



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:04 AM UTC

PDB ID : 9AYU / pdb_00009ayu
Title : Structure of the A type blood alpha-D-galactosamine galactosaminidase
D463A mutant from Flavonifractor plautii
Authors : Worrall, L.J.; Strynadka, N.C.J.
Deposited on : 2024-03-08
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

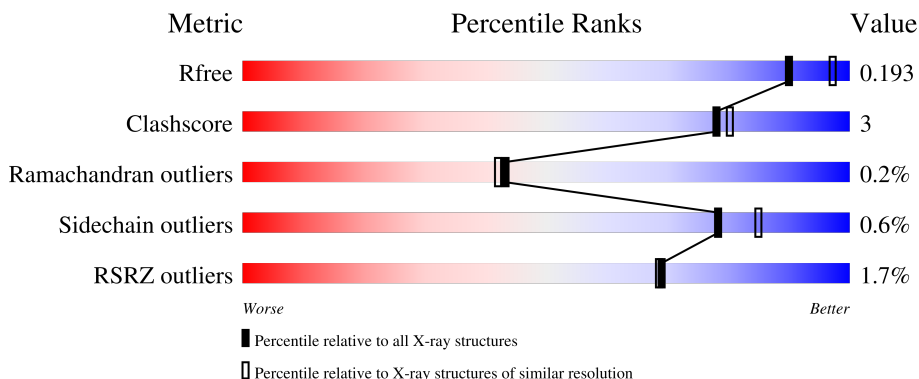
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 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	672	0% 91% 6% .
1	B	672	90% 7% .
1	C	672	0% 91% 6% .
1	D	672	2% 92% 6% .
1	E	672	5% 90% 6% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 28603 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 A type blood alpha-D-galactosamine galactosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	654	Total	C	N	O	S	0	0	0
			5064	3199	832	1009	24			
1	B	654	Total	C	N	O	S	0	7	0
			5125	3241	842	1018	24			
1	C	654	Total	C	N	O	S	0	7	0
			5125	3241	842	1018	24			
1	D	654	Total	C	N	O	S	0	0	0
			5064	3199	832	1009	24			
1	E	654	Total	C	N	O	S	0	0	0
			5064	3199	832	1009	24			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	463	ALA	ASP	conflict	UNP P0DTR5
A	624	ALA	GLU	conflict	UNP P0DTR5
A	625	ALA	LYS	conflict	UNP P0DTR5
B	463	ALA	ASP	conflict	UNP P0DTR5
B	624	ALA	GLU	conflict	UNP P0DTR5
B	625	ALA	LYS	conflict	UNP P0DTR5
C	463	ALA	ASP	conflict	UNP P0DTR5
C	624	ALA	GLU	conflict	UNP P0DTR5
C	625	ALA	LYS	conflict	UNP P0DTR5
D	463	ALA	ASP	conflict	UNP P0DTR5
D	624	ALA	GLU	conflict	UNP P0DTR5
D	625	ALA	LYS	conflict	UNP P0DTR5
E	463	ALA	ASP	conflict	UNP P0DTR5
E	624	ALA	GLU	conflict	UNP P0DTR5
E	625	ALA	LYS	conflict	UNP P0DTR5

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	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
2	E	1	Total Zn 1 1	0	0

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mn 1 1	0	0
3	B	1	Total Mn 1 1	0	0
3	C	1	Total Mn 1 1	0	0
3	D	1	Total Mn 1 1	0	0
3	E	1	Total Mn 1 1	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0
4	E	1	Total Cl 1 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0

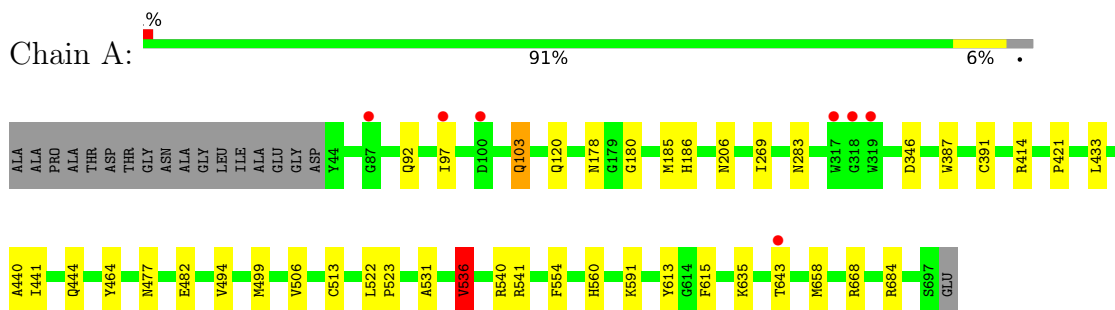
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	661	Total O 661 661	0	0
6	B	715	Total O 715 715	0	0
6	C	576	Total O 576 576	0	0
6	D	562	Total O 562 562	0	0
6	E	560	Total O 560 560	0	0

