



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:33 AM UTC

PDB ID : 4GY7 / pdb_00004gy7
Title : Crystallographic structure analysis of urease from Jack bean (*Canavalia ensiformis*) at 1.49 Å Resolution
Authors : Begum, A.; Banumathi, S.; Choudhary, M.I.; Betzel, C.
Deposited on : 2012-09-05
Resolution : 1.49 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

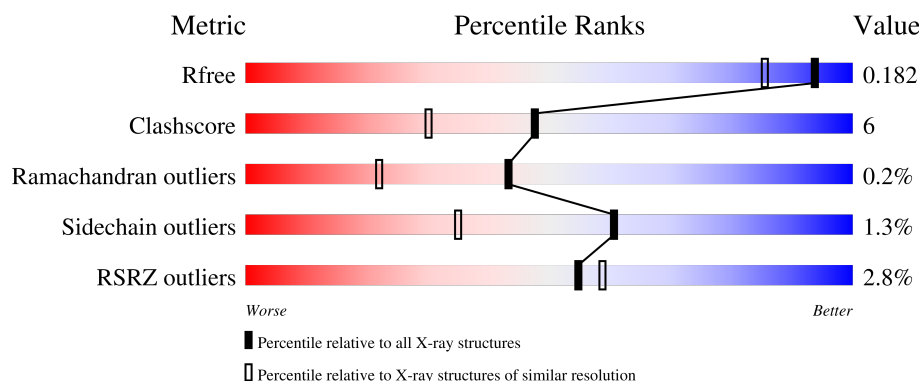
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

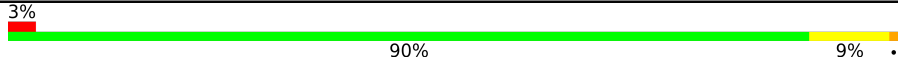
The reported resolution of this entry is 1.49 Å.

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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	840	

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	920	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ACN	A	917	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7468 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.

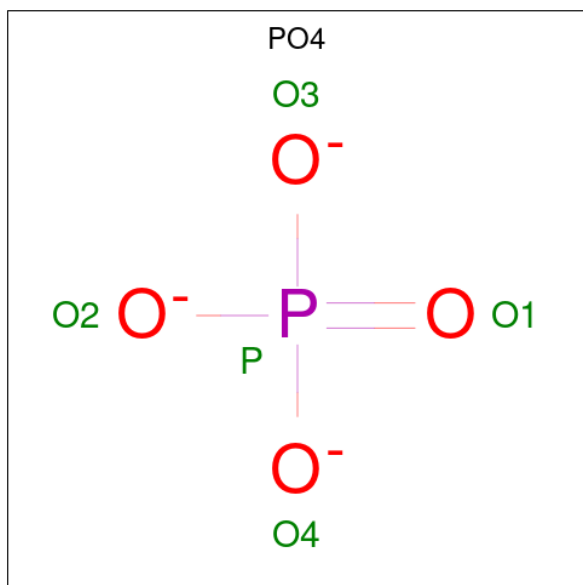
- Molecule 1 is a protein called Urease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	836	Total	C	N	O	S	4	26	0
			6506	4098	1117	1245	46			

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

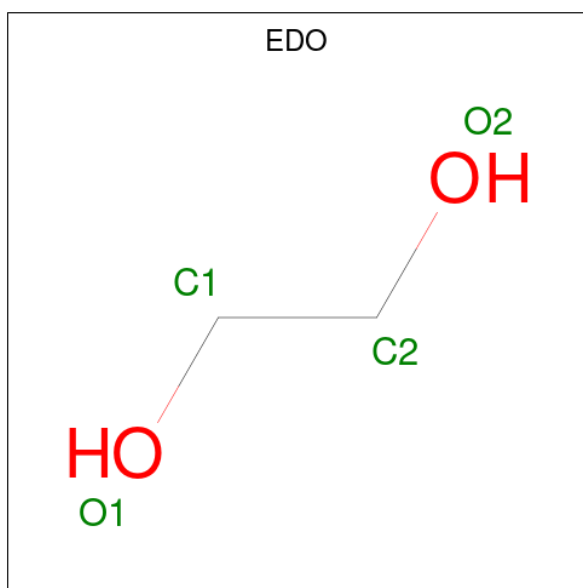
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ni	0	0
			2	2		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



