



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:20 PM GMT

PDB ID : 1JUH
Title : Crystal Structure of Quercetin 2,3-dioxygenase
Authors : Fusetti, F.; Schroeter, K.H.; Steiner, R.A.; Dijkstra, B.W.
Deposited on : 2001-08-24
Resolution : 1.60 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

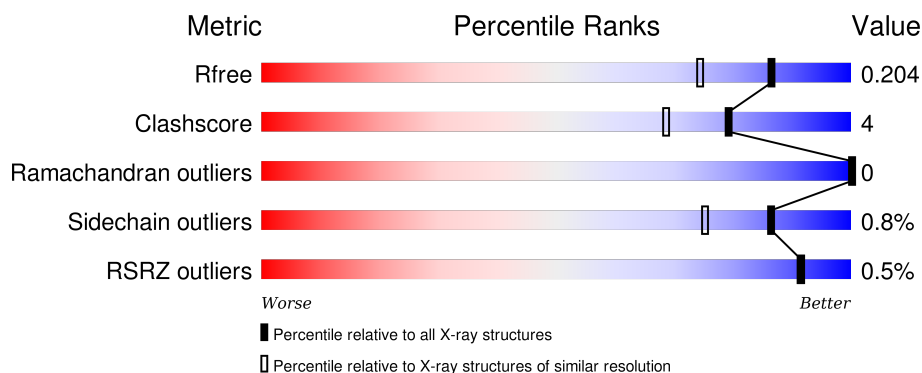
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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}	91344	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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. 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	350	<div> <div>86%</div> <div>9% 5%</div> </div>
1	B	350	<div> <div>91%</div> <div>6% •</div> </div>
1	C	350	<div> <div>91%</div> <div>• 5%</div> </div>
1	D	350	<div> <div>87%</div> <div>8% 6%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	509	-	-	-	X
2	NAG	C	514	-	-	-	X
2	NAG	D	520	-	-	-	X
4	NAG	B	508	-	-	-	X
4	NAG	C	512	-	-	-	X
4	NAG	C	513	-	-	-	X
5	NAG	D	517	-	-	-	X
5	NAG	D	518	-	-	-	X
7	EDO	A	2007	-	-	-	X
7	EDO	A	2009	-	-	-	X
7	EDO	A	2015	-	-	-	X
7	EDO	A	2024	-	-	-	X
7	EDO	A	2028	-	-	-	X
7	EDO	B	2008	-	-	-	X
7	EDO	B	2011	-	-	-	X
7	EDO	B	2013	-	-	-	X
7	EDO	B	2016	-	-	-	X
7	EDO	B	2021	-	-	-	X
7	EDO	B	2033	-	-	-	X
7	EDO	C	2005	-	-	-	X
7	EDO	C	2017	-	-	-	X
7	EDO	C	2022	-	-	X	X
7	EDO	C	2029	-	-	-	X
7	EDO	C	2031	-	-	-	X
7	EDO	D	2012	-	-	-	X
7	EDO	D	2018	-	-	-	X
7	EDO	D	2030	-	-	-	X
7	EDO	D	2034	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12719 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 quercetin 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	11	0
			2613	1664	422	522	5			
1	B	339	Total	C	N	O	S	0	10	0
			2639	1678	425	531	5			
1	C	334	Total	C	N	O	S	0	9	0
			2604	1659	419	521	5			
1	D	330	Total	C	N	O	S	0	9	0
			2579	1644	416	514	5			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 4 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	4	Total	C	N	O	0	0
			50	28	2	20		
4	C	4	Total	C	N	O	0	0
			50	28	2	20		

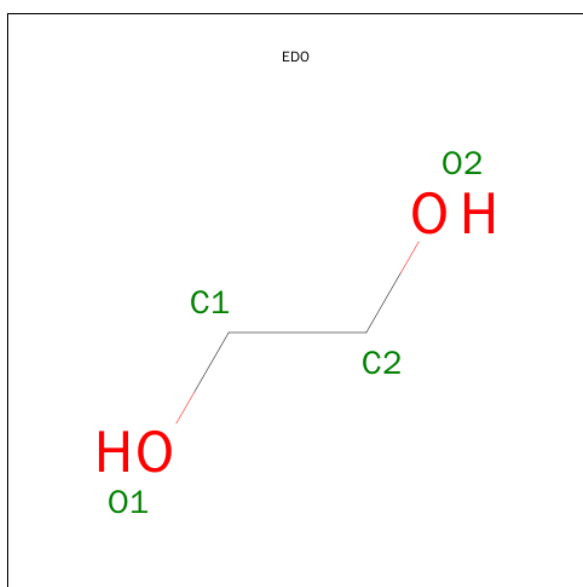
- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cu	0	0
			1	1		
6	A	1	Total	Cu	0	0
			1	1		
6	D	1	Total	Cu	0	0
			1	1		
6	C	1	Total	Cu	0	0
			1	1		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

