Full wwPDB X-ray Structure Validation Report (i)

Oct 18, 2023 – 05:27 AM EDT

PDB ID	:	1JV0
Title	:	THE CRYSTAL STRUCTURE OF THE ZINC(II) ADDUCT OF THE CAI MICHIGAN 1 VARIANT
Authors	:	Briganti, F.; Ferraroni, M.; Chegwidden, W.R.; Scozzafava, A.; Supuran, C.T.; Tilli, S.
Deposited on	:	2001-08-28
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 (i) 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 (i)) were used in the production of this report:

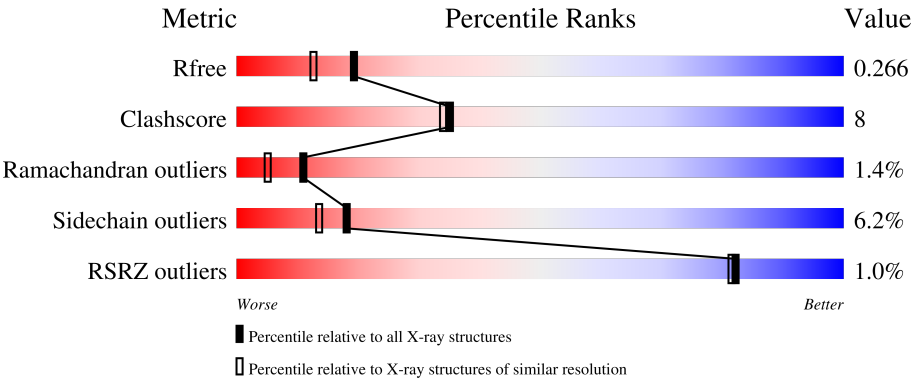
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 <=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	2% 76% 16% 5%
1	B	260	76% 17%

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
4	EDO	A	265	-	X	X	-
4	EDO	B	265	-	X	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4452 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	1	0
			2005	1265	348	389	3			
1	B	256	Total	C	N	O	S	0	3	0
			1990	1258	346	383	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

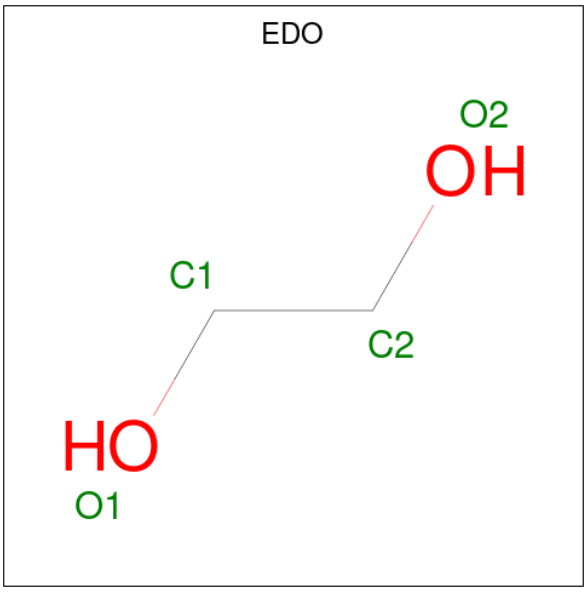
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	3	Total	Zn	0	0
			3	3		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is water.

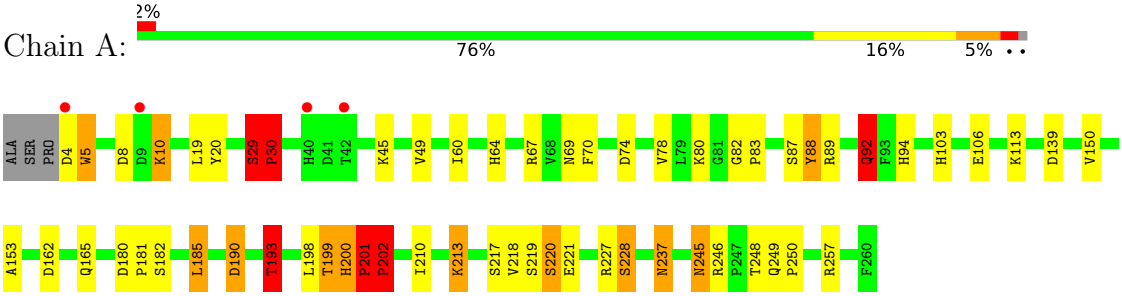
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	233	Total O 233 233	0	0
5	B	207	Total O 207 207	0	0

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.

