



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:16 AM UTC

PDB ID : 5H80 / pdb_00005h80
Title : Biotin Carboxylase domain of single-chain bacterial carboxylase
Authors : Hagmann, A.; Hunkeler, M.; Stuttfeld, E.; Maier, T.
Deposited on : 2015-12-23
Resolution : 1.70 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

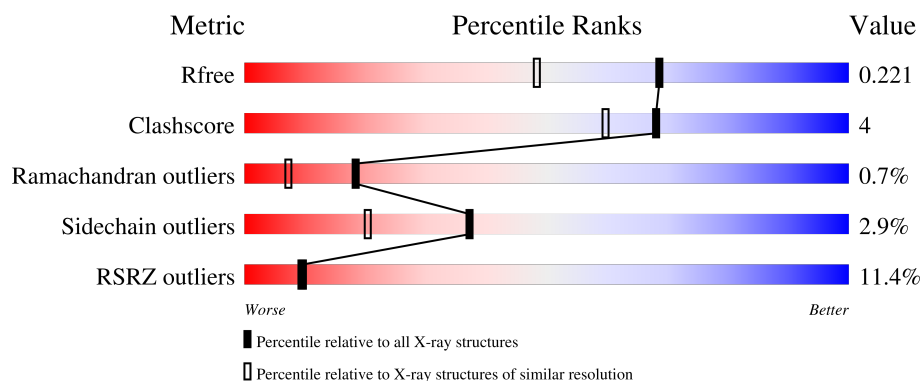
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	494	9% 69% 16% • 13%
1	B	494	11% 70% 15% • 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7305 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 Carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	2	0
			3256	2049	591	609	7			
1	B	426	Total	C	N	O	S	0	2	0
			3235	2040	585	603	7			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-29	MET	-	initiating methionine	UNP Q9RYK2
A	-28	ALA	-	expression tag	UNP Q9RYK2
A	-27	HIS	-	expression tag	UNP Q9RYK2
A	-26	HIS	-	expression tag	UNP Q9RYK2
A	-25	HIS	-	expression tag	UNP Q9RYK2
A	-24	HIS	-	expression tag	UNP Q9RYK2
A	-23	HIS	-	expression tag	UNP Q9RYK2
A	-22	HIS	-	expression tag	UNP Q9RYK2
A	-21	HIS	-	expression tag	UNP Q9RYK2
A	-20	HIS	-	expression tag	UNP Q9RYK2
A	-19	HIS	-	expression tag	UNP Q9RYK2
A	-18	HIS	-	expression tag	UNP Q9RYK2
A	-17	LYS	-	expression tag	UNP Q9RYK2
A	-16	LEU	-	expression tag	UNP Q9RYK2
A	-15	THR	-	expression tag	UNP Q9RYK2
A	-14	SER	-	expression tag	UNP Q9RYK2
A	-13	LEU	-	expression tag	UNP Q9RYK2
A	-12	TYR	-	expression tag	UNP Q9RYK2
A	-11	LYS	-	expression tag	UNP Q9RYK2
A	-10	LYS	-	expression tag	UNP Q9RYK2
A	-9	ALA	-	expression tag	UNP Q9RYK2
A	-8	GLY	-	expression tag	UNP Q9RYK2
A	-7	LEU	-	expression tag	UNP Q9RYK2
A	-6	GLU	-	expression tag	UNP Q9RYK2
A	-5	ASN	-	expression tag	UNP Q9RYK2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	LEU	-	expression tag	UNP Q9RYK2
A	-3	TYR	-	expression tag	UNP Q9RYK2
A	-2	PHE	-	expression tag	UNP Q9RYK2
A	-1	GLN	-	expression tag	UNP Q9RYK2
A	0	GLY	-	expression tag	UNP Q9RYK2
B	-29	MET	-	initiating methionine	UNP Q9RYK2
B	-28	ALA	-	expression tag	UNP Q9RYK2
B	-27	HIS	-	expression tag	UNP Q9RYK2
B	-26	HIS	-	expression tag	UNP Q9RYK2
B	-25	HIS	-	expression tag	UNP Q9RYK2
B	-24	HIS	-	expression tag	UNP Q9RYK2
B	-23	HIS	-	expression tag	UNP Q9RYK2
B	-22	HIS	-	expression tag	UNP Q9RYK2
B	-21	HIS	-	expression tag	UNP Q9RYK2
B	-20	HIS	-	expression tag	UNP Q9RYK2
B	-19	HIS	-	expression tag	UNP Q9RYK2
B	-18	HIS	-	expression tag	UNP Q9RYK2
B	-17	LYS	-	expression tag	UNP Q9RYK2
B	-16	LEU	-	expression tag	UNP Q9RYK2
B	-15	THR	-	expression tag	UNP Q9RYK2
B	-14	SER	-	expression tag	UNP Q9RYK2
B	-13	LEU	-	expression tag	UNP Q9RYK2
B	-12	TYR	-	expression tag	UNP Q9RYK2
B	-11	LYS	-	expression tag	UNP Q9RYK2
B	-10	LYS	-	expression tag	UNP Q9RYK2
B	-9	ALA	-	expression tag	UNP Q9RYK2
B	-8	GLY	-	expression tag	UNP Q9RYK2
B	-7	LEU	-	expression tag	UNP Q9RYK2
B	-6	GLU	-	expression tag	UNP Q9RYK2
B	-5	ASN	-	expression tag	UNP Q9RYK2
B	-4	LEU	-	expression tag	UNP Q9RYK2
B	-3	TYR	-	expression tag	UNP Q9RYK2
B	-2	PHE	-	expression tag	UNP Q9RYK2
B	-1	GLN	-	expression tag	UNP Q9RYK2
B	0	GLY	-	expression tag	UNP Q9RYK2

