



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2017 – 10:55 AM EDT

PDB ID : 1N76
Title : CRYSTAL STRUCTURE OF HUMAN SEMINAL LACTOFERRIN AT 3.4 Å RESOLUTION
Authors : Kumar, J.; Weber, W.; Munchau, S.; Yadav, S.; Singh, S.B.; Sarvanan, K.; Paramsivam, M.; Sharma, S.; Kaur, P.; Bhushan, A.; Srinivasan, A.; Betzel, C.; Singh, T.P.
Deposited on : unknown
Resolution : 3.40 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

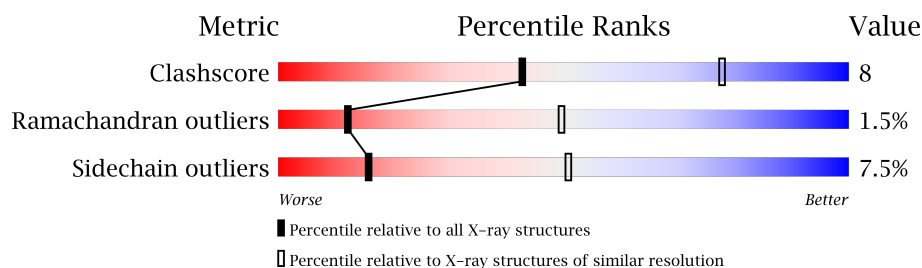
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	690	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5355 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	690	Total	C	N	O	S	0	0	0
			5344	3336	958	1013	37			

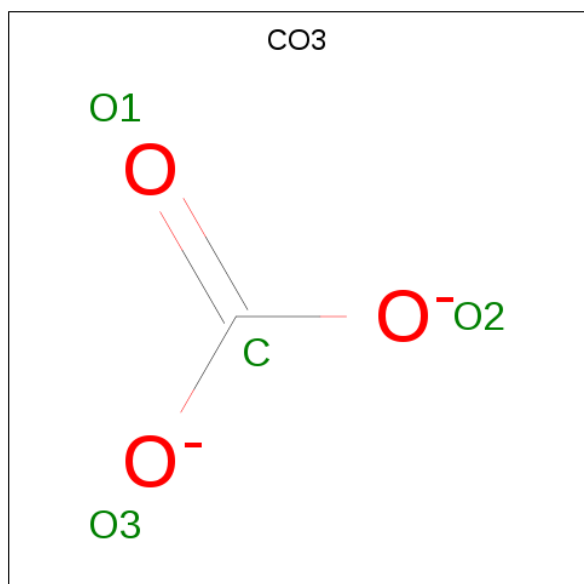
- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 4 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



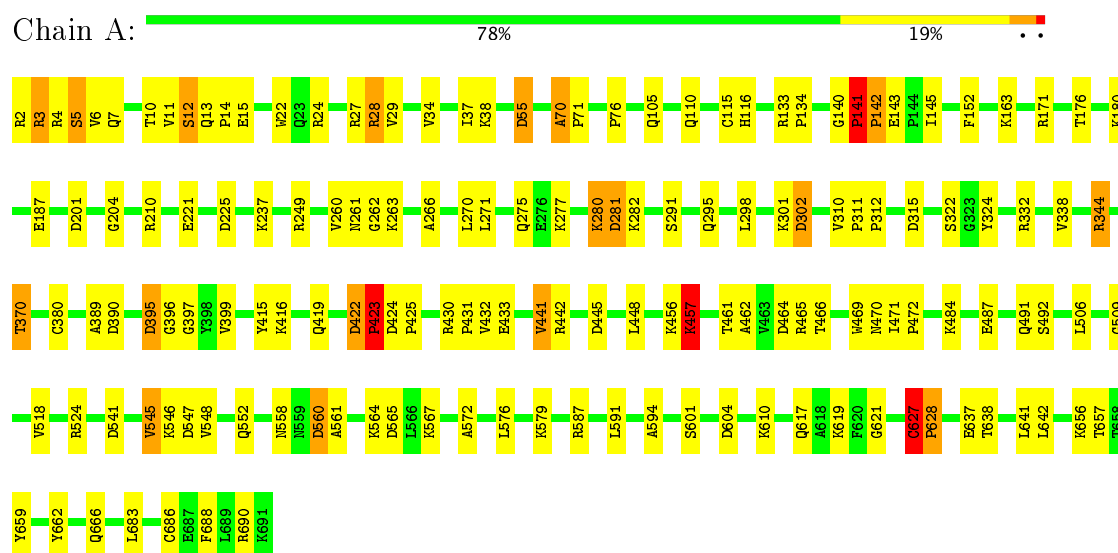
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	1	3		
4	A	1	Total	C	O	0	0
			4	1	3		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