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

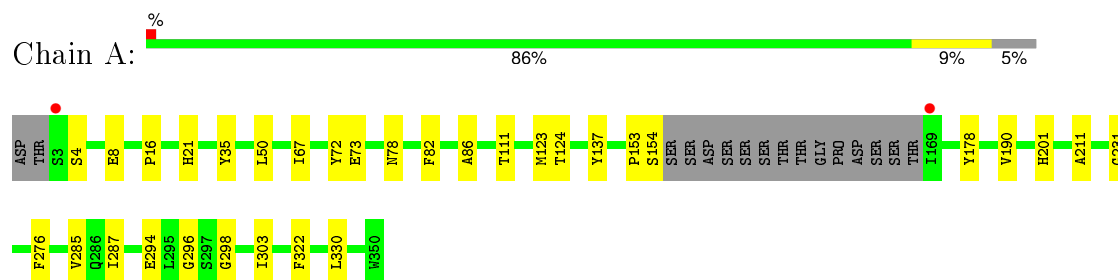
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	457	Total O 459 459	0	2
8	B	425	Total O 426 426	0	1
8	C	439	Total O 440 440	0	1
8	D	433	Total O 434 434	0	1

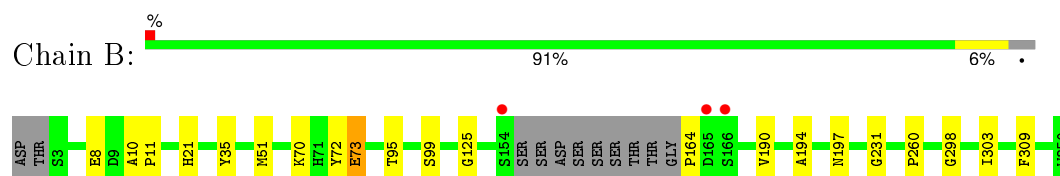
3 Residue-property plots [i](#)

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.

