WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 10:03 AM EST

PDB ID	:	1B7Z
Title	:	STRUCTURE OF OXALATE SUBSTITUTED DIFERRIC MARE LACTO-FERRIN FROM COLOSTRUM
Authors	:	Sharma, A.K.; Singh, T.P.
Deposited on	:	1999-01-26
Resolution	:	2.70 Å(reported)

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

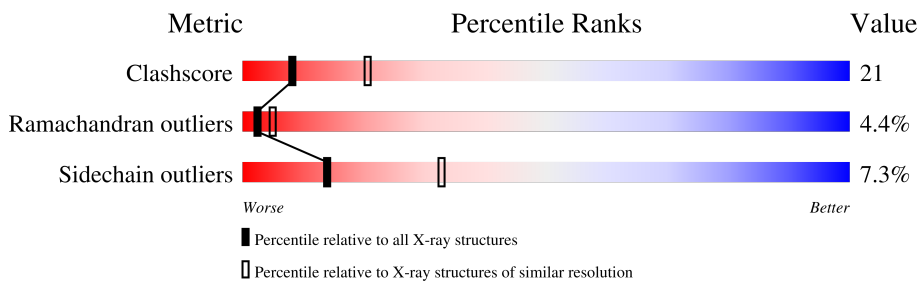|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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	Percentile Ranks	Value
Clashscore		21
Ramachandran outliers		4.4%
Sidechain outliers		7.3%

Worse *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	689	61% 34% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OXL	A	692	-	-	X	-
3	OXL	A	693	-	-	X	-

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 5365 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.
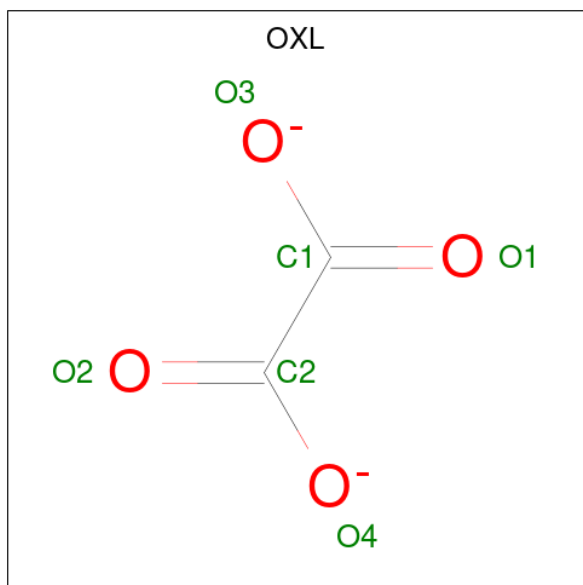
- Molecule 1 is a protein called PROTEIN (LACTOFERRIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	689	Total	C	N	O	S	0	0	0
			5281	3299	937	1008	37			

- 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 OXALATE ION (three-letter code: OXL) (formula: C_2O_4).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	2	4		
3	A	1	Total	C	O	0	0
			6	2	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	70	Total 70	O 70	0	0