Note EDS was not executed.

• Molecule 1: LACTOFERRIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.05 Å 97.51 Å 156.79 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.65 – 3.40	Depositor
% Data completeness (in resolution range)	100.0 (19.65-3.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.217 , 0.266	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5355	wwPDB-VP
Average B, all atoms (Å ²)	52.0	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: NA, 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	1.11	6/5458 (0.1%)	1.04	25/7382 (0.3%)

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	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	ARG	CB-CG	6.45	1.70	1.52
1	A	659	TYR	CE1-CZ	-6.07	1.30	1.38
1	A	324	TYR	CD1-CE1	-5.51	1.31	1.39
1	A	659	TYR	CG-CD2	-5.40	1.32	1.39
1	A	572	ALA	CA-CB	-5.09	1.41	1.52
1	A	389	ALA	CA-CB	-5.04	1.41	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	ARG	NE-CZ-NH1	13.33	126.96	120.30
1	A	28	ARG	NE-CZ-NH2	-11.35	114.63	120.30
1	A	28	ARG	CD-NE-CZ	7.90	134.66	123.60
1	A	180	LYS	CA-CB-CG	7.67	130.28	113.40
1	A	55	ASP	CB-CG-OD2	7.64	125.18	118.30
1	A	28	ARG	CG-CD-NE	7.15	126.82	111.80
1	A	565	ASP	CB-CG-OD2	6.79	124.41	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	A	315	ASP	CB-CG-OD2	6.32	123.99	118.30
1	A	604	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	28	ARG	CA-CB-CG	6.24	127.12	113.40
1	A	560	ASP	CB-CA-C	-6.12	98.16	110.40
1	A	180	LYS	CB-CG-CD	6.12	127.51	111.60
1	A	201	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	76	PRO	N-CD-CG	-5.68	94.68	103.20
1	A	281	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	445	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	457	LYS	CD-CE-NZ	5.38	124.06	111.70
1	A	442	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	A	395	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	464	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	547	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	302	ASP	CB-CG-OD2	5.12	122.90	118.30
1	A	141	PRO	N-CA-C	5.10	125.35	112.10
1	A	390	ASP	CB-CG-OD2	5.07	122.86	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	PRO	Peptide
1	A	627	CYS	Peptide