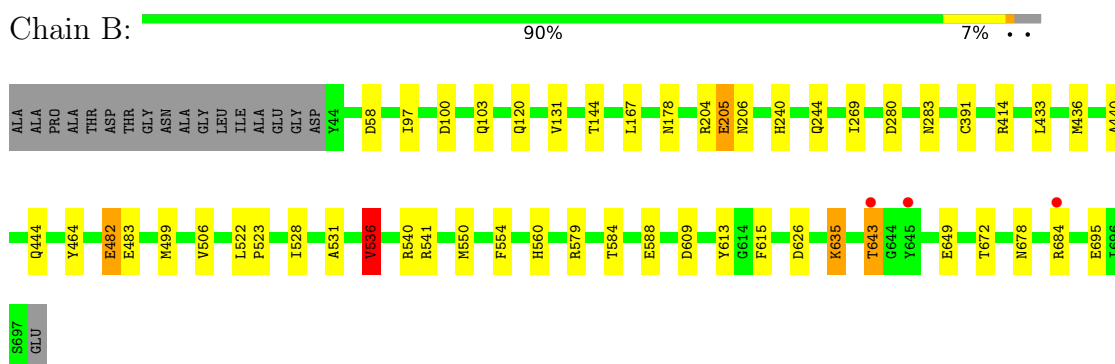
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

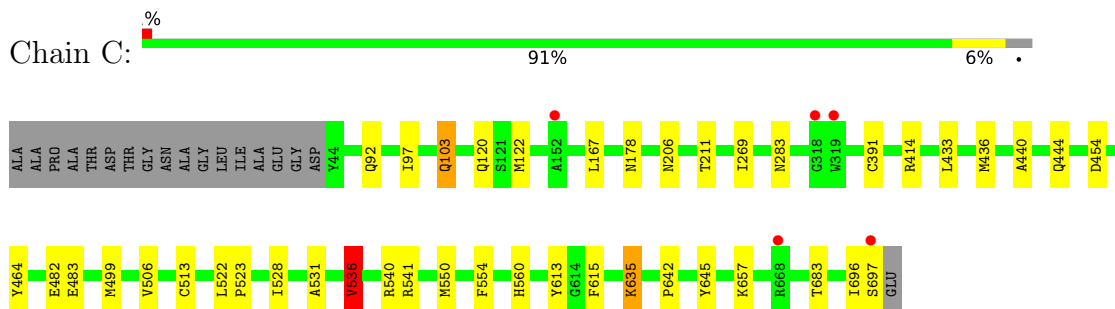
- Molecule 1: A type blood alpha-D-galactosamine galactosaminidase



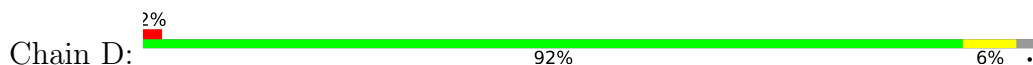
- Molecule 1: A type blood alpha-D-galactosamine galactosaminidase

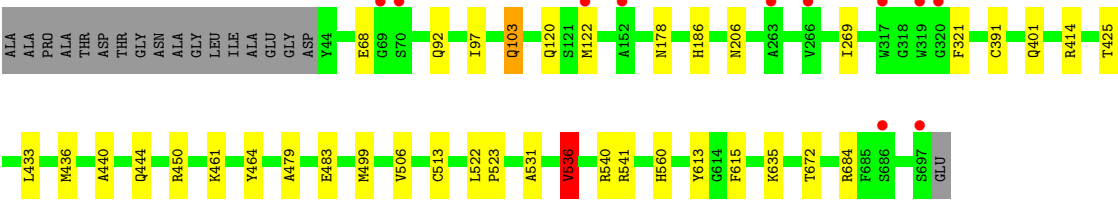


- Molecule 1: A type blood alpha-D-galactosamine galactosaminidase

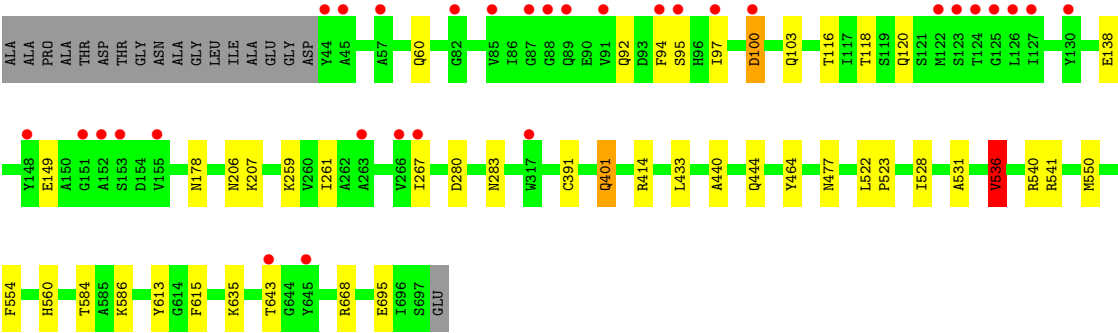
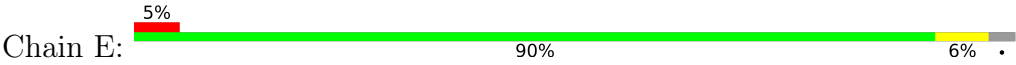