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: PROTEIN (LACTOFERRIN)
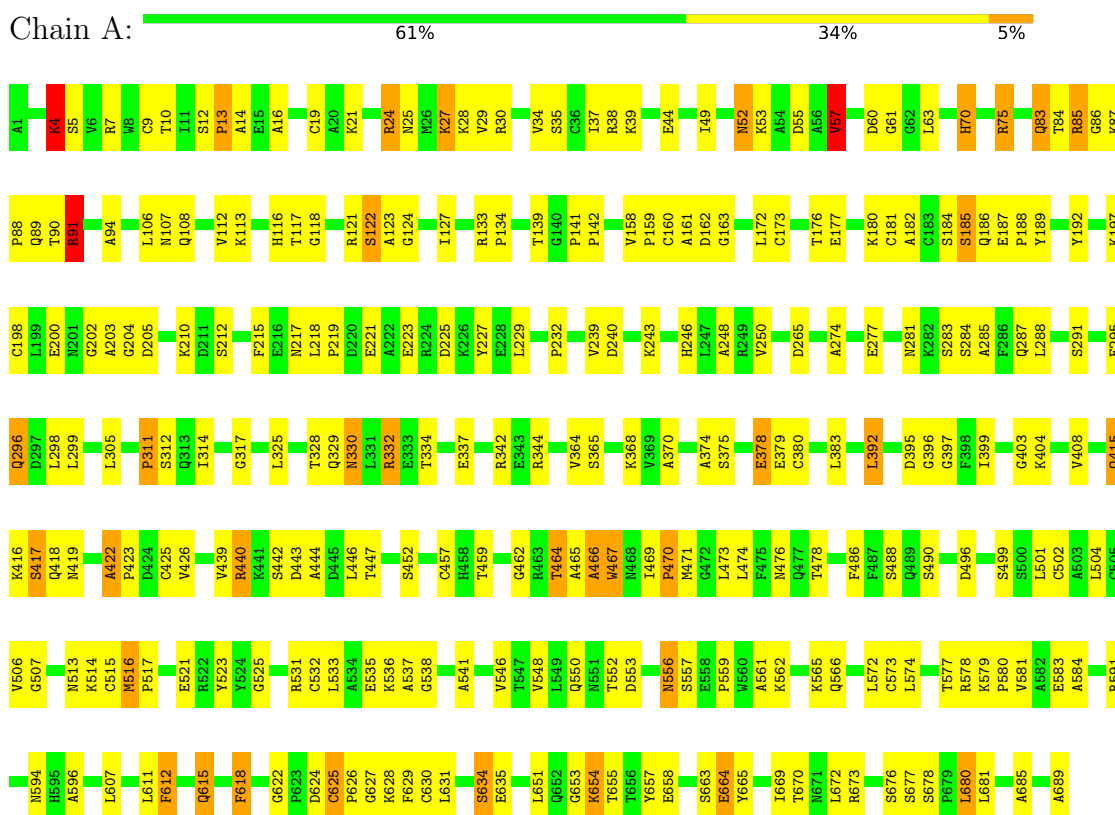
4 Data and refinement statistics ⓘ

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, α, β, γ	84.52Å 99.80Å 103.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.00 – 2.70	Depositor
% Data completeness (in resolution range)	90.0 (17.00-2.70)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.213 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5365	wwPDB-VP
Average B, all atoms (Å^2)	39.0	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: OXL, 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	0.66	0/5392	0.89	6/7298 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	91	ARG	NE-CZ-NH2	7.23	123.92	120.30
1	A	392	LEU	CA-CB-CG	6.66	130.61	115.30
1	A	70	HIS	N-CA-C	5.39	125.56	111.00
1	A	57	VAL	CB-CA-C	-5.26	101.41	111.40
1	A	34	VAL	CB-CA-C	-5.25	101.42	111.40
1	A	312	SER	N-CA-C	5.22	125.09	111.00

There are no chirality outliers.

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	5281	0	5143	221	0
2	A	2	0	0	0	0
3	A	12	0	0	8	0
4	A	70	0	0	5	0
All	All	5365	0	5143	221	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 21.