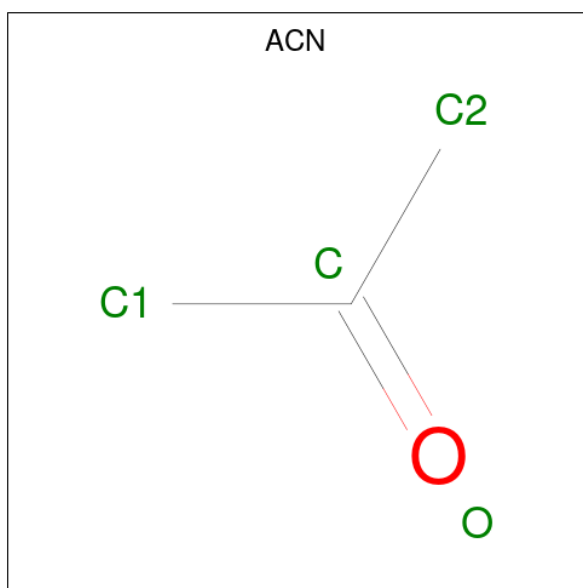
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		

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



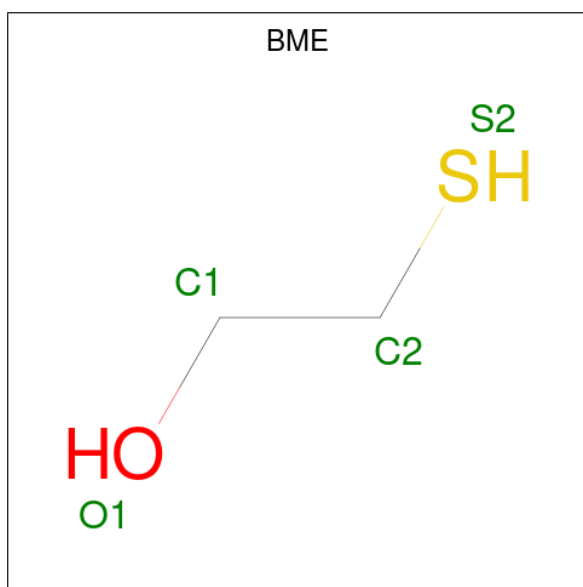
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total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

- Molecule 5 is ACETONE (CCD ID: ACN) (formula: C_3H_6O).



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

- Molecule 6 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C_2H_6OS).



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

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Na	0	0
			2	2		

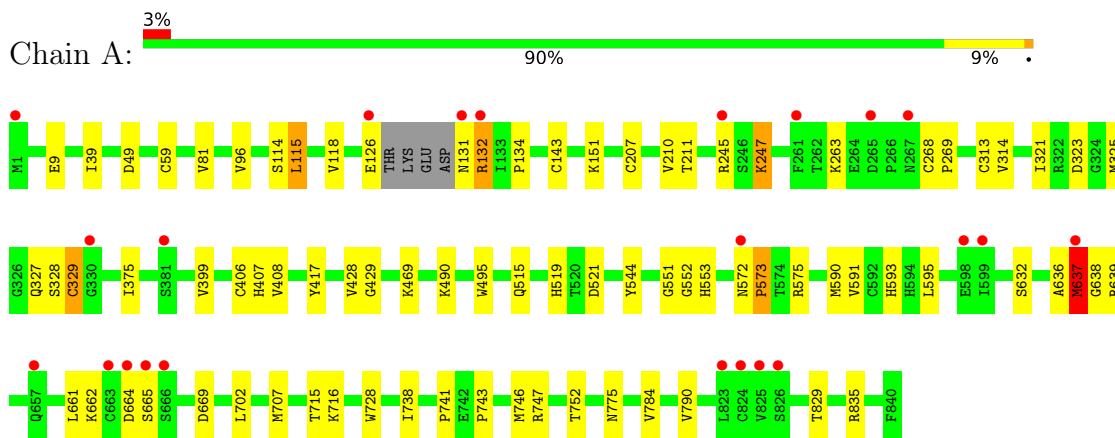
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	872	Total	O	0	0
			872	872		