- Molecule 1: A type blood alpha-D-galactosamine galactosaminidase





● Molecule 1: A type blood alpha-D-galactosamine galactosaminidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.33Å 164.29Å 131.76Å 90.00° 90.20° 90.00°	Depositor
Resolution (Å)	48.90 – 2.00 48.90 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.90-2.00) 99.9 (48.90-2.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.163 , 0.186 0.172 , 0.193	Depositor DCC
R_{free} test set	14623 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	28603	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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, 0.333 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: EDO, MN, CL, ZN

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	0.62	0/5197	0.96	9/7083 (0.1%)
1	B	0.64	1/5263 (0.0%)	1.01	18/7174 (0.3%)
1	C	0.59	0/5263	0.94	10/7174 (0.1%)
1	D	0.60	0/5197	0.94	7/7083 (0.1%)
1	E	0.61	0/5197	0.96	12/7083 (0.2%)
All	All	0.61	1/26117 (0.0%)	0.96	56/35597 (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	3
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	1
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	205	GLU	CD-OE1	5.84	1.36	1.25

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	GLU	CB-CG-CD	14.32	136.95	112.60
1	B	205	GLU	CG-CD-OE2	-14.11	85.96	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	GLU	CG-CD-OE1	13.83	150.22	118.40
1	C	482	GLU	CB-CA-C	-8.15	93.54	110.17
1	E	536	VAL	N-CA-CB	-8.05	96.89	110.65
1	A	482	GLU	CB-CA-C	-7.93	93.98	110.17
1	C	536	VAL	N-CA-CB	-7.85	97.23	110.65
1	D	536	VAL	N-CA-CB	-7.79	97.34	110.65
1	A	536	VAL	N-CA-CB	-7.47	97.88	110.65
1	B	482	GLU	CB-CA-C	-7.47	94.93	110.17
1	E	100	ASP	CA-CB-CG	7.02	119.62	112.60
1	C	683	THR	OG1-CB-CG2	-7.00	95.29	109.30
1	B	536	VAL	N-CA-CB	-6.65	99.28	110.65
1	B	205	GLU	N-CA-CB	6.43	119.79	110.20
1	D	321	PHE	CA-CB-CG	-6.24	107.56	113.80
1	E	103	GLN	CB-CA-C	-5.83	98.52	109.72
1	A	103	GLN	CB-CA-C	-5.83	97.80	109.99
1	E	554	PHE	CA-CB-CG	-5.76	108.04	113.80
1	B	103	GLN	CB-CA-C	-5.75	98.68	109.72
1	A	615	PHE	CA-CB-CG	-5.70	108.10	113.80
1	E	138	GLU	CB-CA-C	-5.67	101.76	110.26
1	C	103	GLN	CB-CA-C	-5.63	98.75	109.95
1	B	615	PHE	CA-CB-CG	-5.61	108.19	113.80
1	A	554	PHE	CA-CB-CG	-5.61	108.19	113.80
1	A	635	LYS	CB-CA-C	-5.59	100.13	109.75
1	B	649	GLU	N-CA-CB	-5.59	101.77	110.55
1	B	100	ASP	CA-CB-CG	5.58	118.18	112.60
1	B	635	LYS	CB-CA-C	-5.56	100.19	109.75
1	C	615	PHE	CA-CB-CG	-5.54	108.26	113.80
1	C	554	PHE	CA-CB-CG	-5.48	108.32	113.80
1	D	615	PHE	CA-CB-CG	-5.46	108.34	113.80
1	D	103	GLN	CB-CA-C	-5.45	98.48	109.55
1	E	615	PHE	CA-CB-CG	-5.44	108.36	113.80
1	A	513	CYS	CB-CA-C	5.41	117.95	109.84
1	E	138	GLU	N-CA-CB	5.39	118.01	109.71
1	D	635	LYS	CB-CA-C	-5.32	100.59	109.75
1	E	401	GLN	CB-CA-C	-5.29	102.58	110.88
1	C	635	LYS	CB-CA-C	-5.27	100.68	109.75
1	E	643	THR	CA-CB-OG1	-5.27	101.69	109.60
1	D	513	CYS	CB-CA-C	5.26	117.73	109.84
1	B	554	PHE	CA-CB-CG	-5.23	108.57	113.80
1	C	482	GLU	CG-CD-OE1	-5.21	106.42	118.40
1	C	513	CYS	CB-CA-C	5.20	117.64	109.84
1	B	584	THR	CA-CB-OG1	-5.18	101.82	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	LEU	N-CA-CB	-5.17	102.36	109.97
1	A	658	MET	CG-SD-CE	5.11	112.15	100.90
1	E	584	THR	CA-CB-OG1	-5.10	101.95	109.60
1	E	635	LYS	CB-CA-C	-5.09	101.00	109.75
1	B	609	ASP	CA-CB-CG	5.08	117.68	112.60
1	B	280	ASP	CA-CB-CG	5.07	117.67	112.60
1	C	167	LEU	N-CA-CB	-5.07	102.52	109.97
1	B	672	THR	CA-CB-OG1	-5.05	102.02	109.60
1	E	280	ASP	CA-CB-CG	5.04	117.64	112.60
1	B	643	THR	CA-CB-OG1	-5.01	102.08	109.60
1	A	643	THR	CA-CB-OG1	-5.01	102.08	109.60
1	D	672	THR	CA-CB-OG1	-5.00	102.10	109.60

