



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:38 PM UTC

PDB ID : 1DLG / pdb_00001dlg
Title : CRYSTAL STRUCTURE OF THE C115S ENTEROBACTER CLOACAE
MURA IN THE UN-LIGANDED STATE
Authors : Schonbrunn, E.; Eschenburg, S.; Krekel, F.; Luger, K.; Amrhein, N.
Deposited on : 1999-12-09
Resolution : 1.90 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

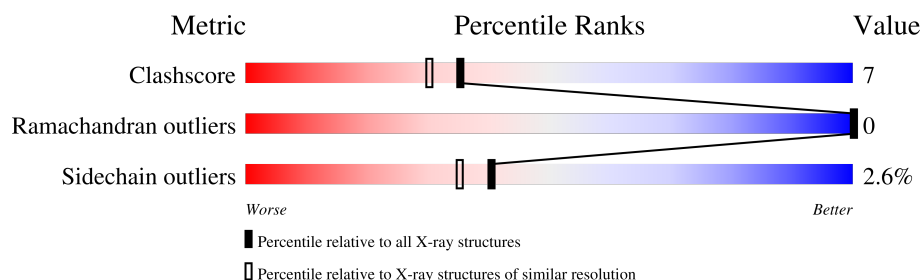
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	419	 84% 15% .
1	B	419	 84% 15% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7466 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.

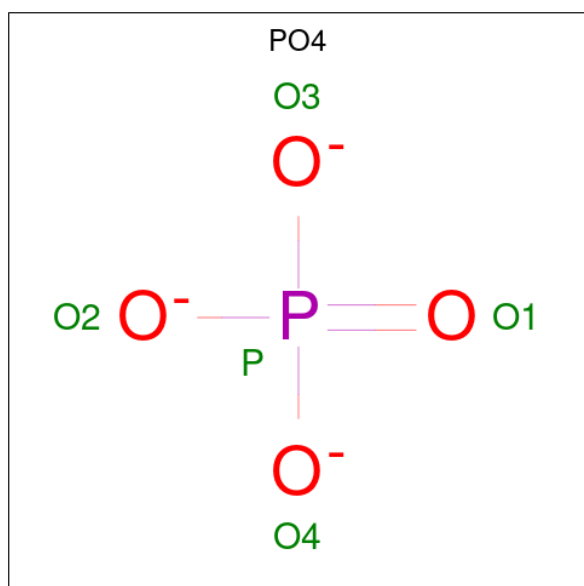
- Molecule 1 is a protein called UDP-N-ACETYLGLUCOSAMINE ENOLPYRUVYL TRANSFERASE MURA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	12	0
			3191	2009	562	606	14			
1	B	419	Total	C	N	O	S	0	13	0
			3193	2013	562	604	14			

There are 4 discrepancies between the modelled and reference sequences:

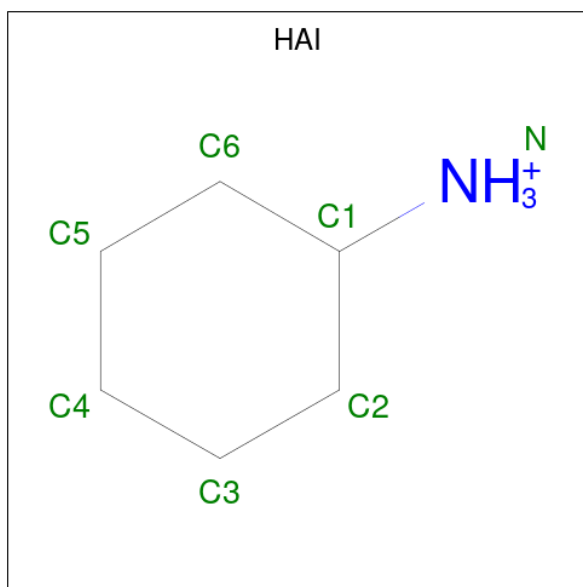
Chain	Residue	Modelled	Actual	Comment	Reference
A	67	IAS	ASN	conflict	UNP P33038
A	115	SER	CYS	engineered mutation	UNP P33038
B	67	IAS	ASN	conflict	UNP P33038
B	115	SER	CYS	engineered mutation	UNP P33038

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 3 is CYCLOHEXYLAMMONIUM ION (CCD ID: HAI) (formula: C₆H₁₄N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 7 6 1	0	0
3	B	1	Total C N 7 6 1	0	0
3	B	1	Total C N 7 6 1	0	0

- Molecule 4 is water.