3 Residue-property plots

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

- Molecule 1: Urease



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	140.66Å 140.66Å 198.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.97 – 1.49 19.97 – 1.49	Depositor EDS
% Data completeness (in resolution range)	97.2 (19.97-1.49) 97.1 (19.97-1.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 1.49Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.151 , 0.165 0.156 , 0.182	Depositor DCC
R_{free} test set	930 reflections (0.50%)	wwPDB-VP
Wilson B-factor (Å ²)	15.3	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7468	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CME, PO4, EDO, BME, NA, NI, ACN, KCX

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	0.44	1/6585 (0.0%)	0.72	1/8906 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	573	PRO	C-O	-5.61	1.17	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	665	SER	N-CA-C	-6.49	102.14	110.19

There are no chirality outliers.

There are no planarity outliers.

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	6506	0	6587	69	0
2	A	2	0	0	0	0
3	A	10	0	0	1	0
4	A	52	0	78	14	0
5	A	20	0	30	11	0
6	A	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	2	0	0	0	0
8	A	872	0	0	10	0
All	All	7468	0	6701	75	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 6.

All (75) 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:573:PRO:HG3	1:A:637:MET:O	1.55	1.04
1:A:131:ASN:O	1:A:132:ARG:HB3	1.53	1.03
1:A:572:ASN:HD21	1:A:639:ARG:H	1.04	1.00
1:A:572:ASN:OD1	1:A:573:PRO:HD3	1.63	0.98
1:A:636:ALA:O	1:A:637:MET:HB2	1.80	0.79
1:A:572:ASN:HD21	1:A:639:ARG:N	1.78	0.78
1:A:572:ASN:ND2	1:A:639:ARG:H	1.80	0.78
1:A:664[B]:ASP:OD2	1:A:669:ASP:HA	1.84	0.75
1:A:263:LYS:NZ	1:A:268:CME:SD	2.59	0.75
1:A:323:ASP:OD1	1:A:329:CME:HZ3	1.89	0.73
1:A:591:VAL:CG1	5:A:917:ACN:C2	2.67	0.73
1:A:572:ASN:OD1	1:A:573:PRO:CD	2.35	0.72
1:A:636:ALA:O	1:A:637:MET:CB	2.38	0.71
1:A:39:ILE:HG21	1:A:81[B]:VAL:HG11	1.74	0.69
1:A:314[B]:VAL:HG11	4:A:909:EDO:H11	1.74	0.69
1:A:835[B]:ARG:HG3	8:A:1314:HOH:O	1.92	0.69
1:A:591:VAL:HG11	5:A:917:ACN:H23	1.75	0.69
1:A:593:HIS:ND1	5:A:915:ACN:H23	2.08	0.68
1:A:329:CME:HE2	1:A:329:CME:HA	1.74	0.68
1:A:591:VAL:CG1	5:A:917:ACN:H23	2.23	0.68
4:A:920:EDO:H21	8:A:1795:HOH:O	1.95	0.67
1:A:268:CME:HE2	1:A:269:PRO:HD2	1.78	0.66
1:A:327:GLN:HE21	1:A:329:CME:HZ2	1.58	0.66
1:A:515:GLN:NE2	1:A:790[B]:VAL:HG13	2.12	0.65
