



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:59 PM UTC

PDB ID : 1LCT / pdb_00001lct
Title : STRUCTURE OF THE RECOMBINANT N-TERMINAL LOBE OF HUMAN LACTOFERRIN AT 2.0 ANGSTROMS RESOLUTION
Authors : Day, C.L.; Anderson, B.F.; Baker, E.N.
Deposited on : 1993-06-19
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 ⓘ 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

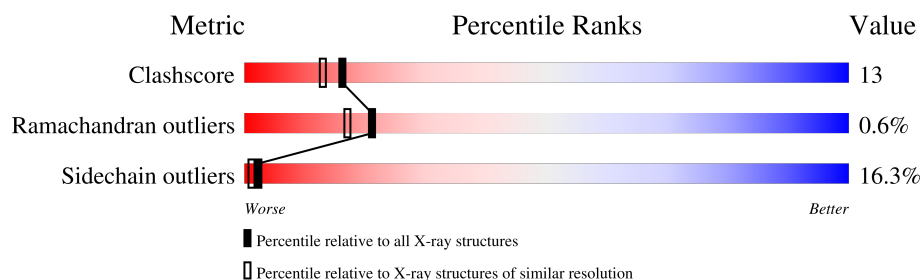
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	333	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2680 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 LACTOFERRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2489	1576	442	458	13			

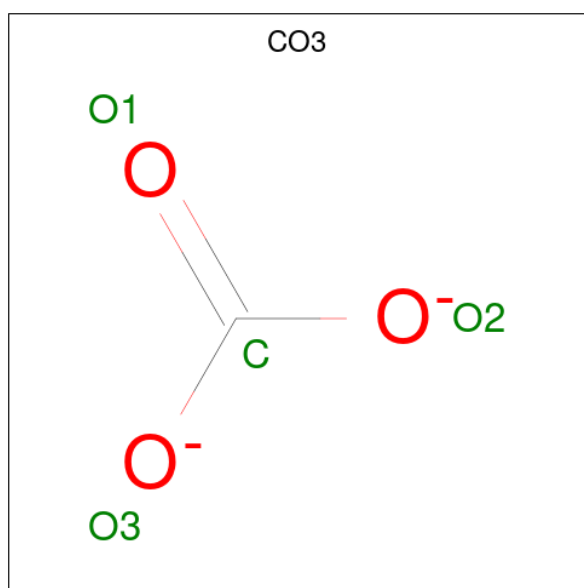
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ASN	GLN	conflict	UNP P02788

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		

- Molecule 3 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	186	Total	O	0	0
			186	186		

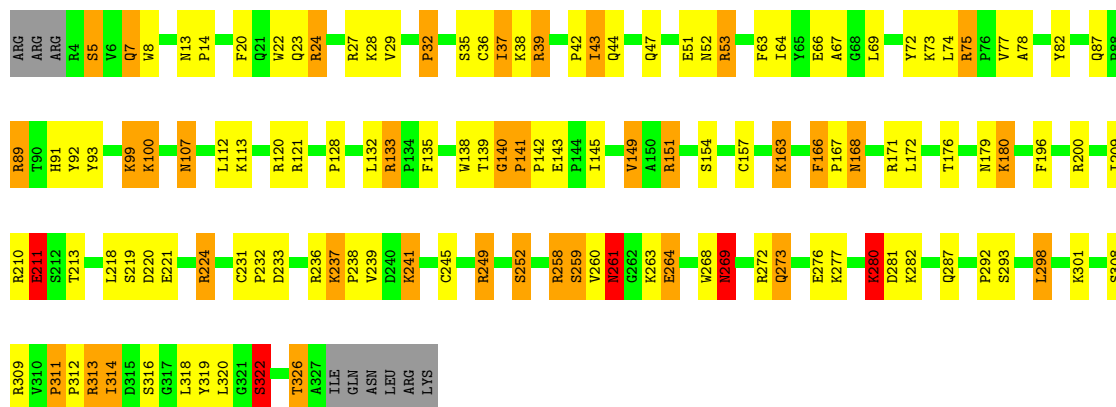
3 Residue-property plots

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: LACTOFERRIN

Chain A: 



