



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 10:09 pm BST

PDB ID : 1CE2  
Title : STRUCTURE OF DIFERRIC BUFFALO LACTOFERRIN AT 2.5A RESOLUTION  
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Deposited on : 1999-03-13  
Resolution : 2.50 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

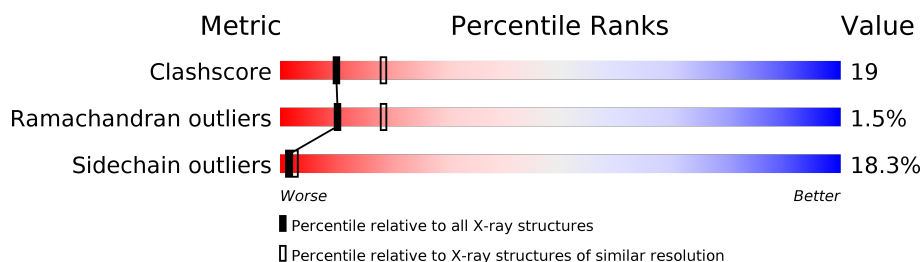
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	689	<div> <div></div> <div>59%</div> <div>33%</div> <div>8%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5415 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 PROTEIN (LACTOFERRIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	689	Total	C	N	O	S	0	0	0
			5314	3334	938	1004	38			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	SER	PHE	SEE REMARK 999	UNP O77698
A	69	ARG	LEU	SEE REMARK 999	UNP O77698
A	145	LEU	PHE	conflict	UNP O77698
A	303	SER	CYS	conflict	UNP O77698

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 3 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



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

- Molecule 4 is water.

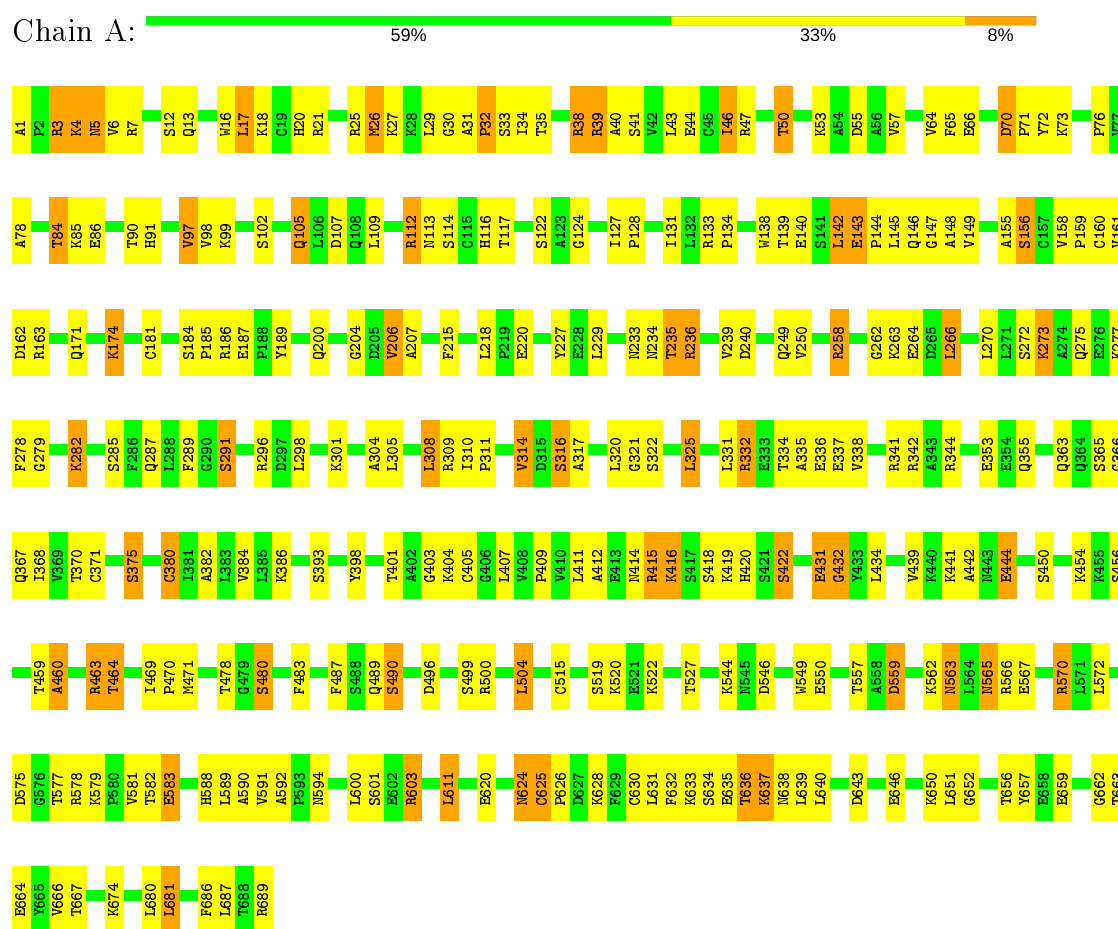
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	91	Total	O	0	0
			91	91		