1:A:835[A]:ARG:NH2	8:A:1797:HOH:O	2.33	0.60
1:A:131:ASN:O	1:A:132:ARG:CB	2.38	0.60
1:A:591:VAL:CG1	5:A:917:ACN:H21	2.32	0.60
1:A:211:THR:H	4:A:904:EDO:H11	1.67	0.59
1:A:210:VAL:HA	4:A:904:EDO:H11	1.85	0.59
1:A:39:ILE:CG2	1:A:81[B]:VAL:HG11	2.34	0.57
5:A:916:ACN:H22	8:A:1795:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:SER:O	1:A:329:CME:HE2	2.05	0.56
1:A:728:TRP:HE1	4:A:920:EDO:H12	1.72	0.55
1:A:829[B]:THR:HG23	8:A:1351:HOH:O	2.06	0.54
1:A:738:ILE:HG13	1:A:741:PRO:HD3	1.89	0.54
1:A:632:SER:O	1:A:638:GLY:HA3	2.08	0.53
1:A:702:LEU:HD11	4:A:922:EDO:H11	1.89	0.53
1:A:325:MET:O	1:A:375:ILE:CD1	2.57	0.53
1:A:775:ASN:HB3	1:A:784[A]:VAL:HG21	1.92	0.52
1:A:211:THR:H	4:A:904:EDO:C1	2.22	0.51
5:A:916:ACN:H23	8:A:1744:HOH:O	2.10	0.51
1:A:314[A]:VAL:HG11	4:A:909:EDO:H22	1.92	0.50
1:A:327:GLN:HE21	1:A:329:CME:CZ	2.24	0.50
1:A:521:ASP:HB3	1:A:553:HIS:CE1	2.48	0.49
1:A:715[B]:THR:HG23	1:A:716:LYS:N	2.28	0.49
1:A:114:SER:O	1:A:115:LEU:HB2	2.14	0.47
1:A:417:TYR:CE1	4:A:920:EDO:H22	2.49	0.47
1:A:9[B]:GLU:HG2	1:A:743:PRO:CG	2.45	0.47
1:A:591:VAL:HG13	5:A:917:ACN:H21	1.97	0.46
4:A:906:EDO:H12	8:A:1744:HOH:O	2.15	0.46
1:A:591:VAL:HG11	5:A:917:ACN:C2	2.37	0.45
1:A:595:LEU:HD21	5:A:915:ACN:H21	1.98	0.45
1:A:637:MET:HE2	1:A:637:MET:HB3	1.73	0.44
1:A:9[B]:GLU:OE2	1:A:747:ARG:NH2	2.48	0.44
1:A:313:CYS:HB3	1:A:321[B]:ILE:HD11	1.98	0.44
1:A:552:GLY:O	1:A:553:HIS:C	2.61	0.44
1:A:637:MET:HG3	3:A:903:PO4:O4	2.17	0.44
1:A:752:THR:CG2	4:A:920:EDO:H12	2.48	0.44
1:A:407:HIS:CE1	1:A:544:TYR:CD2	3.05	0.44
1:A:469:LYS:HE2	1:A:495:TRP:CE2	2.53	0.44
1:A:572:ASN:OD1	1:A:573:PRO:N	2.51	0.44
1:A:81[B]:VAL:CG1	1:A:96:VAL:HB	2.48	0.43
1:A:399:VAL:HG22	1:A:707:MET:SD	2.58	0.43
1:A:519:HIS:CE1	1:A:551:GLY:HA3	2.54	0.43
5:A:915:ACN:H22	8:A:1657:HOH:O	2.18	0.43
1:A:132:ARG:O	1:A:134:PRO:HD3	2.19	0.43
1:A:590:MET:HG2	1:A:595:LEU:HD12	2.02	0.42
1:A:118:VAL:HB	4:A:910:EDO:H22	2.01	0.42
1:A:81[B]:VAL:HG13	1:A:96:VAL:HB	2.02	0.42
1:A:408:VAL:O	1:A:429:GLY:HA3	2.20	0.41
1:A:661:LEU:O	1:A:664[A]:ASP:HB2	2.20	0.41
4:A:920:EDO:C2	8:A:1795:HOH:O	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:KCX:HE2	8:A:1729:HOH:O	2.21	0.41
1:A:747:ARG:CG	4:A:906:EDO:H22	2.51	0.41
1:A:406:CYS:HA	1:A:428:VAL:HB	2.02	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	850/840 (101%)	815 (96%)	33 (4%)	2 (0%)	43 22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	ARG
1	A	637	MET