All (221) 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:465:ALA:HB3	3:A:693:OXL:O3	1.31	1.29
1:A:378:GLU:OE2	4:A:724:HOH:O	1.56	1.21
1:A:141:PRO:HG2	1:A:142:PRO:HD3	1.42	1.01
1:A:465:ALA:CB	3:A:693:OXL:O3	2.16	0.93
1:A:625:CYS:HB3	1:A:626:PRO:HD3	1.51	0.92
1:A:16:ALA:HB2	1:A:38:ARG:HD2	1.54	0.88
1:A:466:ALA:O	1:A:470:PRO:HD2	1.74	0.88
1:A:29:VAL:HG11	1:A:277:GLU:HG2	1.56	0.87
1:A:123:ALA:HB3	3:A:692:OXL:O3	1.76	0.86
1:A:629:PHE:HE1	1:A:631:LEU:HA	1.42	0.84
1:A:185:SER:HB2	1:A:295:GLU:HG2	1.57	0.84
1:A:87:LYS:H	1:A:87:LYS:HD2	1.40	0.83
1:A:624:ASP:HB3	1:A:628:LYS:HG2	1.62	0.82
1:A:580:PRO:HD2	1:A:583:GLU:HG3	1.62	0.81
1:A:552:THR:OG1	1:A:566:GLN:HG2	1.84	0.78
1:A:422:ALA:HB1	1:A:423:PRO:HD2	1.67	0.76
1:A:329:GLN:O	1:A:332:ARG:HG2	1.87	0.75
1:A:83:GLN:HG3	1:A:84:THR:H	1.51	0.74
1:A:516:MET:HG3	1:A:517:PRO:HD2	1.70	0.73
1:A:374:ALA:HB1	1:A:379:GLU:HB3	1.69	0.73
1:A:117:THR:OG1	1:A:124:GLY:HA3	1.89	0.72
1:A:364:VAL:HG13	1:A:628:LYS:HE2	1.71	0.72
1:A:141:PRO:HD2	1:A:334:THR:HG22	1.72	0.71
1:A:7:ARG:HH22	1:A:52:ASN:ND2	1.87	0.71
1:A:504:LEU:HD13	1:A:537:ALA:O	1.91	0.71
1:A:548:VAL:HG11	1:A:581:VAL:HG21	1.73	0.70
1:A:186:GLN:O	1:A:188:PRO:HD3	1.92	0.69
1:A:665:TYR:CE2	1:A:669:ILE:HD11	2.28	0.69
1:A:113:LYS:HB3	1:A:172:LEU:HD11	1.75	0.68
1:A:291:SER:HB3	1:A:298:LEU:HD12	1.75	0.68
1:A:478:THR:HG21	1:A:486:PHE:HE2	1.58	0.68
1:A:502:CYS:O	1:A:514:LYS:HE2	1.95	0.67
1:A:88:PRO:HB3	1:A:305:LEU:HD12	1.74	0.67
1:A:459:THR:OG1	1:A:466:ALA:HB2	1.94	0.67
1:A:7:ARG:HH22	1:A:52:ASN:HD21	1.44	0.66
1:A:496:ASP:HB3	1:A:499:SER:HB3	1.78	0.66
1:A:478:THR:HG21	1:A:486:PHE:CE2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:PHE:CE1	1:A:631:LEU:HA	2.29	0.65
1:A:16:ALA:CB	1:A:38:ARG:HD2	2.25	0.65
1:A:172:LEU:HD13	1:A:203:ALA:O	1.96	0.64
1:A:657:TYR:CE1	1:A:658:GLU:HG3	2.32	0.64
1:A:625:CYS:HB3	1:A:626:PRO:CD	2.27	0.63
1:A:91:ARG:NH2	4:A:701:HOH:O	2.05	0.63
1:A:173:CYS:O	1:A:180:LYS:HE3	1.98	0.63
1:A:403:GLY:HA3	1:A:657:TYR:CD2	2.34	0.63
1:A:83:GLN:OE1	1:A:212:SER:HB3	1.98	0.62
1:A:329:GLN:HA	1:A:332:ARG:HD3	1.80	0.62
1:A:579:LYS:HB3	1:A:583:GLU:CB	2.29	0.62
1:A:84:THR:OG1	1:A:89:GLN:HG3	1.99	0.62
1:A:112:VAL:HG13	1:A:205:ASP:HB2	1.81	0.62
1:A:473:LEU:O	1:A:476:ASN:HB3	1.99	0.62
1:A:9:CYS:HB3	1:A:57:VAL:HG13	1.82	0.61
1:A:29:VAL:HG12	1:A:29:VAL:O	2.01	0.60
1:A:49:ILE:HD11	1:A:57:VAL:HG22	1.84	0.60
