



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:22 PM UTC

PDB ID : 4U6B / pdb_00004u6b
Title : Zg3597, a family 117 glycoside hydrolase, produced by the marine bacterium
Zobellia galactanivorans
Authors : Ficko-Blean, E.
Deposited on : 2014-07-28
Resolution : 2.30 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

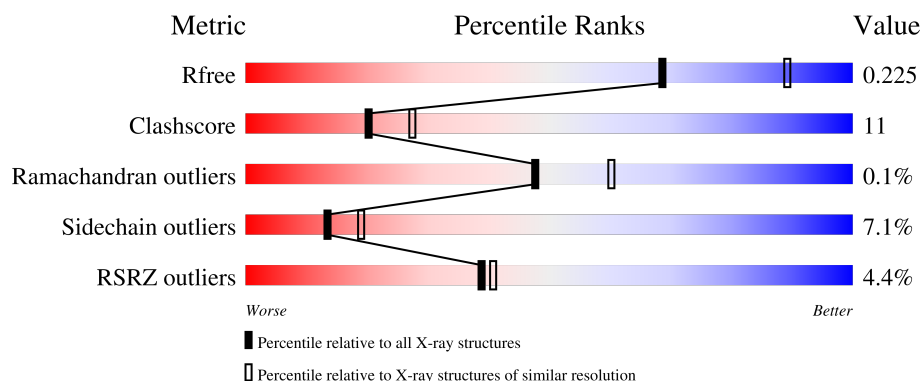
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	433	3% 60% 16% • 21%
1	B	433	4% 61% 15% • • 21%
1	C	433	4% 61% 14% • • 21%
1	D	433	3% 61% 16% • • 21%

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
6	ACY	B	503	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11568 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.

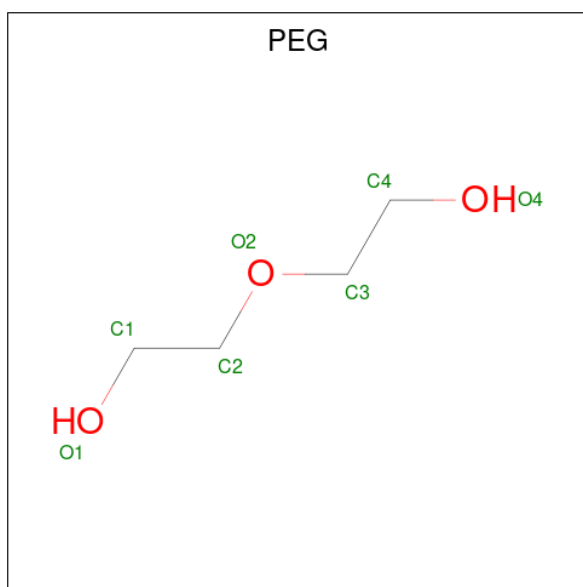
- Molecule 1 is a protein called Conserved hypothetical lipoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	2	0
			2686	1720	447	513	6			
1	B	343	Total	C	N	O	S	0	4	0
			2705	1734	447	518	6			
1	C	342	Total	C	N	O	S	0	3	0
			2693	1729	447	511	6			
1	D	343	Total	C	N	O	S	0	1	0
			2680	1717	442	515	6			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

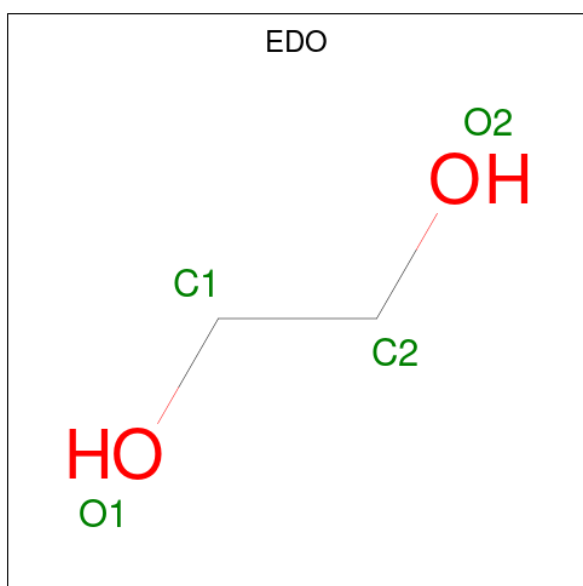
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	B	2	Total	Ca	0	0
			2	2		
2	C	2	Total	Ca	0	0
			2	2		
2	D	2	Total	Ca	0	0
			2	2		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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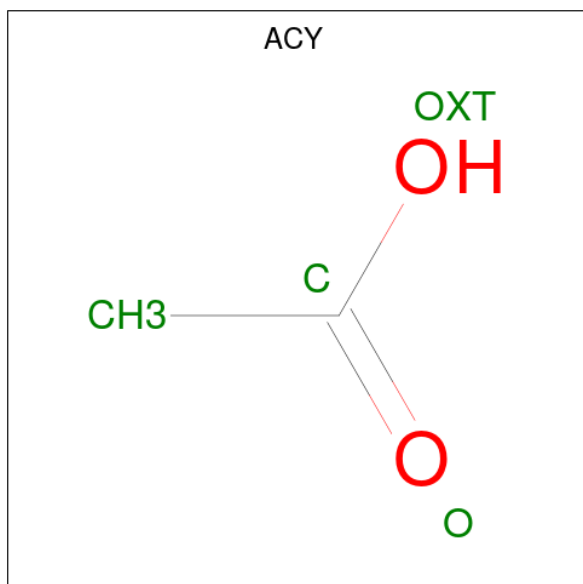
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 6 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



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

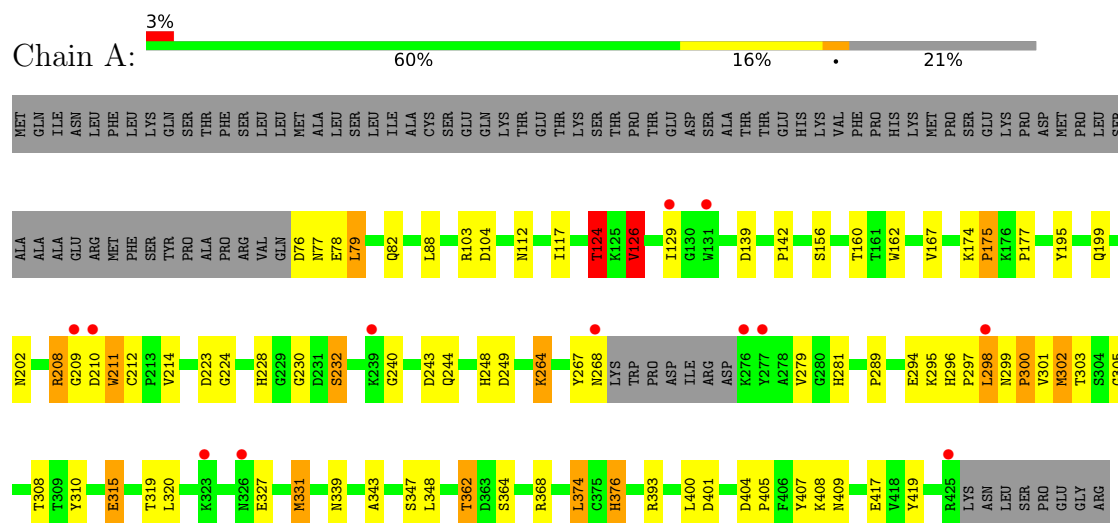
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	168	Total	O	0	7
			175	175		
7	B	173	Total	O	0	7
			180	180		
7	C	185	Total	O	0	10
			195	195		
7	D	175	Total	O	0	12
			187	187		

