Full wwPDB X-ray Structure Validation Report ⓘ

PDB ID	:	3CR9
Title	:	Crystal structure of the complex of Lactoferrin with 6-(Hydroxymethyl)oxane-2,3,4,5-tetrol at 3.49 A resolution
Authors	:	Mir, R.; Kaur, A.; Singh, A.K.; Singh, N.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on	:	2008-04-05
Resolution	:	3.49 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)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36
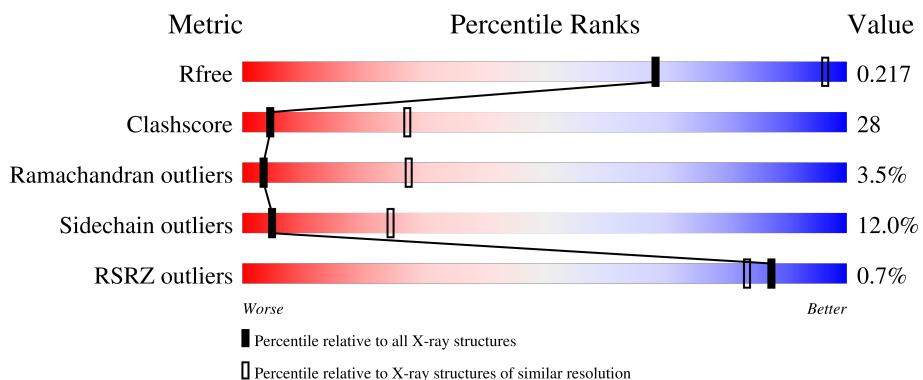
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
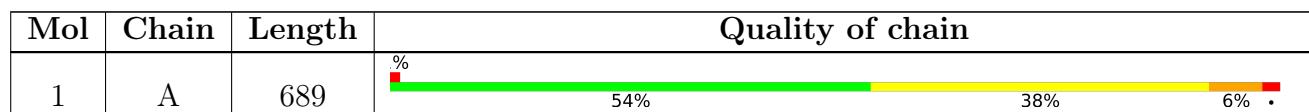
The reported resolution of this entry is 3.49 Å.

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
Rfree		0.217
Clashscore		28
Ramachandran outliers		3.5%
Sidechain outliers		12.0%
RSRZ outliers		0.7%

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))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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% 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.

Mol	Chain	Length	Quality of chain
1	A	689	54% 38% 6% ·

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
2	GLC	A	692	-	-	-	X

2   Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 5295 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.
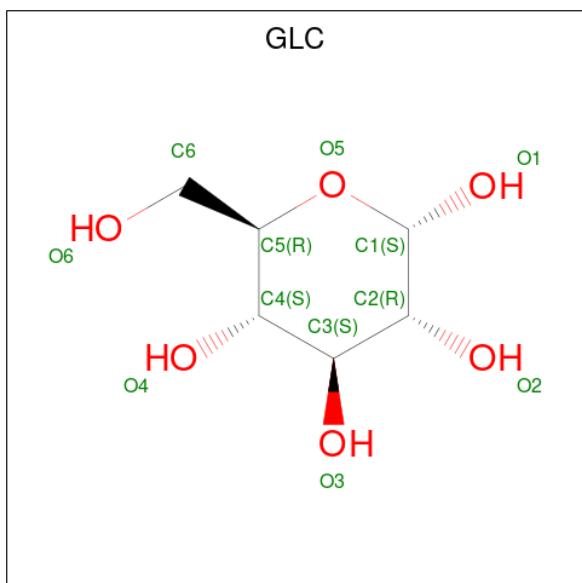
- Molecule 1 is a protein called Lactotransferrin.