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



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

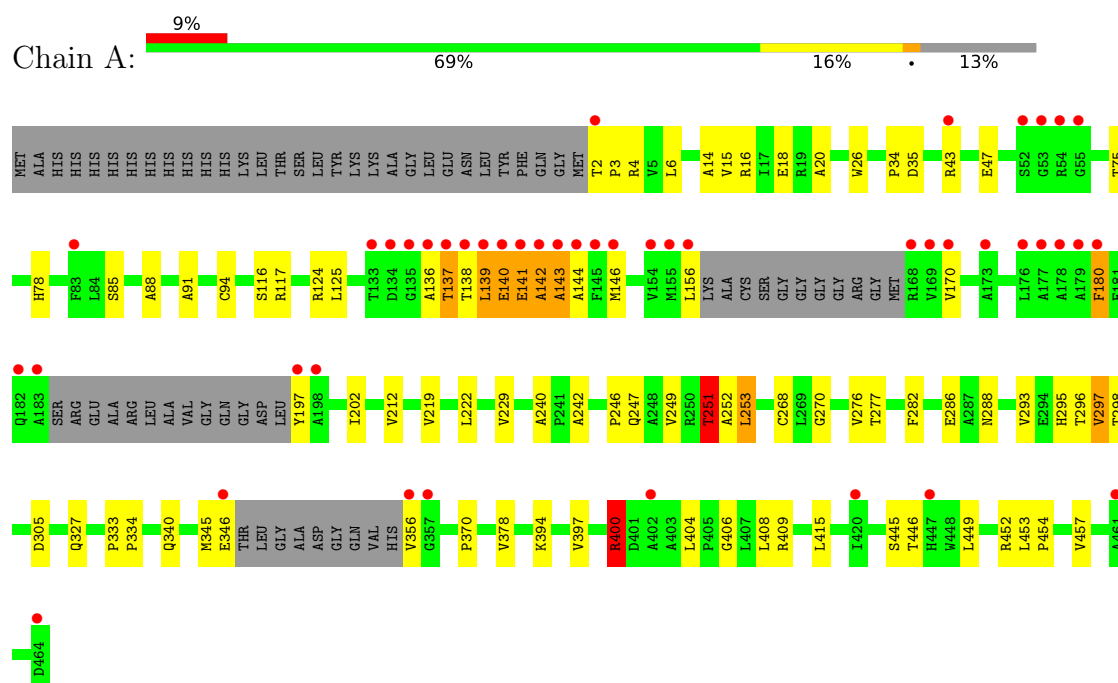
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	412	Total O 412 412	0	0
3	B	374	Total O 374 374	0	0

