



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:51 PM UTC

PDB ID : 1B1X / pdb_00001b1x
Title : STRUCTURE OF DIFERRIC MARE LACTOFERRIN AT 2.62A RESOLUTION
Authors : Sharma, A.K.; Srinivasan, A.; Singh, T.P.
Deposited on : 1998-11-24
Resolution : 2.62 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

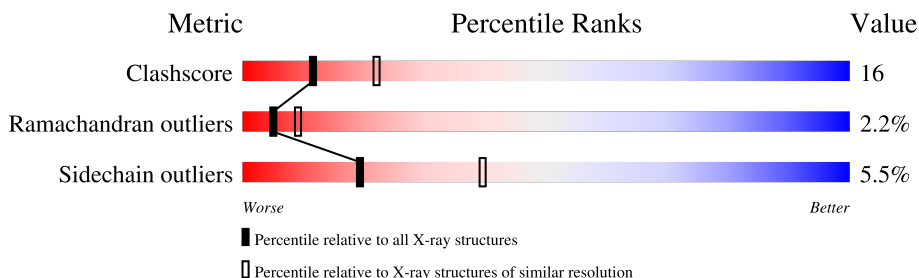
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)

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	 62% 33% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5403 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	689	Total	C	N	O	S	0	0	0
			5281	3299	937	1008	37			

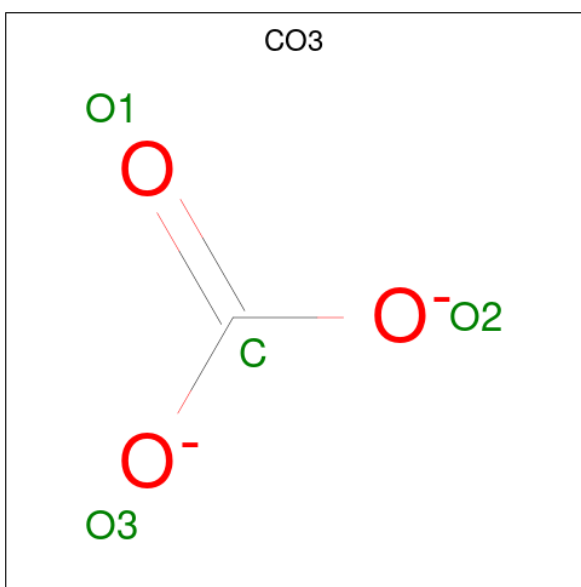
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	GLU	ASP	SEE REMARK 999	UNP O77811
A	269	LYS	ARG	SEE REMARK 999	UNP O77811
A	290	GLY	LYS	SEE REMARK 999	UNP O77811
A	294	GLY	GLU	SEE REMARK 999	UNP O77811
A	295	GLU	ASN	SEE REMARK 999	UNP O77811
A	296	GLN	LYS	SEE REMARK 999	UNP O77811

- 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.

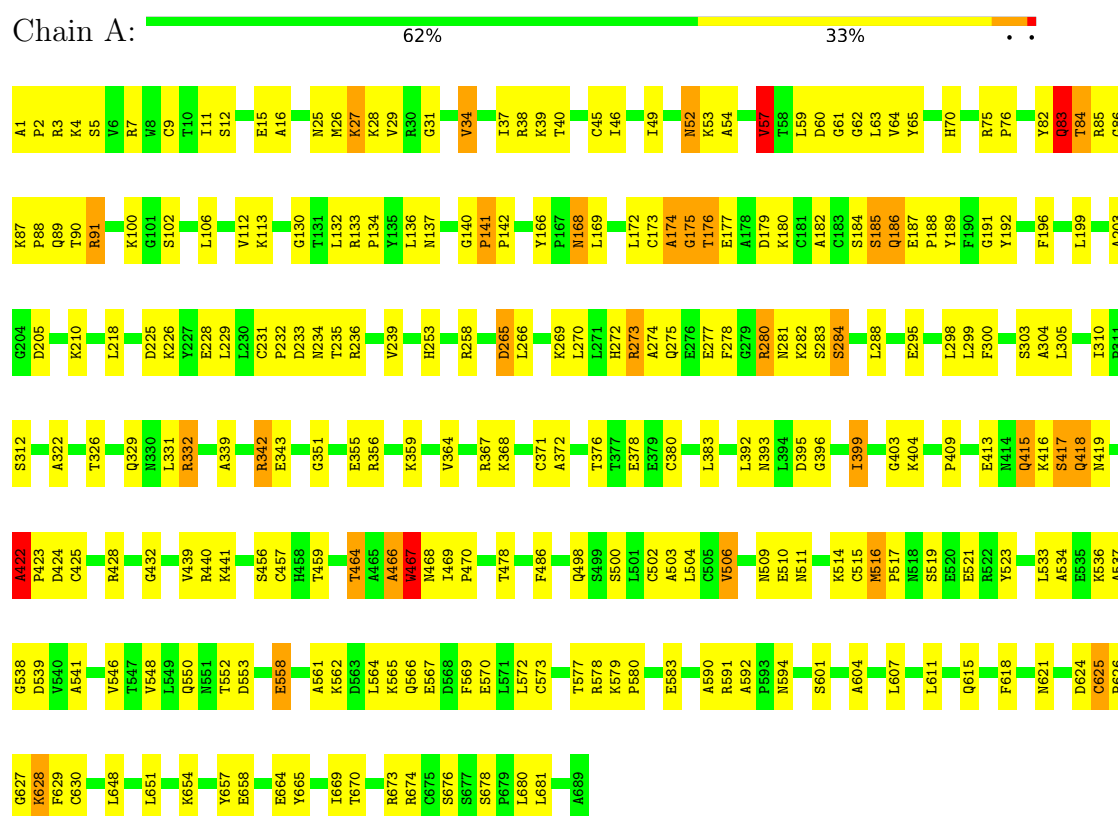
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	112	Total	O	0	0
			112	112		