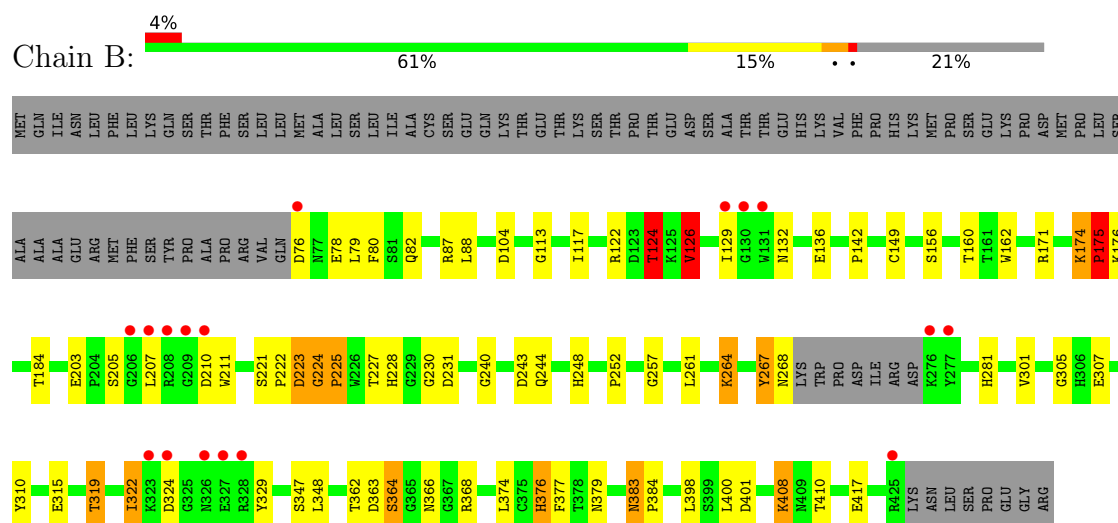
3 Residue-property plots [i](#)

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: Conserved hypothetical lipoprotein