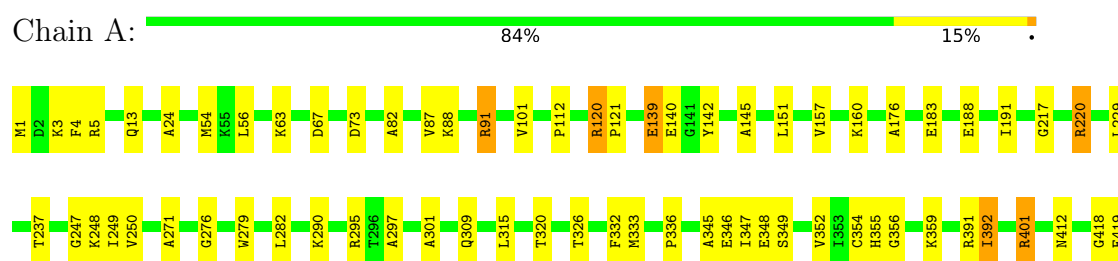
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	550	Total 550	O 550	0	0
4	B	466	Total 466	O 466	0	0

3 Residue-property plots

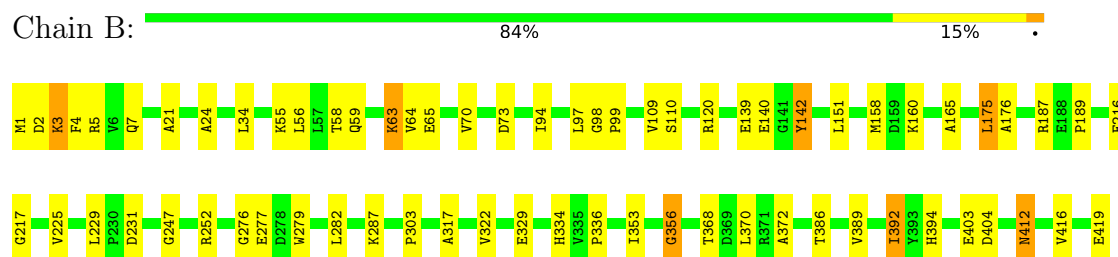
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: UDP-N-ACETYLGLUCOSAMINE ENOLPYRUVYL TRANSFERASE MURA



• Molecule 1: UDP-N-ACETYLGLUCOSAMINE ENOLPYRUVYL TRANSFERASE MURA



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	86.69Å 155.53Å 83.82Å 90.00° 91.82° 90.00°	Depositor
Resolution (Å)	14.97 – 1.90	Depositor
% Data completeness (in resolution range)	98.9 (14.97-1.90)	Depositor
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.173 , 0.197	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7466	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HAI, PO4, IAS

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	0.76	1/3275 (0.0%)	1.06	13/4432 (0.3%)
1	B	0.71	0/3281	1.03	10/4440 (0.2%)
All	All	0.74	1/6556 (0.0%)	1.04	23/8872 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	MET	SD-CE	-5.12	1.66	1.79

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	24	ALA	N-CA-C	-7.62	103.95	113.55
1	B	97	LEU	N-CA-C	7.07	118.64	111.07
1	B	356	GLY	N-CA-C	6.68	119.18	111.36
1	A	120	ARG	N-CA-C	-6.51	101.10	110.08
1	A	349	SER	CB-CA-C	-6.31	109.31	116.63
1	A	247	GLY	N-CA-C	6.12	122.04	112.31
1	B	120	ARG	N-CA-C	-5.93	102.58	109.93
1	A	24	ALA	N-CA-C	-5.65	106.43	113.55
1	B	142	TYR	N-CA-C	5.58	116.74	108.60
1	A	356	GLY	N-CA-C	5.57	117.87	111.36
1	A	87	VAL	CB-CA-C	-5.55	104.83	110.88
1	B	276	GLY	N-CA-C	-5.41	100.36	113.18
1	A	191	ILE	N-CA-C	-5.40	105.45	110.53
1	A	188	GLU	N-CA-C	5.29	115.69	109.60
1	A	151	LEU	N-CA-C	-5.25	103.60	110.53
1	A	139	GLU	N-CA-C	-5.19	100.24	109.06
1	B	70	VAL	N-CA-C	-5.18	100.86	108.11
1	B	247	GLY	N-CA-C	5.15	120.13	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	ALA	CA-C-N	5.12	125.03	119.85
1	A	82	ALA	C-N-CA	5.12	125.03	119.85
1	B	303	PRO	N-CA-C	5.11	118.88	110.55
1	B	151	LEU	N-CA-C	-5.05	104.20	110.41
1	A	88	LYS	N-CA-C	5.01	118.16	111.75