1:A:218:LEU:HB3	1:A:223:GLU:HB2	1.84	0.59
1:A:459:THR:OG1	1:A:466:ALA:CB	2.50	0.59
1:A:229:LEU:HG	1:A:239:VAL:HA	1.84	0.59
1:A:415:GLN:HE22	1:A:594:ASN:HD21	1.51	0.58
1:A:553:ASP:OD1	1:A:565:LYS:HA	2.03	0.58
1:A:634:SER:O	1:A:635:GLU:HB2	2.02	0.58
1:A:141:PRO:CG	1:A:142:PRO:HD3	2.25	0.58
1:A:374:ALA:CB	1:A:379:GLU:HB3	2.33	0.58
1:A:87:LYS:HD2	1:A:87:LYS:N	2.17	0.58
1:A:84:THR:C	1:A:86:GLY:H	2.06	0.58
1:A:94:ALA:CB	1:A:123:ALA:HB2	2.34	0.57
1:A:10:THR:OG1	1:A:38:ARG:HG2	2.04	0.57
1:A:83:GLN:CG	1:A:84:THR:H	2.18	0.57
1:A:665:TYR:O	1:A:669:ILE:HG13	2.05	0.56
1:A:37:ILE:HG22	1:A:38:ARG:N	2.20	0.56
1:A:446:LEU:O	1:A:578:ARG:NH1	2.38	0.56
1:A:506:VAL:HG12	1:A:506:VAL:O	2.05	0.56
1:A:653:GLY:O	1:A:655:THR:HG23	2.05	0.56
1:A:442:SER:O	1:A:444:ALA:N	2.36	0.56
1:A:123:ALA:CB	3:A:692:OXL:O3	2.53	0.56
1:A:673:ARG:HA	1:A:676:SER:O	2.06	0.55
1:A:84:THR:HG21	1:A:87:LYS:O	2.05	0.55
1:A:112:VAL:HG12	1:A:113:LYS:N	2.19	0.55
1:A:112:VAL:CG1	1:A:205:ASP:HB2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ALA:HB1	1:A:123:ALA:CB	2.36	0.54
1:A:452:SER:HA	1:A:486:PHE:CE1	2.42	0.54
1:A:217:ASN:O	1:A:219:PRO:HD3	2.08	0.54
1:A:459:THR:HG22	1:A:525:GLY:C	2.27	0.54
1:A:192:TYR:CD1	1:A:210:LYS:HB2	2.42	0.54
1:A:49:ILE:CD1	1:A:57:VAL:HG22	2.38	0.54
1:A:507:GLY:HA2	1:A:513:ASN:O	2.08	0.54
1:A:625:CYS:C	1:A:630:CYS:SG	2.86	0.54
1:A:133:ARG:N	1:A:134:PRO:CD	2.71	0.53
1:A:629:PHE:HE1	1:A:631:LEU:CA	2.19	0.53
1:A:19:CYS:HA	1:A:299:LEU:HD11	1.91	0.53
1:A:121:ARG:HB3	3:A:692:OXL:C2	2.39	0.53
1:A:625:CYS:HA	1:A:629:PHE:O	2.08	0.53
1:A:53:LYS:O	1:A:53:LYS:HD3	2.09	0.53
1:A:415:GLN:O	1:A:417:SER:N	2.42	0.53
1:A:112:VAL:CG1	1:A:113:LYS:N	2.72	0.53
1:A:122:SER:HB3	1:A:250:VAL:HG11	1.91	0.52
1:A:328:THR:O	1:A:332:ARG:HD2	2.08	0.52
1:A:556:ASN:HB3	1:A:561:ALA:HB1	1.91	0.52
1:A:330:ASN:HB3	4:A:732:HOH:O	2.09	0.52
1:A:579:LYS:HB3	1:A:583:GLU:HB2	1.91	0.52
1:A:189:TYR:CG	1:A:198:CYS:HB2	2.46	0.51
1:A:417:SER:C	1:A:418:GLN:HG3	2.30	0.51
1:A:464:THR:HG23	1:A:665:TYR:CZ	2.45	0.51
1:A:84:THR:O	1:A:85:ARG:HB3	2.10	0.51
1:A:127:ILE:HD12	1:A:248:ALA:HB3	1.92	0.50
1:A:141:PRO:CD	1:A:334:THR:HG22	2.41	0.50
1:A:133:ARG:HB3	1:A:134:PRO:HD3	1.93	0.50
1:A:84:THR:C	1:A:86:GLY:N	2.65	0.50
1:A:447:THR:HA	1:A:572:LEU:HD22	1.94	0.50
1:A:106:LEU:CD2	1:A:232:PRO:HA	2.41	0.50
1:A:466:ALA:O	1:A:470:PRO:CD	2.54	0.49