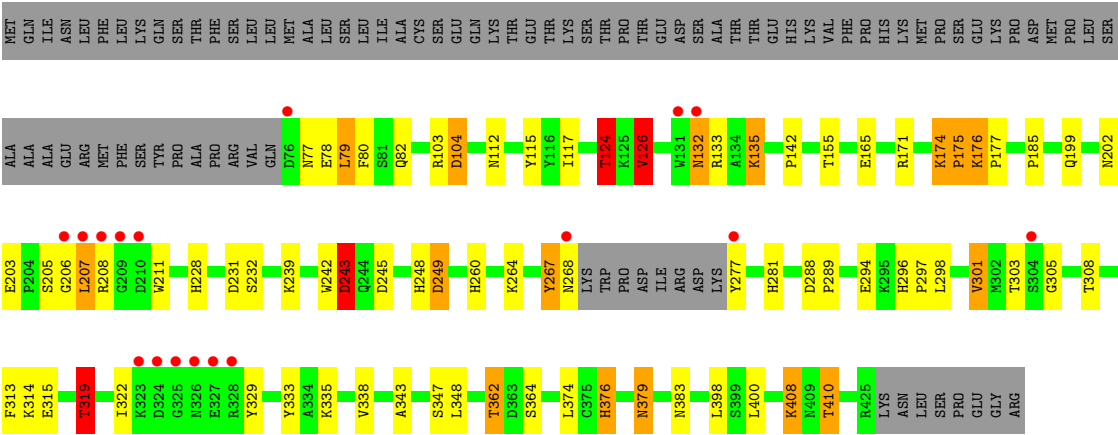


• Molecule 1: Conserved hypothetical lipoprotein

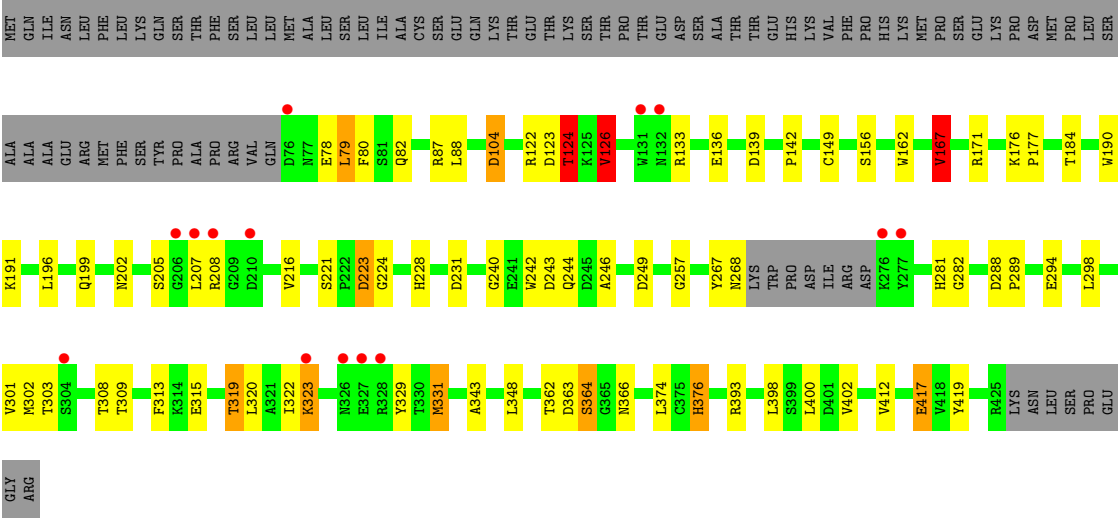


• Molecule 1: Conserved hypothetical lipoprotein





● Molecule 1: Conserved hypothetical lipoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	187.79Å 223.52Å 225.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 30.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.30) 99.7 (30.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.76 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.178 , 0.225 0.178 , 0.225	Depositor DCC
R_{free} test set	5189 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.043 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11568	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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 46.02 % 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 1.2163e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.18	5/2782 (0.2%)	1.21	15/3805 (0.4%)
1	B	1.16	8/2801 (0.3%)	1.25	22/3829 (0.6%)
1	C	1.16	3/2792 (0.1%)	1.21	22/3813 (0.6%)
1	D	1.18	6/2773 (0.2%)	1.24	21/3793 (0.6%)
All	All	1.17	22/11148 (0.2%)	1.23	80/15240 (0.5%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	104	ASP	CA-C	-6.87	1.49	1.53
1	A	160	THR	CA-C	6.10	1.58	1.52
1	C	176	LYS	C-N	5.94	1.40	1.33
1	A	174	LYS	C-O	-5.70	1.17	1.24
1	D	243	ASP	CB-CG	-5.67	1.37	1.52
1	B	227	THR	C-O	-5.60	1.17	1.24
1	B	230	GLY	C-O	-5.57	1.18	1.23
1	D	224	GLY	N-CA	5.56	1.52	1.44
1	D	176	LYS	C-N	5.54	1.40	1.33
1	B	176	LYS	C-N	5.49	1.40	1.33
1	B	222	PRO	C-O	-5.48	1.17	1.24
1	A	224	GLY	N-CA	5.40	1.52	1.44
1	B	417	GLU	N-CA	5.39	1.52	1.46
1	A	230	GLY	C-O	-5.34	1.18	1.24
1	B	126	VAL	C-O	-5.32	1.20	1.24
1	C	203	GLU	C-N	5.31	1.40	1.33
1	C	165	GLU	C-O	-5.25	1.17	1.24
1	B	225	PRO	N-CD	5.20	1.55	1.47
1	D	246	ALA	CA-C	-5.18	1.46	1.52
1	B	160	THR	CA-C	5.08	1.58	1.52
1	A	300	PRO	N-CD	5.04	1.54	1.47
1	D	282	GLY	CA-C	-5.00	1.48	1.52

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	ASP	CA-C-N	-9.38	107.15	121.87
1	A	223	ASP	C-N-CA	-9.38	107.15	121.87
1	C	174	LYS	C-N-CD	8.86	140.10	120.60
1	B	174	LYS	C-N-CD	8.85	140.08	120.60
1	A	174	LYS	C-N-CD	8.67	139.67	120.60
1	D	126	VAL	N-CA-CB	-8.53	102.49	111.87
1	A	299	ASN	C-N-CD	8.35	138.98	120.60
1	B	224	GLY	C-N-CD	8.18	138.59	120.60
1	B	223	ASP	N-CA-C	-7.87	100.73	110.41
1	D	331	MET	CG-SD-CE	-7.70	83.95	100.90
1	D	223	ASP	CA-C-N	-7.53	110.05	121.87
1	D	223	ASP	C-N-CA	-7.53	110.05	121.87
1	B	184	THR	CA-C-N	7.36	127.94	120.14
1	B	184	THR	C-N-CA	7.36	127.94	120.14
1	C	126	VAL	N-CA-CB	-7.23	101.08	111.21
1	C	267	TYR	N-CA-C	7.16	117.43	108.19
1	C	398	LEU	N-CA-C	-7.09	101.80	110.88
1	C	124	THR	N-CA-CB	-6.81	99.71	111.55
1	C	410	THR	CA-C-N	-6.79	116.00	122.66
1	C	410	THR	C-N-CA	-6.79	116.00	122.66
1	B	126	VAL	N-CA-CB	-6.78	104.38	111.64
1	C	207	LEU	N-CA-C	6.76	119.48	111.71
1	D	126	VAL	CB-CA-C	6.73	117.16	109.89
1	D	124	THR	N-CA-CB	-6.68	99.93	111.55
1	C	203	GLU	CA-C-N	-6.66	113.10	119.76
1	C	203	GLU	C-N-CA	-6.66	113.10	119.76
1	C	319	THR	CB-CA-C	-6.44	96.23	109.94
1	B	383	ASN	CA-C-N	6.43	126.05	119.56
1	B	383	ASN	C-N-CA	6.43	126.05	119.56
1	A	267	TYR	N-CA-C	6.39	117.55	108.74
1	C	298	LEU	N-CA-C	6.38	120.76	112.92
1	C	249	ASP	CA-C-N	-6.29	113.03	119.83
1	C	249	ASP	C-N-CA	-6.29	113.03	119.83
1	D	243	ASP	N-CA-CB	-6.29	100.82	110.44
1	B	319	THR	CB-CA-C	-6.26	95.67	109.56
1	B	398	LEU	N-CA-C	-6.24	102.38	111.30
1	A	167	VAL	CB-CA-C	-6.19	101.86	111.26
1	D	171	ARG	CA-C-N	-6.17	114.41	120.52
1	D	171	ARG	C-N-CA	-6.17	114.41	120.52
1	B	267	TYR	N-CA-C	6.12	117.53	108.60
1	B	124	THR	N-CA-CB	-6.10	101.08	111.69
1	D	242	TRP	CA-C-N	6.09	133.40	122.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	242	TRP	C-N-CA	6.09	133.40	122.38
1	D	364	SER	N-CA-C	6.07	117.89	111.28
1	C	175	PRO	CA-N-CD	-6.02	103.07	111.50
1	A	214	VAL	N-CA-C	5.97	117.38	108.54
1	A	126	VAL	N-CA-CB	-5.96	102.86	111.21
1	A	212	CYS	CA-C-N	-5.94	114.15	120.03
1	A	212	CYS	C-N-CA	-5.94	114.15	120.03
1	B	175	PRO	CA-N-CD	-5.92	103.21	111.50
1	D	176	LYS	CA-C-N	-5.90	113.68	119.76
1	D	176	LYS	C-N-CA	-5.90	113.68	119.76
1	B	126	VAL	N-CA-C	-5.89	104.36	109.19
1	A	331	MET	CG-SD-CE	-5.74	88.27	100.90
1	B	176	LYS	CA-C-N	-5.71	113.88	119.76
1	B	176	LYS	C-N-CA	-5.71	113.88	119.76
1	B	171	ARG	CA-C-N	-5.71	114.88	120.98
1	B	171	ARG	C-N-CA	-5.71	114.88	120.98
1	C	104	ASP	N-CA-CB	-5.58	105.46	111.66
1	A	175	PRO	CA-N-CD	-5.52	103.77	111.50
1	B	243	ASP	CB-CG-OD1	-5.52	105.71	118.40
1	C	176	LYS	CA-C-N	-5.50	113.89	119.83
1	C	176	LYS	C-N-CA	-5.50	113.89	119.83
1	A	124	THR	N-CA-CB	-5.49	101.39	111.37
1	B	126	VAL	CB-CA-C	5.48	114.70	109.33
1	C	171	ARG	CA-C-N	-5.46	115.12	120.52
1	C	171	ARG	C-N-CA	-5.46	115.12	120.52
1	B	211	TRP	N-CA-C	-5.37	98.07	107.20
1	A	232	SER	CB-CA-C	-5.31	104.35	111.89
1	D	124	THR	OG1-CB-CG2	5.26	119.81	109.30
1	A	319	THR	CB-CA-C	-5.25	100.56	110.16
1	D	167	VAL	CB-CA-C	-5.22	103.33	111.26
1	D	398	LEU	N-CA-C	-5.22	104.20	110.88
1	C	243	ASP	N-CA-C	5.21	119.39	113.19
1	B	322	ILE	CB-CA-C	-5.17	102.98	110.63
1	D	402	VAL	N-CA-C	-5.15	101.56	108.35
1	D	319	THR	CB-CA-C	-5.11	100.66	109.86
1	D	243	ASP	N-CA-C	5.11	119.50	113.16
1	D	223	ASP	N-CA-C	-5.08	103.98	110.53
1	C	243	ASP	N-CA-CB	-5.04	101.54	110.42