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	3191	0	3272	49	0
1	B	3193	0	3285	48	0
2	A	15	0	0	0	0
2	B	30	0	0	0	0
3	A	7	0	14	0	0
3	B	14	0	28	1	0
4	A	550	0	0	9	0
4	B	466	0	0	15	0
All	All	7466	0	6599	97	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 7.

All (97) 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:348:GLU:HG2	4:A:1128:HOH:O	1.76	0.86
1:B:216:GLU:HG3	4:B:503:HOH:O	1.75	0.86
1:A:401:ARG:HG2	1:A:401:ARG:HH11	1.42	0.85
1:A:347:ILE:HD13	1:A:352:VAL:HG22	1.56	0.85
1:A:91:ARG:HG2	1:A:91:ARG:HH11	1.41	0.84
1:A:4:PHE:CD1	1:A:392:ILE:HG12	2.17	0.79
1:B:1:MET:N	1:B:419:GLU:HB2	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ARG:HG2	4:A:795:HOH:O	1.88	0.73
1:B:63:LYS:HD3	1:B:73:ASP:HB3	1.74	0.70
1:B:252[A]:ARG:CZ	4:B:552:HOH:O	2.39	0.70
1:B:63:LYS:HE2	1:B:65:GLU:OE2	1.92	0.69
1:A:139:GLU:HB2	1:A:142:TYR:CE2	2.28	0.68
1:B:287:LYS:HD3	4:B:858:HOH:O	1.94	0.68
1:B:1:MET:H2	1:B:419:GLU:HB2	1.59	0.67
1:B:99:PRO:HD3	4:B:651:HOH:O	1.97	0.63
1:B:412:ASN:C	1:B:412:ASN:HD22	2.07	0.63
1:B:63:LYS:HE3	4:B:587:HOH:O	1.99	0.63
1:A:1:MET:HE3	1:A:391:ARG:NH1	2.14	0.62
1:B:322[B]:VAL:HG12	1:B:353:ILE:HA	1.81	0.62
1:A:346:GLU:OE1	1:A:355:HIS:HE1	1.83	0.61
1:B:368:THR:HG22	4:B:674:HOH:O	2.03	0.58
1:B:34:LEU:HD22	1:B:175:LEU:HD22	1.84	0.58
1:A:101[A]:VAL:HG11	1:A:145:ALA:HB3	1.86	0.58
1:A:290:LYS:HE3	4:A:1217:HOH:O	2.02	0.58
1:A:347:ILE:CD1	1:A:352:VAL:HG22	2.29	0.58
1:A:401:ARG:HG2	1:A:401:ARG:NH1	2.17	0.56
1:A:120:ARG:NE	1:A:120:ARG:HA	2.21	0.56
1:B:279:TRP:CD1	3:B:1420:HAI:H31	2.41	0.56
1:A:91:ARG:HG2	1:A:91:ARG:NH1	2.17	0.55
1:A:401:ARG:HH11	1:A:401:ARG:CG	2.15	0.54
1:A:295:ARG:HD2	4:A:645:HOH:O	2.06	0.54
1:B:158[A]:MET:HE1	1:B:165:ALA:CB	2.37	0.54
1:B:277:GLU:HB2	4:B:893:HOH:O	2.07	0.54
1:A:160[B]:LYS:HE2	4:A:1028:HOH:O	2.07	0.53
1:A:139:GLU:O	1:A:140:GLU:C	2.50	0.53
1:A:91:ARG:HH11	1:A:91:ARG:CG	2.16	0.52
1:B:187:ARG:NH1	4:B:698:HOH:O	2.42	0.52
1:A:332:PHE:CZ	1:A:352:VAL:HG23	2.44	0.51
1:A:237:THR:OG1	1:A:309[B]:GLN:NE2	2.43	0.51
1:A:295:ARG:NH1	1:A:326:THR:HG21	2.26	0.51
1:B:158[A]:MET:HE1	1:B:165:ALA:HB1	1.92	0.51
1:B:334:HIS:HB3	1:B:372:ALA:HB1	1.92	0.50
1:B:1:MET:H3	1:B:419:GLU:HB2	1.74	0.50
1:A:121:PRO:HD2	4:A:842:HOH:O	2.12	0.50
1:A:359:LYS:HB2	4:A:780:HOH:O	2.12	0.49
1:B:98:GLY:HA3	4:B:651:HOH:O	2.11	0.49
1:B:225:VAL:O	4:B:497:HOH:O	2.19	0.49