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	414	ARG	Sidechain
1	A	668	ARG	Sidechain
1	A	684	ARG	Sidechain
1	B	204	ARG	Sidechain
1	B	414	ARG	Sidechain
1	C	414	ARG	Sidechain
1	C	696	ILE	Peptide
1	D	414	ARG	Sidechain
1	D	68	GLU	Peptide
1	E	414	ARG	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	5064	0	4765	22	0
1	B	5125	0	4810	36	0
1	C	5125	0	4810	26	0
1	D	5064	0	4765	22	0
1	E	5064	0	4765	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	A	24	0	35	1	0
5	B	16	0	24	1	0
5	C	12	0	17	1	0
5	D	12	0	17	2	0
5	E	8	0	11	1	0
6	A	661	0	0	5	0
6	B	715	0	0	16	0
6	C	576	0	0	7	1
6	D	562	0	0	5	1
6	E	560	0	0	14	0
All	All	28603	0	24019	135	1

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 3.

All (135) 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:643:THR:O	6:B:801:HOH:O	1.68	1.09
1:B:626:ASP:HB3	6:B:1294:HOH:O	1.56	1.06
1:D:479:ALA:HB3	6:D:1248:HOH:O	1.61	0.99
1:C:122:MET:HA	1:C:122:MET:HE2	1.48	0.95
1:B:205:GLU:OE1	1:B:240:HIS:ND1	2.10	0.84
1:B:178:ASN:HD22	1:B:206:ASN:HD21	1.25	0.83
1:B:97:ILE:HD11	1:B:120:GLN:HB2	1.61	0.83
1:E:178:ASN:HD22	1:E:206:ASN:HD21	1.27	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:ASN:HD22	1:D:206:ASN:HD21	1.27	0.81
1:B:58:ASP:HB3	6:B:1416:HOH:O	1.80	0.81
1:C:178:ASN:HD22	1:C:206:ASN:HD21	1.27	0.80
1:E:695:GLU:OE2	6:E:801:HOH:O	2.00	0.79
1:A:178:ASN:HD22	1:A:206:ASN:HD21	1.27	0.79
1:D:97:ILE:HD11	1:D:120:GLN:HB2	1.70	0.74
1:E:97:ILE:HD11	1:E:120:GLN:HB2	1.71	0.73
1:D:425:THR:HG22	6:D:1222:HOH:O	1.88	0.73
1:A:97:ILE:HD11	1:A:120:GLN:HB2	1.70	0.72
1:C:97:ILE:HD11	1:C:120:GLN:HB2	1.70	0.72
1:E:668:ARG:HD3	6:E:986:HOH:O	1.90	0.71
1:E:92:GLN:HG2	6:E:1178:HOH:O	1.91	0.70
1:E:118:THR:OG1	6:E:802:HOH:O	2.09	0.70
1:C:657:LYS:NZ	1:D:684:ARG:O	2.24	0.69
1:E:149:GLU:HB2	6:E:816:HOH:O	1.92	0.69
1:B:678:ASN:ND2	6:B:804:HOH:O	2.19	0.68
1:B:464:TYR:CE2	5:B:704:EDO:H21	2.30	0.67
1:B:205:GLU:CD	1:B:240:HIS:HD1	2.02	0.67
1:E:668:ARG:CD	6:E:986:HOH:O	2.43	0.66
1:E:116:THR:OG1	6:E:803:HOH:O	2.12	0.66
1:B:528:ILE:CD1	1:B:550:MET:HG3	2.28	0.64
1:B:97:ILE:CD1	1:B:120:GLN:HB2	2.26	0.63
1:E:586:LYS:HE2	6:E:1320:HOH:O	1.99	0.62
1:A:391:CYS:H	1:A:444:GLN:HE22	1.47	0.62
6:A:1140:HOH:O	1:D:186:HIS:HD2	1.83	0.61
1:E:391:CYS:H	1:E:444:GLN:HE22	1.49	0.61