There are no chirality outliers.

There are no planarity outliers.

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	2686	0	2478	62	0
1	B	2705	0	2502	49	0
1	C	2693	0	2515	73	0
1	D	2680	0	2469	59	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	14	0	20	1	0
4	A	4	0	6	3	0
4	B	12	0	18	3	0
4	C	12	0	18	1	0
4	D	12	0	18	5	0
5	A	1	0	0	0	0
6	B	4	0	3	3	0
7	A	175	0	0	8	0
7	B	180	0	0	7	0
7	C	195	0	0	8	0
7	D	187	0	0	2	1
All	All	11568	0	10047	235	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 11.

All (235) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:THR:O	4:A:505:EDO:H12	1.47	1.12
1:A:320:LEU:HD13	1:A:331:MET:HE1	1.34	1.04
1:A:78:GLU:HG2	1:A:400:LEU:HD23	1.36	1.02
1:D:78:GLU:HG2	1:D:400:LEU:HD23	1.40	1.01
1:D:331:MET:HE2	1:D:331:MET:HA	1.41	1.00
1:A:104:ASP:H	1:A:376:HIS:HD2	1.06	0.96
1:C:314[B]:LYS:HG2	1:C:315:GLU:H	1.30	0.95
3:A:504:PEG:H22	1:C:239:LYS:HG2	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ASN:HD22	1:C:133:ARG:HG3	1.31	0.94
1:C:104:ASP:H	1:C:376:HIS:HD2	0.98	0.93
1:D:104:ASP:H	1:D:376:HIS:HD2	1.05	0.91
1:B:104:ASP:H	1:B:376:HIS:HD2	1.04	0.91
1:C:104:ASP:H	1:C:376:HIS:CD2	1.88	0.91
1:D:133:ARG:NH2	1:D:136:GLU:OE1	2.03	0.90
1:C:314[B]:LYS:CG	1:C:315:GLU:H	1.81	0.89
1:B:210:ASP:HB3	7:B:750:HOH:O	1.73	0.89
1:D:133:ARG:HH21	1:D:136:GLU:CD	1.81	0.88
1:A:320:LEU:HD13	1:A:331:MET:CE	2.03	0.87
1:A:104:ASP:H	1:A:376:HIS:CD2	1.92	0.86
1:C:249:ASP:O	4:C:505:EDO:H22	1.76	0.85
1:C:379:ASN:H	1:C:379:ASN:HD22	1.23	0.85
1:B:379:ASN:OD1	6:B:503:ACY:H1	1.75	0.85
1:B:78:GLU:HG2	1:B:400:LEU:HD23	1.60	0.83
1:A:320:LEU:CD1	1:A:331:MET:HE1	2.08	0.83
1:C:132:ASN:ND2	1:C:133:ARG:HG3	1.93	0.82
1:D:320:LEU:HA	1:D:331:MET:HE1	1.61	0.82
1:D:331:MET:HE2	1:D:331:MET:CA	2.09	0.82
1:A:296:HIS:ND1	1:A:297:PRO:O	2.13	0.81
1:C:362:THR:HG21	7:C:620:HOH:O	1.80	0.81
1:B:364:SER:HB3	1:B:366:ASN:H	1.47	0.80
1:C:80:PHE:O	1:C:408:LYS:HE3	1.81	0.80
1:D:104:ASP:H	1:D:376:HIS:CD2	1.95	0.80
1:D:320:LEU:CB	1:D:331:MET:HE1	2.12	0.80
1:A:78:GLU:HG2	1:A:400:LEU:CD2	2.11	0.79
1:C:78:GLU:HG2	1:C:400:LEU:HD23	1.64	0.79
1:D:87:ARG:HH21	4:D:503:EDO:H21	1.48	0.79
1:B:104:ASP:H	1:B:376:HIS:CD2	1.96	0.78
1:D:78:GLU:HG2	1:D:400:LEU:CD2	2.13	0.76
1:D:320:LEU:CA	1:D:331:MET:HE1	2.17	0.75
1:A:199:GLN:NE2	1:A:249:ASP:H	1.86	0.74
1:A:199:GLN:HE21	1:A:249:ASP:H	1.33	0.74
1:C:124:THR:HG23	1:C:126:VAL:O	1.87	0.73
1:C:199:GLN:NE2	1:C:249:ASP:H	1.85	0.73
1:C:314[B]:LYS:CG	1:C:315:GLU:N	2.48	0.71
1:D:124:THR:HG23	1:D:126:VAL:O	1.90	0.71
1:C:82:GLN:NE2	7:C:749:HOH:O	2.24	0.71
1:A:124:THR:HG23	1:A:126:VAL:O	1.91	0.71
1:B:117:ILE:HD13	1:B:374:LEU:HD11	1.70	0.70
1:A:308:THR:O	4:A:505:EDO:C1	2.35	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:LEU:N	1:D:208:ARG:HA	2.05	0.70
1:C:228:HIS:HE1	1:C:231:ASP:OD1	1.75	0.69
1:D:104:ASP:N	1:D:376:HIS:HD2	1.86	0.69
1:D:320:LEU:HB2	1:D:331:MET:HE1	1.74	0.68
1:A:232:SER:HB3	1:C:175:PRO:HD2	1.76	0.68
1:A:347:SER:HB2	7:A:684:HOH:O	1.94	0.68
1:C:117:ILE:HD13	1:C:374:LEU:HD11	1.76	0.67
1:D:320:LEU:HA	1:D:331:MET:CE	2.24	0.67
1:C:199:GLN:HE21	1:C:249:ASP:H	1.40	0.67
1:C:322:ILE:HD12	1:C:329:TYR:CD1	2.29	0.67
1:C:379:ASN:HD22	1:C:379:ASN:N	1.94	0.66
1:C:207:LEU:N	1:C:208:ARG:HA	2.10	0.66
1:C:315:GLU:OE2	1:C:335[B]:LYS:HD2	1.95	0.65
1:C:124:THR:CG2	1:C:126:VAL:O	2.45	0.65
1:A:408:LYS:NZ	7:A:729:HOH:O	2.30	0.64
1:A:240:GLY:H	1:A:244:GLN:NE2	1.95	0.64
1:B:221:SER:O	1:B:223:ASP:O	2.16	0.64
1:D:82[B]:GLN:NE2	7:D:655:HOH:O	2.30	0.63
1:B:124:THR:HG23	1:B:126:VAL:O	1.98	0.63
1:A:104:ASP:N	1:A:376:HIS:HD2	1.88	0.62
1:A:228:HIS:HD2	7:A:739:HOH:O	1.83	0.62