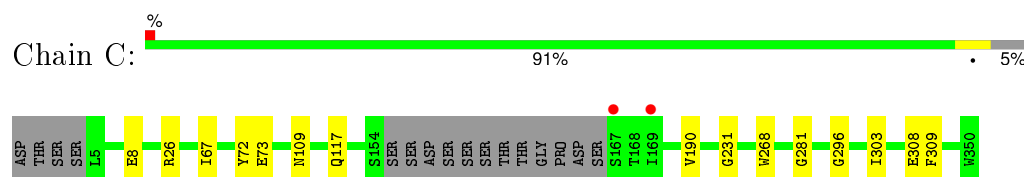
- Molecule 1: quercetin 2,3-dioxygenase



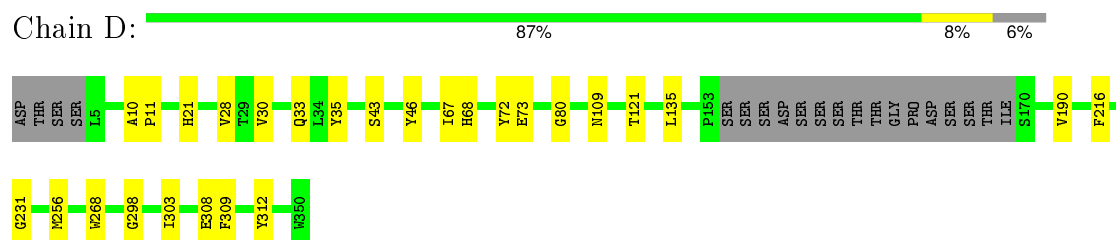
- Molecule 1: quercetin 2,3-dioxygenase



- Molecule 1: quercetin 2,3-dioxygenase



- Molecule 1: quercetin 2,3-dioxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	108.55Å 55.78Å 123.68Å 90.00° 98.31° 90.00°	Depositor
Resolution (Å)	87.20 – 1.60 87.22 – 1.50	Depositor EDS
% Data completeness (in resolution range)	95.1 (87.20-1.60) 94.3 (87.22-1.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 1.50Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.162 , 0.189 0.179 , 0.204	Depositor DCC
R_{free} test set	19549 reflections (10.62%)	DCC
Wilson B-factor (Å ²)	15.7	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 221185 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12719	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MAN, BMA, NAG, CU, 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	0.51	0/2736	0.72	1/3750 (0.0%)
1	B	0.48	0/2758	0.71	2/3781 (0.1%)
1	C	0.48	0/2719	0.69	1/3727 (0.0%)
1	D	0.47	0/2694	0.70	1/3692 (0.0%)
All	All	0.48	0/10907	0.71	5/14950 (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	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	231	GLY	N-CA-C	-6.26	97.46	113.10
1	B	164	PRO	N-CA-CB	5.51	109.92	103.30
1	C	231	GLY	N-CA-C	-5.46	99.46	113.10
1	B	231	GLY	N-CA-C	-5.16	100.19	113.10
1	D	231	GLY	N-CA-C	-5.14	100.25	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	46	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	2613	0	2413	24	0
1	B	2639	0	2431	14	0
1	C	2604	0	2409	13	0
1	D	2579	0	2382	16	0
2	A	56	0	52	0	0
2	B	42	0	39	2	0
2	C	42	0	39	0	0
2	D	42	0	39	0	0
3	A	83	0	70	2	0
4	B	50	0	43	2	0
4	C	50	0	43	1	0
5	D	28	0	25	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	36	0	54	3	0
7	B	32	0	48	8	0
7	C	40	0	60	12	0
7	D	20	0	30	3	0
8	A	459	0	0	7	0
8	B	426	0	0	3	0
8	C	440	0	0	2	0
8	D	434	0	0	1	0
All	All	12719	0	10177	75	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 4.