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	701/678 (103%)	692 (99%)	9 (1%)	61 35

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASP
1	A	115	LEU
1	A	126	GLU
1	A	151	LYS
1	A	245	ARG
1	A	575	ARG
1	A	637	MET
1	A	662	LYS
1	A	746	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	327	GLN
1	A	504	ASN
1	A	524	ASN
1	A	635	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CME	A	207	1	8,9,10	0.87	0	6,9,11	1.48	1 (16%)
1	CME	A	143	1	8,9,10	1.00	0	6,9,11	1.85	1 (16%)
1	CME	A	329	1	8,9,10	1.01	1 (12%)	6,9,11	2.22	2 (33%)
1	KCX	A	490	2,1	10,11,12	0.92	1 (10%)	6,12,14	1.52	1 (16%)
1	KCX	A	247	1	10,11,12	0.99	0	6,12,14	2.84	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CME	A	59[A]	1	8,9,10	0.90	0	6,9,11	1.59	1 (16%)
1	CME	A	139	1	8,9,10	0.90	0	6,9,11	1.08	0
1	CME	A	268	1	8,9,10	0.93	0	6,9,11	0.77	0
1	CME	A	59[B]	1	8,9,10	0.88	0	6,9,11	1.26	1 (16%)
1	CME	A	592	1	8,9,10	0.83	0	6,9,11	0.79	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
1	CME	A	207	1	-	2/5/8/10	-
1	CME	A	143	1	-	1/5/8/10	-
1	CME	A	329	1	-	3/5/8/10	-
1	KCX	A	490	2,1	-	0/9/10/12	-
1	KCX	A	247	1	-	2/9/10/12	-
1	CME	A	59[A]	1	-	3/5/8/10	-
1	CME	A	139	1	-	2/5/8/10	-
1	CME	A	268	1	-	2/5/8/10	-
1	CME	A	59[B]	1	-	1/5/8/10	-
1	CME	A	592	1	-	1/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	490	KCX	OQ1-CX	2.37	1.26	1.21
1	A	329	CME	CB-SG	-2.06	1.74	1.81

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	KCX	CE-NZ-CX	-5.44	112.74	121.98
1	A	329	CME	CB-SG-SD	4.33	115.07	103.86
1	A	247	KCX	OQ1-CX-NZ	-3.88	119.02	124.92
1	A	59[A]	CME	CB-SG-SD	3.64	113.28	103.86
1	A	143	CME	CB-CA-C	-3.55	101.16	110.80
1	A	490	KCX	OQ1-CX-NZ	-3.27	119.95	124.92
1	A	207	CME	CB-SG-SD	3.19	112.10	103.86
1	A	59[B]	CME	CB-SG-SD	2.32	109.86	103.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	CME	CA-CB-SG	-2.02	106.18	114.45

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	59[A]	CME	SD-CE-CZ-OH
1	A	59[B]	CME	SD-CE-CZ-OH
1	A	329	CME	CE-SD-SG-CB
1	A	329	CME	SD-CE-CZ-OH
1	A	59[A]	CME	CE-SD-SG-CB
1	A	139	CME	SD-CE-CZ-OH
1	A	207	CME	SD-CE-CZ-OH
1	A	592	CME	SD-CE-CZ-OH
1	A	247	KCX	CE-CD-CG-CB
1	A	268	CME	SD-CE-CZ-OH
1	A	329	CME	N-CA-CB-SG
1	A	143	CME	CZ-CE-SD-SG
1	A	247	KCX	CA-CB-CG-CD
1	A	59[A]	CME	CZ-CE-SD-SG
1	A	139	CME	CZ-CE-SD-SG
1	A	207	CME	CZ-CE-SD-SG
1	A	268	CME	CZ-CE-SD-SG

