



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:33 AM UTC

PDB ID : 1J9W / pdb_00001j9w
Title : Solution Structure of the CAI Michigan 1 Variant
Authors : Briganti, F.; Ferraroni, M.; Chedwiggen, W.R.; Scozzafava, A.; Supuran, C.T.;
Tilli, S.
Deposited on : 2001-05-29
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

<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

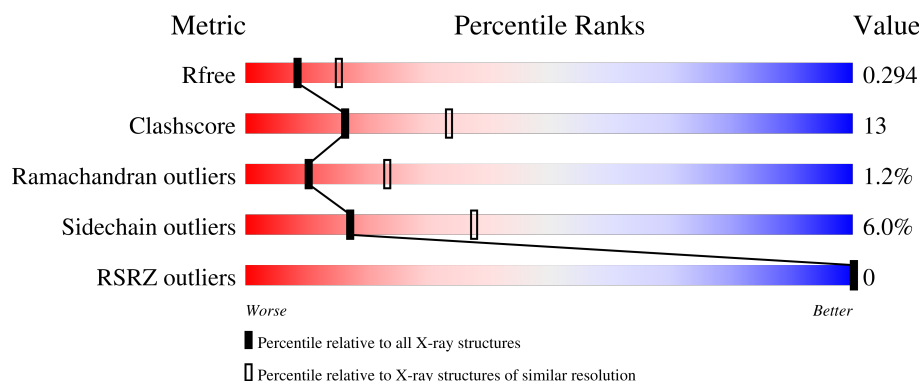
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	260	 66% 27% 5% ..
1	B	260	 58% 32% 7% ..

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
3	EDO	A	401	-	X	-	-
3	EDO	B	402	-	X	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4311 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 CARBONIC ANHYDRASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			1997	1259	347	388	3			
1	B	256	Total	C	N	O	S	0	2	0
			1983	1253	345	382	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	ARG	HIS	engineered mutation	UNP P00915
B	67	ARG	HIS	engineered mutation	UNP P00915

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

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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

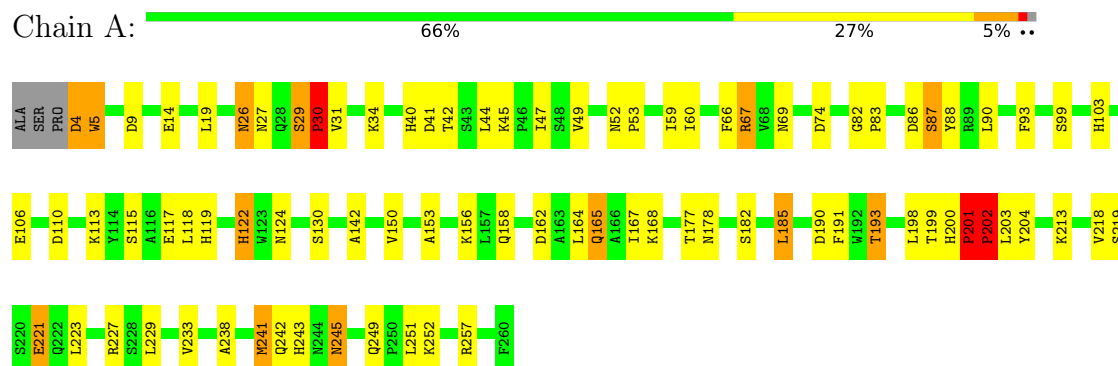
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	154	Total	O	0	0
			154	154		
4	B	167	Total	O	0	0
			167	167		

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: CARBONIC ANHYDRASE I



• Molecule 1: CARBONIC ANHYDRASE I



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.88Å 71.73Å 120.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 15.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.60) 98.8 (15.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.49Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.205 , 0.311 0.199 , 0.294	Depositor DCC
R_{free} test set	979 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	13.1	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4311	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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 21.86 % 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 6.4168e-03. 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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.59	1/2053 (0.0%)	2.00	58/2794 (2.1%)
1	B	0.58	1/2048 (0.0%)	2.04	72/2787 (2.6%)
All	All	0.58	2/4101 (0.0%)	2.02	130/5581 (2.3%)

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	4
1	B	0	3
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	201	PRO	CA-C	-5.99	1.46	1.52
1	B	201	PRO	CA-C	-5.21	1.47	1.52