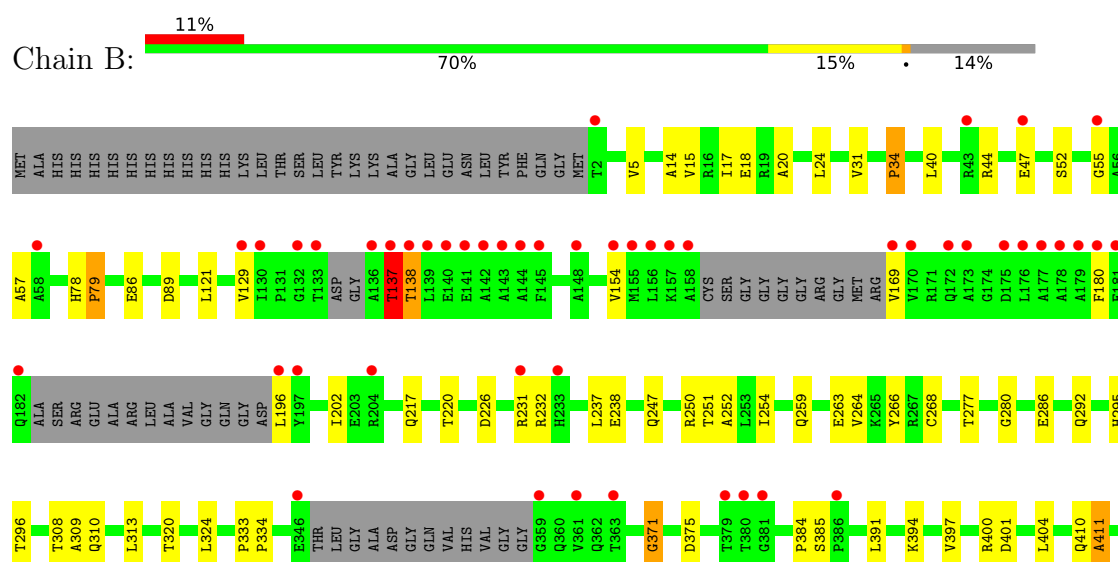
3 Residue-property plots [i](#)

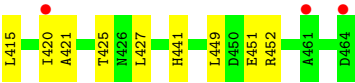
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Carboxylase



• Molecule 1: Carboxylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	138.10Å 138.10Å 97.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	75.74 – 1.70 75.74 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (75.74-1.70) 99.9 (75.74-1.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.149 , 0.184 (Not available) , 0.221	Depositor DCC
R_{free} test set	4741 reflections (4.07%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.694 for H, K, L 0.306 for K, H, -L	Depositor
Outliers	0 of 116229 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7305	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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

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	1.69	37/3323 (1.1%)	1.53	30/4534 (0.7%)
1	B	1.69	42/3301 (1.3%)	1.51	31/4503 (0.7%)
All	All	1.69	79/6624 (1.2%)	1.52	61/9037 (0.7%)