### 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. 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: PROTEIN (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, $\alpha$ , $\beta$ , $\gamma$	77.46 Å 91.03 Å 131.51 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50	Depositor
% Data completeness (in resolution range)	90.0 (15.00-2.50)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.187 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5415	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	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: 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	0.36	0/5426	0.60	0/7345

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	5314	0	5214	200	0
2	A	2	0	0	0	0
3	A	8	0	0	1	0
4	A	91	0	0	4	0
All	All	5415	0	5214	200	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 19.

All (200) 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:415:ARG:HH11	1:A:415:ARG:HG2	1.22	1.02
1:A:625:CYS:HB3	1:A:626:PRO:HD3	1.43	1.00
1:A:563:ASN:HD22	1:A:563:ASN:H	1.04	0.97
1:A:334:THR:HB	1:A:337:GLU:HB2	1.47	0.96
1:A:258:ARG:HB2	1:A:258:ARG:HH11	1.36	0.91
1:A:565:ASN:HD22	1:A:567:GLU:H	1.14	0.89
1:A:258:ARG:NH1	1:A:262:GLY:HA2	1.88	0.88
1:A:415:ARG:NH1	1:A:415:ARG:HG2	1.92	0.84
1:A:39:ARG:HG3	1:A:44:GLU:HB3	1.60	0.83
1:A:625:CYS:HB3	1:A:626:PRO:CD	2.11	0.81
1:A:3:ARG:HA	1:A:263:LYS:HE3	1.65	0.78
1:A:29:LEU:HD13	1:A:29:LEU:O	1.86	0.76
1:A:321:GLY:O	1:A:325:LEU:HB2	1.87	0.75
1:A:102:SER:HB2	1:A:236:ARG:HH22	1.54	0.72
1:A:557:THR:HA	1:A:562:LYS:HD3	1.72	0.71
1:A:91:HIS:HD2	1:A:249:GLN:HG3	1.54	0.71
1:A:565:ASN:ND2	1:A:567:GLU:HB2	2.04	0.71
1:A:107:ASP:H	1:A:234:ASN:ND2	1.90	0.70
1:A:139:THR:OG1	1:A:142:LEU:HB2	1.90	0.70
1:A:102:SER:HB2	1:A:236:ARG:NH2	2.07	0.69
1:A:127:ILE:HB	1:A:128:PRO:HD3	1.74	0.69
1:A:563:ASN:ND2	1:A:563:ASN:H	1.83	0.68
1:A:34:ILE:HD11	1:A:270:LEU:HD11	1.74	0.68
1:A:1:ALA:HB3	1:A:4:LYS:HB2	1.76	0.67
1:A:570:ARG:HG3	1:A:570:ARG:HH11	1.60	0.67
1:A:401:THR:HG23	1:A:681:LEU:HD13	1.75	0.67
1:A:258:ARG:HH11	1:A:262:GLY:HA2	1.60	0.66
1:A:334:THR:HG22	1:A:336:GLU:H	1.61	0.66
1:A:411:LEU:HD12	1:A:611:LEU:HD23	1.76	0.66
1:A:456:SER:OG	1:A:490:SER:HB3	1.95	0.66
1:A:563:ASN:HD22	1:A:563:ASN:N	1.84	0.66
1:A:382:ALA:O	1:A:386:LYS:HG3	1.96	0.66
1:A:200:GLN:OE1	1:A:218:LEU:HD21	1.97	0.65
1:A:565:ASN:ND2	1:A:567:GLU:H	1.92	0.65