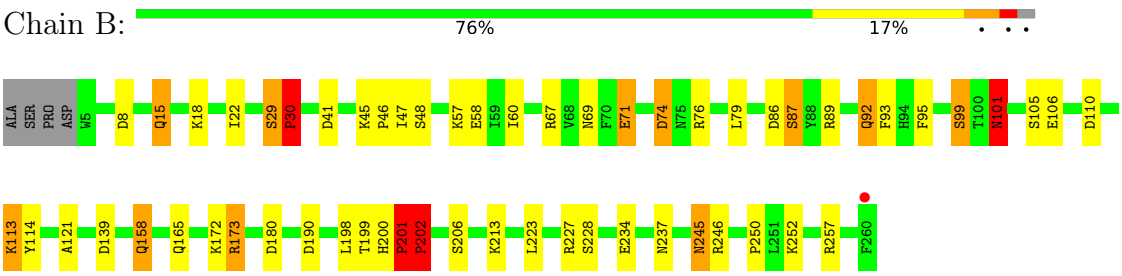
• Molecule 1: CARBONIC ANHYDRASE I

Chain A:



• Molecule 1: CARBONIC ANHYDRASE I

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	62.68Å 71.36Å 120.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.00 14.93 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.00) 84.9 (14.93-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.197 , 0.277 0.191 , 0.266	Depositor DCC
R_{free} test set	1581 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	15.6	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 70.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4452	wwPDB-VP
Average B, all atoms (Å^2)	19.0	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 21.83 % 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 6.4542e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CL, EDO, 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	0.61	0/2066	1.69	35/2813 (1.2%)
1	B	0.59	0/2059	1.70	42/2801 (1.5%)
All	All	0.60	0/4125	1.70	77/5614 (1.4%)

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	4
All	All	0	7

There are no bond length outliers.