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	1

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	334	PRO	CA-C	10.87	1.57	1.51
1	B	320	THR	C-O	8.33	1.33	1.24
1	B	292	GLN	C-O	7.40	1.33	1.23
1	A	14	ALA	N-CA	-7.32	1.37	1.46
1	B	220	THR	C-O	7.27	1.32	1.23
1	B	310	GLN	C-O	7.25	1.32	1.24
1	B	18	GLU	C-O	-7.02	1.16	1.24
1	B	15	VAL	C-O	6.98	1.31	1.24
1	B	334	PRO	CA-C	-6.98	1.48	1.51
1	B	24	LEU	N-CA	-6.93	1.37	1.46
1	A	94	CYS	C-O	6.84	1.31	1.24
1	A	251	THR	CB-CG2	-6.79	1.30	1.52
1	A	20	ALA	CA-C	6.77	1.61	1.52
1	A	296	THR	C-O	6.68	1.31	1.24
1	A	117	ARG	CA-C	6.54	1.61	1.52
1	B	14	ALA	N-CA	-6.52	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	VAL	N-CA	6.49	1.54	1.46
1	A	305	ASP	C-O	6.43	1.31	1.23
1	B	252	ALA	CA-C	6.34	1.60	1.52
1	B	313	LEU	C-O	6.34	1.31	1.24
1	A	415	LEU	N-CA	-6.29	1.38	1.46
1	A	15	VAL	C-O	6.21	1.31	1.24
1	A	282	PHE	N-CA	6.17	1.53	1.45
1	B	226	ASP	C-O	-6.15	1.17	1.24
1	B	31	VAL	C-O	6.07	1.30	1.24
1	B	18	GLU	N-CA	6.07	1.53	1.46
1	B	259	GLN	N-CA	6.04	1.53	1.46
1	B	5	VAL	C-O	6.04	1.30	1.23
1	B	296	THR	N-CA	6.04	1.53	1.46
1	B	250	ARG	N-CA	5.93	1.53	1.46
1	B	410	GLN	C-O	-5.90	1.17	1.24
1	B	86	GLU	C-O	-5.87	1.16	1.24
1	B	129	VAL	N-CA	-5.85	1.39	1.46
1	B	266	TYR	CZ-OH	-5.80	1.25	1.38
1	A	252	ALA	C-O	5.76	1.30	1.24
1	B	79	PRO	N-CA	5.73	1.53	1.47
1	A	394	LYS	C-O	-5.73	1.17	1.24
1	A	293	VAL	C-O	5.67	1.30	1.24
1	A	445	SER	CA-CB	5.67	1.62	1.53
1	B	296	THR	C-O	5.67	1.30	1.24
1	B	371	GLY	C-O	5.63	1.31	1.23
1	A	397	VAL	CA-CB	-5.60	1.47	1.54
1	A	246	PRO	C-O	5.59	1.29	1.23
1	B	333	PRO	CA-C	5.57	1.55	1.52
1	B	89	ASP	C-O	-5.55	1.17	1.24
1	A	222	LEU	N-CA	5.52	1.52	1.46
1	B	401	ASP	N-CA	5.49	1.52	1.45
1	A	240	ALA	CA-C	5.47	1.59	1.52
1	A	446	THR	C-O	-5.46	1.17	1.24
1	A	406	GLY	CA-C	5.43	1.58	1.52
1	A	91	ALA	C-O	-5.41	1.17	1.24
1	B	78	HIS	C-N	5.38	1.38	1.33
1	B	264	VAL	C-O	-5.36	1.17	1.24
1	A	378	VAL	N-CA	5.36	1.52	1.46
1	B	286	GLU	N-CA	5.33	1.52	1.46
1	A	276	VAL	CA-CB	5.33	1.61	1.54
1	B	415	LEU	N-CA	-5.30	1.39	1.46
1	A	370	PRO	CA-C	5.27	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	ALA	N-CA	5.27	1.52	1.46
1	A	277	THR	CA-C	5.24	1.59	1.52
1	B	391	LEU	N-CA	5.24	1.52	1.46
1	A	296	THR	N-CA	5.20	1.52	1.46
1	A	229	VAL	CA-C	5.18	1.58	1.53
1	B	247	GLN	N-CA	-5.18	1.40	1.46
1	B	40	LEU	C-O	-5.16	1.17	1.24
1	B	421	ALA	N-CA	5.14	1.52	1.45
1	B	375	ASP	C-O	5.13	1.30	1.24
1	B	324	LEU	N-CA	-5.11	1.39	1.46
1	A	327	GLN	C-O	5.11	1.29	1.24
1	B	20	ALA	CA-C	5.11	1.59	1.52
1	A	35	ASP	C-O	-5.09	1.16	1.24
1	A	75	THR	C-O	-5.08	1.17	1.23
1	A	219	VAL	N-CA	-5.08	1.40	1.46
1	B	252	ALA	C-O	5.06	1.29	1.24
1	A	298	THR	N-CA	-5.05	1.40	1.46
1	A	88	ALA	CA-C	5.04	1.59	1.52
1	B	44	ARG	CA-C	5.03	1.59	1.52
1	A	6	LEU	CA-C	-5.02	1.46	1.52
1	B	411	ALA	N-CA	-5.01	1.40	1.46