1:A:579:LYS:HD3	1:A:583:GLU:HG2	1.79	0.65
1:A:66:GLU:HG3	4:A:725:HOH:O	1.97	0.65
1:A:114:SER:HB3	1:A:156:SER:HB3	1.79	0.65
1:A:6:VAL:HG23	1:A:266:LEU:HD23	1.79	0.64
1:A:416:LYS:HD2	1:A:646:GLU:HB2	1.79	0.64
1:A:200:GLN:HG3	1:A:227:TYR:OH	1.98	0.64
1:A:116:HIS:ND1	1:A:158:VAL:HG22	2.12	0.64
1:A:65:PHE:HB2	1:A:320:LEU:HD11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:HIS:C	1:A:422:SER:H	2.02	0.63
1:A:31:ALA:HB1	1:A:32:PRO:HD2	1.80	0.62
1:A:91:HIS:CD2	1:A:249:GLN:HG3	2.33	0.62
1:A:469:ILE:HB	1:A:470:PRO:HD3	1.81	0.62
1:A:38:ARG:O	1:A:39:ARG:HD2	2.00	0.62
1:A:370:THR:HG22	1:A:371:CYS:N	2.16	0.61
1:A:5:ASN:HB2	1:A:33:SER:OG	2.01	0.61
1:A:398:TYR:CE2	1:A:463:ARG:HD2	2.36	0.61
1:A:662:GLY:O	1:A:666:VAL:HG23	1.99	0.61
1:A:370:THR:HG21	4:A:755:HOH:O	2.01	0.61
1:A:84:THR:C	1:A:305:LEU:HD21	2.21	0.60
1:A:133:ARG:N	1:A:134:PRO:HD2	2.16	0.60
1:A:334:THR:HG22	1:A:335:ALA:N	2.16	0.60
1:A:289:PHE:CD1	1:A:304:ALA:HB3	2.37	0.59
1:A:380:CYS:O	1:A:384:VAL:HG23	2.02	0.59
1:A:258:ARG:HH12	1:A:262:GLY:HA2	1.67	0.58
1:A:575:ASP:OD1	1:A:577:THR:HB	2.03	0.58
1:A:341:ARG:HD2	1:A:341:ARG:O	2.05	0.57
1:A:496:ASP:O	1:A:499:SER:HB3	2.05	0.57
1:A:97:VAL:HG23	1:A:229:LEU:HD23	1.86	0.56
1:A:375:SER:HB2	4:A:763:HOH:O	2.05	0.56
1:A:143:GLU:HB2	1:A:144:PRO:HD2	1.88	0.56
1:A:229:LEU:HG	1:A:239:VAL:HA	1.88	0.55
1:A:471:MET:HE1	1:A:487:PHE:HE2	1.71	0.55
1:A:109:LEU:HD22	1:A:206:VAL:HG21	1.88	0.55
1:A:215:PHE:HD1	1:A:215:PHE:H	1.55	0.55
1:A:161:VAL:HG12	1:A:162:ASP:N	2.21	0.55
1:A:12:SER:HB3	1:A:185:PRO:HG2	1.89	0.54
1:A:174:LYS:HD2	1:A:189:TYR:OH	2.08	0.54
1:A:139:THR:HG1	1:A:142:LEU:HB2	1.72	0.54
1:A:434:LEU:HD22	1:A:588:HIS:CD2	2.43	0.54
1:A:464:THR:HG21	1:A:592:ALA:HB1	1.88	0.54
1:A:570:ARG:NH1	1:A:570:ARG:HG3	2.22	0.54
1:A:117:THR:OG1	1:A:124:GLY:HA3	2.07	0.53
1:A:638:ASN:HD22	1:A:643:ASP:H	1.57	0.53
1:A:272:SER:HA	1:A:275:GLN:HE21	1.74	0.53
1:A:317:ALA:HB1	1:A:325:LEU:HD11	1.90	0.53
1:A:138:TRP:CZ2	1:A:140:GLU:HG3	2.43	0.53
1:A:233:ASN:OD1	1:A:235:THR:HG23	2.08	0.53
1:A:559:ASP:N	1:A:559:ASP:OD1	2.42	0.53
1:A:258:ARG:HB2	1:A:258:ARG:NH1	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:THR:CG2	1:A:680:LEU:HD23	2.39	0.53
1:A:638:ASN:ND2	1:A:643:ASP:H	2.07	0.52
1:A:107:ASP:H	1:A:234:ASN:HD21	1.55	0.52
1:A:66:GLU:OE2	1:A:332:ARG:NH2	2.42	0.52
1:A:409:PRO:HB2	1:A:651:LEU:HD13	1.92	0.52
1:A:464:THR:HG21	1:A:592:ALA:CB	2.40	0.51