All (75) 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:B:125:GLY:HA3	7:B:2008:EDO:H12	1.44	0.99
1:B:8[A]:GLU:HG2	8:B:2114:HOH:O	1.83	0.78
1:A:50:LEU:HG	8:A:2403:HOH:O	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8[A]:GLU:HG2	8:C:2310:HOH:O	1.87	0.75
1:A:8[A]:GLU:HG2	8:A:2239:HOH:O	1.86	0.74
7:D:2034:EDO:H21	8:D:2314:HOH:O	1.90	0.70
1:B:73[A]:GLU:OE2	7:B:2008:EDO:H11	1.93	0.69
1:B:125:GLY:HA3	7:B:2008:EDO:C1	2.22	0.68
1:C:296:GLY:HA3	7:C:2022:EDO:H21	1.74	0.67
1:D:11:PRO:HD2	1:D:43:SER:OG	1.98	0.64
1:D:256:MET:HB3	7:D:2018:EDO:H22	1.81	0.62
1:C:26:ARG:HD2	8:C:2126:HOH:O	1.98	0.62
4:B:508:NAG:H5	8:B:2352:HOH:O	2.00	0.62
1:D:190:VAL:HG11	5:D:517:NAG:H82	1.83	0.60
2:B:509:NAG:H5	7:B:2023:EDO:H11	1.84	0.60
1:C:26:ARG:HG2	7:C:2032:EDO:H21	1.84	0.59
1:C:296:GLY:CA	7:C:2022:EDO:H21	2.33	0.58
1:A:201:HIS:HB3	1:C:117:GLN:NE2	2.19	0.58
1:A:201:HIS:HB3	1:C:117:GLN:HE22	1.70	0.57
1:C:190:VAL:HG11	4:C:512:NAG:H82	1.87	0.56
1:D:312:TYR:HA	7:D:2018:EDO:H12	1.86	0.56
3:A:610:MAN:H2	8:A:2475:HOH:O	2.04	0.56
1:A:35:TYR:HE1	7:A:2028:EDO:H22	1.70	0.55
1:A:78[A]:ASN:ND2	1:A:124:THR:OG1	2.36	0.55
1:A:16:PRO:HB3	1:A:287:ILE:HG21	1.89	0.55
1:A:211:ALA:HB1	7:A:2001:EDO:H21	1.89	0.55
1:D:30:VAL:HG23	1:D:35:TYR:HE2	1.71	0.54
1:C:281:GLY:O	7:C:2022:EDO:H11	2.08	0.53
1:D:33:GLN:NE2	1:D:35:TYR:OH	2.41	0.53
1:B:260:PRO:HG3	7:B:2013:EDO:H22	1.92	0.51
1:A:276:PHE:HZ	1:A:285[B]:VAL:CG1	2.24	0.49
1:B:99:SER:HB3	7:B:2033:EDO:H12	1.96	0.47
1:A:124:THR:HG22	8:A:2403:HOH:O	2.15	0.46
1:B:95:THR:HG22	1:B:194:ALA:HB3	1.98	0.46
1:B:70:LYS:HE3	8:B:2336:HOH:O	2.15	0.45
1:C:67:ILE:HG23	1:C:109:ASN:HA	1.98	0.45
1:A:137:TYR:O	8:A:2322:HOH:O	2.20	0.45
1:D:30:VAL:CG2	1:D:35:TYR:HE2	2.28	0.45
1:B:303:ILE:HG21	1:B:309:PHE:CD1	2.51	0.45
1:D:80:GLY:HA3	1:D:121:THR:HA	1.97	0.45
1:B:35:TYR:HD2	1:B:51:MET:CE	2.29	0.45
1:A:294:GLU:HG2	8:A:2209:HOH:O	2.17	0.44
1:D:268:TRP:O	1:D:308:GLU:HA	2.17	0.44
1:B:190:VAL:HG11	4:B:507:NAG:H82	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:509:NAG:H5	7:B:2023:EDO:C1	2.47	0.43
1:A:21:HIS:CG	1:A:298:GLY:HA3	2.53	0.43
1:A:4:SER:HA	8:A:2267:HOH:O	2.18	0.43
1:A:82:PHE:CE2	1:A:123:MET:HG2	2.53	0.43
1:C:303:ILE:HG21	1:C:309:PHE:CD1	2.53	0.43
1:D:67:ILE:HG23	1:D:109:ASN:HA	2.00	0.43
1:D:10:ALA:HA	1:D:11:PRO:HD3	1.91	0.43
1:A:67:ILE:CG1	1:A:178:TYR:HB2	2.48	0.42
1:B:197:ASN:HD21	7:B:2011:EDO:C2	2.32	0.42
1:A:190:VAL:HG11	3:A:502:NAG:H82	2.01	0.42
1:A:296:GLY:CA	7:C:2022:EDO:H12	2.50	0.42
1:D:303:ILE:HG21	1:D:309:PHE:CD1	2.54	0.42
1:D:216:PHE:CD1	1:D:216:PHE:N	2.88	0.42
1:C:268:TRP:O	1:C:308:GLU:HA	2.20	0.42
1:D:135:LEU:C	1:D:135:LEU:HD13	2.41	0.42
1:A:322:PHE:CZ	1:A:330:LEU:HB3	2.55	0.41
1:D:21:HIS:CG	1:D:298:GLY:HA3	2.55	0.41
1:C:26:ARG:HA	7:C:2032:EDO:H22	2.03	0.41
1:D:67:ILE:CG2	1:D:68:HIS:N	2.84	0.41
1:A:296:GLY:HA3	7:C:2022:EDO:H12	2.02	0.41
1:B:10:ALA:HA	1:B:11:PRO:HD3	1.93	0.41
1:A:86:ALA:HA	1:A:111:THR:O	2.20	0.41
1:A:35:TYR:CE1	7:A:2028:EDO:H22	2.53	0.41
1:A:153:PRO:O	1:A:154:SER:HB3	2.20	0.40
1:A:303:ILE:HD12	1:A:303:ILE:N	2.37	0.40
1:B:21:HIS:CG	1:B:298:GLY:HA3	2.57	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	341/350 (97%)	331 (97%)	10 (3%)	0	100	100
1	B	345/350 (99%)	336 (97%)	9 (3%)	0	100	100
1	C	339/350 (97%)	329 (97%)	10 (3%)	0	100	100
1	D	335/350 (96%)	329 (98%)	6 (2%)	0	100	100
All	All	1360/1400 (97%)	1325 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	289/294 (98%)	286 (99%)	3 (1%)	82	67
1	B	291/294 (99%)	288 (99%)	3 (1%)	82	67
1	C	287/294 (98%)	284 (99%)	3 (1%)	82	67
1	D	283/294 (96%)	279 (99%)	4 (1%)	74	53
All	All	1150/1176 (98%)	1137 (99%)	13 (1%)	86	63

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	TYR
1	A	73[A]	GLU
1	A	73[B]	GLU
1	B	72	TYR
1	B	73[A]	GLU
1	B	73[B]	GLU
1	C	72	TYR
1	C	73[A]	GLU
1	C	73[B]	GLU
1	D	28	VAL
1	D	72	TYR
1	D	73[A]	GLU
1	D	73[B]	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	117	GLN
1	A	173	GLN
1	B	83	GLN
1	B	173	GLN
1	B	286	GLN
1	C	83	GLN
1	C	117	GLN
1	D	33	GLN
1	D	117	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 ⓘ

17 carbohydrates are modelled in this entry.