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	GLU	N-CA-C	-10.21	100.23	111.36
1	A	14	ALA	N-CA-C	-9.43	101.08	111.36
1	A	78	HIS	CA-C-O	8.87	125.06	119.29
1	A	453	LEU	CA-C-N	-8.15	110.00	119.05
1	A	453	LEU	C-N-CA	-8.15	110.00	119.05
1	B	277	THR	CA-C-N	-8.01	110.47	119.28
1	B	277	THR	C-N-CA	-8.01	110.47	119.28
1	A	295	HIS	N-CA-C	-6.78	103.91	111.71
1	B	427	LEU	N-CA-C	6.67	119.11	111.11
1	A	333	PRO	CA-C-N	6.60	124.47	119.66
1	A	333	PRO	C-N-CA	6.60	124.47	119.66
1	B	295	HIS	N-CA-C	-6.47	104.27	111.71
1	B	309	ALA	O-C-N	6.34	128.60	122.07
1	B	404	LEU	N-CA-C	6.25	122.13	113.45
1	A	116	SER	N-CA-C	6.20	118.04	111.28
1	B	31	VAL	O-C-N	-6.14	116.59	123.03
1	A	251	THR	N-CA-CB	6.05	119.66	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	GLN	N-CA-C	-5.99	105.88	113.43
1	A	94	CYS	CA-C-N	5.97	128.59	120.54
1	A	94	CYS	C-N-CA	5.97	128.59	120.54
1	B	202	ILE	N-CA-CB	5.94	118.16	111.21
1	B	254	ILE	N-CA-C	5.91	116.65	110.62
1	A	333	PRO	O-C-N	5.89	123.92	121.15
1	B	57	ALA	CA-C-N	5.85	128.40	120.38
1	B	57	ALA	C-N-CA	5.85	128.40	120.38
1	B	333	PRO	O-C-N	5.85	123.90	121.15
1	A	452	ARG	NE-CZ-NH2	5.85	124.47	119.20
1	B	55	GLY	CA-C-N	5.82	128.01	120.44
1	B	55	GLY	C-N-CA	5.82	128.01	120.44
1	B	129	VAL	CA-C-N	5.82	131.40	120.11
1	B	129	VAL	C-N-CA	5.82	131.40	120.11
1	A	212	VAL	N-CA-C	5.82	117.73	108.89
1	A	34	PRO	N-CA-C	5.82	122.24	113.81
1	A	139	LEU	N-CA-C	5.71	122.96	110.80
1	B	308	THR	CA-C-N	5.70	127.85	120.44
1	B	308	THR	C-N-CA	5.70	127.85	120.44
1	A	400	ARG	NE-CZ-NH2	5.70	124.33	119.20
1	A	270	GLY	CA-C-O	-5.65	115.21	121.37
1	B	252	ALA	N-CA-C	5.63	117.10	111.07
1	B	394	LYS	CG-CD-CE	5.60	124.18	111.30
1	A	85	SER	N-CA-C	5.59	119.20	112.38
1	B	292	GLN	N-CA-C	5.52	118.70	110.14
1	B	280	GLY	CA-C-O	5.50	124.90	118.96
1	B	251	THR	N-CA-C	-5.49	105.38	111.36
1	B	385	SER	CA-C-N	-5.46	115.26	120.83
1	B	385	SER	C-N-CA	-5.46	115.26	120.83
1	A	404	LEU	N-CA-C	5.43	120.31	113.25
1	A	242	ALA	O-C-N	5.42	126.03	121.31
1	B	451	GLU	N-CA-C	5.42	117.95	111.71
1	A	295	HIS	O-C-N	5.35	128.48	122.22
1	A	16	ARG	CA-C-O	5.33	126.60	120.90
1	A	408	LEU	CA-C-N	5.30	127.34	120.44
1	A	408	LEU	C-N-CA	5.30	127.34	120.44
1	A	409	ARG	N-CA-C	-5.24	105.46	111.07
1	B	415	LEU	N-CA-C	5.24	117.90	111.82
1	B	34	PRO	N-CA-C	5.23	121.55	113.75
1	A	252	ALA	N-CA-C	5.21	117.04	111.36
1	A	251	THR	OG1-CB-CG2	5.13	119.56	109.30
1	B	441	HIS	N-CA-C	5.12	119.62	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17	ILE	CA-C-O	-5.09	115.66	120.95
1	A	143	ALA	N-CA-C	5.07	117.47	111.33