1:C:78:GLU:HG2	1:C:400:LEU:CD2	2.30	0.62
1:C:314[B]:LYS:HD3	1:C:335[B]:LYS:NZ	2.15	0.62
1:A:175:PRO:HD2	1:C:232:SER:HB3	1.81	0.61
1:B:78:GLU:HG2	1:B:400:LEU:CD2	2.29	0.61
1:C:104:ASP:N	1:C:376:HIS:HD2	1.83	0.60
1:B:80:PHE:O	1:B:408:LYS:HE3	2.02	0.60
1:D:124:THR:HG21	1:D:142:PRO:HG3	1.84	0.60
1:C:347:SER:HB2	7:C:679:HOH:O	2.01	0.60
1:A:117:ILE:HD13	1:A:374:LEU:HD11	1.84	0.59
1:D:78:GLU:CG	1:D:400:LEU:HD23	2.24	0.59
1:C:348:LEU:CD1	1:D:419:TYR:CE2	2.87	0.58
1:A:281:HIS:HE1	1:A:305:GLY:O	1.87	0.57
1:A:368:ARG:HD3	1:A:401:ASP:OD2	2.04	0.57
1:A:243:ASP:OD2	1:A:295:LYS:NZ	2.35	0.57
1:D:320:LEU:CD1	1:D:331:MET:HE1	2.35	0.57
1:A:302:MET:HE1	1:A:310:TYR:OH	2.05	0.57
1:D:322:ILE:HD12	1:D:329:TYR:CD1	2.40	0.56
1:A:77:ASN:ND2	1:A:343:ALA:O	2.35	0.56
1:A:124:THR:CG2	1:A:126:VAL:O	2.52	0.56
1:A:298:LEU:HD22	1:A:298:LEU:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:GLN:NE2	1:D:249:ASP:H	2.04	0.56
1:B:113:GLY:O	4:B:506:EDO:H12	2.06	0.55
1:B:368:ARG:HD3	1:B:401:ASP:OD2	2.06	0.55
1:D:221:SER:O	1:D:223:ASP:O	2.24	0.55
1:C:383:ASN:OD1	1:C:383:ASN:C	2.50	0.54
1:B:368:ARG:NH2	1:B:401:ASP:OD1	2.37	0.54
1:D:124:THR:CG2	1:D:126:VAL:O	2.56	0.54
1:C:362:THR:HG23	1:C:364:SER:HB3	1.90	0.54
1:C:228:HIS:CE1	1:C:231:ASP:OD1	2.60	0.54
1:A:362:THR:CG2	1:A:364:SER:HB3	2.38	0.54
1:B:122:ARG:HB2	1:B:149:CYS:SG	2.47	0.54
1:A:76:ASP:HA	7:A:683[A]:HOH:O	2.08	0.53
1:B:322:ILE:HD12	1:B:329:TYR:CD1	2.44	0.53
1:B:87[B]:ARG:NH1	7:B:603:HOH:O	2.41	0.53
1:B:310:TYR:HE1	4:B:504:EDO:H11	1.74	0.52
1:B:124:THR:CG2	1:B:126:VAL:O	2.57	0.52
1:A:362:THR:HG23	1:A:364:SER:HB3	1.92	0.51
1:C:348:LEU:HD13	1:D:419:TYR:CE2	2.44	0.51
1:D:320:LEU:CD1	1:D:331:MET:CE	2.89	0.51
1:C:79:LEU:CD1	1:C:313:PHE:CZ	2.93	0.51
1:D:257:GLY:HA2	1:D:363:ASP:OD2	2.10	0.51
1:A:296:HIS:CG	1:A:297:PRO:HD2	2.46	0.51
1:A:296:HIS:CE1	1:A:297:PRO:O	2.64	0.50
1:B:364:SER:HB2	7:B:698:HOH:O	2.11	0.50
1:C:79:LEU:HD11	1:C:313:PHE:CZ	2.47	0.50
4:B:504:EDO:H12	7:B:733:HOH:O	2.10	0.50
1:D:240:GLY:H	1:D:244:GLN:NE2	2.09	0.50
1:A:232:SER:HB2	1:C:176:LYS:HG3	1.94	0.50
1:B:82:GLN:NE2	7:B:727:HOH:O	2.43	0.50
1:C:408:LYS:NZ	7:C:683:HOH:O	2.45	0.49
1:C:206:GLY:C	1:C:208:ARG:CB	2.85	0.49
1:C:77:ASN:ND2	1:C:343:ALA:O	2.39	0.49
1:D:281:HIS:CD2	1:D:308:THR:OG1	2.65	0.49
1:C:103:ARG:HB2	1:C:376:HIS:CD2	2.48	0.49
1:D:87:ARG:HE	4:D:503:EDO:C2	2.26	0.49
1:C:288:ASP:OD1	1:C:289:PRO:HD2	2.12	0.49
1:C:379:ASN:H	1:C:379:ASN:ND2	2.03	0.49
1:A:362:THR:HG21	7:A:709:HOH:O	2.12	0.49
1:D:267:TYR:O	1:D:268:ASN:HB2	2.13	0.48
1:B:257:GLY:HA2	1:B:363:ASP:OD2	2.13	0.48
1:D:87:ARG:NH2	4:D:503:EDO:H21	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:TRP:NE1	1:D:191:LYS:HD2	2.28	0.48
1:A:195:TYR:CZ	1:A:289:PRO:HG3	2.49	0.48
1:B:240:GLY:H	1:B:244:GLN:NE2	2.11	0.48
1:C:132:ASN:HD22	1:C:133:ARG:CG	2.15	0.48
1:C:314[B]:LYS:HG3	1:C:315:GLU:N	2.28	0.48
1:D:320:LEU:HD13	1:D:331:MET:CE	2.44	0.48
1:A:320:LEU:CD1	1:A:331:MET:CE	2.79	0.48
1:A:78:GLU:CG	1:A:400:LEU:HD23	2.25	0.48
1:D:80:PHE:CD2	1:D:80:PHE:C	2.91	0.48
1:D:167:VAL:HG23	7:D:682:HOH:O	2.13	0.48
1:C:135:LYS:HE3	7:C:682:HOH:O	2.13	0.48
1:A:327:GLU:OE1	1:B:347:SER:HB2	2.14	0.47
1:D:309:THR:O	1:D:319:THR:HG23	2.14	0.47
1:B:78:GLU:CG	1:B:400:LEU:HD23	2.40	0.47
1:C:294:GLU:HB3	7:C:717:HOH:O	2.14	0.47
1:B:267:TYR:O	1:B:268:ASN:HB2	2.15	0.47
1:A:82[A]:GLN:NE2	1:A:409:ASN:HB2	2.29	0.47
1:C:301:VAL:HG22	1:C:338:VAL:O	2.15	0.47
1:D:122:ARG:HB2	1:D:149:CYS:SG	2.54	0.47
1:B:364:SER:CB	1:B:366:ASN:H	2.24	0.47
1:A:310:TYR:HE1	4:A:505:EDO:H21	1.79	0.47
1:B:364:SER:HB3	1:B:366:ASN:N	2.22	0.47
1:C:281:HIS:HE1	1:C:305:GLY:O	1.97	0.46