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	PRO	CA-C-O	-19.46	92.34	120.56
1	B	29	SER	O-C-N	17.38	141.31	121.32
1	B	201	PRO	CA-C-O	-17.34	95.42	120.56
1	B	202	PRO	CA-N-CD	-14.98	91.02	112.00
1	A	202	PRO	CA-N-CD	-13.74	92.26	111.50
1	A	29	SER	O-C-N	13.03	136.31	121.32
1	A	201	PRO	O-C-N	-12.24	107.01	121.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	LYS	CA-CB-CG	11.77	137.64	114.10
1	A	29	SER	CA-C-O	-11.49	104.42	120.16
1	A	4	ASP	CA-CB-CG	10.45	123.05	112.60
1	A	30	PRO	CA-N-CD	-10.22	97.69	112.00
1	B	201	PRO	O-C-N	-9.78	109.92	121.46
1	B	29	SER	CA-C-O	-9.32	107.39	120.16
1	A	165	GLN	O-C-N	-9.16	110.15	122.43
1	A	74	ASP	CA-CB-CG	9.05	121.65	112.60
1	A	165	GLN	CB-CA-C	8.93	128.97	110.31
1	B	29	SER	N-CA-C	8.34	128.24	109.81
1	A	4	ASP	CA-C-N	8.13	137.07	121.54
1	A	4	ASP	C-N-CA	8.13	137.07	121.54
1	B	237	ASN	OD1-CG-ND2	-8.10	114.50	122.60
1	A	162	ASP	CA-CB-CG	8.00	120.60	112.60
1	B	8	ASP	CA-CB-CG	7.86	120.46	112.60
1	A	49	VAL	CA-C-O	7.75	128.52	120.39
1	B	176	PHE	CA-CB-CG	7.71	121.50	113.80
1	A	14	GLU	CA-CB-CG	7.63	129.37	114.10
1	A	201	PRO	C-N-CD	-7.60	103.88	120.60
1	B	151	GLY	CA-C-O	-7.56	115.69	120.91
1	B	195	PRO	CA-C-O	-7.56	112.41	121.48
1	A	26	ASN	OD1-CG-ND2	-7.49	115.11	122.60
1	B	30	PRO	N-CA-C	-7.43	97.17	112.47
1	B	245	ASN	CA-CB-CG	7.42	120.03	112.60
1	A	66	PHE	CA-CB-CG	7.42	121.22	113.80
1	A	9	ASP	CA-CB-CG	-7.40	105.20	112.60
1	A	164	LEU	CA-C-O	7.34	128.41	119.31
1	B	250	PRO	CA-C-O	-7.20	113.13	121.34
1	A	5	TRP	N-CA-CB	7.03	122.36	110.49
1	B	66	PHE	CA-C-O	-6.93	113.54	121.58
1	B	202	PRO	N-CA-C	6.93	126.74	112.47
1	A	165	GLN	CA-C-O	6.75	127.69	119.38
1	B	64	HIS	CA-CB-CG	-6.70	107.10	113.80
1	A	90	LEU	CA-C-O	-6.67	113.86	121.19
1	B	158	GLN	CA-C-O	-6.63	113.52	120.55
1	A	165	GLN	CA-C-N	6.62	133.32	121.66
1	A	165	GLN	C-N-CA	6.62	133.32	121.66
1	A	165	GLN	N-CA-CB	-6.57	99.48	110.39
1	B	69	ASN	CA-CB-CG	-6.53	106.07	112.60
1	B	26	ASN	CA-CB-CG	-6.52	106.08	112.60
1	A	14	GLU	CB-CG-CD	6.51	123.66	112.60
1	A	30	PRO	N-CA-CB	6.50	110.07	103.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	PRO	N-CA-C	6.49	118.61	110.70
1	A	165	GLN	N-CA-C	-6.38	104.76	112.54
1	B	108	THR	CA-C-O	-6.37	113.66	121.11
1	A	249	GLN	CG-CD-NE2	6.34	125.91	116.40
1	B	146	VAL	CA-C-O	-6.32	113.76	120.39
1	B	15	GLN	CB-CA-C	-6.30	99.57	110.09
1	B	30	PRO	CA-N-CD	-6.28	103.21	112.00
1	A	42	THR	CB-CA-C	-6.23	101.10	110.88
1	B	15	GLN	CA-CB-CG	6.23	126.55	114.10
1	B	38	THR	N-CA-CB	6.22	119.13	110.17
1	B	190	ASP	CA-C-O	-6.18	114.22	120.96
1	A	40	HIS	CA-CB-CG	6.13	119.93	113.80
1	B	226	PHE	CA-CB-CG	6.07	119.87	113.80
1	B	101	ASN	CB-CA-C	6.04	120.88	110.01
1	B	201	PRO	CB-CA-C	6.02	118.26	110.92