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	GLU	Mainchain

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	3256	0	3209	33	0
1	B	3235	0	3197	12	0
2	A	20	0	30	2	0
2	B	8	0	12	1	0
3	A	412	0	0	3	1
3	B	374	0	0	3	0
All	All	7305	0	6448	47	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 4.

All (47) 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:139:LEU:HD22	1:A:180:PHE:CE1	1.96	0.99
1:A:141:GLU:O	1:A:144:ALA:N	2.01	0.93
1:A:138:THR:OG1	1:A:141:GLU:HG3	1.76	0.85
1:A:138:THR:OG1	1:A:141:GLU:CG	2.33	0.76
2:B:501:EDO:H11	3:B:685:HOH:O	1.85	0.76
1:B:137:THR:OG1	1:B:138:THR:N	2.22	0.70
1:A:141:GLU:OE1	1:A:141:GLU:C	2.37	0.67
1:A:141:GLU:O	1:A:142:ALA:C	2.39	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:PHE:HD2	1:A:180:PHE:C	2.06	0.63
1:A:180:PHE:C	1:A:180:PHE:CD2	2.77	0.63
1:A:141:GLU:OE1	1:A:142:ALA:N	2.34	0.60
1:B:397[A]:VAL:HG21	1:B:411:ALA:HA	1.84	0.60
1:A:137:THR:HG23	1:A:139:LEU:HG	1.85	0.59
1:A:400:ARG:HH21	1:A:400:ARG:HG2	1.68	0.56
1:A:124:ARG:NH1	2:A:504:EDO:O1	2.41	0.54
1:A:156:LEU:O	1:A:197:TYR:N	2.41	0.53
1:A:4:ARG:NH2	1:A:47:GLU:OE1	2.37	0.52
1:A:141:GLU:O	1:A:143:ALA:N	2.43	0.51
1:A:286:GLU:HG2	1:A:288:ASN:HD21	1.76	0.51
1:A:141:GLU:C	1:A:143:ALA:N	2.69	0.50
1:B:180:PHE:O	1:B:196:LEU:HD11	2.11	0.50
1:A:139:LEU:HD22	1:A:180:PHE:CZ	2.46	0.49
1:A:124:ARG:NH2	3:A:608:HOH:O	2.45	0.49
1:B:452:ARG:NH1	3:B:611:HOH:O	2.45	0.48
1:A:136:ALA:O	1:A:137:THR:HB	2.14	0.48
1:B:449:LEU:HD23	1:B:449:LEU:C	2.39	0.48
1:A:249:VAL:HG12	1:A:253:LEU:HD22	1.96	0.48
1:A:449:LEU:C	1:A:449:LEU:HD23	2.40	0.47
1:B:137:THR:HG22	1:B:196:LEU:O	2.14	0.47
1:A:247:GLN:O	1:A:251:THR:HG23	2.14	0.47
1:B:371:GLY:O	1:B:397[B]:VAL:HA	2.14	0.47
1:B:420:ILE:HD12	1:B:425:THR:HG21	1.97	0.47
1:A:297[A]:VAL:HG13	1:A:340:GLN:HB2	1.97	0.46
1:A:3:PRO:HG2	1:A:26:TRP:CD2	2.51	0.45
1:B:237:LEU:C	1:B:238:GLU:HG3	2.39	0.45
1:A:454:PRO:HA	1:A:457:VAL:HG22	1.98	0.45
1:A:400:ARG:HH21	1:A:400:ARG:CG	2.31	0.44
1:A:146:MET:HE1	1:A:170:VAL:HG12	2.00	0.43
2:A:503:EDO:O2	3:A:602:HOH:O	2.21	0.43
1:B:121:LEU:HD11	1:B:263:GLU:HG2	2.00	0.43
1:A:449:LEU:HD23	1:A:449:LEU:O	2.18	0.42
1:B:52:SER:HB3	3:B:941:HOH:O	2.18	0.42
1:A:345:MET:O	1:A:346:GLU:HB3	2.20	0.42
1:B:231:ARG:O	1:B:232:ARG:C	2.62	0.41
1:A:286:GLU:HG2	1:A:288:ASN:ND2	2.36	0.41
1:A:43:ARG:NE	3:A:612:HOH:O	2.53	0.40
1:A:136:ALA:O	1:A:137:THR:CB	2.69	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)
3:A:731:HOH:O	3:A:932:HOH:O[6_554]	2.00	0.20

