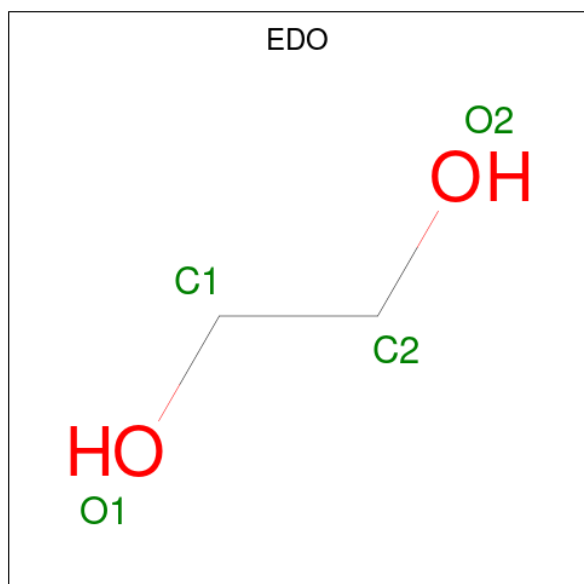
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Chain	Residue	Modelled	Actual	Comment	Reference
C	449	HIS	-	expression tag	UNP G8UMQ6
C	450	HIS	-	expression tag	UNP G8UMQ6
C	451	HIS	-	expression tag	UNP G8UMQ6
C	452	HIS	-	expression tag	UNP G8UMQ6
C	453	HIS	-	expression tag	UNP G8UMQ6
C	454	HIS	-	expression tag	UNP G8UMQ6
D	20	MET	-	initiating methionine	UNP G8UMQ6
D	447	LEU	-	expression tag	UNP G8UMQ6
D	448	GLU	-	expression tag	UNP G8UMQ6
D	449	HIS	-	expression tag	UNP G8UMQ6
D	450	HIS	-	expression tag	UNP G8UMQ6
D	451	HIS	-	expression tag	UNP G8UMQ6
D	452	HIS	-	expression tag	UNP G8UMQ6
D	453	HIS	-	expression tag	UNP G8UMQ6
D	454	HIS	-	expression tag	UNP G8UMQ6

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 10 2 6 2	0	0
3	A	1	Total C H O 10 2 6 2	0	0
3	A	1	Total C H O 10 2 6 2	0	0
3	B	1	Total C H O 10 2 6 2	0	0
3	B	1	Total C H O 10 2 6 2	0	0
3	C	1	Total C H O 10 2 6 2	0	0
3	C	1	Total C H O 10 2 6 2	0	0
3	C	1	Total C H O 10 2 6 2	0	0
3	D	1	Total C H O 10 2 6 2	0	0
3	D	1	Total C H O 10 2 6 2	0	0
3	D	1	Total C H O 10 2 6 2	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Na 1 1	0	0

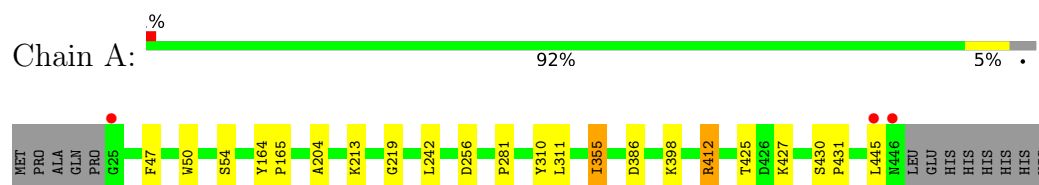
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	450	Total O 450 450	0	0
5	B	410	Total O 410 410	0	0
5	C	508	Total O 508 508	0	0
5	D	438	Total O 438 438	0	0

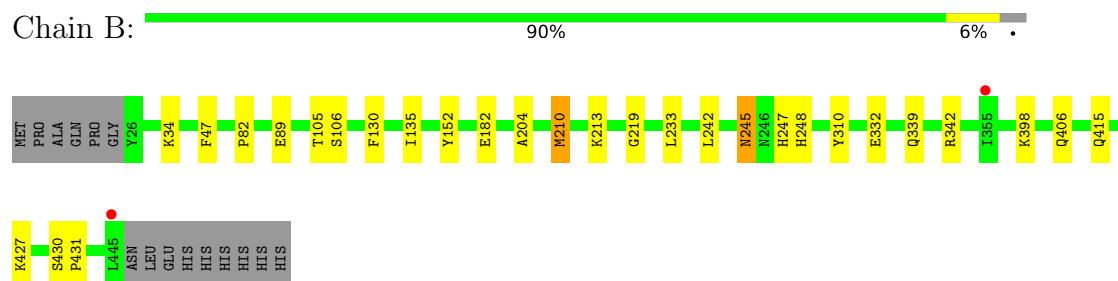
3 Residue-property plots [i](#)

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.