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

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 alpha-D-glucopyranose (three-letter code: GLC) (formula: $C_6H_{12}O_6$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 12	C 6	O 6	0	0
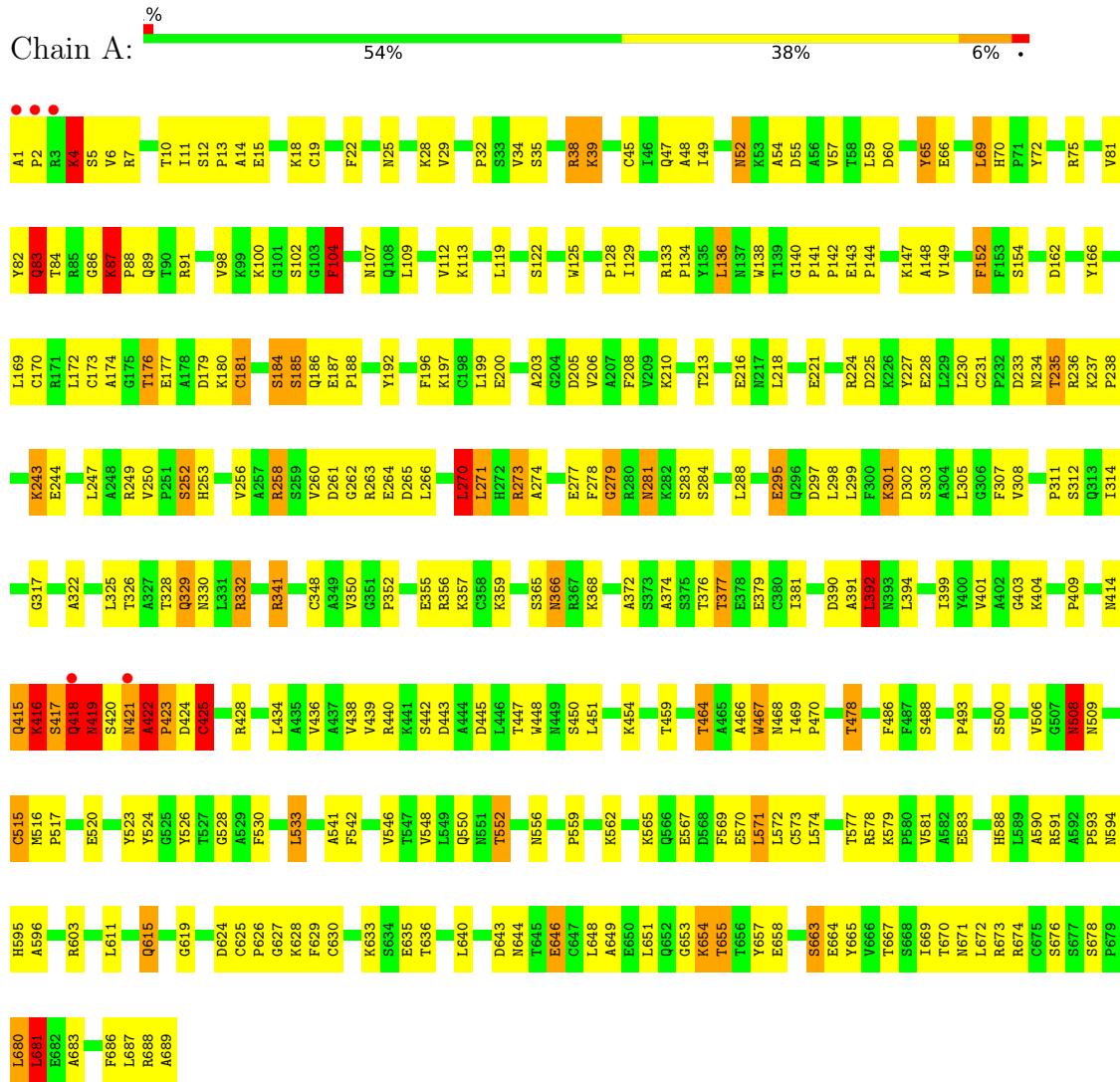
- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 1: Lactotransferrin

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.95Å 99.50Å 102.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.49 19.96 – 3.50	Depositor EDS
% Data completeness (in resolution range)	81.4 (20.00-3.49) 86.5 (19.96-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 3.52Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.226 0.195 , 0.217	Depositor DCC
R_{free} test set	530 reflections (5.32%)	wwPDB-VP
Wilson B-factor (Å^2)	66.0	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 45.2	EDS
L-test for twinning [2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.032 for -h,l,k	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5295	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, 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	0.61	2/5392 (0.0%)	1.01	29/7298 (0.4%)