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



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	85.17Å 99.50Å 103.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.62	Depositor
% Data completeness (in resolution range)	87.8 (10.00-2.62)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.194 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5403	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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: FE, CO3

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	0.75	3/5392 (0.1%)	1.21	55/7298 (0.8%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	432	GLY	C-N	-6.21	1.25	1.33
1	A	91	ARG	C-N	-5.19	1.26	1.33
1	A	191	GLY	C-N	-5.17	1.27	1.33

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	VAL	N-CA-C	-10.34	100.50	110.42
1	A	141	PRO	N-CA-C	9.95	122.84	110.70
1	A	312	SER	N-CA-C	9.68	121.91	111.36
1	A	368	LYS	N-CA-C	-8.92	101.48	111.82
1	A	351	GLY	CA-C-N	8.83	129.39	119.32
1	A	351	GLY	C-N-CA	8.83	129.39	119.32
1	A	399	ILE	N-CA-C	-7.40	101.84	111.09
1	A	284	SER	N-CA-C	-7.36	105.22	114.56
1	A	70	HIS	N-CA-C	7.07	125.43	109.81
1	A	174	ALA	N-CA-C	-7.03	97.78	109.24
1	A	509	ASN	N-CA-C	6.95	118.86	111.28
1	A	57	VAL	CB-CA-C	-6.84	101.27	111.80
1	A	140	GLY	CA-C-N	6.75	127.34	120.38
1	A	140	GLY	C-N-CA	6.75	127.34	120.38
1	A	503	ALA	N-CA-C	6.58	118.53	111.36
1	A	82	TYR	N-CA-C	6.36	118.21	109.18
1	A	467	TRP	N-CA-C	6.34	124.31	110.80
1	A	519	SER	N-CA-C	6.34	120.58	112.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	367	ARG	N-CA-C	6.31	120.32	112.24
1	A	46	ILE	N-CA-C	-6.29	104.38	110.42
1	A	558	GLU	N-CA-C	-6.19	101.78	109.64
1	A	371	CYS	N-CA-C	6.11	119.50	109.85
1	A	31	GLY	CA-C-N	6.04	126.40	119.93
1	A	31	GLY	C-N-CA	6.04	126.40	119.93
1	A	425	CYS	N-CA-C	6.00	121.21	111.37
1	A	569	PHE	N-CA-C	5.97	119.13	109.40
1	A	218	LEU	CA-C-N	5.83	125.94	119.87
1	A	218	LEU	C-N-CA	5.83	125.94	119.87
1	A	282	LYS	N-CA-C	-5.77	104.68	110.97
1	A	304	ALA	N-CA-C	-5.76	102.38	110.50
1	A	511	ASN	N-CA-C	5.74	119.47	111.90
1	A	137	ASN	N-CA-C	-5.70	104.25	110.91
1	A	456	SER	N-CA-C	5.63	118.65	109.24
1	A	601	SER	CA-C-N	5.60	128.58	120.79
1	A	601	SER	C-N-CA	5.60	128.58	120.79
1	A	40	THR	N-CA-C	5.52	120.12	113.17
1	A	186	GLN	N-CA-C	-5.51	105.36	111.36
1	A	418	GLN	N-CA-C	5.49	117.30	107.80
1	A	621	ASN	N-CA-C	-5.38	105.42	112.41
1	A	235	THR	N-CA-C	-5.36	101.26	109.41
1	A	510	GLU	N-CA-C	-5.29	107.37	112.97
1	A	372	ALA	N-CA-C	-5.27	101.06	109.23
1	A	590	ALA	N-CA-C	5.26	116.20	107.73
1	A	275	GLN	CB-CA-C	-5.25	102.64	110.88
1	A	140	GLY	N-CA-C	-5.20	101.73	112.34
1	A	628	LYS	N-CA-C	5.18	119.87	113.50
1	A	422	ALA	CA-C-N	-5.17	115.56	120.83
1	A	422	ALA	C-N-CA	-5.17	115.56	120.83
1	A	548	VAL	N-CA-C	-5.16	105.57	110.42
1	A	468	ASN	N-CA-C	5.10	119.79	111.37
1	A	674	ARG	N-CA-C	-5.06	105.89	111.71
1	A	506	VAL	CB-CA-C	-5.04	105.18	110.62
1	A	175	GLY	N-CA-C	-5.02	101.28	113.18
1	A	604	ALA	N-CA-C	5.02	117.14	111.11
1	A	226	LYS	N-CA-C	-5.00	106.96	113.16