1:A:40:ALA:HA	1:A:186:ARG:NH2	2.26	0.51
1:A:145:LEU:O	1:A:149:VAL:HG23	2.11	0.51
1:A:370:THR:CG2	1:A:371:CYS:N	2.74	0.51
1:A:404:LYS:HD3	1:A:657:TYR:OH	2.11	0.51
1:A:155:ALA:HB2	1:A:171:GLN:HE21	1.76	0.50
1:A:527:THR:HG21	1:A:636:THR:O	2.10	0.50
1:A:412:ALA:HB2	1:A:651:LEU:HD21	1.93	0.50
1:A:353:GLU:OE1	1:A:637:LYS:HD2	2.12	0.50
1:A:625:CYS:C	1:A:630:CYS:SG	2.90	0.50
1:A:566:ARG:HD2	4:A:734:HOH:O	2.11	0.49
1:A:105:GLN:HE22	1:A:236:ARG:HD2	1.77	0.49
1:A:311:PRO:O	1:A:314:VAL:HG13	2.12	0.49
1:A:344:ARG:HB2	1:A:368:ILE:O	2.13	0.49
1:A:415:ARG:HH11	1:A:415:ARG:CG	2.07	0.49
1:A:444:GLU:OE1	1:A:444:GLU:HA	2.11	0.49
1:A:85:LYS:N	1:A:305:LEU:HD21	2.26	0.49
1:A:341:ARG:HH12	1:A:603:ARG:HH21	1.60	0.49
1:A:107:ASP:N	1:A:234:ASN:HD21	2.11	0.48
1:A:634:SER:O	1:A:635:GLU:HG2	2.13	0.48
1:A:105:GLN:HA	1:A:105:GLN:HE21	1.78	0.48
1:A:565:ASN:HD22	1:A:567:GLU:N	1.96	0.48
1:A:625:CYS:CB	1:A:626:PRO:CD	2.89	0.48
1:A:334:THR:CG2	1:A:335:ALA:N	2.76	0.48
1:A:78:ALA:N	1:A:310:ILE:HD12	2.29	0.48
1:A:184:SER:HB2	1:A:185:PRO:HD2	1.96	0.48
1:A:366:GLY:O	1:A:367:GLN:HB2	2.12	0.48
1:A:50:THR:HG21	1:A:72:TYR:HB3	1.96	0.48
1:A:113:ASN:HB3	1:A:204:GLY:HA2	1.95	0.47
1:A:420:HIS:C	1:A:422:SER:N	2.66	0.47
1:A:624:ASN:OD1	1:A:624:ASN:N	2.47	0.47
1:A:138:TRP:HB2	1:A:148:ALA:CB	2.44	0.47
1:A:39:ARG:HG3	1:A:44:GLU:OE1	2.15	0.47
1:A:450:SER:O	1:A:454:LYS:HE2	2.14	0.47
1:A:625:CYS:O	1:A:626:PRO:C	2.51	0.47
1:A:258:ARG:CB	1:A:258:ARG:HH11	2.19	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ALA:HB3	1:A:386:LYS:HD2	1.96	0.47
1:A:174:LYS:HD2	1:A:189:TYR:CZ	2.50	0.47
1:A:76:PRO:HB2	1:A:310:ILE:HD13	1.96	0.47
1:A:557:THR:HA	1:A:562:LYS:CD	2.43	0.47
1:A:127:ILE:O	1:A:131:ILE:HD12	2.14	0.47
1:A:39:ARG:CG	1:A:44:GLU:HB3	2.39	0.47
1:A:38:ARG:O	1:A:39:ARG:CD	2.63	0.47
1:A:273:LYS:HA	1:A:273:LYS:HD3	1.42	0.47
1:A:308:LEU:HD13	1:A:686:PHE:CE1	2.50	0.46
1:A:4:LYS:HB3	1:A:4:LYS:HE2	1.73	0.46
1:A:215:PHE:CD1	1:A:215:PHE:N	2.82	0.46
1:A:262:GLY:O	1:A:263:LYS:HB2	2.16	0.46
1:A:27:LYS:HA	1:A:27:LYS:HD2	1.64	0.46
1:A:496:ASP:HB3	1:A:499:SER:HB2	1.98	0.46
1:A:1:ALA:C	1:A:3:ARG:H	2.17	0.46
1:A:401:THR:HG22	1:A:680:LEU:HD23	1.97	0.46
1:A:114:SER:OG	1:A:116:HIS:CE1	2.69	0.46
1:A:46:ILE:O	1:A:50:THR:HG23	2.16	0.46
1:A:155:ALA:CB	1:A:171:GLN:HE21	2.29	0.46
1:A:637:LYS:HE3	1:A:637:LYS:HB2	1.61	0.46
1:A:442:ALA:O	1:A:444:GLU:N	2.49	0.45
1:A:365:SER:O	1:A:368:ILE:HD12	2.17	0.45