1	B	191	PHE	CA-C-O	6.01	128.19	121.40
1	A	67	ARG	CD-NE-CZ	6.01	132.81	124.40
1	A	93	PHE	CA-CB-CG	6.00	119.80	113.80
1	B	47	ILE	O-C-N	-5.99	116.28	122.63
1	A	122	HIS	CA-CB-CG	5.99	119.79	113.80
1	A	30	PRO	N-CD-CG	5.98	112.17	103.20
1	B	101	ASN	CA-CB-CG	5.97	118.57	112.60
1	B	93	PHE	CA-CB-CG	5.94	119.74	113.80
1	A	241	MET	CA-C-O	-5.93	115.23	122.41
1	A	42	THR	N-CA-CB	5.93	118.60	110.01
1	A	118	LEU	CA-C-O	-5.91	114.04	120.36
1	B	72	ASP	N-CA-C	5.88	117.49	110.44
1	B	92	GLN	OE1-CD-NE2	-5.85	116.75	122.60
1	A	30	PRO	N-CA-C	5.83	124.49	112.47
1	A	257	ARG	NE-CZ-NH1	5.83	127.33	121.50
1	B	61	ASN	CA-CB-CG	5.82	118.42	112.60
1	A	156	LYS	O-C-N	-5.78	114.68	122.43
1	B	30	PRO	CB-CA-C	5.72	121.00	111.56
1	A	158	GLN	N-CA-CB	5.67	118.19	109.91
1	A	93	PHE	CA-C-O	-5.64	114.51	121.11
1	A	27	ASN	OD1-CG-ND2	-5.60	117.00	122.60
1	B	218	VAL	CA-C-O	-5.59	115.43	121.19
1	B	175	PRO	CA-C-O	-5.59	115.05	121.36
1	B	103	HIS	N-CA-C	5.53	118.51	107.62
1	B	232	ASN	CA-CB-CG	-5.50	107.10	112.60
1	A	52	ASN	CA-C-N	5.49	125.32	119.28
1	A	52	ASN	C-N-CA	5.49	125.32	119.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	11	ASN	OD1-CG-ND2	-5.49	117.11	122.60
1	B	69	ASN	OD1-CG-ND2	-5.48	117.12	122.60
1	A	257	ARG	CA-C-O	-5.47	114.47	120.43
1	B	86[A]	ASP	CA-CB-CG	-5.47	107.13	112.60
1	B	86[B]	ASP	CA-CB-CG	-5.47	107.13	112.60
1	A	200	HIS	O-C-N	5.46	127.59	121.32
1	B	153	ALA	CA-C-O	-5.45	115.20	121.19
1	A	200	HIS	CA-CB-CG	5.44	119.24	113.80
1	A	238	ALA	CB-CA-C	5.42	118.56	109.89
1	B	251	LEU	CA-C-N	5.36	129.78	122.34
1	B	251	LEU	C-N-CA	5.36	129.78	122.34
1	A	87	SER	CA-C-O	-5.35	114.50	120.54
1	B	24	ASN	OD1-CG-ND2	-5.34	117.26	122.60
1	B	75	ASN	CA-CB-CG	-5.33	107.27	112.60
1	B	87	SER	CA-C-N	5.33	130.93	122.94
1	B	87	SER	C-N-CA	5.33	130.93	122.94
1	B	200	HIS	O-C-N	5.33	127.45	121.32
1	A	249	GLN	OE1-CD-NE2	-5.31	117.29	122.60
1	A	4	ASP	CA-C-O	5.31	129.82	120.80
1	B	210	ILE	CA-C-O	-5.30	113.80	120.69
1	B	29	SER	CB-CA-C	-5.29	99.75	110.17
1	B	215	SER	N-CA-C	5.28	118.25	110.59
1	A	156	LYS	CA-C-O	5.27	125.87	119.38
1	A	200	HIS	CA-C-N	-5.25	114.97	120.38
1	A	200	HIS	C-N-CA	-5.25	114.97	120.38
1	B	104	GLY	N-CA-C	5.24	125.59	113.18
1	B	96	HIS	CA-CB-CG	-5.21	108.59	113.80
1	B	147	LEU	CB-CA-C	5.20	119.02	109.46
1	B	240	PRO	CA-C-O	-5.19	115.53	121.56
1	B	64	HIS	N-CA-C	-5.15	106.96	114.12
1	B	74	ASP	CB-CA-C	-5.15	100.44	109.71
1	B	202	PRO	O-C-N	-5.15	115.69	122.64
1	B	40	HIS	CA-CB-CG	-5.12	108.68	113.80
1	B	47	ILE	CA-C-N	5.12	129.98	122.77
1	B	47	ILE	C-N-CA	5.12	129.98	122.77
1	B	217	SER	CB-CA-C	5.12	118.24	109.80
1	B	67	ARG	CD-NE-CZ	5.07	131.50	124.40
1	B	229	LEU	CA-C-N	-5.05	115.12	122.65
1	B	229	LEU	C-N-CA	-5.05	115.12	122.65