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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	422	ALA	CA-CB	7.89	1.69	1.52
1	A	418	GLN	CA-C	6.00	1.68	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	PHE	CB-CG-CD2	-9.35	114.26	120.80
1	A	136	LEU	CA-CB-CG	8.75	135.43	115.30
1	A	508	ASN	N-CA-CB	8.53	125.96	110.60
1	A	646	GLU	CA-CB-CG	8.30	131.67	113.40
1	A	104	PHE	CB-CA-C	-8.30	93.80	110.40
1	A	104	PHE	CB-CG-CD1	7.89	126.33	120.80
1	A	422	ALA	N-CA-CB	7.86	121.10	110.10
1	A	417	SER	N-CA-C	7.75	131.94	111.00
1	A	83	GLN	CA-CB-CG	6.95	128.69	113.40
1	A	681	LEU	CA-CB-CG	6.95	131.28	115.30
1	A	392	LEU	CA-CB-CG	6.63	130.56	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	GLY	N-CA-C	-6.61	96.57	113.10
1	A	247	LEU	CA-CB-CG	6.60	130.47	115.30
1	A	508	ASN	CB-CA-C	-6.54	97.31	110.40
1	A	417	SER	CA-C-N	-6.40	103.12	117.20
1	A	104	PHE	N-CA-CB	6.06	121.51	110.60
1	A	83	GLN	N-CA-CB	6.06	121.50	110.60
1	A	417	SER	C-N-CA	5.86	136.34	121.70
1	A	270	LEU	CA-CB-CG	5.82	128.69	115.30
1	A	366	ASN	N-CA-CB	5.56	120.61	110.60
1	A	83	GLN	CB-CA-C	-5.55	99.29	110.40
1	A	418	GLN	CA-C-N	-5.45	105.21	117.20
1	A	523	TYR	CA-CB-CG	5.34	123.55	113.40
1	A	87	LYS	N-CA-CB	-5.28	101.10	110.60
1	A	416	LYS	CD-CE-NZ	5.23	123.73	111.70
1	A	418	GLN	N-CA-C	5.20	125.05	111.00
1	A	230	LEU	CA-CB-CG	5.17	127.20	115.30
1	A	271	LEU	CA-CB-CG	-5.14	103.49	115.30
1	A	533	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	418	GLN	Mainchain

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	5146	296	0
2	A	12	0	12	3	0
3	A	2	0	0	0	0
All	All	5295	0	5158	296	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 28.