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	5281	0	5143	167	0
2	A	2	0	0	0	0
3	A	8	0	0	0	0
4	A	112	0	0	3	0
All	All	5403	0	5143	167	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 16.

All (167) 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:16:ALA:HB2	1:A:38:ARG:HD2	1.47	0.95
1:A:625:CYS:HB3	1:A:626:PRO:HD3	1.51	0.93
1:A:580:PRO:HD2	1:A:583:GLU:HG3	1.50	0.93
1:A:84:THR:HG21	1:A:89:GLN:HG3	1.61	0.81
1:A:466:ALA:O	1:A:470:PRO:HD2	1.80	0.80
1:A:7:ARG:HH22	1:A:52:ASN:ND2	1.79	0.80
1:A:579:LYS:HB3	1:A:583:GLU:HB2	1.62	0.80
1:A:376:THR:HG22	1:A:517:PRO:HG2	1.64	0.79
1:A:83:GLN:HG3	1:A:84:THR:H	1.47	0.78
1:A:29:VAL:HG11	1:A:277:GLU:HG2	1.66	0.76
1:A:329:GLN:HA	1:A:332:ARG:HD3	1.67	0.76
1:A:364:VAL:HG13	1:A:628:LYS:HE2	1.66	0.75
1:A:87:LYS:HD2	1:A:87:LYS:H	1.52	0.74
1:A:100:LYS:HG2	1:A:228:GLU:HG3	1.70	0.74
1:A:422:ALA:HB1	1:A:423:PRO:HD2	1.72	0.70
1:A:141:PRO:HG2	1:A:142:PRO:HD3	1.74	0.69
1:A:83:GLN:CG	1:A:84:THR:H	2.06	0.68
1:A:16:ALA:CB	1:A:38:ARG:HD2	2.22	0.68
1:A:37:ILE:HG23	1:A:53:LYS:HZ2	1.60	0.67
1:A:49:ILE:HD11	1:A:57:VAL:HG22	1.75	0.67
1:A:88:PRO:HB3	1:A:305:LEU:HD12	1.77	0.67
1:A:504:LEU:HD13	1:A:537:ALA:O	1.95	0.66
1:A:624:ASP:HB3	1:A:628:LYS:HG2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:ALA:HB3	1:A:2:PRO:HD3	1.78	0.66
1:A:415:GLN:HE22	1:A:594:ASN:HD21	1.44	0.65
1:A:615:GLN:HE22	1:A:648:LEU:H	1.45	0.65
1:A:657:TYR:CE1	1:A:658:GLU:HG3	2.32	0.64
1:A:651:LEU:O	1:A:654:LYS:HG2	1.98	0.64
1:A:185:SER:HB2	1:A:295:GLU:HG2	1.80	0.64
1:A:113:LYS:HB3	1:A:172:LEU:HD11	1.79	0.64
1:A:552:THR:OG1	1:A:566:GLN:HG2	1.98	0.63
1:A:187:GLU:OE2	1:A:189:TYR:HB2	1.99	0.63
1:A:573:CYS:SG	1:A:579:LYS:HG2	2.39	0.63
1:A:4:LYS:HG3	1:A:5:SER:H	1.64	0.62
1:A:112:VAL:HG13	1:A:205:ASP:HB2	1.82	0.62
1:A:678:SER:OG	1:A:681:LEU:HB2	2.00	0.62
1:A:440:ARG:HH21	1:A:536:LYS:HA	1.65	0.62
1:A:409:PRO:O	1:A:651:LEU:HD11	2.00	0.62
1:A:25:ASN:O	1:A:29:VAL:HG23	2.00	0.61
1:A:579:LYS:CB	1:A:583:GLU:HB2	2.28	0.61
1:A:87:LYS:HD2	1:A:87:LYS:N	2.14	0.61
1:A:84:THR:C	1:A:86:GLY:H	2.08	0.61
1:A:166:TYR:HB2	1:A:169:LEU:HD12	1.84	0.59
1:A:274:ALA:HB1	1:A:288:LEU:HD22	1.83	0.59
1:A:403:GLY:HA3	1:A:657:TYR:CD2	2.38	0.59
1:A:534:ALA:C	1:A:536:LYS:H	2.11	0.58
1:A:579:LYS:HB3	1:A:583:GLU:CB	2.32	0.58
1:A:174:ALA:O	1:A:188:PRO:HD2	2.04	0.57
1:A:280:ARG:NH2	1:A:303:SER:HA	2.19	0.57
1:A:625:CYS:C	1:A:630:CYS:SG	2.88	0.57
1:A:49:ILE:CD1	1:A:57:VAL:HG22	2.34	0.57
1:A:45:CYS:O	1:A:49:ILE:HG13	2.05	0.56