1:A:439:VAL:HG21	1:A:572:LEU:HD21	1.95	0.49
1:A:685:ALA:O	1:A:689:ALA:HB2	2.12	0.49
1:A:457:CYS:SG	1:A:538:GLY:HA3	2.53	0.49
1:A:39:LYS:HB3	1:A:44:GLU:HB3	1.94	0.49
1:A:200:GLU:HG3	1:A:227:TYR:OH	2.13	0.48
1:A:364:VAL:HG12	1:A:618:PHE:CE2	2.48	0.48
1:A:7:ARG:HA	1:A:35:SER:HB3	1.95	0.48
1:A:118:GLY:HA2	1:A:159:PRO:HD2	1.95	0.48
1:A:422:ALA:CB	1:A:423:PRO:HD2	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:THR:O	1:A:469:ILE:HG12	2.13	0.48
1:A:465:ALA:HB3	3:A:693:OXL:C1	2.29	0.48
1:A:399:ILE:HD11	1:A:596:ALA:HB3	1.95	0.48
1:A:37:ILE:HG22	1:A:38:ARG:H	1.78	0.48
1:A:556:ASN:HD22	1:A:557:SER:N	2.11	0.48
1:A:12:SER:HB3	1:A:184:SER:HB2	1.96	0.48
1:A:422:ALA:HB1	1:A:423:PRO:CD	2.40	0.47
1:A:334:THR:OG1	1:A:337:GLU:HG3	2.14	0.47
1:A:83:GLN:HE21	1:A:84:THR:N	2.11	0.47
1:A:618:PHE:CD2	1:A:629:PHE:HB3	2.49	0.47
1:A:84:THR:O	1:A:84:THR:HG22	2.15	0.47
1:A:88:PRO:O	1:A:89:GLN:HG2	2.14	0.47
1:A:426:VAL:HG12	1:A:426:VAL:O	2.15	0.47
1:A:28:LYS:NZ	1:A:285:ALA:HB1	2.30	0.47
1:A:478:THR:CG2	1:A:486:PHE:HE2	2.27	0.47
1:A:533:LEU:HB2	1:A:541:ALA:HB2	1.96	0.47
1:A:116:HIS:CD2	1:A:158:VAL:HG22	2.51	0.46
1:A:556:ASN:HD22	1:A:557:SER:H	1.62	0.46
1:A:94:ALA:HB2	1:A:123:ALA:HB2	1.96	0.46
1:A:75:ARG:NH1	1:A:314:ILE:O	2.48	0.46
1:A:440:ARG:HH21	1:A:536:LYS:HA	1.79	0.46
1:A:552:THR:O	1:A:553:ASP:HB2	2.15	0.46
1:A:548:VAL:HB	1:A:581:VAL:HG11	1.99	0.45
1:A:94:ALA:CB	1:A:123:ALA:CB	2.94	0.45
1:A:665:TYR:CD2	1:A:669:ILE:HD11	2.51	0.45
1:A:13:PRO:O	1:A:14:ALA:C	2.54	0.45
1:A:274:ALA:HB1	1:A:288:LEU:HD22	1.98	0.45
1:A:577:THR:HG22	1:A:578:ARG:N	2.32	0.45
1:A:580:PRO:HD2	1:A:583:GLU:CG	2.42	0.45
1:A:329:GLN:HA	1:A:332:ARG:CD	2.44	0.45
1:A:60:ASP:O	1:A:61:GLY:C	2.55	0.45
1:A:546:VAL:CG1	1:A:550:GLN:NE2	2.80	0.45
1:A:651:LEU:HB3	1:A:654:LYS:O	2.16	0.45
1:A:466:ALA:O	1:A:467:TRP:C	2.55	0.45
1:A:553:ASP:OD2	1:A:566:GLN:HG3	2.17	0.45
1:A:325:LEU:HD23	1:A:325:LEU:HA	1.81	0.44
1:A:470:PRO:HG2	1:A:471:MET:H	1.81	0.44
1:A:611:LEU:O	1:A:615:GLN:HG2	2.16	0.44
1:A:182:ALA:H	1:A:187:GLU:HB2	1.82	0.44
1:A:395:ASP:O	1:A:396:GLY:C	2.54	0.44
1:A:189:TYR:HE1	1:A:197:LYS:HB3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:ASP:CG	1:A:566:GLN:HG3	2.38	0.44
1:A:83:GLN:CG	1:A:84:THR:N	2.81	0.44
1:A:84:THR:CB	1:A:87:LYS:O	2.65	0.44
1:A:678:SER:OG	1:A:681:LEU:HB2	2.18	0.44
1:A:296:GLN:NE2	4:A:757:HOH:O	2.51	0.44
1:A:523:TYR:CD2	1:A:532:CYS:HB2	2.53	0.44