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	201	PRO	Peptide,Mainchain
1	A	29	SER	Peptide,Mainchain
1	B	201	PRO	Peptide,Mainchain
1	B	29	SER	Peptide

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	1997	0	1897	41	0
1	B	1983	0	1896	60	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	4	0	5	3	0
3	B	4	0	5	5	0
4	A	154	0	0	6	0
4	B	167	0	0	2	0
All	All	4311	0	3803	101	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (101) 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:60[A]:ILE:HG21	1:B:67:ARG:NH1	1.61	1.15
1:B:60[A]:ILE:HG21	1:B:67:ARG:HH11	1.29	0.94
1:B:190:ASP:HB3	1:B:213:LYS:HD2	1.56	0.87
1:B:60[A]:ILE:CG2	1:B:67:ARG:HH11	1.91	0.84
1:A:229:LEU:HB3	1:A:241:MET:HE3	1.63	0.78
1:A:30:PRO:HG3	1:A:106:GLU:HB3	1.66	0.78
1:B:60[A]:ILE:CG2	1:B:67:ARG:NH1	2.46	0.76
1:A:67:ARG:HH21	1:A:69:ASN:HD21	1.33	0.76
1:A:115:SER:HB3	1:A:223:LEU:HD11	1.66	0.75
1:B:60[A]:ILE:HG21	1:B:67:ARG:HH12	1.51	0.75
1:A:67:ARG:NH2	1:A:69:ASN:HD21	1.86	0.74
1:B:67:ARG:NH1	1:B:69:ASN:HD21	1.86	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ASP:HB3	1:B:76:ARG:H	1.53	0.73
1:B:199:THR:H	3:B:402:EDO:H21	1.55	0.72
1:A:153:ALA:HA	1:A:219:SER:HB3	1.71	0.70
1:B:198:LEU:HD23	3:B:402:EDO:H12	1.72	0.70
1:A:182:SER:HA	1:A:185:LEU:HD22	1.76	0.67
1:A:190:ASP:HB2	1:A:213:LYS:HD3	1.77	0.66
1:A:198:LEU:HA	3:A:401:EDO:H21	1.80	0.63
1:B:29:SER:O	1:B:199:THR:HG22	1.99	0.62
1:A:198:LEU:HD12	1:A:204:TYR:H	1.65	0.61
1:A:199:THR:H	3:A:401:EDO:H12	1.66	0.61
1:B:74:ASP:HB2	4:B:498:HOH:O	2.04	0.58
1:B:60[B]:ILE:CD1	1:B:69:ASN:HD22	2.16	0.58
1:B:153:ALA:HA	1:B:219:SER:HB3	1.84	0.58
1:B:27:ASN:HD22	1:B:254:ARG:HD3	1.70	0.57
1:A:4:ASP:HA	4:A:550:HOH:O	2.04	0.56
1:B:47:ILE:HD12	1:B:79:LEU:HD11	1.87	0.56
1:B:60[B]:ILE:HD12	1:B:69:ASN:ND2	2.21	0.56
1:B:202:PRO:HD2	1:B:203:LEU:H	1.72	0.55
1:A:245:ASN:H	1:A:245:ASN:HD22	1.55	0.53
1:A:45:LYS:O	1:A:82:GLY:HA2	2.08	0.53
1:A:153:ALA:CA	1:A:219:SER:HB3	2.39	0.52
1:B:198:LEU:HA	3:B:402:EDO:H12	1.90	0.52
1:B:219:SER:OG	1:B:222:GLN:HG3	2.10	0.52
1:B:53:PRO:O	1:B:178:ASN:HA	2.10	0.52
1:A:165:GLN:HB2	4:A:478:HOH:O	2.10	0.51
1:B:118:LEU:O	1:B:145:GLY:HA2	2.10	0.51
1:B:101:ASN:HB2	1:B:223:LEU:CD1	2.42	0.50
1:B:47:ILE:HG22	1:B:189:LEU:HD13	1.93	0.50
1:B:202:PRO:HD2	1:B:203:LEU:N	2.27	0.50
1:B:101:ASN:HB3	1:B:227:ARG:HH22	1.77	0.49
1:B:74:ASP:OD2	1:B:76:ARG:NE	2.45	0.49
1:B:193:THR:HG22	1:B:257:ARG:HB2	1.94	0.49
1:B:128:TYR:CZ	1:B:137:LYS:HG3	2.49	0.48
1:A:221:GLU:HG2	4:A:418:HOH:O	2.13	0.48
1:B:60[B]:ILE:HD12	1:B:69:ASN:HD22	1.78	0.48