1:A:84:THR:HG21	1:A:89:GLN:CG	2.35	0.56
1:A:415:GLN:HE22	1:A:594:ASN:ND2	2.04	0.56
1:A:29:VAL:HG21	1:A:278:PHE:HZ	1.71	0.56
1:A:355:GLU:O	1:A:359:LYS:HG2	2.07	0.55
1:A:521:GLU:OE2	1:A:523:TYR:HB2	2.07	0.55
1:A:265:ASP:O	1:A:269:LYS:HG3	2.07	0.55
1:A:625:CYS:HB3	1:A:626:PRO:CD	2.31	0.55
1:A:506:VAL:O	1:A:506:VAL:HG12	2.06	0.54
1:A:106:LEU:CD2	1:A:232:PRO:HA	2.38	0.54
1:A:133:ARG:HB3	1:A:134:PRO:HD3	1.89	0.54
1:A:133:ARG:N	1:A:134:PRO:CD	2.70	0.53
1:A:376:THR:HG22	1:A:517:PRO:CG	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:VAL:HG12	1:A:29:VAL:O	2.07	0.53
1:A:172:LEU:HD13	1:A:203:ALA:O	2.09	0.53
1:A:546:VAL:CG1	1:A:550:GLN:HE21	2.22	0.53
1:A:228:GLU:OE1	1:A:236:ARG:HD3	2.09	0.53
1:A:106:LEU:HD23	1:A:232:PRO:HA	1.89	0.53
1:A:329:GLN:O	1:A:332:ARG:HG2	2.09	0.53
1:A:132:LEU:O	1:A:136:LEU:HG	2.09	0.53
1:A:29:VAL:HG21	1:A:278:PHE:CZ	2.44	0.52
1:A:186:GLN:O	1:A:188:PRO:HD3	2.10	0.52
1:A:459:THR:OG1	1:A:466:ALA:CB	2.58	0.52
1:A:561:ALA:O	1:A:564:LEU:HG	2.09	0.52
1:A:176:THR:OG1	1:A:179:ASP:HB2	2.10	0.52
1:A:84:THR:C	1:A:86:GLY:N	2.68	0.51
1:A:415:GLN:O	1:A:417:SER:N	2.44	0.51
1:A:459:THR:OG1	1:A:466:ALA:HB3	2.11	0.50
1:A:59:LEU:HD22	1:A:63:LEU:HD12	1.93	0.50
1:A:516:MET:HG3	1:A:517:PRO:HD2	1.93	0.50
1:A:175:GLY:HA3	1:A:180:LYS:HA	1.92	0.49
1:A:417:SER:C	1:A:418:GLN:HG3	2.37	0.49
1:A:364:VAL:HG12	1:A:618:PHE:CZ	2.48	0.49
1:A:502:CYS:O	1:A:514:LYS:HE2	2.13	0.49
1:A:396:GLY:HA2	1:A:399:ILE:HD12	1.95	0.49
1:A:464:THR:O	1:A:469:ILE:HG12	2.12	0.49
1:A:669:ILE:O	1:A:673:ARG:HG3	2.13	0.49
1:A:283:SER:OG	1:A:284:SER:N	2.46	0.48
1:A:611:LEU:O	1:A:615:GLN:HG2	2.13	0.48
1:A:580:PRO:HD2	1:A:583:GLU:CG	2.32	0.48
1:A:439:VAL:HG12	1:A:539:ASP:O	2.14	0.48
1:A:665:TYR:O	1:A:669:ILE:HG13	2.13	0.48
1:A:356:ARG:O	1:A:359:LYS:HB2	2.13	0.48
1:A:424:ASP:O	1:A:428:ARG:N	2.46	0.48
1:A:322:ALA:O	1:A:326:THR:HG23	2.13	0.47
1:A:3:ARG:HG2	1:A:266:LEU:HD11	1.96	0.47
1:A:9:CYS:HB3	1:A:57:VAL:HG13	1.95	0.47
1:A:60:ASP:O	1:A:61:GLY:C	2.57	0.47
1:A:395:ASP:O	1:A:396:GLY:C	2.57	0.47
1:A:102:SER:OG	1:A:236:ARG:NH2	2.46	0.47
1:A:552:THR:HA	1:A:564:LEU:HB2	1.97	0.47
1:A:53:LYS:O	1:A:53:LYS:HD3	2.15	0.47
1:A:192:TYR:CD1	1:A:210:LYS:HB2	2.49	0.46
1:A:192:TYR:CE1	1:A:210:LYS:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:LYS:HB2	1:A:570:GLU:HG3	1.95	0.46
1:A:478:THR:HG21	1:A:486:PHE:CE2	2.51	0.46
1:A:577:THR:HG22	1:A:578:ARG:N	2.31	0.46
1:A:15:GLU:HG2	1:A:299:LEU:HD23	1.98	0.46
1:A:62:GLY:O	1:A:65:TYR:HB3	2.15	0.46