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	30	PRO	CA-N-CD	-17.50	87.00	111.50
1	A	257	ARG	NE-CZ-NH1	16.10	128.35	120.30
1	B	67	ARG	NE-CZ-NH2	15.47	128.04	120.30
1	A	202	PRO	CA-N-CD	-13.34	92.82	111.50
1	B	202	PRO	CA-N-CD	-13.29	92.90	111.50
1	A	30	PRO	CA-CB-CG	-12.03	81.15	104.00
1	B	139	ASP	CB-CG-OD1	11.71	128.84	118.30
1	B	30	PRO	CA-N-CD	-11.52	95.38	111.50
1	B	74	ASP	CB-CG-OD1	-10.34	108.99	118.30
1	A	30	PRO	CB-CA-C	10.13	137.33	112.00
1	B	173	ARG	NE-CZ-NH2	-9.58	115.51	120.30
1	B	101	ASN	CB-CA-C	9.21	128.83	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	93	PHE	CB-CG-CD2	8.87	127.01	120.80
1	A	162	ASP	CB-CG-OD2	8.85	126.27	118.30
1	B	92	GLN	CA-CB-CG	8.77	132.69	113.40
1	A	89	ARG	NE-CZ-NH2	-8.53	116.03	120.30
1	B	234	GLU	OE1-CD-OE2	-8.14	113.53	123.30
1	A	201	PRO	CA-C-O	-8.07	100.83	120.20
1	B	114	TYR	CB-CG-CD2	-7.98	116.21	121.00
1	A	80	LYS	CA-CB-CG	7.96	130.92	113.40
1	B	29	SER	CA-C-O	-7.87	103.57	120.10
1	A	139	ASP	CB-CG-OD1	7.52	125.07	118.30
1	B	74	ASP	CB-CG-OD2	7.46	125.02	118.30
1	A	246	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	B	246	ARG	NE-CZ-NH1	7.35	123.98	120.30
1	B	257	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	B	89	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	A	74	ASP	CB-CG-OD1	7.06	124.66	118.30
1	A	88	TYR	CB-CG-CD2	-6.96	116.82	121.00
1	B	86[A]	ASP	CB-CG-OD2	6.82	124.44	118.30
1	B	86[B]	ASP	CB-CG-OD2	6.82	124.44	118.30
1	A	248	THR	CA-CB-CG2	-6.79	102.90	112.40
1	B	67	ARG	NE-CZ-NH1	-6.74	116.93	120.30
1	B	93	PHE	CB-CG-CD1	-6.65	116.14	120.80
1	A	5	TRP	N-CA-CB	6.55	122.38	110.60
1	A	92	GLN	N-CA-CB	-6.52	98.86	110.60
1	A	200	HIS	CA-CB-CG	6.51	124.66	113.60
1	B	227	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	A	20	TYR	CB-CG-CD1	-6.50	117.10	121.00
1	B	202	PRO	N-CA-C	6.42	128.80	112.10
1	B	201	PRO	C-N-CD	-6.34	106.65	120.60
1	B	110	ASP	CB-CG-OD2	6.33	124.00	118.30
1	B	201	PRO	CA-C-O	-6.29	105.10	120.20
1	B	86[A]	ASP	CA-CB-CG	6.25	127.16	113.40
1	B	86[B]	ASP	CA-CB-CG	6.25	127.16	113.40
1	A	221	GLU	OE1-CD-OE2	-6.24	115.81	123.30
1	A	8	ASP	CB-CG-OD1	6.18	123.86	118.30
1	A	180	ASP	CB-CG-OD1	6.06	123.75	118.30
1	A	237	ASN	CB-CG-OD1	6.05	133.71	121.60
1	B	74	ASP	CB-CA-C	-6.04	98.31	110.40
1	B	41	ASP	CB-CG-OD1	6.03	123.73	118.30
1	A	190	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	A	74	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	A	228	SER	CA-CB-OG	-5.90	95.26	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	227	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	A	193	THR	CB-CA-C	-5.77	96.02	111.60
1	B	95	PHE	CB-CG-CD2	5.63	124.74	120.80
1	B	180	ASP	CB-CG-OD2	-5.63	113.24	118.30
1	A	201	PRO	C-N-CD	-5.57	108.34	120.60
1	A	220	SER	N-CA-CB	-5.54	102.19	110.50
1	B	121	ALA	N-CA-CB	5.48	117.77	110.10
1	A	88	TYR	CB-CG-CD1	5.45	124.27	121.00
1	A	257	ARG	NH1-CZ-NH2	-5.42	113.44	119.40
1	B	101	ASN	O-C-N	-5.40	114.06	122.70
1	A	199	THR	CA-CB-CG2	-5.33	104.94	112.40
1	A	49	VAL	N-CA-CB	5.24	123.02	111.50
1	B	99	SER	N-CA-CB	5.21	118.32	110.50
1	B	99	SER	CB-CA-C	-5.20	100.21	110.10
1	B	139	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	B	228	SER	CB-CA-C	-5.16	100.30	110.10
1	B	74	ASP	CA-CB-CG	-5.11	102.16	113.40
1	B	237	ASN	OD1-CG-ND2	-5.08	110.21	121.90
1	B	71	GLU	OE1-CD-OE2	-5.08	117.20	123.30
1	A	4	ASP	C-N-CA	5.06	134.35	121.70
1	B	206	SER	N-CA-CB	-5.04	102.94	110.50
1	B	87	SER	CB-CA-C	5.03	119.66	110.10
1	A	29	SER	CA-C-N	-5.01	103.06	117.10

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
1	B	201	PRO	Peptide,Mainchain
1	B	29	SER	Peptide,Mainchain

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	2005	0	1910	35	0
1	B	1990	0	1903	28	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
4	A	4	0	5	4	0
4	B	4	0	5	6	0
5	A	233	0	0	6	0
5	B	207	0	0	4	0
All	All	4452	0	3823	64	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 8.