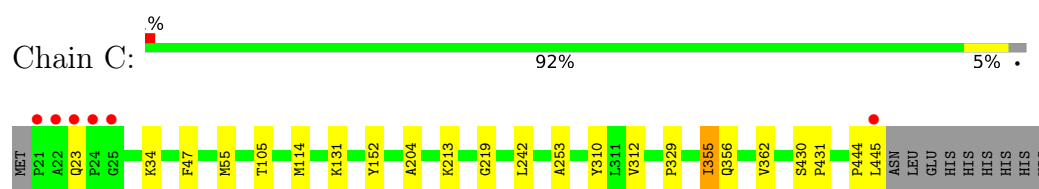
- Molecule 1: Alpha-L-fucosidase



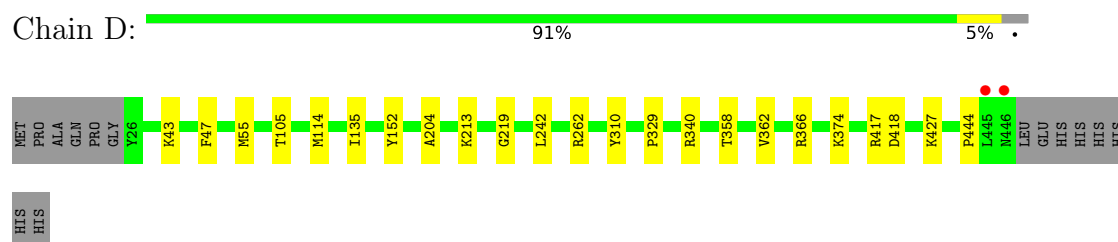
- Molecule 1: Alpha-L-fucosidase



- Molecule 1: Alpha-L-fucosidase



- Molecule 1: Alpha-L-fucosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.91Å 147.91Å 197.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.02 – 1.84 47.02 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.02-1.84) 90.7 (47.02-1.84)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.92 (at 1.84Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.162 , 0.188 0.162 , 0.187	Depositor DCC
R_{free} test set	213058 reflections (0.93%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	28870	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.20 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.2893e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

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

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	0.35	0/3507	0.65	1/4757 (0.0%)
1	B	0.34	0/3487	0.62	0/4730
1	C	0.36	0/3529	0.65	1/4788 (0.0%)
1	D	0.35	0/3510	0.62	0/4761
All	All	0.35	0/14033	0.64	2/19036 (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	D	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	C	114	MET	CG-SD-CE	-5.24	91.81	100.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	262	ARG	Sidechain
1	D	340	ARG	Sidechain
1	D	366	ARG	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	3416	3323	3320	13	0
1	B	3396	3292	3301	18	0
1	C	3436	3346	3342	14	0
1	D	3419	3322	3324	13	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	12	18	18	0	0
3	B	8	12	12	0	0
3	C	12	18	18	0	0
3	D	12	18	18	0	0
4	C	1	0	0	0	0
5	A	450	0	0	2	0
5	B	410	0	0	3	0
5	C	508	0	0	3	0
5	D	438	0	0	5	0
All	All	15521	13349	13353	58	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 2.