1:A:3:LYS:HE3	1:A:418:GLY:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:GLY:HA3	1:A:279:TRP:CE2	2.48	0.48
1:B:252[A]:ARG:HD2	4:B:1218:HOH:O	2.12	0.48
1:B:139:GLU:O	1:B:140:GLU:C	2.56	0.48
1:A:315:LEU:HD21	1:A:345:ALA:HB2	1.96	0.48
1:A:91:ARG:NH1	1:A:91:ARG:CG	2.75	0.48
1:A:13:GLN:HA	1:A:248:LYS:O	2.14	0.47
1:B:4:PHE:CD1	1:B:392:ILE:HG12	2.49	0.47
1:B:63:LYS:HD3	1:B:73:ASP:CB	2.42	0.47
1:B:329:GLU:HA	4:B:544:HOH:O	2.16	0.46
1:A:101[B]:VAL:HG21	1:A:145:ALA:HB3	1.97	0.46
1:B:2:ASP:HA	1:B:416:VAL:O	2.15	0.46
1:B:58:THR:OG1	1:B:64[B]:VAL:CG1	2.64	0.46
1:B:142:TYR:C	1:B:142:TYR:CD1	2.93	0.46
1:B:3:LYS:HD2	1:B:419:GLU:HA	1.98	0.46
1:A:320:THR:OG1	1:A:355:HIS:HD2	1.99	0.45
1:B:394:HIS:HB2	4:B:630:HOH:O	2.16	0.45
1:A:401:ARG:NH1	1:A:401:ARG:CG	2.74	0.45
1:A:333:MET:O	1:A:336:PRO:HD2	2.16	0.45
1:A:139:GLU:HB2	1:A:142:TYR:CZ	2.50	0.45
1:A:5[B]:ARG:NH1	4:A:676:HOH:O	2.49	0.44
1:B:176:ALA:O	1:B:217:GLY:HA3	2.18	0.44
1:A:112:PRO:CD	4:A:636:HOH:O	2.65	0.44
1:B:55[B]:LYS:HG3	4:B:423:HOH:O	2.17	0.44
1:B:59:GLN:HE21	1:B:59:GLN:HA	1.83	0.44
1:B:94:ILE:HD12	1:B:109[A]:VAL:HG21	1.99	0.43
1:A:297:ALA:HB3	1:A:301:ALA:CB	2.49	0.43
1:A:176:ALA:O	1:A:217:GLY:HA3	2.18	0.43
1:B:403:GLU:HG2	1:B:404:ASP:N	2.34	0.43
1:A:142:TYR:CD1	1:A:142:TYR:C	2.96	0.43
1:B:56:LEU:C	1:B:56:LEU:HD23	2.45	0.42
1:A:332:PHE:CE2	1:A:352:VAL:HG23	2.53	0.42
1:B:282:LEU:C	1:B:282:LEU:HD23	2.44	0.42
1:B:317:ALA:O	1:B:356:GLY:HA3	2.20	0.42
1:B:389:VAL:HG12	1:B:392:ILE:CD1	2.50	0.42
1:A:271:ALA:HB1	1:A:282:LEU:HG	2.02	0.42
1:B:187:ARG:CZ	4:B:488:HOH:O	2.68	0.42
1:A:4:PHE:CD1	1:A:392:ILE:CG1	2.96	0.42
1:B:389:VAL:O	1:B:392:ILE:HD13	2.20	0.42
1:B:5:ARG:NH2	1:B:386:THR:HG21	2.34	0.41
1:A:63:LYS:HB2	1:A:73:ASP:HB3	2.02	0.41
1:A:157:VAL:HG22	1:A:183:GLU:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:THR:OG1	1:B:64[B]:VAL:HG12	2.21	0.41
1:A:249:ILE:HG12	1:A:250:VAL:N	2.35	0.40
1:B:21:ALA:HB2	1:B:231:ASP:HA	2.03	0.40
1:B:7:GLN:OE1	1:B:386:THR:OG1	2.32	0.40
1:A:320:THR:HA	1:A:354:CYS:O	2.21	0.40
1:B:160:LYS:HA	1:B:160:LYS:HD3	1.83	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	427/419 (102%)	421 (99%)	6 (1%)	0	100	100
1	B	428/419 (102%)	425 (99%)	3 (1%)	0	100	100
All	All	855/838 (102%)	846 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	341/329 (104%)	334 (98%)	7 (2%)	47	44
1	B	342/329 (104%)	332 (97%)	10 (3%)	37	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	683/658 (104%)	666 (98%)	17 (2%)	40 37