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	133.00Å 58.30Å 58.30Å 90.00° 114.70° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.184 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2680	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

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: CO3, FE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.32	3/2553 (0.1%)	1.95	69/3457 (2.0%)

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	1	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	ARG	N-CA	-5.37	1.41	1.46
1	A	280	LYS	N-CA	-5.09	1.39	1.46
1	A	53	ARG	NE-CZ	5.06	1.38	1.33

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	311	PRO	O-C-N	10.15	125.98	121.31
1	A	53	ARG	N-CA-CB	9.36	124.05	110.47
1	A	326	THR	CA-C-N	9.14	138.15	121.70
1	A	326	THR	C-N-CA	9.14	138.15	121.70
1	A	211	GLU	N-CA-C	9.09	121.19	111.28
1	A	52	ASN	N-CA-C	8.72	123.86	113.23
1	A	239	VAL	N-CA-C	8.62	121.83	111.05
1	A	322	SER	CA-C-N	8.40	130.02	120.53
1	A	322	SER	C-N-CA	8.40	130.02	120.53
1	A	312	PRO	O-C-N	8.21	132.85	122.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	LEU	N-CA-CB	8.04	121.86	110.36
1	A	36	CYS	N-CA-C	7.80	121.12	108.41
1	A	221	GLU	N-CA-CB	-7.39	98.84	110.22
1	A	77	VAL	N-CA-C	7.33	117.83	111.90
1	A	326	THR	N-CA-CB	7.25	122.74	110.49
1	A	261	ASN	CB-CA-C	-7.20	102.21	111.86
1	A	141	PRO	N-CA-CB	6.99	107.11	103.19
1	A	273	GLN	CB-CA-C	-6.86	99.19	110.85
1	A	269	ASN	CA-CB-CG	6.82	119.42	112.60
1	A	149	VAL	N-CA-C	6.57	117.32	110.62
1	A	260	VAL	CB-CA-C	-6.57	102.06	111.19
1	A	220	ASP	CA-C-N	6.56	129.72	120.28
1	A	220	ASP	C-N-CA	6.56	129.72	120.28
1	A	179	ASN	CA-CB-CG	-6.51	106.09	112.60
1	A	38	LYS	N-CA-CB	6.48	120.72	110.55
1	A	66	GLU	N-CA-CB	-6.46	100.28	110.22
1	A	211	GLU	N-CA-CB	6.37	119.49	110.12
1	A	326	THR	CB-CA-C	6.37	123.09	110.42
1	A	269	ASN	N-CA-CB	6.34	120.10	110.28
1	A	20	PHE	CA-CB-CG	-6.18	107.62	113.80
1	A	168	ASN	N-CA-CB	-6.14	101.10	110.12
1	A	224	ARG	CB-CA-C	6.09	122.09	110.27
1	A	151	ARG	CB-CA-C	6.07	121.37	109.72
1	A	128	PRO	N-CA-CB	6.02	109.95	103.33
1	A	236	ARG	NE-CZ-NH2	-6.00	113.80	119.20
1	A	211	GLU	CB-CA-C	-5.95	100.92	110.79
1	A	232	PRO	N-CA-CB	5.89	108.80	103.20
1	A	107	ASN	CA-CB-CG	5.81	118.41	112.60
1	A	69	LEU	CB-CA-C	-5.80	100.23	109.80
1	A	258	ARG	N-CA-CB	5.70	118.52	110.36
1	A	135	PHE	CB-CA-C	-5.70	100.54	110.17
1	A	245	CYS	N-CA-CB	-5.67	100.47	110.90
1	A	264	GLU	CB-CG-CD	5.62	122.15	112.60
1	A	22	TRP	CA-C-N	5.55	127.65	120.44
1	A	22	TRP	C-N-CA	5.55	127.65	120.44
1	A	236	ARG	CD-NE-CZ	5.54	132.16	124.40
1	A	32	PRO	CB-CA-C	5.51	117.65	110.92
1	A	5	SER	CB-CA-C	-5.51	99.45	110.42
1	A	52	ASN	CA-C-O	-5.49	113.81	120.12
1	A	236	ARG	NE-CZ-NH1	5.36	126.86	121.50
1	A	64	ILE	N-CA-C	-5.34	104.38	111.05
1	A	151	ARG	CA-C-O	5.34	125.53	119.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	A	24	ARG	N-CA-CB	5.31	118.51	110.28
1	A	171	ARG	N-CA-C	5.31	117.48	111.11
1	A	157	CYS	N-CA-CB	5.30	119.43	110.69
1	A	149	VAL	N-CA-CB	5.24	117.67	110.54
1	A	149	VAL	CA-C-N	5.23	128.26	120.31
1	A	149	VAL	C-N-CA	5.23	128.26	120.31
1	A	326	THR	O-C-N	5.22	129.54	122.59
1	A	239	VAL	O-C-N	5.21	127.14	121.87
1	A	154	SER	N-CA-CB	5.20	117.86	110.16
1	A	43	ILE	N-CA-C	5.16	115.38	110.53
1	A	100	LYS	CB-CA-C	5.13	118.43	109.65
1	A	63	PHE	CA-CB-CG	-5.12	108.68	113.80
1	A	121	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	A	99	LYS	CB-CA-C	5.07	118.09	109.53
1	A	36	CYS	CA-C-N	5.00	129.40	123.19
1	A	36	CYS	C-N-CA	5.00	129.40	123.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	326	THR	CA