1:A:177:PRO:HA	1:A:202:ASN:OD1	2.16	0.46
1:C:104:ASP:O	1:C:185:PRO:HD2	2.16	0.46
1:B:117:ILE:HD13	1:B:374:LEU:CD1	2.44	0.46
1:B:379:ASN:OD1	6:B:503:ACY:CH3	2.58	0.46
1:A:315:GLU:H	1:A:315:GLU:HG3	1.51	0.46
1:C:78:GLU:CG	1:C:400:LEU:HD23	2.43	0.45
1:C:115:TYR:O	1:C:155:THR:HA	2.16	0.45
1:C:174:LYS:HA	1:C:175:PRO:HA	1.70	0.45
1:C:124:THR:HG21	1:C:142:PRO:HG3	1.99	0.45
1:C:248:HIS:HB2	1:C:264:LYS:HG2	1.99	0.45
1:B:156:SER:HB2	1:B:162:TRP:CD2	2.52	0.45
1:B:224:GLY:HA3	1:B:225:PRO:HA	1.85	0.45
1:B:377:PHE:HD1	6:B:503:ACY:H2	1.82	0.45
1:A:339:ASN:HA	7:A:741:HOH:O	2.17	0.44
1:B:117:ILE:HG12	1:B:162:TRP:CZ3	2.52	0.44
1:C:308:THR:HB	1:C:319:THR:CG2	2.46	0.44
1:D:228:HIS:HE1	1:D:231:ASP:OD1	2.00	0.44
1:B:87[B]:ARG:HD2	7:B:603:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:TYR:OH	1:C:335[B]:LYS:HD3	2.17	0.44
1:B:268:ASN:HD22	1:B:268:ASN:HA	1.61	0.44
1:D:123:ASP:O	4:D:505:EDO:O1	2.36	0.44
1:A:320:LEU:HB2	1:A:331:MET:HE1	2.00	0.44
1:B:281:HIS:HE1	1:B:305:GLY:O	2.00	0.44
1:B:88:LEU:HD23	1:B:88:LEU:HA	1.84	0.44
1:D:364:SER:HB3	1:D:366:ASN:H	1.83	0.44
1:C:314[B]:LYS:HD3	1:C:335[B]:LYS:HZ2	1.82	0.43
1:D:364:SER:C	1:D:366:ASN:H	2.25	0.43
1:D:320:LEU:HD13	1:D:331:MET:HE3	2.00	0.43
1:D:288:ASP:OD1	1:D:289:PRO:HD2	2.19	0.43
1:A:79:LEU:HD12	1:A:79:LEU:HA	1.75	0.43
1:A:88:LEU:HD21	1:A:393:ARG:HB2	1.99	0.43
1:B:228:HIS:HE1	1:B:231:ASP:OD1	2.01	0.43
1:B:408:LYS:NZ	7:B:675:HOH:O	2.50	0.43
1:C:308:THR:HB	1:C:319:THR:HG21	1.99	0.43
1:D:88:LEU:HD21	1:D:393:ARG:HB2	1.99	0.43
1:B:383:ASN:HA	1:B:384:PRO:HD3	1.77	0.43
1:C:117:ILE:HD13	1:C:374:LEU:CD1	2.46	0.43
1:C:348:LEU:HD12	1:D:419:TYR:CE2	2.53	0.43
1:A:103:ARG:HB2	1:A:376:HIS:CD2	2.53	0.43
1:A:124:THR:HG21	1:A:142:PRO:HG3	2.00	0.43
1:A:248:HIS:HB2	1:A:264:LYS:HG2	2.01	0.43
1:D:331:MET:HA	1:D:331:MET:CE	2.29	0.43
1:A:117:ILE:CD1	1:A:374:LEU:HD11	2.49	0.43
1:C:177:PRO:HA	1:C:202:ASN:OD1	2.18	0.43
1:D:156:SER:HB2	1:D:162:TRP:CD2	2.54	0.43
1:C:79:LEU:HD11	1:C:313:PHE:CE2	2.53	0.43
1:B:174:LYS:HA	1:B:175:PRO:HA	1.68	0.42
1:D:79:LEU:HD13	1:D:313:PHE:CZ	2.54	0.42
1:B:248:HIS:HB2	1:B:264:LYS:HG2	2.01	0.42
1:C:207:LEU:N	1:C:208:ARG:CA	2.81	0.42
1:C:362:THR:CG2	1:C:364:SER:HB3	2.49	0.42
1:C:379:ASN:N	1:C:379:ASN:ND2	2.64	0.42
1:A:300:PRO:HB2	1:A:302:MET:O	2.19	0.42
1:A:296:HIS:CG	1:A:297:PRO:CD	3.03	0.42
1:B:124:THR:HG21	1:B:142:PRO:HG3	2.01	0.42
1:C:242:TRP:CG	1:C:243:ASP:N	2.88	0.42
1:D:133:ARG:NH2	1:D:136:GLU:CD	2.64	0.42
1:D:177:PRO:HA	1:D:202:ASN:OD1	2.20	0.42
1:A:77:ASN:HA	7:A:738:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:LEU:O	1:D:216:VAL:HA	2.20	0.42
1:B:76:ASP:OD1	1:B:76:ASP:N	2.53	0.41
1:C:211:TRP:HZ3	1:C:245:ASP:OD1	2.02	0.41
1:B:329:TYR:HD2	1:B:347:SER:HA	1.85	0.41
1:D:123:ASP:O	4:D:505:EDO:C1	2.68	0.41
1:B:104:ASP:N	1:B:376:HIS:HD2	1.89	0.41
7:C:767:HOH:O	1:D:417:GLU:HG3	2.19	0.41
1:D:323:LYS:N	1:D:323:LYS:HD2	2.36	0.41
1:A:156:SER:HB2	1:A:162:TRP:CD2	2.55	0.41
1:D:79:LEU:HD23	1:D:343:ALA:CB	2.50	0.41
1:A:208:ARG:HB2	1:A:209:GLY:H	1.74	0.41
1:A:210:ASP:O	1:A:211:TRP:HB2	2.21	0.41
1:B:252:PRO:HA	1:B:261:LEU:HA	2.02	0.41
1:C:267:TYR:O	1:C:277:TYR:HA	2.20	0.41
1:C:296:HIS:CG	1:C:297:PRO:HD2	2.56	0.41
1:A:302:MET:HG2	7:A:697:HOH:O	2.19	0.40
1:A:419:TYR:CE2	1:B:348:LEU:HD12	2.55	0.40
1:A:268:ASN:HD22	1:A:268:ASN:HA	1.62	0.40
1:C:260:HIS:HE1	7:C:766:HOH:O	2.03	0.40
1:A:82[A]:GLN:HE21	1:A:407:TYR:C	2.29	0.40
1:A:404:ASP:HA	1:A:405:PRO:HD2	1.92	0.40
1:C:348:LEU:HD12	1:D:419:TYR:CD2	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	Interatomic distance (Å)	Clash overlap (Å)
7:D:601:HOH:O	7:D:601:HOH:O[2_555]	2.02	0.18