All (58) 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:D:418:ASP:OD1	5:D:601:HOH:O	1.83	0.96
1:D:417:ARG:NH2	5:D:601:HOH:O	2.06	0.87
1:C:312:VAL:HG22	1:C:355[B]:ILE:HD11	1.56	0.87
1:D:417:ARG:CZ	5:D:601:HOH:O	2.43	0.61
1:A:386:ASP:O	1:A:427:LYS:HD2	2.01	0.61
1:D:43:LYS:NZ	1:D:358:THR:O	2.38	0.56
1:C:355[A]:ILE:HG13	1:C:356:GLN:N	2.21	0.56
1:B:406:GLN:NE2	5:B:604:HOH:O	2.27	0.56
1:B:332:GLU:OE1	5:B:601:HOH:O	2.18	0.54
1:C:34:LYS:HD2	5:C:986:HOH:O	2.06	0.54
1:B:210:MET:CE	1:B:245:ASN:OD1	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LEU:HD21	1:A:355[A]:ILE:HD11	1.91	0.53
1:A:412:ARG:NH2	5:D:601:HOH:O	2.39	0.53
1:A:445:LEU:HD11	5:A:913:HOH:O	2.10	0.51
1:B:210:MET:HE3	1:B:245:ASN:OD1	2.11	0.51
1:D:374:LYS:NZ	5:D:603:HOH:O	2.36	0.49
1:B:89:GLU:OE2	5:B:602:HOH:O	2.19	0.49
1:A:430:SER:HB3	1:A:431:PRO:HA	1.95	0.49
1:B:182:GLU:H	1:B:182:GLU:CD	2.17	0.48
1:C:312:VAL:HG22	1:C:355[B]:ILE:CD1	2.38	0.47
1:C:23:GLN:HB3	1:C:253:ALA:HA	1.96	0.47
1:C:213:LYS:O	1:C:219:GLY:HA3	2.15	0.47
1:B:213:LYS:O	1:B:219:GLY:HA3	2.14	0.47
1:A:164:TYR:CD1	1:A:165:PRO:HA	2.50	0.47
1:C:204:ALA:HA	1:C:242:LEU:O	2.15	0.46
1:C:362:VAL:HG11	1:C:444:PRO:HD2	1.96	0.46
1:B:82:PRO:HD2	1:B:130:PHE:CD1	2.51	0.46
1:A:50:TRP:HD1	1:A:54[A]:SER:HG	1.63	0.46
1:A:311:LEU:HD21	1:A:355[A]:ILE:CD1	2.45	0.46
1:C:105:THR:HA	1:C:152:TYR:HB3	1.98	0.45
1:B:233:LEU:C	1:B:233:LEU:HD23	2.36	0.45
1:B:82:PRO:HD2	1:B:130:PHE:CG	2.52	0.45
1:A:213:LYS:O	1:A:219:GLY:HA3	2.17	0.45
1:D:55[B]:MET:HA	1:D:329:PRO:HB3	1.98	0.44
1:A:204:ALA:HA	1:A:242:LEU:O	2.17	0.44
1:C:445:LEU:HD21	5:C:830:HOH:O	2.18	0.44
1:C:55:MET:HA	1:C:329:PRO:HB3	2.00	0.43
1:D:362:VAL:HG11	1:D:444:PRO:HD2	2.00	0.43
1:B:247:HIS:O	1:B:248:HIS:HB2	2.18	0.43
1:D:204:ALA:HA	1:D:242:LEU:O	2.18	0.43
1:D:114:MET:O	1:D:135:ILE:HG12	2.18	0.42
1:B:106:SER:HA	1:B:135:ILE:HD11	2.01	0.42
1:C:329:PRO:HB2	5:C:602:HOH:O	2.19	0.42
1:D:55[A]:MET:HA	1:D:329:PRO:HB3	2.01	0.42
1:D:105:THR:HA	1:D:152:TYR:HB3	2.01	0.42
1:B:398:LYS:HD2	1:B:415:GLN:OE1	2.19	0.42
1:D:213:LYS:O	1:D:219:GLY:HA3	2.19	0.42
1:B:204:ALA:HA	1:B:242:LEU:O	2.20	0.42
1:D:417:ARG:NH1	1:D:417:ARG:HG2	2.35	0.41
1:A:256:ASP:O	1:A:281:PRO:HD2	2.20	0.41
1:B:105:THR:HA	1:B:152:TYR:HB3	2.03	0.41
1:B:339:GLN:HG3	1:B:342:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:LYS:HA	1:A:398:LYS:HD2	1.97	0.41
1:B:245:ASN:HD22	1:B:245:ASN:C	2.24	0.41
1:B:430:SER:HB3	1:B:431:PRO:HA	2.03	0.41
1:C:430:SER:HB3	1:C:431:PRO:HA	2.01	0.41
1:A:425:THR:HG21	5:A:945:HOH:O	2.22	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	422/435 (97%)	410 (97%)	12 (3%)	0	100	100
1	B	419/435 (96%)	408 (97%)	11 (3%)	0	100	100
1	C	425/435 (98%)	412 (97%)	13 (3%)	0	100	100
1	D	422/435 (97%)	411 (97%)	11 (3%)	0	100	100
All	All	1688/1740 (97%)	1641 (97%)	47 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	359/369 (97%)	355 (99%)	4 (1%)	70	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	357/369 (97%)	351 (98%)	6 (2%)	56 41
1	C	361/369 (98%)	356 (99%)	5 (1%)	62 50
1	D	360/369 (98%)	357 (99%)	3 (1%)	79 72
All	All	1437/1476 (97%)	1419 (99%)	18 (1%)	70 53