1:A:200:GLU:C	1:A:202:GLY:H	2.21	0.43
1:A:651:LEU:O	1:A:654:LYS:HG2	2.18	0.43
1:A:217:ASN:C	1:A:219:PRO:HD3	2.38	0.43
1:A:628:LYS:O	1:A:629:PHE:HB2	2.19	0.43
1:A:664:GLU:N	1:A:664:GLU:CD	2.71	0.43
1:A:60:ASP:O	1:A:63:LEU:N	2.50	0.43
1:A:113:LYS:HB2	1:A:204:GLY:HA2	1.99	0.43
1:A:243:LYS:O	1:A:246:HIS:CE1	2.72	0.43
1:A:85:ARG:HG2	1:A:85:ARG:O	2.18	0.43
1:A:612:PHE:HD1	1:A:612:PHE:HA	1.68	0.43
1:A:672:LEU:HD23	1:A:672:LEU:HA	1.84	0.43
1:A:4:LYS:CG	1:A:5:SER:H	2.32	0.43
1:A:127:ILE:HD12	1:A:248:ALA:CB	2.48	0.43
1:A:531:ARG:O	1:A:535:GLU:N	2.51	0.43
1:A:83:GLN:HE21	1:A:84:THR:CA	2.32	0.43
1:A:344:ARG:HD3	1:A:370:ALA:CB	2.49	0.43
1:A:27:LYS:HD3	1:A:28:LYS:N	2.33	0.43
1:A:283:SER:OG	1:A:284:SER:N	2.52	0.43
1:A:364:VAL:CG1	1:A:618:PHE:CE2	3.02	0.43
1:A:574:LEU:HD23	1:A:574:LEU:HA	1.90	0.43
1:A:440:ARG:NH2	1:A:536:LYS:HA	2.34	0.42
1:A:680:LEU:HD23	1:A:680:LEU:HA	1.84	0.42
1:A:317:GLY:HA2	1:A:325:LEU:HD11	2.01	0.42
1:A:83:GLN:HE21	1:A:84:THR:C	2.23	0.42
1:A:107:ASN:OD1	1:A:108:GLN:HG3	2.18	0.42
1:A:459:THR:HG22	1:A:525:GLY:O	2.19	0.42
1:A:490:SER:HB2	1:A:501:LEU:HA	2.01	0.42
1:A:4:LYS:HD2	1:A:4:LYS:HA	1.50	0.42
1:A:465:ALA:CA	3:A:693:OXL:O3	2.67	0.42
1:A:298:LEU:O	1:A:299:LEU:HB2	2.19	0.42
1:A:197:LYS:HA	1:A:197:LYS:HD2	1.62	0.42
1:A:470:PRO:O	1:A:473:LEU:N	2.53	0.42
1:A:83:GLN:HE21	1:A:85:ARG:N	2.17	0.41
1:A:573:CYS:SG	1:A:579:LYS:HG2	2.59	0.41
1:A:7:ARG:HB2	1:A:55:ASP:OD2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:PHE:HZ	1:A:240:ASP:HA	1.85	0.41
1:A:474:LEU:C	1:A:476:ASN:N	2.72	0.41
1:A:365:SER:O	1:A:368:LYS:HG3	2.20	0.41
1:A:4:LYS:HG3	1:A:5:SER:H	1.85	0.41
1:A:452:SER:HA	1:A:486:PHE:HE1	1.83	0.41
1:A:622:GLY:O	1:A:625:CYS:HB2	2.21	0.41
1:A:25:ASN:O	1:A:29:VAL:HG23	2.21	0.41
1:A:459:THR:H	1:A:466:ALA:HB2	1.85	0.41
1:A:10:THR:HG21	1:A:16:ALA:HA	2.03	0.41
1:A:344:ARG:HD3	1:A:370:ALA:HB3	2.01	0.41
1:A:618:PHE:CD1	1:A:618:PHE:N	2.86	0.41
1:A:611:LEU:HD23	1:A:611:LEU:HA	1.92	0.41
1:A:653:GLY:N	4:A:738:HOH:O	2.08	0.40
1:A:21:LYS:O	1:A:24:ARG:HB3	2.21	0.40
1:A:380:CYS:O	1:A:383:LEU:HB2	2.22	0.40
1:A:161:ALA:O	1:A:163:GLY:N	2.54	0.40
1:A:189:TYR:HD1	1:A:189:TYR:HA	1.76	0.40
1:A:521:GLU:OE2	1:A:523:TYR:HB2	2.22	0.40
1:A:121:ARG:HB3	3:A:692:OXL:O4	2.21	0.40
1:A:397:GLY:HA3	1:A:462:GLY:O	2.21	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%)	579 (84%)	78 (11%)	30 (4%)	2	5