1:A:534:ALA:C	1:A:536:LYS:N	2.74	0.46
1:A:11:ILE:HA	1:A:39:LYS:O	2.15	0.45
1:A:673:ARG:HA	1:A:676:SER:O	2.16	0.45
1:A:84:THR:CB	1:A:87:LYS:O	2.64	0.45
1:A:231:CYS:HB2	1:A:233:ASP:OD1	2.16	0.45
1:A:422:ALA:HB1	1:A:423:PRO:CD	2.42	0.45
1:A:553:ASP:OD1	1:A:565:LYS:HA	2.17	0.45
1:A:577:THR:HG22	1:A:578:ARG:H	1.82	0.45
1:A:229:LEU:HG	1:A:239:VAL:HA	1.97	0.45
1:A:4:LYS:HD2	1:A:4:LYS:HA	1.68	0.45
1:A:37:ILE:HG22	1:A:38:ARG:N	2.30	0.45
1:A:464:THR:HG21	1:A:592:ALA:HB1	1.99	0.45
1:A:54:ALA:O	1:A:258:ARG:NH2	2.50	0.45
1:A:88:PRO:HB3	1:A:305:LEU:CD1	2.45	0.45
1:A:459:THR:H	1:A:466:ALA:CB	2.29	0.45
1:A:3:ARG:CG	1:A:266:LEU:HD11	2.47	0.44
1:A:84:THR:O	1:A:85:ARG:HB3	2.18	0.44
1:A:85:ARG:O	1:A:85:ARG:HG2	2.16	0.44
1:A:173:CYS:O	1:A:180:LYS:HE3	2.17	0.44
1:A:26:MET:HE1	1:A:273:ARG:HB3	1.98	0.44
1:A:27:LYS:HD3	1:A:28:LYS:N	2.33	0.44
1:A:533:LEU:HB2	1:A:541:ALA:HB2	2.00	0.44
1:A:553:ASP:CG	1:A:566:GLN:HG3	2.42	0.44
1:A:12:SER:HB3	1:A:184:SER:HB2	2.00	0.44
1:A:439:VAL:HG21	1:A:572:LEU:HD21	2.00	0.44
1:A:196:PHE:O	1:A:199:LEU:HB3	2.18	0.43
1:A:298:LEU:C	1:A:300:PHE:H	2.27	0.43
1:A:466:ALA:O	1:A:467:TRP:C	2.62	0.43
1:A:422:ALA:CB	1:A:423:PRO:HD2	2.47	0.43
1:A:625:CYS:CB	1:A:626:PRO:HD3	2.37	0.43
1:A:76:PRO:HB2	1:A:310:ILE:CD1	2.49	0.42
1:A:130:GLY:HA2	1:A:331:LEU:HD21	2.00	0.42
1:A:625:CYS:HA	1:A:629:PHE:O	2.18	0.42
1:A:342:ARG:HG3	1:A:342:ARG:HH11	1.84	0.42
1:A:83:GLN:HE21	1:A:84:THR:CA	2.32	0.42
1:A:339:ALA:O	1:A:343:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:678:SER:HB2	4:A:799:HOH:O	2.19	0.42
1:A:173:CYS:HB3	1:A:187:GLU:OE1	2.20	0.42
1:A:272:HIS:CD2	4:A:732:HOH:O	2.72	0.42
1:A:415:GLN:NE2	1:A:594:ASN:ND2	2.67	0.42
1:A:415:GLN:HE21	1:A:415:GLN:H	1.68	0.42
1:A:457:CYS:SG	1:A:538:GLY:HA3	2.60	0.42
1:A:60:ASP:HA	1:A:253:HIS:CD2	2.55	0.41
1:A:280:ARG:HD2	1:A:305:LEU:HD23	2.02	0.41
1:A:380:CYS:O	1:A:383:LEU:HB2	2.20	0.41
1:A:34:VAL:HG22	1:A:270:LEU:HD11	2.02	0.41
1:A:234:ASN:HA	4:A:754:HOH:O	2.19	0.41
1:A:76:PRO:HB2	1:A:310:ILE:HD13	2.02	0.41
1:A:83:GLN:CG	1:A:84:THR:N	2.78	0.41
1:A:651:LEU:HB3	1:A:654:LYS:O	2.21	0.41
1:A:168:ASN:O	1:A:168:ASN:ND2	2.54	0.40
1:A:182:ALA:H	1:A:187:GLU:HB2	1.87	0.40
1:A:393:ASN:ND2	1:A:413:GLU:OE2	2.54	0.40
1:A:84:THR:O	1:A:86:GLY:N	2.55	0.40
1:A:176:THR:N	1:A:179:ASP:HB2	2.36	0.40
1:A:459:THR:HG23	1:A:466:ALA:HB2	2.04	0.40
1:A:657:TYR:CD1	1:A:657:TYR:C	2.99	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%)	620 (90%)	52 (8%)	15 (2%)	5 9