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	NAG	A	502	1,3	14,14,15	0.62	0	15,19,21	0.80	1 (6%)
3	NAG	A	503	3	14,14,15	0.61	0	15,19,21	0.70	1 (6%)
3	BMA	A	604	3	11,11,12	0.40	0	14,15,17	0.49	0
3	MAN	A	605	3	11,11,12	0.51	0	14,15,17	0.56	0
3	MAN	A	606	3	11,11,12	0.49	0	14,15,17	0.70	1 (7%)
3	MAN	A	607	3	11,11,12	0.50	0	14,15,17	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	A	610	3	11,11,12	0.53	0	14,15,17	0.65	1 (7%)
4	NAG	B	507	1,4	14,14,15	0.56	0	15,19,21	0.82	1 (6%)
4	NAG	B	508	4	14,14,15	0.49	0	15,19,21	0.85	1 (6%)
4	BMA	B	608	4	11,11,12	0.63	0	14,15,17	0.37	0
4	MAN	B	609	4	11,11,12	0.55	0	14,15,17	0.44	0
4	NAG	C	512	1,4	14,14,15	0.50	0	15,19,21	0.65	0
4	NAG	C	513	4	14,14,15	0.44	0	15,19,21	0.59	0
4	BMA	C	601	4	11,11,12	0.52	0	14,15,17	0.30	0
4	MAN	C	603	4	11,11,12	0.66	0	14,15,17	0.49	0
5	NAG	D	517	1,5	14,14,15	0.57	0	15,19,21	0.71	1 (6%)
5	NAG	D	518	5	14,14,15	0.61	0	15,19,21	0.57	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	NAG	A	502	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	503	3	-	0/6/23/26	0/1/1/1
3	BMA	A	604	3	-	0/2/19/22	0/1/1/1
3	MAN	A	605	3	-	0/2/19/22	0/1/1/1
3	MAN	A	606	3	-	0/2/19/22	0/1/1/1
3	MAN	A	607	3	-	0/2/19/22	0/1/1/1
3	MAN	A	610	3	-	0/2/19/22	0/1/1/1
4	NAG	B	507	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	508	4	-	0/6/23/26	0/1/1/1
4	BMA	B	608	4	-	0/2/19/22	0/1/1/1
4	MAN	B	609	4	-	0/2/19/22	0/1/1/1
4	NAG	C	512	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	513	4	-	0/6/23/26	0/1/1/1
4	BMA	C	601	4	-	0/2/19/22	0/1/1/1
4	MAN	C	603	4	-	0/2/19/22	0/1/1/1
5	NAG	D	517	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	518	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	507	NAG	C2-N2-C7	-2.46	119.88	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	NAG	C2-N2-C7	-2.38	119.98	123.04
4	B	508	NAG	C2-N2-C7	-2.28	120.10	123.04
5	D	517	NAG	C2-N2-C7	-2.20	120.22	123.04
3	A	503	NAG	C2-N2-C7	-2.11	120.33	123.04
3	A	606	MAN	C1-O5-C5	2.10	114.91	112.25
3	A	610	MAN	C1-O5-C5	2.16	114.99	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	NAG	1	0
3	A	610	MAN	1	0
4	B	507	NAG	1	0
4	B	508	NAG	1	0
4	C	512	NAG	1	0
5	D	517	NAG	1	0