1:B:45:LYS:HB3	1:B:46:PRO:HD2	1.96	0.48
1:A:150:VAL:HA	1:A:218:VAL:O	2.14	0.47
1:A:177:THR:HB	4:A:443:HOH:O	2.14	0.47
1:A:30:PRO:HG3	1:A:106:GLU:CB	2.40	0.47
1:B:101:ASN:HB2	1:B:223:LEU:HD12	1.95	0.47
1:B:200:HIS:HB2	1:B:201:PRO:HD2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:ASN:OD1	1:B:170:LYS:HA	2.15	0.47
1:B:27:ASN:ND2	1:B:254:ARG:HD3	2.29	0.47
1:B:38:THR:HG22	1:B:256:VAL:HB	1.96	0.47
1:B:168:LYS:HG2	4:B:408:HOH:O	2.15	0.47
1:B:45:LYS:O	1:B:82:GLY:HA2	2.15	0.46
1:A:53:PRO:HB2	1:A:178:ASN:HD22	1.80	0.46
1:A:227:ARG:NH2	4:A:428:HOH:O	2.48	0.46
1:B:230:LEU:HB3	1:B:232:ASN:OD1	2.14	0.46
1:B:16:TRP:CZ3	1:B:200:HIS:HA	2.50	0.46
1:B:128:TYR:CE1	1:B:137:LYS:HG3	2.51	0.46
1:A:86:ASP:HB2	4:A:547:HOH:O	2.15	0.46
1:A:60:ILE:HD12	1:A:69:ASN:ND2	2.31	0.46
1:B:200:HIS:HB2	1:B:201:PRO:CD	2.46	0.45
1:B:51:TYR:HD2	1:B:182:SER:H	1.65	0.45
1:B:242:GLN:HB2	1:B:243:HIS:HD2	1.82	0.45
1:A:59:ILE:HG12	1:A:167:ILE:HD13	1.99	0.45
1:A:242:GLN:HB3	1:A:243:HIS:HD2	1.81	0.45
1:B:198:LEU:CD2	3:B:402:EDO:H12	2.43	0.45
1:A:199:THR:H	3:A:401:EDO:C1	2.30	0.44
1:B:192:TRP:CZ3	1:B:213:LYS:HA	2.52	0.44
1:B:201:PRO:HA	1:B:203:LEU:HG	1.98	0.44
1:A:103:HIS:CG	1:A:113:LYS:HD3	2.53	0.44
1:B:245:ASN:HD22	1:B:245:ASN:H	1.66	0.44
1:A:41:ASP:HB3	1:A:44:LEU:HG	1.99	0.44
1:B:13:PRO:HA	1:B:16:TRP:CD2	2.53	0.44
1:B:60[B]:ILE:HD12	1:B:67:ARG:HH12	1.82	0.44
1:B:185:LEU:HB3	1:B:186:PRO:HD2	2.00	0.43
1:A:88:TYR:CE2	1:A:124:ASN:HB2	2.54	0.43
1:A:117:GLU:HG2	1:A:119:HIS:CD2	2.54	0.43
1:A:202:PRO:HD2	1:A:203:LEU:H	1.84	0.42
1:B:55:THR:O	1:B:56:ALA:C	2.62	0.42
1:A:34:LYS:HA	1:A:110:ASP:OD1	2.19	0.42
1:B:29:SER:HB2	1:B:197:SER:OG	2.20	0.42
1:B:199:THR:OG1	3:B:402:EDO:H21	2.20	0.42
1:A:31:VAL:HG11	1:A:251:LEU:CD1	2.50	0.42
1:A:202:PRO:HD2	1:A:203:LEU:N	2.35	0.42
1:B:88:TYR:CE2	1:B:124:ASN:HB2	2.55	0.42
1:B:60[A]:ILE:HD13	1:B:173:ARG:CZ	2.50	0.42
1:A:198:LEU:HD12	1:A:204:TYR:N	2.34	0.41
1:A:47:ILE:HG12	1:A:191:PHE:CE2	2.55	0.41
1:A:168:LYS:HA	1:A:168:LYS:HD2	1.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:LEU:HB3	1:B:186:PRO:CD	2.50	0.41
1:A:83:PRO:HG3	1:A:193:THR:HG21	2.02	0.41
1:B:127:LYS:HB3	1:B:128:TYR:CE2	2.56	0.41
1:B:60[A]:ILE:CG2	1:B:67:ARG:HG3	2.51	0.41
1:A:26:ASN:HA	1:A:252:LYS:HG3	2.03	0.41
1:A:122:HIS:HB2	1:A:142:ALA:HB3	2.02	0.40
1:B:72:ASP:O	1:B:89:ARG:NH1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	255/260 (98%)	237 (93%)	15 (6%)	3 (1%)	10	23
1	B	256/260 (98%)	243 (95%)	10 (4%)	3 (1%)	10	23
All	All	511/520 (98%)	480 (94%)	25 (5%)	6 (1%)	10	23