1:E:401:GLN:HG3	6:E:874:HOH:O	2.01	0.60
1:C:391:CYS:H	1:C:444:GLN:HE22	1.48	0.59
1:B:391:CYS:H	1:B:444:GLN:HE22	1.50	0.59
1:C:464:TYR:CE2	5:C:704:EDO:H21	2.38	0.59
1:D:391:CYS:H	1:D:444:GLN:HE22	1.49	0.58
1:C:528:ILE:CD1	1:C:550:MET:HG3	2.34	0.58
1:D:461:LYS:HE2	5:D:704:EDO:H22	1.86	0.57
1:E:464:TYR:CE2	5:E:704:EDO:H21	2.40	0.57
1:E:528:ILE:CD1	1:E:550:MET:HG3	2.34	0.57
1:D:97:ILE:CD1	1:D:120:GLN:HB2	2.35	0.56
1:A:464:TYR:CE2	5:A:704:EDO:H21	2.39	0.56
1:D:464:TYR:CE2	5:D:704:EDO:H21	2.41	0.56
1:E:97:ILE:CD1	1:E:120:GLN:HB2	2.34	0.56
1:E:261:ILE:HG12	1:E:267:ILE:HD11	1.88	0.56
1:D:436:MET:SD	1:D:483:GLU:HG2	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:ILE:CD1	1:C:120:GLN:HB2	2.36	0.55
1:C:122:MET:HA	1:C:122:MET:CE	2.28	0.55
1:A:97:ILE:CD1	1:A:120:GLN:HB2	2.34	0.54
1:C:436:MET:SD	1:C:483:GLU:HG2	2.47	0.54
1:A:283:ASN:CG	6:A:847:HOH:O	2.51	0.53
1:B:283:ASN:CG	6:B:835:HOH:O	2.51	0.52
1:B:695:GLU:OE2	6:B:802:HOH:O	2.18	0.52
1:B:588:GLU:OE1	6:B:803:HOH:O	2.19	0.51
1:D:92:GLN:HA	6:D:1218:HOH:O	2.10	0.51
1:A:591:LYS:NZ	6:A:821:HOH:O	2.43	0.50
1:D:97:ILE:HD11	1:D:120:GLN:CB	2.40	0.50
1:C:283:ASN:CG	6:C:827:HOH:O	2.55	0.50
1:D:541:ARG:HD3	1:D:613:TYR:CZ	2.47	0.49
1:E:97:ILE:HD11	1:E:120:GLN:CB	2.41	0.49
1:B:635:LYS:HE2	6:B:814:HOH:O	2.13	0.48
1:B:528:ILE:HD12	1:B:550:MET:HG3	1.95	0.48
1:C:642:PRO:O	6:C:801:HOH:O	2.20	0.48
1:B:528:ILE:HD11	1:B:550:MET:HG3	1.94	0.48
1:C:528:ILE:HD12	1:C:550:MET:HG3	1.96	0.48
1:C:269:ILE:C	1:C:269:ILE:HD12	2.39	0.48
1:B:391:CYS:H	1:B:444:GLN:NE2	2.12	0.47
1:C:536:VAL:HG13	1:C:540:ARG:CZ	2.44	0.47
1:C:541:ARG:HD3	1:C:613:TYR:CZ	2.49	0.47
1:E:536:VAL:HG13	1:E:540:ARG:CZ	2.44	0.47
1:A:536:VAL:HG13	1:A:540:ARG:CZ	2.44	0.47
1:B:436:MET:SD	1:B:483:GLU:HG2	2.54	0.47
1:A:92:GLN:HA	6:A:963:HOH:O	2.15	0.47
1:B:269:ILE:HD12	1:B:269:ILE:C	2.40	0.47
1:B:482:GLU:CD	6:B:805:HOH:O	2.57	0.47
1:C:391:CYS:H	1:C:444:GLN:NE2	2.12	0.47
1:D:499:MET:HB3	1:D:506:VAL:HG21	1.97	0.47
1:E:60:GLN:HE22	1:E:95:SER:HA	1.79	0.47
1:C:97:ILE:HD11	1:C:120:GLN:CB	2.40	0.47
1:D:401:GLN:HG3	6:D:938:HOH:O	2.14	0.47
1:B:536:VAL:HG13	1:B:540:ARG:CZ	2.45	0.47
1:A:269:ILE:C	1:A:269:ILE:HD12	2.39	0.46
1:D:269:ILE:C	1:D:269:ILE:HD12	2.40	0.46