5.6 Ligand geometry

Of 49 ligands modelled in this entry, 4 are monoatomic - leaving 45 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	$\# Z > 2$
7	EDO	A	2001	-	3,3,3	0.51	0	2,2,2	0.17	0
7	EDO	A	2007	-	3,3,3	0.29	0	2,2,2	0.50	0
7	EDO	A	2009	-	3,3,3	0.50	0	2,2,2	0.41	0
7	EDO	A	2015	-	3,3,3	0.43	0	2,2,2	0.56	0
7	EDO	A	2020	-	3,3,3	0.49	0	2,2,2	0.40	0
7	EDO	A	2024	-	3,3,3	0.41	0	2,2,2	0.36	0
7	EDO	A	2025	-	3,3,3	0.50	0	2,2,2	0.35	0
7	EDO	A	2026	-	3,3,3	0.40	0	2,2,2	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	A	2028	-	3,3,3	0.39	0	2,2,2	0.44	0
2	NAG	A	501	1	14,14,15	0.55	0	15,19,21	0.62	0
2	NAG	A	504	1	14,14,15	0.56	0	15,19,21	0.80	1 (6%)
2	NAG	A	505	1	14,14,15	0.55	0	15,19,21	0.69	0
2	NAG	A	521	1	14,14,15	0.71	0	15,19,21	0.65	0
7	EDO	B	2002	-	3,3,3	0.55	0	2,2,2	0.43	0
7	EDO	B	2008	-	3,3,3	0.60	0	2,2,2	0.42	0
7	EDO	B	2011	-	3,3,3	0.50	0	2,2,2	0.31	0
7	EDO	B	2013	-	3,3,3	0.50	0	2,2,2	0.39	0
7	EDO	B	2016	-	3,3,3	0.44	0	2,2,2	0.53	0
7	EDO	B	2021	-	3,3,3	0.65	0	2,2,2	0.23	0
7	EDO	B	2023	-	3,3,3	0.58	0	2,2,2	0.31	0
7	EDO	B	2033	-	3,3,3	0.46	0	2,2,2	0.45	0
2	NAG	B	506	1	14,14,15	0.53	0	15,19,21	0.66	0
2	NAG	B	509	1	14,14,15	0.68	0	15,19,21	0.76	1 (6%)
2	NAG	B	510	1	14,14,15	0.65	0	15,19,21	0.72	1 (6%)
7	EDO	C	2003	-	3,3,3	0.56	0	2,2,2	0.37	0
7	EDO	C	2005	-	3,3,3	0.43	0	2,2,2	0.48	0
7	EDO	C	2006	-	3,3,3	0.46	0	2,2,2	0.38	0
7	EDO	C	2014	-	3,3,3	0.39	0	2,2,2	0.50	0
7	EDO	C	2017	-	3,3,3	0.56	0	2,2,2	0.35	0
7	EDO	C	2022	-	3,3,3	0.38	0	2,2,2	0.40	0
7	EDO	C	2027	-	3,3,3	0.36	0	2,2,2	0.40	0
7	EDO	C	2029	-	3,3,3	0.58	0	2,2,2	0.30	0
7	EDO	C	2031	-	3,3,3	0.66	0	2,2,2	0.29	0
7	EDO	C	2032	-	3,3,3	0.46	0	2,2,2	0.38	0
2	NAG	C	511	1	14,14,15	0.45	0	15,19,21	0.70	0
2	NAG	C	514	1	14,14,15	0.60	0	15,19,21	0.81	1 (6%)
2	NAG	C	515	1	14,14,15	0.53	0	15,19,21	0.82	0
7	EDO	D	2004	-	3,3,3	0.51	0	2,2,2	0.48	0
7	EDO	D	2012	-	3,3,3	0.40	0	2,2,2	0.51	0
7	EDO	D	2018	-	3,3,3	0.47	0	2,2,2	0.28	0
7	EDO	D	2030	-	3,3,3	0.41	0	2,2,2	0.44	0
7	EDO	D	2034	-	3,3,3	0.47	0	2,2,2	0.39	0
2	NAG	D	516	1	14,14,15	0.47	0	15,19,21	0.65	0
2	NAG	D	519	1	14,14,15	0.73	1 (7%)	15,19,21	0.62	0
2	NAG	D	520	1	14,14,15	0.59	0	15,19,21	0.79	1 (6%)