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	ARG
1	A	220	ARG
1	A	229	LEU
1	A	392	ILE
1	A	401	ARG
1	A	412	ASN
1	A	419	GLU
1	B	3	LYS
1	B	63	LYS
1	B	110	SER
1	B	175	LEU
1	B	189	PRO
1	B	229	LEU
1	B	336	PRO
1	B	370	LEU
1	B	392	ILE
1	B	412	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	76	ASN
1	A	79	ASN
1	A	106	GLN
1	A	108	GLN
1	A	355	HIS
1	B	13	GLN
1	B	23	ASN
1	B	59	GLN
1	B	253	ASN
1	B	307	GLN
1	B	412	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	IAS	B	67	1	6,7,8	1.08	0	3,8,10	1.14	0
1	IAS	A	67	1	6,7,8	0.97	0	3,8,10	1.34	1 (33%)

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	IAS	B	67	1	-	0/7/7/8	-
1	IAS	A	67	1	-	0/7/7/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	IAS	OD1-CG-CB	-2.22	118.93	125.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	PO4	B	1501	-	4,4,4	1.74	1 (25%)	6,6,6	0.47	0
3	HAI	A	1424	-	7,7,7	0.92	0	8,8,8	1.70	2 (25%)
2	PO4	B	1507	-	4,4,4	1.72	1 (25%)	6,6,6	0.45	0
2	PO4	B	1506	-	4,4,4	1.63	0	6,6,6	0.45	0
2	PO4	B	1509	-	4,4,4	1.69	1 (25%)	6,6,6	0.45	0
2	PO4	A	1503	-	4,4,4	1.55	1 (25%)	6,6,6	0.51	0
2	PO4	B	1504	-	4,4,4	1.51	0	6,6,6	0.48	0
3	HAI	B	1422	-	7,7,7	1.18	1 (14%)	8,8,8	1.67	1 (12%)
2	PO4	B	1508	-	4,4,4	1.76	2 (50%)	6,6,6	0.45	0
2	PO4	A	1502	-	4,4,4	1.95	2 (50%)	6,6,6	0.49	0
2	PO4	A	1500	-	4,4,4	1.62	0	6,6,6	0.48	0
3	HAI	B	1420	-	7,7,7	1.31	1 (14%)	8,8,8	2.53	2 (25%)

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	HAI	A	1424	-	-	-	0/1/1/1
3	HAI	B	1420	-	-	-	0/1/1/1
3	HAI	B	1422	-	-	-	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1502	PO4	P-O4	-2.42	1.47	1.54
3	B	1420	HAI	C5-C6	2.41	1.59	1.53
3	B	1422	HAI	C5-C4	2.35	1.60	1.51
2	B	1501	PO4	P-O4	-2.15	1.48	1.54
2	B	1508	PO4	P-O3	-2.14	1.48	1.54
2	A	1503	PO4	P-O2	-2.12	1.48	1.54
2	B	1507	PO4	P-O3	-2.04	1.48	1.54
2	A	1502	PO4	P-O3	-2.03	1.48	1.54
2	B	1508	PO4	P-O4	-2.01	1.48	1.54
2	B	1509	PO4	P-O4	-2.00	1.48	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1420	HAI	C6-C1-C2	5.57	115.95	110.29
3	B	1420	HAI	C5-C6-C1	3.65	116.72	111.77
3	B	1422	HAI	C6-C1-C2	3.53	113.87	110.29
3	A	1424	HAI	C2-C1-N	2.92	119.86	111.17
3	A	1424	HAI	C6-C1-N	2.63	119.00	111.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1420	HAI	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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.