All (64) 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:199:THR:H	4:B:265:EDO:H12	1.30	0.91
1:A:30:PRO:HG2	1:A:106:GLU:HB3	1.68	0.75
1:B:245:ASN:HD22	1:B:245:ASN:H	1.34	0.74
1:A:190:ASP:HB2	1:A:213:LYS:HD2	1.71	0.72
1:B:101:ASN:C	1:B:101:ASN:HD22	1.94	0.71
1:B:74:ASP:HB3	1:B:76:ARG:H	1.58	0.68
1:A:198:LEU:HA	4:A:265:EDO:H12	1.76	0.68
1:B:15[A]:GLN:HE21	1:B:18:LYS:HD2	1.59	0.67
1:A:10:LYS:HB3	5:A:476:HOH:O	1.96	0.66
1:A:193:THR:HG23	1:A:210:ILE:HD13	1.76	0.66
1:A:29:SER:HB3	1:A:30:PRO:CD	2.27	0.65
1:A:67:ARG:HD3	5:A:471:HOH:O	1.96	0.65
1:B:30:PRO:HG3	1:B:106:GLU:HB3	1.79	0.65
1:B:45:LYS:HB3	1:B:46:PRO:HD2	1.80	0.63
1:A:245:ASN:H	1:A:245:ASN:HD22	1.44	0.63
1:A:92:GLN:HE22	1:A:94:HIS:HD1	1.46	0.63
1:B:15[A]:GLN:NE2	1:B:18:LYS:HD2	2.14	0.62
1:A:182:SER:HA	1:A:185[B]:LEU:HD23	1.82	0.60
1:B:8:ASP:HB3	5:B:1414:HOH:O	2.00	0.60
1:B:101:ASN:HB2	1:B:223:LEU:HD13	1.84	0.59
1:A:64:HIS:HD2	5:A:398:HOH:O	1.85	0.58
1:A:83:PRO:HG3	1:A:193:THR:HG21	1.86	0.58
1:B:172:LYS:HD3	5:B:1453:HOH:O	2.04	0.57
1:A:103:HIS:CD2	1:A:113:LYS:HD3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LYS:HE3	1:B:71:GLU:HG2	1.88	0.55
1:A:45:LYS:O	1:A:82:GLY:HA2	2.08	0.53
1:B:60[B]:ILE:HD12	1:B:69:ASN:HD22	1.74	0.52
1:B:190:ASP:HB3	1:B:213:LYS:HD2	1.91	0.52
1:A:199:THR:H	4:A:265:EDO:H21	1.76	0.51
1:A:70:PHE:CZ	1:A:181:PRO:HG3	2.45	0.51
1:A:30:PRO:CG	1:A:106:GLU:HB3	2.38	0.49
1:A:92:GLN:NE2	1:A:94:HIS:HD1	2.10	0.49
1:A:29:SER:HB3	1:A:30:PRO:HD2	1.95	0.48
1:B:105:SER:O	1:B:113:LYS:HE3	2.14	0.48
1:A:199:THR:H	4:A:265:EDO:C1	2.27	0.48
1:B:101:ASN:HB2	1:B:223:LEU:CD1	2.44	0.48
4:B:265:EDO:H11	5:B:1384:HOH:O	2.14	0.47
1:B:200:HIS:HB2	1:B:201:PRO:HD2	1.96	0.47
1:B:199:THR:H	4:B:265:EDO:C1	2.16	0.47
1:A:78:VAL:HA	1:A:88:TYR:O	2.16	0.46
1:B:58:GLU:OE1	1:B:60[B]:ILE:HD11	2.15	0.46
1:A:30:PRO:HD2	1:A:199:THR:CG2	2.46	0.46
1:B:60[A]:ILE:HD13	1:B:173:ARG:CZ	2.47	0.45
1:A:193:THR:HB	5:A:359:HOH:O	2.17	0.44
1:B:74:ASP:HB2	5:B:1320:HOH:O	2.16	0.44
1:A:181:PRO:O	1:A:185[B]:LEU:HD23	2.18	0.44
1:A:200:HIS:HB2	1:A:201:PRO:CD	2.48	0.44
1:B:47:ILE:HD12	1:B:79:LEU:HD11	1.99	0.43
1:A:30:PRO:HD2	1:A:199:THR:HG22	2.00	0.43
1:A:92:GLN:HE21	1:A:92:GLN:C	2.22	0.43
1:A:237:ASN:HB3	5:A:492:HOH:O	2.19	0.43
1:A:182:SER:HA	1:A:185[B]:LEU:CD2	2.48	0.43
1:B:22:ILE:HD12	1:B:22:ILE:HA	1.89	0.43
1:A:153:ALA:HA	1:A:219:SER:HB3	2.00	0.42
1:B:199:THR:N	4:B:265:EDO:H12	2.14	0.42
1:A:30:PRO:O	1:A:249:GLN:N	2.52	0.42
1:A:150:VAL:HA	1:A:218:VAL:O	2.20	0.42
1:A:60:ILE:HD12	1:A:69:ASN:ND2	2.35	0.41
1:B:158:GLN:HE21	1:B:158:GLN:HB3	1.56	0.41
1:B:199:THR:OG1	4:B:265:EDO:H12	2.20	0.41
1:B:198:LEU:HA	4:B:265:EDO:H21	2.01	0.41
1:A:250:PRO:HG2	5:A:354:HOH:O	2.20	0.41
1:B:250:PRO:HB2	1:B:252:LYS:HG2	2.03	0.40
1:A:199:THR:H	4:A:265:EDO:C2	2.34	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	256/260 (98%)	240 (94%)	12 (5%)	4 (2%)	9 4
1	B	257/260 (99%)	242 (94%)	12 (5%)	3 (1%)	13 7
All	All	513/520 (99%)	482 (94%)	24 (5%)	7 (1%)	11 5

