



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1CE2 / pdb_00001ce2
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

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

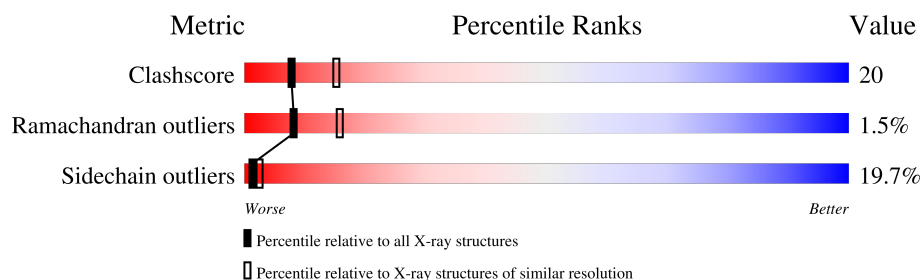
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (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 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	689	

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 (CCD ID: FE) (formula: Fe).

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

- 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		
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		

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	77.46Å 91.03Å 131.51Å 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 ²)	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	0.43	0/5426	0.95	24/7345 (0.3%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	627	ASP	N-CA-C	9.19	121.06	111.14
1	A	368	ILE	N-CA-C	-7.75	103.30	110.82
1	A	186	ARG	N-CA-C	-6.71	104.82	112.87
1	A	507	GLY	N-CA-C	-6.59	102.43	112.84
1	A	688	THR	N-CA-C	-6.47	104.64	113.30
1	A	56	ALA	N-CA-C	6.18	118.69	108.99
1	A	70	ASP	N-CA-C	5.93	122.92	109.81
1	A	102	SER	N-CA-C	-5.72	103.10	110.19
1	A	371	CYS	N-CA-C	5.68	118.81	109.72
1	A	391	ALA	N-CA-C	5.65	116.01	108.38
1	A	127	ILE	CB-CA-C	-5.50	108.47	113.70
1	A	582	THR	N-CA-C	-5.43	106.66	113.72
1	A	501	LEU	N-CA-C	-5.42	106.62	113.18
1	A	656	THR	N-CA-C	-5.41	103.56	110.53
1	A	70	ASP	CA-C-N	-5.39	113.63	119.24
1	A	70	ASP	C-N-CA	-5.39	113.63	119.24
1	A	578	ARG	N-CA-C	-5.36	101.44	109.95
1	A	421	SER	N-CA-C	-5.25	106.12	113.37
1	A	685	ALA	N-CA-C	-5.18	105.64	111.28
1	A	211	GLU	N-CA-C	5.03	117.41	111.33
1	A	625	CYS	CA-C-N	-5.02	114.02	119.24
1	A	625	CYS	C-N-CA	-5.02	114.02	119.24
1	A	616	ALA	N-CA-C	-5.02	107.11	113.18
1	A	595	HIS	N-CA-C	-5.00	103.45	110.50

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	210	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	210	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 20.