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	424/494 (86%)	409 (96%)	12 (3%)	3 (1%)	18	7
1	B	418/494 (85%)	406 (97%)	9 (2%)	3 (1%)	18	7
All	All	842/988 (85%)	815 (97%)	21 (2%)	6 (1%)	18	7

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	THR
1	A	142	ALA
1	A	268	CYS
1	B	268	CYS
1	B	137	THR
1	B	138	THR

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	326/371 (88%)	314 (96%)	12 (4%)	30	14
1	B	325/371 (88%)	317 (98%)	8 (2%)	42	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	651/742 (88%)	631 (97%)	20 (3%)	37	18

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	125	LEU
1	A	140	GLU
1	A	141	GLU
1	A	180	PHE
1	A	202	ILE
1	A	251	THR
1	A	253	LEU
1	A	297[A]	VAL
1	A	297[B]	VAL
1	A	356	VAL
1	A	400	ARG
1	B	34	PRO
1	B	47	GLU
1	B	79	PRO
1	B	137	THR
1	B	154	VAL
1	B	169	VAL
1	B	384	PRO
1	B	400	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	HIS
1	A	447	HIS
1	A	459	GLN
1	B	72	HIS
1	B	360	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 ligands 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	$\# Z > 2$
2	EDO	A	504	-	3,3,3	0.27	0	2,2,2	0.40	0
2	EDO	A	503	-	3,3,3	0.58	0	2,2,2	0.62	0
2	EDO	A	505	-	3,3,3	0.43	0	2,2,2	0.97	0
2	EDO	A	501	-	3,3,3	0.33	0	2,2,2	0.46	0
2	EDO	B	501	-	3,3,3	0.42	0	2,2,2	0.56	0
2	EDO	A	502	-	3,3,3	0.43	0	2,2,2	0.52	0
2	EDO	B	502	-	3,3,3	0.88	0	2,2,2	0.50	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	504	-	-	0/1/1/1	-
2	EDO	A	503	-	-	0/1/1/1	-
2	EDO	A	505	-	-	0/1/1/1	-
2	EDO	A	501	-	-	1/1/1/1	-
2	EDO	B	501	-	-	1/1/1/1	-
2	EDO	A	502	-	-	1/1/1/1	-
2	EDO	B	502	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	502	EDO	O1-C1-C2-O2
2	B	501	EDO	O1-C1-C2-O2
2	A	501	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	504	EDO	1	0
2	A	503	EDO	1	0
2	B	501	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	430/494 (87%)	0.68	45 (10%)	11 11	10, 29, 66, 93	2 (0%)
1	B	426/494 (86%)	0.77	53 (12%)	8 8	11, 29, 62, 106	2 (0%)
All	All	856/988 (86%)	0.72	98 (11%)	10 9	10, 29, 64, 106	4 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	142	ALA	7.2
1	A	139	LEU	7.2