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
7	EDO	A	2001	-	-	0/1/1/1	0/0/0/0
7	EDO	A	2007	-	-	0/1/1/1	0/0/0/0
7	EDO	A	2009	-	-	0/1/1/1	0/0/0/0
7	EDO	A	2015	-	-	0/1/1/1	0/0/0/0
7	EDO	A	2020	-	-	0/1/1/1	0/0/0/0
7	EDO	A	2024	-	-	0/1/1/1	0/0/0/0
7	EDO	A	2025	-	-	0/1/1/1	0/0/0/0
7	EDO	A	2026	-	-	0/1/1/1	0/0/0/0
7	EDO	A	2028	-	-	0/1/1/1	0/0/0/0
2	NAG	A	501	1	-	0/6/23/26	0/1/1/1
2	NAG	A	504	1	-	0/6/23/26	0/1/1/1
2	NAG	A	505	1	-	0/6/23/26	0/1/1/1
2	NAG	A	521	1	-	0/6/23/26	0/1/1/1
7	EDO	B	2002	-	-	0/1/1/1	0/0/0/0
7	EDO	B	2008	-	-	0/1/1/1	0/0/0/0
7	EDO	B	2011	-	-	0/1/1/1	0/0/0/0
7	EDO	B	2013	-	-	0/1/1/1	0/0/0/0
7	EDO	B	2016	-	-	0/1/1/1	0/0/0/0
7	EDO	B	2021	-	-	0/1/1/1	0/0/0/0
7	EDO	B	2023	-	-	0/1/1/1	0/0/0/0
7	EDO	B	2033	-	-	0/1/1/1	0/0/0/0
2	NAG	B	506	1	-	0/6/23/26	0/1/1/1
2	NAG	B	509	1	-	0/6/23/26	0/1/1/1
2	NAG	B	510	1	-	0/6/23/26	0/1/1/1
7	EDO	C	2003	-	-	0/1/1/1	0/0/0/0
7	EDO	C	2005	-	-	0/1/1/1	0/0/0/0
7	EDO	C	2006	-	-	0/1/1/1	0/0/0/0
7	EDO	C	2014	-	-	0/1/1/1	0/0/0/0
7	EDO	C	2017	-	-	0/1/1/1	0/0/0/0
7	EDO	C	2022	-	-	0/1/1/1	0/0/0/0
7	EDO	C	2027	-	-	0/1/1/1	0/0/0/0
7	EDO	C	2029	-	-	0/1/1/1	0/0/0/0
7	EDO	C	2031	-	-	0/1/1/1	0/0/0/0
7	EDO	C	2032	-	-	0/1/1/1	0/0/0/0
2	NAG	C	511	1	-	0/6/23/26	0/1/1/1
2	NAG	C	514	1	-	0/6/23/26	0/1/1/1
2	NAG	C	515	1	-	0/6/23/26	0/1/1/1
7	EDO	D	2004	-	-	0/1/1/1	0/0/0/0
7	EDO	D	2012	-	-	0/1/1/1	0/0/0/0
7	EDO	D	2018	-	-	0/1/1/1	0/0/0/0
7	EDO	D	2030	-	-	0/1/1/1	0/0/0/0
7	EDO	D	2034	-	-	0/1/1/1	0/0/0/0
2	NAG	D	516	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	519	1	-	0/6/23/26	0/1/1/1
2	NAG	D	520	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	519	NAG	C1-C2	2.07	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	514	NAG	C2-N2-C7	-2.67	119.61	123.04
2	D	520	NAG	C2-N2-C7	-2.52	119.81	123.04
2	A	504	NAG	C2-N2-C7	-2.50	119.83	123.04
2	B	509	NAG	C2-N2-C7	-2.27	120.13	123.04
2	B	510	NAG	C2-N2-C7	-2.02	120.44	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2001	EDO	1	0
7	A	2028	EDO	2	0
7	B	2008	EDO	3	0
7	B	2011	EDO	1	0
7	B	2013	EDO	1	0
7	B	2023	EDO	2	0
7	B	2033	EDO	1	0
2	B	509	NAG	2	0
7	C	2022	EDO	10	0
7	C	2032	EDO	2	0
7	D	2018	EDO	2	0
7	D	2034	EDO	1	0

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	334/350 (95%)	-0.74	2 (0%) 90 90	11, 15, 25, 44	0
1	B	339/350 (96%)	-0.73	3 (0%) 85 85	12, 17, 27, 49	0
1	C	334/350 (95%)	-0.69	2 (0%) 90 90	10, 17, 28, 50	0
1	D	330/350 (94%)	-0.72	0 100 100	12, 18, 27, 47	0
All	All	1337/1400 (95%)	-0.72	7 (0%) 91 91	10, 17, 27, 50	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	169	ILE	3.4
1	A	3	SER	3.1
1	B	166	SER	2.9
1	C	167	SER	2.8
1	B	154	SER	2.3
1	C	169	ILE	2.1
1	B	165	ASP	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 ⓘ

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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	B	508	14/15	0.83	0.17	11.29	29,34,37,40	0
4	NAG	C	513	14/15	0.91	0.09	7.52	21,29,32,39	0
4	NAG	C	512	14/15	0.95	0.09	4.73	20,23,32,33	0
5	NAG	D	518	14/15	0.92	0.08	2.85	24,27,33,33	0
5	NAG	D	517	14/15	0.93	0.10	2.47	22,27,36,38	0
3	NAG	A	503	14/15	0.95	0.07	1.95	20,26,34,35	0
4	NAG	B	507	14/15	0.95	0.08	1.16	20,22,28,30	0
3	NAG	A	502	14/15	0.95	0.07	0.83	20,23,30,32	0
4	BMA	C	601	11/12	0.77	0.14	-	41,42,43,43	0
3	MAN	A	610	11/12	0.75	0.30	-	45,46,48,48	0
3	MAN	A	606	11/12	0.82	0.20	-	37,40,42,45	0
4	MAN	B	609	11/12	0.67	0.39	-	46,48,52,53	0
4	BMA	B	608	11/12	0.70	0.28	-	42,43,46,47	0
4	MAN	C	603	11/12	0.76	0.15	-	39,42,45,46	0
3	MAN	A	605	11/12	0.83	0.20	-	42,43,46,47	0
3	BMA	A	604	11/12	0.88	0.13	-	36,38,40,42	0
3	MAN	A	607	11/12	0.71	0.24	-	43,46,46,48	0