5.2 Too-close contacts ⓘ

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	5344	0	5201	82	0
2	A	1	0	0	0	0
3	A	2	0	0	0	0
4	A	8	0	0	0	0
All	All	5355	0	5201	82	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 (82) 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:561:ALA:HA	1:A:564:LYS:HE3	1.16	1.08
1:A:561:ALA:CA	1:A:564:LYS:HE3	1.90	1.02
1:A:2:ARG:O	1:A:263:LYS:HE2	1.61	1.00
1:A:3:ARG:HG3	1:A:266:ALA:HB2	1.44	0.98
1:A:560:ASP:O	1:A:564:LYS:HG3	1.70	0.90
1:A:10:THR:HG22	1:A:11:VAL:N	1.90	0.87
1:A:561:ALA:HA	1:A:564:LYS:CE	2.04	0.86
1:A:260:VAL:HG23	1:A:261:ASN:H	1.41	0.86
1:A:560:ASP:O	1:A:564:LYS:CG	2.24	0.84
1:A:2:ARG:O	1:A:263:LYS:CE	2.26	0.83
1:A:141:PRO:O	1:A:143:GLU:N	2.21	0.73
1:A:10:THR:CG2	1:A:15:GLU:HB3	2.21	0.70
1:A:3:ARG:HG3	1:A:266:ALA:CB	2.21	0.68
1:A:260:VAL:HG23	1:A:261:ASN:N	2.07	0.68
1:A:10:THR:HG23	1:A:15:GLU:HB3	1.79	0.65
1:A:561:ALA:N	1:A:564:LYS:HE3	2.13	0.63
1:A:10:THR:CG2	1:A:11:VAL:N	2.62	0.63
1:A:560:ASP:O	1:A:564:LYS:HG2	1.99	0.62
1:A:70:ALA:HB3	1:A:71:PRO:HD3	1.81	0.61
1:A:422:ASP:O	1:A:424:ASP:N	2.34	0.60
1:A:2:ARG:O	1:A:263:LYS:NZ	2.36	0.59
1:A:4:ARG:O	1:A:5:SER:CB	2.50	0.58
1:A:545:VAL:HG23	1:A:546:LYS:N	2.17	0.58
1:A:295:GLN:HB3	1:A:298:LEU:HD21	1.86	0.58
1:A:441:VAL:HG12	1:A:541:ASP:O	2.02	0.58
1:A:10:THR:HG22	1:A:12:SER:H	1.69	0.58
1:A:4:ARG:O	1:A:5:SER:HB2	2.05	0.56
1:A:291:SER:HB3	1:A:298:LEU:CD1	2.35	0.56
1:A:548:VAL:HG23	1:A:552:GLN:HE21	1.72	0.55
1:A:484:LYS:HD2	1:A:487:GLU:OE2	2.07	0.54
1:A:344:ARG:HD3	1:A:370:THR:CG2	2.37	0.54
1:A:10:THR:HG22	1:A:11:VAL:H	1.68	0.54
1:A:627:CYS:HB3	1:A:628:PRO:CD	2.38	0.53
1:A:187:GLU:O	1:A:187:GLU:HG3	2.08	0.52
1:A:29:VAL:O	1:A:29:VAL:HG12	2.10	0.51
1:A:3:ARG:O	1:A:4:ARG:CG	2.59	0.51
1:A:34:VAL:O	1:A:34:VAL:HG13	2.11	0.51
1:A:461:THR:O	1:A:462:ALA:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:CYS:O	1:A:690:ARG:HG2	2.11	0.51
1:A:466:THR:HG21	1:A:594:ALA:HB1	1.93	0.50
1:A:7:GLN:O	1:A:55:ASP:HB2	2.12	0.49
1:A:140:GLY:O	1:A:141:PRO:O	2.30	0.49
1:A:548:VAL:HG23	1:A:552:GLN:NE2	2.27	0.49
1:A:141:PRO:CB	1:A:142:PRO:CD	2.91	0.48
1:A:492:SER:HA	1:A:506:LEU:HD12	1.97	0.47
1:A:310:VAL:HG22	1:A:688:PHE:CZ	2.49	0.47
1:A:311:PRO:HA	1:A:312:PRO:HD3	1.84	0.47
1:A:133:ARG:N	1:A:134:PRO:CD	2.78	0.46
1:A:260:VAL:CG2	1:A:261:ASN:N	2.78	0.46
1:A:13:GLN:HB3	1:A:14:PRO:HD3	1.98	0.46
1:A:116:HIS:N	1:A:116:HIS:CD2	2.83	0.46
1:A:461:THR:HG22	1:A:465:ARG:HD3	1.97	0.45
1:A:395:ASP:O	1:A:397:GLY:N	2.49	0.45
1:A:3:ARG:CG	1:A:266:ALA:HB2	2.32	0.45
1:A:3:ARG:O	1:A:4:ARG:HG3	2.16	0.44
1:A:457:LYS:HA	1:A:491:GLN:O	2.17	0.44
1:A:576:LEU:HD21	1:A:591:LEU:HD22	1.99	0.44
1:A:271:LEU:O	1:A:275:GLN:HB2	2.16	0.44
1:A:105:GLN:HA	1:A:105:GLN:NE2	2.32	0.44
1:A:627:CYS:HB3	1:A:628:PRO:HD2	1.99	0.44
1:A:301:LYS:HD3	1:A:302:ASP:N	2.34	0.43
1:A:627:CYS:CB	1:A:628:PRO:CD	2.96	0.43
1:A:558:ASN:ND2	1:A:638:THR:OG1	2.50	0.43
1:A:656:LYS:HE2	1:A:662:TYR:HA	2.00	0.43
1:A:471:ILE:HB	1:A:472:PRO:HD3	2.01	0.42
1:A:115:CYS:SG	1:A:204:GLY:HA3	2.59	0.42
1:A:110:GLN:HB2	1:A:152:PHE:CE1	2.55	0.42
1:A:262:GLY:O	1:A:263:LYS:C	2.56	0.42
1:A:424:ASP:HA	1:A:425:PRO:HD3	1.92	0.42
1:A:37:ILE:CG2	1:A:38:LYS:N	2.82	0.42
1:A:469:TRP:O	1:A:470:ASN:C	2.58	0.42
1:A:22:TRP:CZ2	1:A:270:LEU:HD11	2.55	0.42
1:A:29:VAL:HG11	1:A:277:LYS:HD3	2.01	0.42
1:A:399:VAL:HG12	1:A:399:VAL:O	2.20	0.42
1:A:344:ARG:HD3	1:A:370:THR:HG22	2.02	0.41
1:A:415:TYR:O	1:A:416:LYS:C	2.58	0.41
1:A:509:GLY:O	1:A:524:ARG:HG3	2.21	0.41
1:A:395:ASP:O	1:A:396:GLY:C	2.58	0.41
1:A:422:ASP:O	1:A:423:PRO:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ARG:HA	1:A:431:PRO:HD3	1.94	0.40
1:A:617:GLN:O	1:A:621:GLY:HA3	2.22	0.40
1:A:641:LEU:O	1:A:642:LEU:HB2	2.22	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	688/690 (100%)	620 (90%)	58 (8%)	10 (2%)	12	49