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	2489	0	2401	64	0
2	A	1	0	0	0	0
3	A	4	0	0	0	0
4	A	186	0	0	12	0
All	All	2680	0	2401	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 13.

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:A:314:ILE:HG23	4:A:664:HOH:O	1.49	1.09
1:A:82:TYR:CE2	1:A:252:SER:HB3	2.10	0.86
1:A:120:ARG:HG2	4:A:638:HOH:O	1.75	0.86
1:A:269:ASN:HB2	1:A:272:ARG:HH21	1.43	0.83
1:A:39:ARG:HG3	1:A:44:GLN:HB3	1.60	0.83
1:A:32:PRO:CG	1:A:273:GLN:HG3	2.13	0.79
1:A:23:GLN:O	1:A:27:ARG:HG3	1.81	0.79
1:A:43:ILE:O	1:A:47:GLN:HG3	1.84	0.77
1:A:91:HIS:CD2	1:A:249:ARG:HD3	2.23	0.74
1:A:218:LEU:O	1:A:224:ARG:NH1	2.21	0.73
1:A:237:LYS:HD2	4:A:602:HOH:O	1.89	0.71
1:A:272:ARG:NE	4:A:662:HOH:O	2.23	0.71
1:A:93:TYR:HB2	1:A:211:GLU:HG3	1.75	0.69
1:A:99:LYS:HE3	4:A:599:HOH:O	1.94	0.68
1:A:53:ARG:O	1:A:53:ARG:HG3	1.93	0.68
1:A:138:TRP:HA	4:A:642:HOH:O	1.96	0.66
1:A:73:LYS:O	1:A:259:SER:HB2	1.96	0.65
1:A:82:TYR:HE2	1:A:252:SER:HB3	1.60	0.63
1:A:93:TYR:CE2	1:A:249:ARG:HG3	2.33	0.63
1:A:7:GLN:HG2	1:A:35:SER:OG	2.00	0.61
1:A:32:PRO:HG3	1:A:273:GLN:HG3	1.83	0.60
1:A:89:ARG:NH2	1:A:211:GLU:OE1	2.26	0.59
1:A:92:TYR:HB2	1:A:211:GLU:OE2	2.03	0.59
1:A:276:GLU:HA	1:A:276:GLU:OE1	2.03	0.58
1:A:138:TRP:NE1	1:A:143:GLU:O	2.28	0.56
1:A:143:GLU:OE2	1:A:151:ARG:NH2	2.39	0.56
1:A:75:ARG:NH1	1:A:314:ILE:O	2.40	0.54
1:A:219:SER:HA	4:A:650:HOH:O	2.07	0.54
1:A:269:ASN:O	1:A:273:GLN:HG2	2.08	0.53
1:A:287:GLN:HG3	4:A:655:HOH:O	2.08	0.53
1:A:272:ARG:HD3	4:A:660:HOH:O	2.08	0.53
1:A:238:PRO:HD2	1:A:241:LYS:HG3	1.90	0.53
1:A:292:PRO:HD2	1:A:298:LEU:HD22	1.92	0.52
1:A:32:PRO:HG2	1:A:273:GLN:HG3	1.89	0.52
1:A:280:LYS:O	1:A:281:ASP:HB2	2.09	0.52
1:A:139:THR:O	1:A:140:GLY:O	2.27	0.51
1:A:231:CYS:HB2	1:A:233:ASP:OD1	2.12	0.49
1:A:268:TRP:CG	1:A:309:ARG:HD2	2.48	0.48
1:A:168:ASN:HB2	4:A:682:HOH:O	2.14	0.47
1:A:13:ASN:HB3	1:A:14:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:TYR:CE2	1:A:249:ARG:CG	2.98	0.47
1:A:233:ASP:OD1	1:A:233:ASP:N	2.40	0.47
1:A:67:ALA:O	1:A:72:TYR:HB2	2.14	0.47