1:A:431:GLU:O	1:A:432:GLY:O	2.35	0.45
1:A:478:THR:HG22	1:A:480:SER:H	1.80	0.45
1:A:565:ASN:HD21	1:A:567:GLU:HB2	1.81	0.45
1:A:620:GLU:HG2	1:A:646:GLU:HG3	1.99	0.45
1:A:143:GLU:HG3	1:A:147:GLY:HA3	1.98	0.45
1:A:279:GLY:O	1:A:282:LYS:HB2	2.17	0.44
1:A:109:LEU:CD2	1:A:206:VAL:HG21	2.48	0.44
1:A:25:ARG:NH2	1:A:285:SER:OG	2.50	0.44
1:A:589:LEU:O	1:A:590:ALA:HB2	2.17	0.44
1:A:463:ARG:NH2	3:A:693:CO3:O1	2.51	0.44
1:A:441:LYS:HD2	1:A:570:ARG:CZ	2.48	0.44
1:A:114:SER:O	1:A:156:SER:HB3	2.18	0.44
1:A:159:PRO:O	1:A:160:CYS:SG	2.76	0.43
1:A:185:PRO:C	1:A:187:GLU:N	2.71	0.43
1:A:489:GLN:HB3	1:A:504:LEU:HD13	1.99	0.43
1:A:544:LYS:HE3	1:A:546:ASP:HB2	2.00	0.43
1:A:291:SER:HB3	1:A:298:LEU:HG	2.00	0.43
1:A:334:THR:HB	1:A:337:GLU:CB	2.33	0.43
1:A:7:ARG:NH2	1:A:55:ASP:OD1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:VAL:HG12	1:A:99:LYS:N	2.32	0.43
1:A:624:ASN:HB3	1:A:628:LYS:HB2	2.01	0.43
1:A:70:ASP:O	1:A:71:PRO:C	2.57	0.43
1:A:26:MET:HE1	1:A:278:PHE:HE2	1.84	0.43
1:A:549:TRP:CZ2	1:A:582:THR:HG22	2.53	0.43
1:A:161:VAL:CG1	1:A:162:ASP:N	2.81	0.43
1:A:577:THR:CG2	1:A:578:ARG:N	2.82	0.42
1:A:5:ASN:O	1:A:263:LYS:HE2	2.18	0.42
1:A:18:LYS:HD2	1:A:298:LEU:HB2	2.01	0.42
1:A:439:VAL:HG11	1:A:572:LEU:HD11	2.02	0.42
1:A:341:ARG:NH1	1:A:603:ARG:HH21	2.16	0.42
1:A:639:LEU:O	1:A:640:LEU:HB2	2.19	0.42
1:A:316:SER:O	1:A:320:LEU:HG	2.20	0.42
1:A:432:GLY:HA2	1:A:594:ASN:OD1	2.19	0.42
1:A:632:PHE:O	1:A:643:ASP:HA	2.19	0.42
1:A:16:TRP:CE2	1:A:20:HIS:NE2	2.86	0.42
1:A:3:ARG:CA	1:A:263:LYS:HE3	2.43	0.42
1:A:311:PRO:HD2	1:A:314:VAL:HG11	2.02	0.42
1:A:109:LEU:O	1:A:112:ARG:HB2	2.20	0.42
1:A:105:GLN:NE2	1:A:236:ARG:HD2	2.35	0.41
1:A:113:ASN:CB	1:A:204:GLY:HA2	2.50	0.41
1:A:97:VAL:HG12	1:A:207:ALA:HB3	2.02	0.41
1:A:310:ILE:HA	1:A:311:PRO:HD3	1.93	0.41
1:A:6:VAL:CG2	1:A:266:LEU:HD23	2.49	0.41
1:A:546:ASP:O	1:A:550:GLU:HG3	2.21	0.41
1:A:133:ARG:N	1:A:134:PRO:CD	2.83	0.41
1:A:159:PRO:O	1:A:160:CYS:CB	2.68	0.41
1:A:3:ARG:HA	1:A:263:LYS:CE	2.45	0.41
1:A:17:LEU:O	1:A:21:ARG:HG3	2.21	0.41
1:A:370:THR:CG2	1:A:371:CYS:H	2.34	0.41
1:A:5:ASN:ND2	1:A:35:THR:OG1	2.51	0.40
1:A:258:ARG:HB2	1:A:262:GLY:HA2	2.03	0.40
1:A:403:GLY:C	1:A:405:CYS:H	2.25	0.40
1:A:459:THR:O	1:A:460:ALA:HB2	2.21	0.40
1:A:600:LEU:HA	1:A:600:LEU:HD23	1.78	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	687/689 (100%)	625 (91%)	52 (8%)	10 (2%)	10	18