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	LYS

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Mol	Chain	Res	Type
1	A	70	HIS
1	A	176	THR
1	A	177	GLU
1	A	417	SER
1	A	422	ALA
1	A	467	TRP
1	A	562	LYS
1	A	24	ARG
1	A	139	THR
1	A	281	ASN
1	A	443	ASP
1	A	584	ALA
1	A	627	GLY
1	A	122	SER
1	A	162	ASP
1	A	221	GLU
1	A	464	THR
1	A	625	CYS
1	A	425	CYS
1	A	488	SER
1	A	419	ASN
1	A	466	ALA
1	A	634	SER
1	A	663	SER
1	A	311	PRO
1	A	416	LYS
1	A	654	LYS
1	A	470	PRO
1	A	559	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	565/565 (100%)	524 (93%)	41 (7%)	14	33

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	13	PRO
1	A	27	LYS
1	A	30	ARG
1	A	52	ASN
1	A	57	VAL
1	A	75	ARG
1	A	83	GLN
1	A	85	ARG
1	A	90	THR
1	A	91	ARG
1	A	160	CYS
1	A	181	CYS
1	A	185	SER
1	A	225	ASP
1	A	265	ASP
1	A	287	GLN
1	A	296	GLN
1	A	311	PRO
1	A	330	ASN
1	A	332	ARG
1	A	342	ARG
1	A	375	SER
1	A	378	GLU
1	A	392	LEU
1	A	404	LYS
1	A	408	VAL
1	A	415	GLN
1	A	440	ARG
1	A	515	CYS
1	A	516	MET
1	A	556	ASN
1	A	591	ARG
1	A	607	LEU
1	A	612	PHE
1	A	615	GLN
1	A	618	PHE
1	A	664	GLU
1	A	670	THR
1	A	677	SER
1	A	680	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	83	GLN
1	A	137	ASN
1	A	201	ASN
1	A	330	ASN
1	A	415	GLN
1	A	511	ASN
1	A	513	ASN
1	A	550	GLN
1	A	556	ASN
1	A	615	GLN
1	A	621	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 monosaccharides 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	OXL	A	693	2	5,5,5	1.56	1 (20%)	6,6,6	2.02	2 (33%)
3	OXL	A	692	2	5,5,5	1.57	1 (20%)	6,6,6	2.11	2 (33%)

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
3	OXL	A	693	2	-	1/4/4/4	-
3	OXL	A	692	2	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	692	OXL	O3-C1	-2.74	1.22	1.30
3	A	693	OXL	O3-C1	-2.51	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	692	OXL	O4-C2-O2	3.82	132.34	123.61
3	A	693	OXL	O4-C2-O2	3.65	131.96	123.61
3	A	693	OXL	O2-C2-C1	-2.61	112.41	120.78
3	A	692	OXL	O2-C2-C1	-2.47	112.86	120.78

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	693	OXL	O3-C1-C2-O4

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	693	OXL	4	0
3	A	692	OXL	4	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.