1:A:292:PRO:HD2	1:A:298:LEU:CD2	2.46	0.46
1:A:209:ILE:HD12	1:A:213:THR:HB	1.97	0.45
1:A:37:ILE:HG13	1:A:53:ARG:O	2.17	0.45
1:A:311:PRO:O	1:A:314:ILE:HB	2.17	0.45
1:A:316:SER:O	1:A:319:TYR:HB3	2.16	0.45
1:A:8:TRP:N	1:A:35:SER:O	2.34	0.45
1:A:113:LYS:HB3	1:A:172:LEU:HD11	1.99	0.44
1:A:37:ILE:HD11	1:A:53:ARG:CZ	2.48	0.44
1:A:163:LYS:HE2	1:A:180:LYS:O	2.18	0.43
1:A:196:PHE:O	1:A:200:ARG:HG3	2.18	0.43
1:A:141:PRO:HA	1:A:142:PRO:C	2.43	0.42
1:A:93:TYR:O	1:A:210:ARG:HA	2.20	0.42
1:A:196:PHE:CZ	1:A:200:ARG:HD3	2.54	0.42
1:A:258:ARG:NH1	1:A:261:ASN:O	2.53	0.41
1:A:42:PRO:HD2	4:A:675:HOH:O	2.19	0.41
1:A:78:ALA:HA	1:A:308:SER:O	2.21	0.41
1:A:166:PHE:N	1:A:167:PRO:HD3	2.36	0.41
1:A:89:ARG:HH22	1:A:211:GLU:CD	2.21	0.40
1:A:319:TYR:O	1:A:322:SER:HB2	2.21	0.40
1:A:231:CYS:SG	1:A:237:LYS:HD3	2.61	0.40
1:A:318:LEU:HB2	4:A:614:HOH:O	2.21	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	322/333 (97%)	305 (95%)	15 (5%)	2 (1%)	21 17

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	GLY
1	A	326	THR

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	258/275 (94%)	216 (84%)	42 (16%)	2 1

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	7	GLN
1	A	24	ARG
1	A	28	LYS
1	A	29	VAL
1	A	37	ILE
1	A	39	ARG
1	A	51	GLU
1	A	75	ARG
1	A	87	GLN
1	A	89	ARG
1	A	100	LYS
1	A	107	ASN
1	A	112	LEU
1	A	132	LEU
1	A	133	ARG
1	A	145	ILE
1	A	149	VAL
1	A	163	LYS
1	A	166	PHE
1	A	176	THR
1	A	180	LYS
1	A	211	GLU

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Mol	Chain	Res	Type
1	A	237	LYS
1	A	241	LYS
1	A	249	ARG
1	A	252	SER
1	A	259	SER
1	A	261	ASN
1	A	263	LYS
1	A	264	GLU
1	A	269	ASN
1	A	277	LYS
1	A	280	LYS
1	A	282	LYS
1	A	293	SER
1	A	298	LEU
1	A	301	LYS
1	A	313	ARG
1	A	314	ILE
1	A	320	LEU
1	A	322	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	91	HIS
1	A	105	GLN
1	A	107	ASN
1	A	186	GLN
1	A	234	ASN
1	A	261	ASN
1	A	287	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	CO3	A	401	2	3,3,3	1.03	0	2,3,3	1.36	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.