1:D:391:CYS:H	1:D:444:GLN:NE2	2.11	0.46
1:A:185:MET:HG2	1:A:421:PRO:HG2	1.97	0.46
1:D:536:VAL:HG13	1:D:540:ARG:CZ	2.45	0.46
1:A:477:ASN:ND2	6:A:813:HOH:O	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:541:ARG:HD3	1:B:613:TYR:CZ	2.51	0.45
1:D:450:ARG:HD3	6:D:952:HOH:O	2.17	0.45
1:A:97:ILE:HD11	1:A:120:GLN:CB	2.40	0.45
1:C:92:GLN:HA	6:C:1167:HOH:O	2.16	0.45
1:C:499:MET:HB3	1:C:506:VAL:HG21	1.98	0.45
1:E:149:GLU:CB	6:E:816:HOH:O	2.59	0.45
1:E:259:LYS:HD2	1:E:267:ILE:HD12	1.99	0.45
1:E:541:ARG:HD3	1:E:613:TYR:CZ	2.51	0.45
1:B:635:LYS:CE	6:B:814:HOH:O	2.65	0.45
1:E:283:ASN:CG	6:E:889:HOH:O	2.60	0.45
1:E:391:CYS:H	1:E:444:GLN:NE2	2.12	0.44
1:A:499:MET:HB3	1:A:506:VAL:HG21	1.98	0.44
1:A:541:ARG:HD3	1:A:613:TYR:CZ	2.52	0.44
1:B:482:GLU:OE1	6:B:805:HOH:O	2.21	0.44
1:B:499:MET:HB3	1:B:506:VAL:HG21	2.00	0.44
1:E:528:ILE:HD12	1:E:550:MET:HG3	1.99	0.44
1:B:522:LEU:N	1:B:523:PRO:CD	2.81	0.44
1:C:433:LEU:HB3	1:C:440:ALA:HB1	2.00	0.44
1:A:391:CYS:H	1:A:444:GLN:NE2	2.14	0.43
1:C:454:ASP:OD2	6:C:804:HOH:O	2.21	0.43
1:B:283:ASN:ND2	6:B:835:HOH:O	2.51	0.43
1:C:211:THR:OG1	6:C:803:HOH:O	2.20	0.43
1:D:522:LEU:N	1:D:523:PRO:CD	2.81	0.43
1:B:58:ASP:CB	6:B:1416:HOH:O	2.52	0.43
1:E:522:LEU:N	1:E:523:PRO:CD	2.82	0.43
1:A:522:LEU:N	1:A:523:PRO:CD	2.82	0.42
1:C:522:LEU:N	1:C:523:PRO:CD	2.82	0.42
1:A:433:LEU:HB3	1:A:440:ALA:HB1	2.01	0.42
1:B:97:ILE:HD11	1:B:120:GLN:CB	2.39	0.42
1:C:283:ASN:ND2	6:C:827:HOH:O	2.52	0.42
1:B:131:VAL:O	1:B:144:THR:HA	2.19	0.42
1:D:433:LEU:HB3	1:D:440:ALA:HB1	2.02	0.42
1:C:645:TYR:OH	6:C:802:HOH:O	2.20	0.41
1:A:186:HIS:HD2	6:B:1207:HOH:O	2.02	0.41
1:E:94:PHE:HB2	6:E:1238:HOH:O	2.19	0.41
1:B:433:LEU:HB3	1:B:440:ALA:HB1	2.02	0.41
1:E:207:LYS:NZ	6:E:836:HOH:O	2.54	0.41
1:B:579:ARG:HE	1:E:477:ASN:ND2	2.18	0.41
1:B:684:ARG:HA	6:B:1112:HOH:O	2.20	0.41
1:E:92:GLN:HA	6:E:1219:HOH:O	2.19	0.41
1:A:346:ASP:HA	1:A:387:TRP:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:GLY:HA3	1:A:206:ASN:HA	2.03	0.40
1:A:441:ILE:CG2	1:A:494:VAL:HG11	2.52	0.40
1:B:244:GLN:HG2	6:B:1217:HOH:O	2.22	0.40
1:E:433:LEU:HB3	1:E:440:ALA:HB1	2.04	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	Interatomic distance (Å)	Clash overlap (Å)
6:C:1302:HOH:O	6:D:1228:HOH:O[1_655]	1.94	0.26