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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	EDO	C	2022	4/4	0.83	0.29	23.85	31,32,33,41	0
7	EDO	C	2031	4/4	0.94	0.13	18.31	18,23,25,27	0
2	NAG	B	509	14/15	0.92	0.14	15.32	22,27,35,35	0
7	EDO	B	2008	4/4	0.85	0.24	12.55	36,40,41,42	0
2	NAG	C	514	14/15	0.86	0.14	12.43	25,30,37,39	0
7	EDO	A	2028	4/4	0.88	0.21	12.15	45,45,46,47	0
7	EDO	A	2009	4/4	0.80	0.16	10.40	39,39,40,45	0
7	EDO	A	2007	4/4	0.86	0.17	9.20	33,38,38,39	0
7	EDO	B	2016	4/4	0.76	0.18	8.60	38,39,40,41	0
7	EDO	C	2029	4/4	0.92	0.13	7.88	24,28,30,33	0
7	EDO	D	2018	4/4	0.94	0.13	7.35	22,29,32,32	0
7	EDO	B	2013	4/4	0.55	0.19	6.02	45,45,46,47	0
7	EDO	D	2034	4/4	0.90	0.23	5.62	30,31,34,35	0
7	EDO	D	2030	4/4	0.87	0.12	5.51	40,43,43,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	EDO	C	2017	4/4	0.81	0.12	5.14	34,37,38,42	0
7	EDO	B	2033	4/4	0.89	0.11	4.05	37,38,39,39	0
7	EDO	A	2024	4/4	0.92	0.08	3.90	40,42,43,44	0
7	EDO	B	2011	4/4	0.90	0.10	3.71	30,32,34,36	0
7	EDO	B	2021	4/4	0.78	0.11	3.57	31,32,33,36	0
7	EDO	A	2015	4/4	0.83	0.11	3.52	31,32,34,34	0
2	NAG	D	520	14/15	0.90	0.11	3.50	30,33,40,42	0
7	EDO	C	2005	4/4	0.98	0.09	2.86	20,21,22,24	0
7	EDO	D	2012	4/4	0.87	0.10	2.05	38,38,39,40	0
7	EDO	B	2023	4/4	0.90	0.11	1.79	26,30,33,33	0
7	EDO	A	2020	4/4	0.83	0.15	1.57	36,38,40,40	0
2	NAG	D	519	14/15	0.94	0.07	1.36	22,24,29,29	0
2	NAG	A	504	14/15	0.93	0.07	1.35	22,25,34,34	0
7	EDO	C	2027	4/4	0.91	0.07	1.18	48,48,48,50	0
2	NAG	A	521	14/15	0.95	0.10	1.07	16,24,28,30	0
7	EDO	A	2001	4/4	0.94	0.07	0.62	19,20,23,23	0
2	NAG	D	516	14/15	0.93	0.09	0.34	27,31,35,36	0
2	NAG	A	505	14/15	0.92	0.07	0.32	28,31,35,36	0
6	CU	C	403	1/1	1.00	0.07	0.17	18,18,18,18	0
7	EDO	B	2002	4/4	0.97	0.05	-0.30	15,17,18,18	0
7	EDO	C	2006	4/4	0.95	0.06	-0.30	23,24,25,26	0
7	EDO	C	2014	4/4	0.95	0.06	-0.36	32,33,34,35	0
6	CU	B	402	1/1	1.00	0.05	-0.61	17,17,17,17	0
7	EDO	C	2003	4/4	0.97	0.06	-0.64	17,18,19,21	0
7	EDO	D	2004	4/4	0.98	0.06	-0.93	17,18,19,19	0
6	CU	A	401	1/1	1.00	0.06	-	16,16,16,16	0
7	EDO	A	2025	4/4	0.78	0.22	-	53,53,54,54	0
2	NAG	C	515	14/15	0.82	0.15	-	34,39,43,45	0
2	NAG	B	506	14/15	0.94	0.07	-	23,28,31,34	0
7	EDO	A	2026	4/4	0.83	0.09	-	46,46,46,46	0
6	CU	D	404	1/1	1.00	0.04	-	17,17,17,17	0
7	EDO	C	2032	4/4	0.77	0.14	-	47,47,48,50	0
2	NAG	B	510	14/15	0.80	0.20	-	36,42,45,47	0
2	NAG	A	501	14/15	0.95	0.06	-	24,27,30,32	0
2	NAG	C	511	14/15	0.90	0.09	-	25,30,38,39	0

6.5 Other polymers ⓘ

There are no such residues in this entry.