All (296) 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:66:GLU:HA	1:A:69:LEU:HD23	1.34	1.07
1:A:417:SER:OG	1:A:418:GLN:N	1.91	1.03
1:A:422:ALA:HB3	1:A:423:PRO:HD2	1.34	1.03
1:A:419:ASN:HD22	1:A:420:SER:N	1.57	1.01
1:A:422:ALA:HB3	1:A:423:PRO:CD	1.90	1.00
1:A:89:GLN:HE22	1:A:249:ARG:HH21	1.00	0.99
1:A:104:PHE:HZ	1:A:205:ASP:HB3	1.23	0.99
1:A:4:LYS:HG3	1:A:5:SER:H	1.28	0.97
1:A:466:ALA:O	1:A:470:PRO:HD2	1.65	0.96
1:A:419:ASN:ND2	1:A:420:SER:H	1.65	0.94
1:A:45:CYS:O	1:A:49:ILE:HG12	1.67	0.94
1:A:258:ARG:NH1	1:A:262:GLY:HA2	1.83	0.93
1:A:422:ALA:O	1:A:423:PRO:O	1.87	0.92
1:A:420:SER:C	1:A:422:ALA:H	1.71	0.92
1:A:376:THR:HG22	1:A:517:PRO:HG2	1.53	0.89
1:A:281:ASN:O	1:A:281:ASN:ND2	2.06	0.88
1:A:314:ILE:HD11	1:A:683:ALA:HB1	1.55	0.88
1:A:49:ILE:HD13	1:A:54:ALA:HB3	1.56	0.88
1:A:420:SER:OG	1:A:422:ALA:HB2	1.73	0.88
1:A:89:GLN:HE22	1:A:249:ARG:NH2	1.72	0.87
1:A:422:ALA:CB	1:A:423:PRO:CD	2.52	0.86
1:A:678:SER:HB3	1:A:681:LEU:HD22	1.58	0.86
1:A:550:GLN:HE22	1:A:644:ASN:HD22	1.20	0.85
1:A:243:LYS:HG2	1:A:244:GLU:OE1	1.75	0.85
1:A:7:ARG:HH22	1:A:52:ASN:ND2	1.75	0.83
1:A:419:ASN:HD22	1:A:420:SER:H	0.84	0.83
1:A:341:ARG:HG3	1:A:341:ARG:HH11	1.44	0.82
1:A:243:LYS:H	1:A:243:LYS:HD2	1.44	0.80
1:A:548:VAL:O	1:A:552:THR:HG23	1.80	0.80
1:A:615:GLN:HE22	1:A:648:LEU:H	1.30	0.80
1:A:65:TYR:HD2	1:A:328:THR:HG21	1.47	0.79
1:A:136:LEU:HD23	1:A:152:PHE:HD2	1.45	0.79
1:A:104:PHE:CZ	1:A:205:ASP:HB3	2.13	0.78
1:A:89:GLN:NE2	1:A:249:ARG:HH21	1.81	0.78
1:A:221:GLU:HA	1:A:224:ARG:NH1	1.99	0.78
1:A:258:ARG:HH12	1:A:262:GLY:HA2	1.48	0.77
1:A:571:LEU:HD21	1:A:581:VAL:HA	1.65	0.77
1:A:271:LEU:HD22	1:A:307:PHE:CZ	2.20	0.76
1:A:65:TYR:CD2	1:A:328:THR:HG21	2.21	0.76
1:A:141:PRO:HG2	1:A:142:PRO:HD3	1.67	0.75
1:A:678:SER:H	1:A:681:LEU:HD23	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:GLU:O	1:A:359:LYS:HG2	1.88	0.73
1:A:624:ASP:HB3	1:A:628:LYS:HG2	1.69	0.73
1:A:420:SER:C	1:A:422:ALA:N	2.35	0.72
1:A:440:ARG:NH1	1:A:443:ASP:OD2	2.23	0.71
1:A:196:PHE:HZ	1:A:218:LEU:HD11	1.55	0.71
1:A:107:ASN:CG	1:A:234:ASN:OD1	2.30	0.71
1:A:65:TYR:CD1	1:A:65:TYR:C	2.64	0.70
1:A:66:GLU:HA	1:A:69:LEU:CD2	2.17	0.70
1:A:419:ASN:ND2	1:A:420:SER:N	2.30	0.70
1:A:669:ILE:HA	1:A:672:LEU:HD12	1.74	0.70
1:A:329:GLN:HA	1:A:332:ARG:HD3	1.74	0.70
1:A:221:GLU:HA	1:A:224:ARG:HH11	1.56	0.70
1:A:29:VAL:HG11	1:A:277:GLU:HG2	1.73	0.69
1:A:421:ASN:ND2	1:A:646:GLU:OE2	2.25	0.69