All (210) 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:HG2	1:A:415:ARG:HH11	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:HG2	1:A:415:ARG:NH1	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:O	1:A:29:LEU:HD13	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:91:HIS:HD2	1:A:249:GLN:HG3	1.54	0.71
1:A:557:THR:HA	1:A:562:LYS:HD3	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:A:563:ASN:ND2	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:420:HIS:C	1:A:422:SER:H	2.02	0.67
1:A:570:ARG:HH11	1:A:570:ARG:HG3	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:22:TRP:HE1	1:A:26:MET:HE3	1.60	0.65
1:A:84:THR:C	1:A:305:LEU:HD21	2.21	0.65
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:66:GLU:HG3	4:A:725:HOH:O	1.97	0.65
1:A:579:LYS:HD3	1:A:583:GLU:HG2	1.79	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
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: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:370:THR:HG22	1:A:371:CYS:N	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ARG:O	1:A:341:ARG:HD2	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: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:625:CYS:C	1:A:630:CYS:SG	2.90	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:HG3	1:A:570:ARG:NH1	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:OD1	1:A:559:ASP:N	2.42	0.53
1:A:258:ARG:HB2	1:A:258:ARG:NH1	2.16	0.53
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:22:TRP:NE1	1:A:26:MET:HE3	2.24	0.52
1:A:420:HIS:C	1:A:422:SER:N	2.66	0.52
1:A:66:GLU:OE2	1:A:332:ARG:NH2	2.42	0.52
1:A:107:ASP:H	1:A:234:ASN:HD21	1.55	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:1:ALA:C	1:A:3:ARG:H	2.17	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:625:CYS:O	1:A:626:PRO:C	2.51	0.50
1:A:412:ALA:HB2	1:A:651:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:GLU:OE1	1:A:637:LYS:HD2	2.12	0.50
1:A:471:MET:HE1	1:A:487:PHE:HE2	1.77	0.49
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:HE21	1:A:105:GLN:HA	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:78:ALA:N	1:A:310:ILE:HD12	2.29	0.48
1:A:334:THR:CG2	1:A:335:ALA:N	2.76	0.48
1:A:184:SER:HB2	1:A:185:PRO:HD2	1.96	0.48
1:A:185:PRO:C	1:A:187:GLU:N	2.71	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: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:258:ARG:HH11	1:A:258:ARG:CB	2.19	0.47
1:A:317:ALA:HB3	1:A:386:LYS:HD2	1.96	0.47
1:A:76:PRO:HB2	1:A:310:ILE:HD13	1.96	0.47
1:A:174:LYS:HD2	1:A:189:TYR:CZ	2.50	0.47
1:A:557:THR:HA	1:A:562:LYS:CD	2.43	0.47
1:A:39:ARG:CG	1:A:44:GLU:HB3	2.39	0.47
1:A:127:ILE:O	1:A:131:ILE:HD12	2.14	0.47
1:A:38:ARG:O	1:A:39:ARG:CD	2.63	0.47
1:A:273:LYS:HD3	1:A:273:LYS:HA	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:70:ASP:O	1:A:71:PRO:C	2.57	0.46
1:A:27:LYS:HA	1:A:27:LYS:HD2	1.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:ASP:HB3	1:A:499:SER:HB2	1.98	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:403:GLY:C	1:A:405:CYS:H	2.25	0.45
1:A:279:GLY:O	1:A:282:LYS:HB2	2.17	0.44
1:A:25:ARG:NH2	1:A:285:SER:OG	2.50	0.44
1:A:109:LEU:CD2	1:A:206:VAL:HG21	2.48	0.44
1:A:463:ARG:NH2	3:A:693:CO3:O1	2.51	0.44
1:A:589:LEU:O	1:A:590:ALA:HB2	2.17	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: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:7:ARG:NH2	1:A:55:ASP:OD1	2.50	0.43
1:A:98:VAL:HG12	1:A:99:LYS:N	2.32	0.43
1:A:334:THR:HB	1:A:337:GLU:CB	2.33	0.43
1:A:483:PHE:C	1:A:485:GLU:H	2.25	0.43
1:A:280:LYS:C	1:A:282:LYS:H	2.27	0.43
1:A:624:ASN:HB3	1:A:628:LYS:HB2	2.01	0.43
1:A:185:PRO:C	1:A:187:GLU:H	2.27	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:341:ARG:NH1	1:A:603:ARG:HH21	2.16	0.42
1:A:439:VAL:HG11	1:A:572:LEU:HD11	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3:ARG:CA	1:A:263:LYS:HE3	2.43	0.42
1:A:16:TRP:CE2	1:A:20:HIS:NE2	2.86	0.42
1:A:77:VAL:C	1:A:310:ILE:HD12	2.45	0.42
1:A:311:PRO:HD2	1:A:314:VAL:HG11	2.02	0.42
1:A:125:TRP:C	1:A:128:PRO:HD2	2.44	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:97:VAL:HG12	1:A:207:ALA:HB3	2.02	0.41
1:A:113:ASN:CB	1:A:204:GLY:HA2	2.50	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:301:LYS:HZ3	1:A:302:ASP:N	2.18	0.41
1:A:556:SER:C	1:A:557:THR:HG23	2.44	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:3:ARG:HA	1:A:263:LYS:CE	2.45	0.41
1:A:159:PRO:O	1:A:160:CYS:CB	2.68	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:1:ALA:C	1:A:3:ARG:N	2.79	0.40
1:A:458:HIS:HE1	1:A:471:MET:HE3	1.85	0.40
1:A:5:ASN:ND2	1:A:35:THR:OG1	2.51	0.40
1:A:558:ALA:O	1:A:559:ASP:C	2.64	0.40
1:A:258:ARG:HB2	1:A:262:GLY:HA2	2.03	0.40
1:A:600:LEU:HD23	1:A:600:LEU:HA	1.78	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	8 16

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 ⓘ

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%)	457 (80%)	112 (20%)	1 2

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	4	LYS
1	A	5	ASN
1	A	13	GLN
1	A	17	LEU
1	A	26	MET
1	A	27	LYS
1	A	38	ARG
1	A	41	SER
1	A	43	LEU
1	A	46	ILE

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Mol	Chain	Res	Type
1	A	47	ARG
1	A	50	THR
1	A	53	LYS
1	A	57	VAL
1	A	64	VAL
1	A	73	LYS
1	A	77	VAL
1	A	84	THR
1	A	85	LYS
1	A	86	GLU
1	A	90	THR
1	A	97	VAL
1	A	105	GLN
1	A	131	ILE
1	A	142	LEU
1	A	143	GLU
1	A	146	GLN
1	A	156	SER
1	A	163	ARG
1	A	164	GLN
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	280	LYS
1	A	282	LYS
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

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Mol	Chain	Res	Type
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	360	GLN
1	A	363	GLN
1	A	375	SER
1	A	380	CYS
1	A	388	GLU
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	420	HIS
1	A	422	SER
1	A	427	LEU
1	A	430	THR
1	A	431	GLU
1	A	444	GLU
1	A	480	SER
1	A	483	PHE
1	A	490	SER
1	A	500	ARG
1	A	504	LEU
1	A	514	LYS
1	A	515	CYS
1	A	520	LYS
1	A	559	ASP
1	A	563	ASN
1	A	567	GLU
1	A	570	ARG
1	A	583	GLU
1	A	591	VAL
1	A	601	SER
1	A	603	ARG

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Mol	Chain	Res	Type
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	673	LYS
1	A	674	LYS
1	A	681	LEU
1	A	687	LEU
1	A	689	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	105	GLN
1	A	108	GLN
1	A	113	ASN
1	A	116	HIS
1	A	171	GLN
1	A	217	ASN
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	420	HIS
1	A	545	ASN
1	A	563	ASN
1	A	565	ASN
1	A	588	HIS
1	A	638	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	3,3,3	2.09	1 (33%)	2,3,3	0.79	0
3	CO3	A	692	2	3,3,3	1.89	1 (33%)	2,3,3	0.66	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	693	CO3	O1-C	3.58	1.38	1.25
3	A	692	CO3	O1-C	3.18	1.36	1.25

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 [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.