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	432	GLY
1	A	625	CYS
1	A	464	THR
1	A	652	GLY
1	A	122	SER
1	A	519	SER
1	A	30	GLY
1	A	460	ALA
1	A	581	VAL
1	A	32	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	569/569 (100%)	465 (82%)	104 (18%)	1	3

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG

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Mol	Chain	Res	Type
1	A	4	LYS
1	A	5	ASN
1	A	13	GLN
1	A	17	LEU
1	A	26	MET
1	A	38	ARG
1	A	39	ARG
1	A	41	SER
1	A	43	LEU
1	A	46	ILE
1	A	47	ARG
1	A	50	THR
1	A	53	LYS
1	A	57	VAL
1	A	64	VAL
1	A	70	ASP
1	A	73	LYS
1	A	84	THR
1	A	86	GLU
1	A	90	THR
1	A	97	VAL
1	A	105	GLN
1	A	112	ARG
1	A	142	LEU
1	A	143	GLU
1	A	146	GLN
1	A	156	SER
1	A	163	ARG
1	A	174	LYS
1	A	181	CYS
1	A	206	VAL
1	A	220	GLU
1	A	235	THR
1	A	236	ARG
1	A	240	ASP
1	A	250	VAL
1	A	258	ARG
1	A	264	GLU
1	A	266	LEU
1	A	273	LYS
1	A	277	LYS
1	A	282	LYS

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Mol	Chain	Res	Type
1	A	287	GLN
1	A	291	SER
1	A	296	ARG
1	A	301	LYS
1	A	308	LEU
1	A	309	ARG
1	A	314	VAL
1	A	316	SER
1	A	322	SER
1	A	325	LEU
1	A	331	LEU
1	A	332	ARG
1	A	338	VAL
1	A	342	ARG
1	A	355	GLN
1	A	363	GLN
1	A	375	SER
1	A	380	CYS
1	A	393	SER
1	A	407	LEU
1	A	414	ASN
1	A	415	ARG
1	A	416	LYS
1	A	418	SER
1	A	419	LYS
1	A	422	SER
1	A	431	GLU
1	A	444	GLU
1	A	463	ARG
1	A	480	SER
1	A	483	PHE
1	A	490	SER
1	A	500	ARG
1	A	504	LEU
1	A	515	CYS
1	A	520	LYS
1	A	522	LYS
1	A	559	ASP
1	A	563	ASN
1	A	565	ASN
1	A	570	ARG
1	A	583	GLU

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Mol	Chain	Res	Type
1	A	591	VAL
1	A	601	SER
1	A	603	ARG
1	A	611	LEU
1	A	624	ASN
1	A	631	LEU
1	A	633	LYS
1	A	636	THR
1	A	637	LYS
1	A	650	LYS
1	A	656	THR
1	A	659	GLU
1	A	663	THR
1	A	664	GLU
1	A	667	THR
1	A	674	LYS
1	A	681	LEU
1	A	687	LEU
1	A	689	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	23	GLN
1	A	105	GLN
1	A	113	ASN
1	A	116	HIS
1	A	171	GLN
1	A	234	ASN
1	A	281	ASN
1	A	287	GLN
1	A	330	ASN
1	A	355	GLN
1	A	359	GLN
1	A	414	ASN
1	A	563	ASN
1	A	565	ASN
1	A	638	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 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	$\# Z  > 2$
3	CO3	A	693	2	0,3,3	0.00	-	0,3,3	0.00	-
3	CO3	A	692	2	0,3,3	0.00	-	0,3,3	0.00	-

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	693	CO3	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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.