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	PRO
1	A	202	PRO
1	B	30	PRO
1	B	102	GLU
1	A	5	TRP
1	B	202	PRO

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	218/225 (97%)	208 (95%)	10 (5%)	24	49
1	B	217/225 (96%)	199 (92%)	18 (8%)	10	23
All	All	435/450 (97%)	407 (94%)	28 (6%)	17	35

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	87	SER
1	A	99	SER
1	A	130	SER
1	A	185	LEU
1	A	193	THR
1	A	201	PRO
1	A	221	GLU
1	A	233	VAL
1	A	245	ASN
1	B	8	ASP
1	B	15	GLN
1	B	22	ILE
1	B	29	SER
1	B	50	SER
1	B	60[A]	ILE
1	B	60[B]	ILE
1	B	67	ARG
1	B	86[A]	ASP
1	B	86[B]	ASP
1	B	101	ASN
1	B	158	GLN
1	B	165	GLN
1	B	187	SER
1	B	201	PRO
1	B	217	SER
1	B	241	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	245	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	26	ASN
1	A	27	ASN
1	A	69	ASN
1	A	158	GLN
1	A	178	ASN
1	A	200	HIS
1	A	245	ASN
1	B	27	ASN
1	B	69	ASN
1	B	158	GLN
1	B	178	ASN
1	B	237	ASN
1	B	245	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EDO	A	401	2	3,3,3	2.50	2 (66%)	2,2,2	1.53	0
3	EDO	B	402	2	3,3,3	2.48	2 (66%)	2,2,2	1.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	401	2	-	1/1/1/1	-
3	EDO	B	402	2	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	EDO	O2-C2	3.18	1.58	1.42
3	B	402	EDO	O2-C2	3.16	1.58	1.42
3	B	402	EDO	O1-C1	2.80	1.56	1.42
3	A	401	EDO	O1-C1	2.72	1.56	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	EDO	O1-C1-C2-O2
3	B	402	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	EDO	3	0
3	B	402	EDO	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	257/260 (98%)	-0.33	0 100 100	8, 21, 40, 53	0
1	B	256/260 (98%)	-0.34	0 100 100	9, 20, 33, 42	2 (0%)
All	All	513/520 (98%)	-0.33	0 100 100	8, 21, 36, 53	2 (0%)

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
3	EDO	A	401	4/4	0.91	0.13	13,14,15,16	0
3	EDO	B	402	4/4	0.96	0.07	7,7,8,9	0
2	ZN	A	261	1/1	0.99	0.02	16,16,16,16	0
2	ZN	B	262	1/1	1.00	0.01	18,18,18,18	0

6.5 Other polymers ⓘ

There are no such residues in this entry.