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	329	CME	5	0
1	A	247	KCX	1	0
1	A	268	CME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 4 are monoatomic - leaving 21 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	ACN	A	914	-	3,3,3	0.36	0	3,3,3	0.77	0
4	EDO	A	908	-	3,3,3	0.43	0	2,2,2	0.37	0
5	ACN	A	916	-	3,3,3	0.38	0	3,3,3	0.71	0
6	BME	A	919	-	3,3,3	0.38	0	2,2,2	1.75	0
3	PO4	A	923	-	4,4,4	0.94	0	6,6,6	0.52	0
4	EDO	A	906	-	3,3,3	0.50	0	2,2,2	0.24	0
4	EDO	A	921	-	3,3,3	0.42	0	2,2,2	0.48	0
3	PO4	A	903	2	4,4,4	1.07	0	6,6,6	0.49	0
4	EDO	A	920	-	3,3,3	0.41	0	2,2,2	1.06	0
4	EDO	A	907	-	3,3,3	0.41	0	2,2,2	0.32	0
4	EDO	A	922	-	3,3,3	0.47	0	2,2,2	0.32	0
4	EDO	A	904	-	3,3,3	0.37	0	2,2,2	0.59	0
4	EDO	A	913	-	3,3,3	0.44	0	2,2,2	0.34	0
5	ACN	A	915	-	3,3,3	0.40	0	3,3,3	1.58	1 (33%)
5	ACN	A	917	-	3,3,3	0.27	0	3,3,3	0.59	0
4	EDO	A	905	-	3,3,3	0.43	0	2,2,2	0.19	0
4	EDO	A	910	-	3,3,3	0.41	0	2,2,2	0.45	0
4	EDO	A	911	-	3,3,3	0.41	0	2,2,2	0.38	0
4	EDO	A	912	-	3,3,3	0.47	0	2,2,2	0.21	0
5	ACN	A	918	-	3,3,3	0.41	0	3,3,3	0.68	0
4	EDO	A	909	-	3,3,3	0.44	0	2,2,2	0.21	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	920	-	-	1/1/1/1	-
4	EDO	A	922	-	-	1/1/1/1	-
4	EDO	A	906	-	-	1/1/1/1	-
6	BME	A	919	-	-	0/1/1/1	-
4	EDO	A	921	-	-	0/1/1/1	-
4	EDO	A	908	-	-	1/1/1/1	-
4	EDO	A	905	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	904	-	-	1/1/1/1	-
4	EDO	A	910	-	-	0/1/1/1	-
4	EDO	A	911	-	-	1/1/1/1	-
4	EDO	A	913	-	-	1/1/1/1	-
4	EDO	A	912	-	-	1/1/1/1	-
4	EDO	A	907	-	-	1/1/1/1	-
4	EDO	A	909	-	-	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(°)
5	A	915	ACN	C2-C-C1	-2.52	101.61	117.52