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	PHE
1	A	310	TYR
1	A	355[A]	ILE
1	A	355[B]	ILE
1	B	34	LYS
1	B	47	PHE
1	B	210	MET
1	B	245	ASN
1	B	310	TYR
1	B	427	LYS
1	C	47	PHE
1	C	131	LYS
1	C	310	TYR
1	C	355[A]	ILE
1	C	355[B]	ILE
1	D	47	PHE
1	D	310	TYR
1	D	427	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	136	HIS
1	B	248	HIS

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	$\# Z > 2$
3	EDO	B	502	-	3,3,3	0.45	0	2,2,2	0.73	0
3	EDO	D	503	-	3,3,3	0.48	0	2,2,2	0.21	0
3	EDO	C	502	-	3,3,3	0.51	0	2,2,2	0.12	0
3	EDO	A	502	-	3,3,3	0.49	0	2,2,2	0.25	0
3	EDO	D	504	-	3,3,3	0.49	0	2,2,2	0.32	0
3	EDO	B	501	-	3,3,3	0.54	0	2,2,2	0.41	0
3	EDO	D	502	-	3,3,3	0.50	0	2,2,2	0.13	0
3	EDO	C	504	-	3,3,3	0.46	0	2,2,2	0.61	0
3	EDO	A	503	-	3,3,3	0.51	0	2,2,2	0.09	0
3	EDO	A	504	-	3,3,3	0.64	0	2,2,2	0.26	0
3	EDO	C	503	-	3,3,3	0.51	0	2,2,2	0.25	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
3	EDO	B	502	-	-	0/1/1/1	-
3	EDO	D	503	-	-	1/1/1/1	-
3	EDO	C	502	-	-	0/1/1/1	-
3	EDO	A	502	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	504	-	-	0/1/1/1	-
3	EDO	B	501	-	-	1/1/1/1	-
3	EDO	D	502	-	-	1/1/1/1	-
3	EDO	C	504	-	-	1/1/1/1	-
3	EDO	A	503	-	-	0/1/1/1	-
3	EDO	A	504	-	-	1/1/1/1	-
3	EDO	C	503	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	503	EDO	O1-C1-C2-O2
3	B	501	EDO	O1-C1-C2-O2
3	A	504	EDO	O1-C1-C2-O2
3	D	502	EDO	O1-C1-C2-O2
3	C	504	EDO	O1-C1-C2-O2

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	422/435 (97%)	-0.60	3 (0%) 84 90	15, 36, 55, 112	2 (0%)
1	B	420/435 (96%)	-0.49	2 (0%) 87 92	18, 39, 62, 79	1 (0%)
1	C	425/435 (97%)	-0.69	6 (1%) 73 80	14, 31, 48, 173	2 (0%)
1	D	421/435 (96%)	-0.58	2 (0%) 87 92	17, 37, 56, 118	3 (0%)
All	All	1688/1740 (97%)	-0.59	13 (0%) 82 89	14, 36, 58, 173	8 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	22	ALA	9.7
1	C	24	PRO	8.2
1	B	445	LEU	6.5
1	C	23	GLN	6.4
1	C	21	PRO	5.5
1	D	446	ASN	4.9
1	C	445	LEU	4.4
1	D	445	LEU	4.4
1	A	446	ASN	4.3
1	C	25	GLY	3.8
1	A	25	GLY	3.4
1	A	445	LEU	3.2
1	B	355	ILE	2.2

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, 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(\AA^2)	Q<0.9
2	ZN	D	501	1/1	0.39	0.23	249,249,249,249	0
2	ZN	C	501	1/1	0.57	0.26	173,173,173,173	0
3	EDO	A	503	4/4	0.79	0.18	41,56,68,68	0
3	EDO	D	503	4/4	0.92	0.10	43,52,56,56	0
3	EDO	C	504	4/4	0.93	0.08	41,49,54,54	0
3	EDO	A	504	4/4	0.94	0.10	37,44,49,49	0
3	EDO	D	504	4/4	0.94	0.09	39,47,55,59	0
3	EDO	D	502	4/4	0.95	0.07	32,38,43,46	0
3	EDO	A	502	4/4	0.96	0.08	31,38,42,46	0
3	EDO	B	501	4/4	0.96	0.08	37,45,48,49	0
3	EDO	B	502	4/4	0.97	0.06	32,39,43,47	0
3	EDO	C	502	4/4	0.97	0.07	30,36,40,42	0
4	NA	C	505	1/1	0.97	0.07	43,43,43,43	0
3	EDO	C	503	4/4	0.99	0.04	29,35,41,44	0
2	ZN	A	501	1/1	1.00	0.04	28,28,28,28	1

6.5 Other polymers [i](#)

There are no such residues in this entry.