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	341/433 (79%)	322 (94%)	18 (5%)	1 (0%)	36	46
1	B	343/433 (79%)	327 (95%)	15 (4%)	1 (0%)	36	46
1	C	341/433 (79%)	327 (96%)	14 (4%)	0	100	100
1	D	340/433 (78%)	328 (96%)	12 (4%)	0	100	100
All	All	1365/1732 (79%)	1304 (96%)	59 (4%)	2 (0%)	48	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	211	TRP
1	B	132	ASN

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	274/366 (75%)	254 (93%)	20 (7%)	13	18
1	B	277/366 (76%)	257 (93%)	20 (7%)	13	18
1	C	277/366 (76%)	260 (94%)	17 (6%)	17	24
1	D	274/366 (75%)	254 (93%)	20 (7%)	13	18
All	All	1102/1464 (75%)	1025 (93%)	77 (7%)	13	19

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LEU
1	A	112	ASN
1	A	124	THR
1	A	126	VAL
1	A	129	ILE
1	A	139	ASP
1	A	208	ARG
1	A	264	LYS
1	A	279	VAL

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Mol	Chain	Res	Type
1	A	294	GLU
1	A	298	LEU
1	A	301	VAL
1	A	302	MET
1	A	303	THR
1	A	315	GLU
1	A	348	LEU
1	A	362	THR
1	A	374	LEU
1	A	376	HIS
1	A	417	GLU
1	B	79	LEU
1	B	124	THR
1	B	126	VAL
1	B	129	ILE
1	B	136	GLU
1	B	175	PRO
1	B	203	GLU
1	B	205	SER
1	B	207	LEU
1	B	264	LYS
1	B	301	VAL
1	B	307	GLU
1	B	315	GLU
1	B	319	THR
1	B	324	ASP
1	B	362	THR
1	B	364	SER
1	B	376	HIS
1	B	408	LYS
1	B	410	THR
1	C	79	LEU
1	C	112	ASN
1	C	124	THR
1	C	126	VAL
1	C	132	ASN
1	C	135	LYS
1	C	205	SER
1	C	243	ASP
1	C	268	ASN
1	C	301	VAL
1	C	303	THR

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Mol	Chain	Res	Type
1	C	319	THR
1	C	362	THR
1	C	376	HIS
1	C	379	ASN
1	C	408	LYS
1	C	410	THR
1	D	79	LEU
1	D	124	THR
1	D	126	VAL
1	D	139	ASP
1	D	167	VAL
1	D	184	THR
1	D	205	SER
1	D	294	GLU
1	D	298	LEU
1	D	301	VAL
1	D	302	MET
1	D	303	THR
1	D	315	GLU
1	D	323	LYS
1	D	348	LEU
1	D	362	THR
1	D	374	LEU
1	D	376	HIS
1	D	412	VAL
1	D	417	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	95	ASN
1	A	199	GLN
1	A	244	GLN
1	A	268	ASN
1	A	281	HIS
1	A	376	HIS
1	A	382	ASN
1	A	422	GLN
1	B	94	ASN
1	B	95	ASN
1	B	228	HIS