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	906	EDO	O1-C1-C2-O2
4	A	908	EDO	O1-C1-C2-O2
4	A	920	EDO	O1-C1-C2-O2
4	A	905	EDO	O1-C1-C2-O2
4	A	909	EDO	O1-C1-C2-O2
4	A	904	EDO	O1-C1-C2-O2
4	A	911	EDO	O1-C1-C2-O2
4	A	922	EDO	O1-C1-C2-O2
4	A	907	EDO	O1-C1-C2-O2
4	A	913	EDO	O1-C1-C2-O2
4	A	912	EDO	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	916	ACN	2	0
4	A	906	EDO	2	0
3	A	903	PO4	1	0
4	A	920	EDO	5	0
4	A	922	EDO	1	0
4	A	904	EDO	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	915	ACN	3	0
5	A	917	ACN	6	0
4	A	910	EDO	1	0
4	A	909	EDO	2	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	827/840 (98%)	-0.21	23 (2%) 55 59	5, 12, 25, 57	32 (3%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	131	ASN	8.2
1	A	637	MET	7.0
1	A	572	ASN	6.2
1	A	666	SER	5.6
1	A	825	VAL	5.4
1	A	330	GLY	4.3
1	A	663	CYS	3.7
1	A	245	ARG	3.6
1	A	823	LEU	3.6
1	A	665	SER	3.6
1	A	824	CYS	3.5
1	A	126	GLU	3.1
1	A	826	SER	3.1
1	A	664[A]	ASP	3.0
1	A	132	ARG	2.8
1	A	599	ILE	2.5
1	A	1	MET	2.4
1	A	381	SER	2.4
1	A	265	ASP	2.3
1	A	261	PHE	2.3
1	A	598	GLU	2.3
1	A	657	GLN	2.0
1	A	267	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CME	A	329	10/11	0.74	0.29	6,24,39,51	5
1	KCX	A	247	12/13	0.85	0.16	16,20,28,29	0
1	CME	A	59[A]	10/11	0.86	0.19	13,15,42,45	10
1	CME	A	59[B]	10/11	0.86	0.19	12,14,35,35	10
1	CME	A	143	10/11	0.87	0.16	19,23,46,53	2
1	CME	A	268	10/11	0.90	0.17	21,28,61,64	0
1	CME	A	207	10/11	0.91	0.14	18,19,30,40	2
1	CME	A	592	10/11	0.92	0.10	12,18,28,30	5
1	CME	A	139	10/11	0.96	0.08	16,17,28,36	7
1	KCX	A	490	12/13	0.98	0.04	8,9,10,11	0

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
7	NA	A	924	1/1	0.67	0.29	46,46,46,46	0
5	ACN	A	915	4/4	0.73	0.15	31,32,35,35	0
5	ACN	A	917	4/4	0.74	0.27	51,53,53,54	0
3	PO4	A	923	5/5	0.75	0.29	60,62,65,68	4
5	ACN	A	916	4/4	0.77	0.22	53,53,54,54	0
4	EDO	A	911	4/4	0.77	0.21	27,29,34,34	0
5	ACN	A	918	4/4	0.77	0.18	22,30,31,35	0
4	EDO	A	909	4/4	0.77	0.15	29,29,30,37	0
4	EDO	A	912	4/4	0.79	0.23	27,40,41,43	0
4	EDO	A	907	4/4	0.80	0.17	35,36,44,48	0
5	ACN	A	914	4/4	0.82	0.16	41,41,42,43	0
4	EDO	A	908	4/4	0.82	0.24	56,57,59,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	BME	A	919	4/4	0.82	0.17	33,45,51,71	0
4	EDO	A	906	4/4	0.82	0.20	24,31,32,35	0
7	NA	A	925	1/1	0.82	0.28	48,48,48,48	0
4	EDO	A	910	4/4	0.83	0.16	49,50,50,54	0
4	EDO	A	921	4/4	0.85	0.13	41,46,48,51	0
4	EDO	A	922	4/4	0.85	0.21	26,30,35,40	0
4	EDO	A	920	4/4	0.86	0.21	18,23,26,31	0
4	EDO	A	904	4/4	0.88	0.14	27,29,33,42	0
3	PO4	A	903	5/5	0.91	0.14	10,12,22,23	5
4	EDO	A	905	4/4	0.91	0.10	31,36,39,43	0
4	EDO	A	913	4/4	0.94	0.16	19,25,29,43	0
2	NI	A	902	1/1	1.00	0.02	9,9,9,9	0
2	NI	A	901	1/1	1.00	0.01	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.