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	PRO
1	B	202	PRO
1	A	5	TRP
1	A	202	PRO
1	B	30	PRO
1	B	201	PRO
1	A	201	PRO

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	220/225 (98%)	205 (93%)	15 (7%)	16 11
1	B	218/225 (97%)	204 (94%)	14 (6%)	17 13
All	All	438/450 (97%)	409 (93%)	29 (7%)	18 12

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	19	LEU
1	A	30	PRO
1	A	87	SER
1	A	92	GLN
1	A	165	GLN
1	A	185[A]	LEU
1	A	185[B]	LEU
1	A	193	THR
1	A	202	PRO
1	A	213	LYS
1	A	217	SER
1	A	220	SER
1	A	228	SER
1	A	245	ASN
1	B	15[A]	GLN
1	B	15[B]	GLN
1	B	30	PRO
1	B	48	SER
1	B	87	SER
1	B	92	GLN
1	B	99	SER
1	B	101	ASN
1	B	113	LYS
1	B	158	GLN
1	B	165	GLN
1	B	201	PRO
1	B	202	PRO
1	B	245	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	92	GLN
1	A	158	GLN
1	A	178	ASN
1	A	245	ASN
1	B	101	ASN
1	B	158	GLN
1	B	178	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 9 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	$\#\|Z\| > 2$
4	EDO	A	265	2	3,3,3	2.28	2 (66%)	2,2,2	0.48	0
4	EDO	B	265	2	3,3,3	2.33	2 (66%)	2,2,2	1.13	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
4	EDO	A	265	2	-	1/1/1/1	-
4	EDO	B	265	2	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	265	EDO	O2-C2	3.07	1.57	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	265	EDO	O2-C2	3.03	1.57	1.42
4	B	265	EDO	O1-C1	2.61	1.55	1.42
4	A	265	EDO	O1-C1	2.32	1.54	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
4	A	265	EDO	O1-C1-C2-O2
4	B	265	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	265	EDO	4	0
4	B	265	EDO	6	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, 95^{th} 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%)	-0.29	4 (1%)	72	70	8, 18, 34, 62	0
1	B	256/260 (98%)	-0.39	1 (0%)	92	92	7, 17, 31, 38	0
All	All	513/520 (98%)	-0.34	5 (0%)	82	81	7, 17, 33, 62	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	42	THR	3.3
1	A	9	ASP	2.9
1	A	40	HIS	2.6
1	A	4	ASP	2.2
1	B	260	PHE	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 monosaccharides 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, 95^{th} 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	CL	B	1266	1/1	0.94	0.09	43,43,43,43	1
2	ZN	B	264	1/1	0.96	0.05	29,29,29,29	1
2	ZN	A	264	1/1	0.96	0.06	28,28,28,28	1
4	EDO	A	265	4/4	0.96	0.20	40,41,42,44	0
3	CL	B	263	1/1	0.98	0.04	19,19,19,19	0
4	EDO	B	265	4/4	0.98	0.12	23,23,26,28	0
3	CL	A	263	1/1	0.99	0.06	27,27,27,27	0
2	ZN	B	261	1/1	1.00	0.02	12,12,12,12	0
2	ZN	B	262	1/1	1.00	0.08	20,20,20,20	0
2	ZN	A	262	1/1	1.00	0.06	22,22,22,22	0
2	ZN	A	261	1/1	1.00	0.02	14,14,14,14	0

6.5 Other polymers (i)

There are no such residues in this entry.