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	70	ALA
1	A	141	PRO
1	A	142	PRO
1	A	423	PRO
1	A	628	PRO
1	A	280	LYS
1	A	419	GLN
1	A	637	GLU
1	A	545	VAL

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	575/575 (100%)	532 (92%)	43 (8%)	16	51

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	6	VAL
1	A	12	SER
1	A	24	ARG
1	A	27	ARG
1	A	28	ARG
1	A	141	PRO
1	A	145	ILE
1	A	163	LYS
1	A	171	ARG
1	A	176	THR
1	A	210	ARG
1	A	221	GLU
1	A	225	ASP
1	A	237	LYS
1	A	249	ARG
1	A	280	LYS
1	A	281	ASP
1	A	282	LYS
1	A	322	SER
1	A	332	ARG
1	A	338	VAL
1	A	370	THR
1	A	380	CYS
1	A	422	ASP
1	A	423	PRO
1	A	432	VAL
1	A	433	GLU
1	A	441	VAL
1	A	448	LEU
1	A	456	LYS
1	A	457	LYS
1	A	518	VAL
1	A	567	LYS
1	A	579	LYS
1	A	587	ARG

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Mol	Chain	Res	Type
1	A	601	SER
1	A	610	LYS
1	A	619	LYS
1	A	627	CYS
1	A	657	THR
1	A	666	GLN
1	A	683	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	105	GLN
1	A	165	GLN
1	A	329	GLN
1	A	330	ASN
1	A	552	GLN
1	A	558	ASN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 3 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	CO3	A	695	3	0,3,3	0.00	-	0,3,3	0.00	-
4	CO3	A	696	3	0,3,3	0.00	-	0,3,3	0.00	-

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	CO3	A	695	3	-	0/0/0/0	0/0/0/0
4	CO3	A	696	3	-	0/0/0/0	0/0/0/0

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.