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	ALA
1	A	467	TRP
1	A	562	LYS
1	A	176	THR
1	A	177	GLU
1	A	83	GLN
1	A	416	LYS
1	A	417	SER
1	A	464	THR
1	A	627	GLY
1	A	466	ALA
1	A	281	ASN
1	A	419	ASN
1	A	280	ARG
1	A	625	CYS

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	565/565 (100%)	534 (94%)	31 (6%)	19	39

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LYS
1	A	34	VAL
1	A	52	ASN
1	A	57	VAL
1	A	75	ARG
1	A	83	GLN
1	A	84	THR
1	A	90	THR
1	A	91	ARG
1	A	168	ASN
1	A	185	SER
1	A	225	ASP

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Mol	Chain	Res	Type
1	A	265	ASP
1	A	273	ARG
1	A	332	ARG
1	A	342	ARG
1	A	378	GLU
1	A	392	LEU
1	A	404	LYS
1	A	415	GLN
1	A	498	GLN
1	A	500	SER
1	A	515	CYS
1	A	516	MET
1	A	558	GLU
1	A	567	GLU
1	A	591	ARG
1	A	607	LEU
1	A	664	GLU
1	A	670	THR
1	A	680	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	52	ASN
1	A	137	ASN
1	A	201	ASN
1	A	272	HIS
1	A	313	GLN
1	A	330	ASN
1	A	415	GLN
1	A	513	ASN
1	A	550	GLN
1	A	556	ASN
1	A	615	GLN
1	A	642	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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	3,3,3	0.77	0	2,3,3	1.28	0
3	CO3	A	692	2	3,3,3	0.37	0	2,3,3	0.99	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.