1	B	169	VAL	6.7
1	A	356	VAL	6.4
1	A	197	TYR	6.2
1	A	137	THR	6.1
1	B	158	ALA	6.0
1	B	136	ALA	5.9
1	A	177	ALA	5.8
1	B	156	LEU	5.6
1	A	136	ALA	5.4
1	B	139	LEU	5.3
1	A	169	VAL	5.1
1	B	142	ALA	4.9
1	B	180	PHE	4.9
1	B	138	THR	4.6
1	A	133	THR	4.5
1	B	182	GLN	4.3
1	A	143	ALA	4.3
1	B	143	ALA	4.3
1	B	157	LYS	4.3
1	A	138	THR	4.2
1	A	179	ALA	4.2
1	A	180	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	197	TYR	4.2
1	B	177	ALA	4.0
1	A	198	ALA	3.9
1	A	135	GLY	3.9
1	B	204	ARG	3.9
1	B	133	THR	3.8
1	B	179	ALA	3.6
1	A	83	PHE	3.6
1	A	156	LEU	3.6
1	B	379	THR	3.5
1	A	357	GLY	3.5
1	B	137	THR	3.5
1	B	178	ALA	3.4
1	B	196	LEU	3.4
1	B	181	GLU	3.4
1	A	178	ALA	3.4
1	A	134	ASP	3.4
1	A	176	LEU	3.3
1	B	145	PHE	3.3
1	A	168	ARG	3.3
1	A	183	ALA	3.2
1	B	359	GLY	3.0
1	B	140	GLU	3.0
1	B	420	ILE	3.0
1	A	144	ALA	3.0
1	A	43	ARG	2.9
1	B	148	ALA	2.9
1	B	47	GLU	2.8
1	A	55	GLY	2.8
1	B	173	ALA	2.7
1	A	155	MET	2.7
1	B	154	VAL	2.7
1	A	2	THR	2.7
1	B	176	LEU	2.6
1	A	140	GLU	2.6
1	B	461	ALA	2.6
1	A	53	GLY	2.6
1	A	141	GLU	2.6
1	B	346	GLU	2.6
1	B	381	GLY	2.6
1	A	154	VAL	2.6
1	B	58	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	144	ALA	2.5
1	B	464	ASP	2.5
1	A	346	GLU	2.5
1	A	182	GLN	2.5
1	B	363	THR	2.5
1	B	155	MET	2.4
1	A	461	ALA	2.4
1	A	464	ASP	2.4
1	B	55	GLY	2.4
1	B	132	GLY	2.3
1	B	380	THR	2.3
1	B	170	VAL	2.3
1	B	141	GLU	2.3
1	B	43	ARG	2.3
1	A	170	VAL	2.3
1	B	386	PRO	2.3
1	A	54	ARG	2.2
1	A	146	MET	2.2
1	A	173	ALA	2.2
1	A	402	ALA	2.2
1	B	175	ASP	2.2
1	B	172	GLN	2.2
1	A	420	ILE	2.2
1	B	231	ARG	2.1
1	A	52	SER	2.1
1	B	129	VAL	2.1
1	B	2	THR	2.0
1	A	145	PHE	2.0
1	B	130	ILE	2.0
1	B	361	VAL	2.0
1	A	447	HIS	2.0
1	B	233	HIS	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 [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
2	EDO	A	503	4/4	0.75	0.19	45,53,57,67	0
2	EDO	A	504	4/4	0.84	0.15	53,56,57,58	0
2	EDO	A	502	4/4	0.88	0.17	38,45,49,55	0
2	EDO	A	505	4/4	0.89	0.14	38,41,43,50	0
2	EDO	A	501	4/4	0.91	0.12	39,40,43,46	0
2	EDO	B	501	4/4	0.91	0.15	37,37,46,47	0
2	EDO	B	502	4/4	0.91	0.14	27,28,30,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.