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Mol	Chain	Res	Type
1	B	244	GLN
1	B	268	ASN
1	B	281	HIS
1	B	339	ASN
1	B	376	HIS
1	B	382	ASN
1	B	422	GLN
1	C	94	ASN
1	C	95	ASN
1	C	132	ASN
1	C	199	GLN
1	C	228	HIS
1	C	260	HIS
1	C	281	HIS
1	C	306	HIS
1	C	376	HIS
1	C	379	ASN
1	C	422	GLN
1	D	94	ASN
1	D	95	ASN
1	D	228	HIS
1	D	244	GLN
1	D	248	HIS
1	D	260	HIS
1	D	268	ASN
1	D	281	HIS
1	D	376	HIS
1	D	382	ASN
1	D	422	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 22 ligands modelled in this entry, 9 are monoatomic - leaving 13 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	PEG	A	503	-	6,6,6	0.50	0	5,5,5	0.59	0
3	PEG	A	504	-	6,6,6	0.49	0	5,5,5	0.66	0
4	EDO	B	506	-	3,3,3	0.50	0	2,2,2	0.73	0
4	EDO	B	504	-	3,3,3	0.27	0	2,2,2	0.66	0
4	EDO	D	503	-	3,3,3	0.52	0	2,2,2	0.45	0
4	EDO	B	505	-	3,3,3	0.61	0	2,2,2	0.33	0
4	EDO	C	503	-	3,3,3	0.67	0	2,2,2	0.04	0
4	EDO	D	505	-	3,3,3	0.62	0	2,2,2	0.23	0
6	ACY	B	503	-	3,3,3	0.47	0	3,3,3	1.99	1 (33%)
4	EDO	C	504	-	3,3,3	0.55	0	2,2,2	0.37	0
4	EDO	C	505	-	3,3,3	0.35	0	2,2,2	0.29	0
4	EDO	D	504	-	3,3,3	0.54	0	2,2,2	0.47	0
4	EDO	A	505	-	3,3,3	0.27	0	2,2,2	0.82	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	PEG	A	503	-	-	3/4/4/4	-
3	PEG	A	504	-	-	2/4/4/4	-
4	EDO	B	506	-	-	1/1/1/1	-
4	EDO	B	504	-	-	1/1/1/1	-
4	EDO	D	503	-	-	1/1/1/1	-
4	EDO	B	505	-	-	1/1/1/1	-
4	EDO	C	503	-	-	0/1/1/1	-
4	EDO	D	505	-	-	1/1/1/1	-
4	EDO	C	504	-	-	0/1/1/1	-
4	EDO	C	505	-	-	0/1/1/1	-
4	EDO	D	504	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	505	-	-	1/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	503	ACY	O-C-CH3	-2.73	111.32	122.53

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	PEG	O1-C1-C2-O2
3	A	503	PEG	O2-C3-C4-O4
4	A	505	EDO	O1-C1-C2-O2
3	A	504	PEG	O2-C3-C4-O4
4	B	504	EDO	O1-C1-C2-O2
4	B	505	EDO	O1-C1-C2-O2
4	B	506	EDO	O1-C1-C2-O2
4	D	505	EDO	O1-C1-C2-O2
3	A	503	PEG	C1-C2-O2-C3
4	D	503	EDO	O1-C1-C2-O2
3	A	504	PEG	C4-C3-O2-C2
4	D	504	EDO	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	504	PEG	1	0
4	B	506	EDO	1	0
4	B	504	EDO	2	0
4	D	503	EDO	3	0
4	D	505	EDO	2	0
6	B	503	ACY	3	0
4	C	505	EDO	1	0
4	A	505	EDO	3	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	343/433 (79%)	-0.18	12 (3%)	47 49	17, 36, 70, 101	2 (0%)
1	B	343/433 (79%)	-0.17	17 (4%)	34 35	12, 35, 74, 122	4 (1%)
1	C	342/433 (78%)	-0.24	17 (4%)	34 35	14, 34, 70, 114	3 (0%)
1	D	343/433 (79%)	-0.17	14 (4%)	41 43	18, 36, 71, 111	1 (0%)
All	All	1371/1732 (79%)	-0.19	60 (4%)	39 41	12, 36, 73, 122	10 (0%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	207	LEU	4.8
1	C	208	ARG	4.2
1	B	327	GLU	4.1
1	C	326	ASN	3.9
1	B	207	LEU	3.6
1	A	276	LYS	3.6
1	C	323	LYS	3.6
1	C	327	GLU	3.5
1	B	277	TYR	3.5
1	C	324	ASP	3.5
1	A	425	ARG	3.5
1	B	131	TRP	3.4
1	C	268	ASN	3.4
1	B	208	ARG	3.3
1	D	131	TRP	3.3
1	B	209	GLY	3.3
1	C	76	ASP	3.2
1	C	277	TYR	3.2
1	C	209	GLY	3.2
1	C	132	ASN	3.1
1	D	277	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	328	ARG	3.1
1	D	276	LYS	3.0
1	A	298	LEU	3.0
1	A	209	GLY	3.0
1	D	304	SER	3.0
1	A	210	ASP	2.9
1	B	210	ASP	2.9
1	B	276	LYS	2.8
1	C	328	ARG	2.8
1	C	206	GLY	2.7
1	C	210	ASP	2.7
1	C	207	LEU	2.7
1	B	323	LYS	2.7
1	B	324	ASP	2.6
1	D	132	ASN	2.6
1	A	323	LYS	2.5
1	D	323	LYS	2.5
1	D	208	ARG	2.5
1	A	268	ASN	2.5
1	C	131	TRP	2.5
1	A	277	TYR	2.5
1	D	206	GLY	2.5
1	B	129	ILE	2.4
1	D	326	ASN	2.4
1	A	131	TRP	2.4
1	D	327	GLU	2.3
1	D	76	ASP	2.3
1	B	130	GLY	2.2
1	D	210	ASP	2.2
1	A	129	ILE	2.2
1	B	425	ARG	2.1
1	A	326	ASN	2.1
1	B	206	GLY	2.1
1	C	325	GLY	2.1
1	A	239	LYS	2.1
1	B	328	ARG	2.1
1	C	304	SER	2.1
1	B	326	ASN	2.0
1	B	76	ASP	2.0

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	EDO	C	503	4/4	0.73	0.26	66,66,74,83	0
4	EDO	B	506	4/4	0.76	0.21	66,73,74,78	0
4	EDO	D	505	4/4	0.76	0.25	68,69,70,78	0
4	EDO	C	504	4/4	0.77	0.17	73,76,79,80	0
4	EDO	D	504	4/4	0.79	0.19	69,72,77,77	0
4	EDO	B	505	4/4	0.82	0.23	54,55,66,71	0
3	PEG	A	504	7/7	0.83	0.23	63,81,92,93	0
6	ACY	B	503	4/4	0.83	0.20	57,66,69,70	0
4	EDO	D	503	4/4	0.85	0.16	70,72,79,80	0
3	PEG	A	503	7/7	0.86	0.20	62,72,84,87	0
5	NA	A	506	1/1	0.90	0.18	66,66,66,66	0
4	EDO	C	505	4/4	0.92	0.14	41,43,46,47	0
4	EDO	A	505	4/4	0.95	0.12	48,50,53,54	0
4	EDO	B	504	4/4	0.97	0.11	38,44,45,52	0
2	CA	C	501	1/1	0.99	0.02	45,45,45,45	0
2	CA	D	501	1/1	0.99	0.03	46,46,46,46	0
2	CA	A	501	1/1	0.99	0.02	49,49,49,49	0
2	CA	B	501	1/1	0.99	0.02	40,40,40,40	0
2	CA	B	502	1/1	1.00	0.02	27,27,27,27	0
2	CA	D	502	1/1	1.00	0.01	29,29,29,29	0
2	CA	A	502	1/1	1.00	0.01	27,27,27,27	0
2	CA	C	502	1/1	1.00	0.01	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.