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	652/672 (97%)	626 (96%)	25 (4%)	1 (0%)	43	42
1	B	659/672 (98%)	636 (96%)	22 (3%)	1 (0%)	43	42
1	C	659/672 (98%)	635 (96%)	23 (4%)	1 (0%)	43	42
1	D	652/672 (97%)	629 (96%)	22 (3%)	1 (0%)	43	42
1	E	652/672 (97%)	629 (96%)	22 (3%)	1 (0%)	43	42
All	All	3274/3360 (97%)	3155 (96%)	114 (4%)	5 (0%)	43	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	531	ALA
1	B	531	ALA
1	C	531	ALA
1	D	531	ALA
1	E	531	ALA

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	535/545 (98%)	532 (99%)	3 (1%)	78	85
1	B	540/545 (99%)	538 (100%)	2 (0%)	84	89
1	C	540/545 (99%)	535 (99%)	5 (1%)	70	78
1	D	535/545 (98%)	531 (99%)	4 (1%)	76	82
1	E	535/545 (98%)	532 (99%)	3 (1%)	78	85
All	All	2685/2725 (98%)	2668 (99%)	17 (1%)	78	85

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	536	VAL
1	A	560	HIS
1	B	536	VAL
1	B	560	HIS
1	C	103	GLN
1	C	536	VAL
1	C	560	HIS
1	C	635	LYS
1	C	697	SER
1	D	103	GLN
1	D	122	MET
1	D	536	VAL
1	D	560	HIS
1	E	100	ASP
1	E	536	VAL
1	E	560	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	ASN

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Mol	Chain	Res	Type
1	A	186	HIS
1	A	444	GLN
1	B	178	ASN
1	B	186	HIS
1	B	444	GLN
1	B	666	ASN
1	C	178	ASN
1	C	444	GLN
1	D	178	ASN
1	D	186	HIS
1	D	402	GLN
1	D	444	GLN
1	E	60	GLN
1	E	103	GLN
1	E	178	ASN
1	E	186	HIS
1	E	444	GLN
1	E	477	ASN

5.3.3 RNA [i](#)

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 33 ligands modelled in this entry, 15 are monoatomic - leaving 18 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	$\# Z > 2$
5	EDO	C	705	3	3,3,3	0.21	0	2,2,2	0.20	0
5	EDO	E	705	3	3,3,3	0.23	0	2,2,2	0.05	0
5	EDO	A	705	3	3,3,3	0.12	0	2,2,2	0.23	0
5	EDO	A	709	-	3,3,3	0.46	0	2,2,2	0.18	0
5	EDO	A	706	-	3,3,3	0.36	0	2,2,2	0.16	0
5	EDO	B	706	-	3,3,3	0.50	0	2,2,2	0.30	0
5	EDO	A	704	-	3,3,3	0.61	0	2,2,2	0.32	0
5	EDO	C	706	-	3,3,3	0.38	0	2,2,2	0.27	0
5	EDO	D	704	-	3,3,3	0.74	0	2,2,2	0.52	0
5	EDO	B	705	-	3,3,3	0.41	0	2,2,2	0.39	0
5	EDO	D	705	-	3,3,3	0.60	0	2,2,2	0.44	0
5	EDO	A	707	-	3,3,3	0.32	0	2,2,2	0.31	0
5	EDO	C	704	-	3,3,3	0.64	0	2,2,2	0.33	0
5	EDO	A	708	-	3,3,3	0.29	0	2,2,2	0.13	0
5	EDO	B	707	-	3,3,3	0.25	0	2,2,2	0.13	0
5	EDO	B	704	-	3,3,3	0.62	0	2,2,2	0.54	0
5	EDO	E	704	-	3,3,3	0.57	0	2,2,2	0.50	0
5	EDO	D	706	3	3,3,3	0.25	0	2,2,2	0.29	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
5	EDO	C	705	3	-	0/1/1/1	-
5	EDO	E	705	3	-	1/1/1/1	-
5	EDO	A	705	3	-	0/1/1/1	-
5	EDO	A	709	-	-	0/1/1/1	-
5	EDO	A	706	-	-	0/1/1/1	-
5	EDO	B	706	-	-	0/1/1/1	-
5	EDO	A	704	-	-	0/1/1/1	-
5	EDO	C	706	-	-	0/1/1/1	-
5	EDO	D	704	-	-	1/1/1/1	-
5	EDO	B	705	-	-	1/1/1/1	-
5	EDO	D	705	-	-	0/1/1/1	-
5	EDO	A	707	-	-	0/1/1/1	-
5	EDO	C	704	-	-	1/1/1/1	-
5	EDO	A	708	-	-	0/1/1/1	-
5	EDO	B	707	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	704	-	-	1/1/1/1	-
5	EDO	E	704	-	-	1/1/1/1	-
5	EDO	D	706	3	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	704	EDO	O1-C1-C2-O2
5	B	705	EDO	O1-C1-C2-O2
5	B	704	EDO	O1-C1-C2-O2
5	E	705	EDO	O1-C1-C2-O2
5	C	704	EDO	O1-C1-C2-O2
5	E	704	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	704	EDO	1	0
5	D	704	EDO	2	0
5	C	704	EDO	1	0
5	B	704	EDO	1	0
5	E	704	EDO	1	0

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

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	654/672 (97%)	-0.40	7 (1%) 78 77	13, 22, 49, 65	0
1	B	654/672 (97%)	-0.50	3 (0%) 87 87	10, 19, 40, 62	7 (1%)
1	C	654/672 (97%)	-0.28	5 (0%) 82 82	13, 25, 52, 71	7 (1%)
1	D	654/672 (97%)	-0.14	11 (1%) 69 68	16, 27, 56, 75	0
1	E	654/672 (97%)	-0.13	31 (4%) 36 35	12, 24, 67, 95	0
All	All	3270/3360 (97%)	-0.29	57 (1%) 69 68	10, 24, 53, 95	14 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	152	ALA	5.2
1	E	151	GLY	4.7
1	C	697	SER	4.3
1	A	317	TRP	3.9
1	E	122	MET	3.8
1	D	70	SER	3.6
1	D	69	GLY	3.5
1	E	153	SER	3.4
1	B	643	THR	3.3
1	E	88	GLY	3.3
1	C	318[A]	GLY	3.2
1	E	87	GLY	3.2
1	E	100	ASP	3.1
1	E	267	ILE	3.0
1	D	152	ALA	3.0
1	E	317	TRP	2.9
1	D	317	TRP	2.9
1	E	155	VAL	2.8
1	D	686	SER	2.8
1	E	124	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	668	ARG	2.6
1	E	148	TYR	2.6
1	A	319	TRP	2.6
1	E	97	ILE	2.5
1	D	122	MET	2.5
1	A	643	THR	2.5
1	E	263	ALA	2.5
1	E	126	LEU	2.5
1	C	152	ALA	2.5
1	D	320	GLY	2.5
1	B	645	TYR	2.5
1	E	91	VAL	2.4
1	E	643	THR	2.4
1	D	266	VAL	2.4
1	E	85	VAL	2.4
1	E	127	ILE	2.4
1	D	697	SER	2.4
1	E	645	TYR	2.3
1	E	123	SER	2.3
1	E	266	VAL	2.3
1	E	45	ALA	2.2
1	B	684	ARG	2.2
1	E	82	GLY	2.2
1	E	125	GLY	2.2
1	C	319[A]	TRP	2.2
1	E	89	GLN	2.1
1	A	87	GLY	2.1
1	D	319	TRP	2.1
1	D	263	ALA	2.1
1	E	44	TYR	2.1
1	A	97	ILE	2.1
1	E	94	PHE	2.1
1	E	57	ALA	2.1
1	E	95	SER	2.1
1	A	100	ASP	2.0
1	A	318	GLY	2.0
1	E	130	TYR	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 oligosaccharides 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. 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(Å ²)	Q<0.9
5	EDO	D	704	4/4	0.76	0.24	44,47,49,49	0
5	EDO	C	704	4/4	0.82	0.19	41,44,46,49	0
5	EDO	A	704	4/4	0.89	0.22	36,38,44,44	0
5	EDO	B	706	4/4	0.92	0.12	42,43,46,46	0
5	EDO	A	709	4/4	0.92	0.10	26,27,28,30	0
5	EDO	B	704	4/4	0.92	0.12	31,32,33,34	0
5	EDO	E	704	4/4	0.92	0.13	29,34,36,37	0
5	EDO	D	706	4/4	0.93	0.10	28,33,35,36	0
4	CL	C	703	1/1	0.93	0.08	25,25,25,25	0
5	EDO	B	705	4/4	0.94	0.11	22,31,37,49	0
4	CL	E	703	1/1	0.94	0.06	22,22,22,22	0
5	EDO	C	705	4/4	0.95	0.09	27,30,31,31	0
4	CL	B	703	1/1	0.95	0.06	22,22,22,22	0
5	EDO	A	708	4/4	0.96	0.07	24,26,28,30	0
5	EDO	E	705	4/4	0.96	0.07	26,30,31,32	0
5	EDO	B	707	4/4	0.97	0.06	21,25,27,28	0
5	EDO	D	705	4/4	0.97	0.06	21,22,22,22	0
5	EDO	A	706	4/4	0.97	0.06	19,19,19,20	0
4	CL	D	703	1/1	0.97	0.05	25,25,25,25	0
5	EDO	C	706	4/4	0.97	0.06	21,22,22,25	0
5	EDO	A	707	4/4	0.98	0.05	21,22,22,23	0
5	EDO	A	705	4/4	0.98	0.06	20,22,23,24	0
2	ZN	E	701	1/1	0.98	0.03	21,21,21,21	0
3	MN	E	702	1/1	0.99	0.07	31,31,31,31	0
4	CL	A	703	1/1	0.99	0.04	21,21,21,21	0
2	ZN	A	701	1/1	0.99	0.02	21,21,21,21	0
3	MN	B	702	1/1	0.99	0.12	38,38,38,38	0
3	MN	C	702	1/1	0.99	0.08	32,32,32,32	0
3	MN	D	702	1/1	0.99	0.07	32,32,32,32	0
3	MN	A	702	1/1	1.00	0.06	27,27,27,27	0
2	ZN	C	701	1/1	1.00	0.03	21,21,21,21	0
2	ZN	D	701	1/1	1.00	0.02	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	B	701	1/1	1.00	0.02	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.