1:A:65:TYR:C	1:A:65:TYR:HD1	1.95	0.69
1:A:314:ILE:CD1	1:A:683:ALA:HB1	2.22	0.69
1:A:352:PRO:HG3	1:A:520:GLU:OE1	1.93	0.69
1:A:420:SER:OG	1:A:422:ALA:CB	2.40	0.69
1:A:653:GLY:O	1:A:655:THR:HG23	1.92	0.69
1:A:11:ILE:HG13	1:A:15:GLU:OE2	1.93	0.69
1:A:100:LYS:HG2	1:A:228:GLU:HG3	1.74	0.68
1:A:1:ALA:HB3	1:A:2:PRO:HD3	1.75	0.68
1:A:414:ASN:ND2	1:A:649:ALA:HB2	2.08	0.68
1:A:233:ASP:OD1	1:A:235:THR:HG23	1.94	0.68
1:A:185:SER:OG	1:A:295:GLU:HB3	1.94	0.68
1:A:329:GLN:O	1:A:332:ARG:HG2	1.95	0.67
1:A:469:ILE:HG21	1:A:590:ALA:HB3	1.74	0.67
1:A:415:GLN:NE2	1:A:594:ASN:HD21	1.93	0.67
1:A:414:ASN:HD22	1:A:649:ALA:HB2	1.60	0.66
1:A:59:LEU:HD12	1:A:256:VAL:HG11	1.77	0.66
1:A:60:ASP:HA	1:A:253:HIS:CD2	2.31	0.65
1:A:13:PRO:HD3	1:A:38:ARG:HH22	1.61	0.65
1:A:83:GLN:HG2	1:A:88:PRO:HG3	1.78	0.65
1:A:104:PHE:CE2	1:A:112:VAL:HG11	2.32	0.65
1:A:376:THR:HG22	1:A:517:PRO:CG	2.26	0.65
1:A:258:ARG:HB2	1:A:258:ARG:HH11	1.62	0.65
1:A:546:VAL:CG1	1:A:550:GLN:HE21	2.11	0.64
1:A:341:ARG:HG3	1:A:341:ARG:NH1	2.09	0.64
1:A:228:GLU:OE1	1:A:236:ARG:HD3	1.97	0.64
1:A:174:ALA:O	1:A:188:PRO:HD2	1.96	0.64
1:A:104:PHE:H	1:A:104:PHE:HD1	1.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLN:NE2	1:A:249:ARG:NH2	2.42	0.63
1:A:200:GLU:HG3	1:A:227:TYR:OH	1.98	0.63
1:A:25:ASN:O	1:A:29:VAL:HG23	1.99	0.62
1:A:274:ALA:HB1	1:A:288:LEU:HD22	1.80	0.62
1:A:401:VAL:HG11	1:A:680:LEU:HD13	1.80	0.62
1:A:439:VAL:HG21	1:A:572:LEU:HD21	1.81	0.62
1:A:113:LYS:HB3	1:A:172:LEU:HD11	1.81	0.62
1:A:409:PRO:O	1:A:651:LEU:HD11	2.00	0.62
1:A:678:SER:HB3	1:A:681:LEU:CD2	2.30	0.62
1:A:571:LEU:HD23	1:A:571:LEU:N	2.14	0.62
1:A:4:LYS:CG	1:A:5:SER:H	2.07	0.61
1:A:530:PHE:O	1:A:533:LEU:HB3	1.99	0.60
1:A:11:ILE:HD13	1:A:184:SER:HB3	1.84	0.60
1:A:141:PRO:O	1:A:142:PRO:C	2.40	0.60
1:A:579:LYS:HB3	1:A:583:GLU:HB2	1.82	0.60
1:A:172:LEU:HD13	1:A:203:ALA:O	2.01	0.59
1:A:422:ALA:O	1:A:423:PRO:C	2.39	0.59
1:A:19:CYS:O	1:A:22:PHE:HB3	2.03	0.59
1:A:283:SER:OG	1:A:284:SER:N	2.36	0.59
1:A:625:CYS:HA	1:A:629:PHE:O	2.03	0.58
1:A:49:ILE:HD13	1:A:54:ALA:CB	2.31	0.58
1:A:401:VAL:CG1	1:A:680:LEU:HD13	2.34	0.58
1:A:438:VAL:HG12	1:A:533:LEU:HD21	1.86	0.58
1:A:221:GLU:CA	1:A:224:ARG:NH1	2.67	0.58
1:A:32:PRO:CD	1:A:273:ARG:HG3	2.34	0.58
1:A:4:LYS:HG3	1:A:5:SER:N	2.10	0.58
1:A:39:LYS:HD2	1:A:48:ALA:HB2	1.84	0.58
1:A:420:SER:O	1:A:422:ALA:N	2.36	0.58
1:A:636:THR:HA	1:A:643:ASP:OD2	2.03	0.58
1:A:421:ASN:O	1:A:422:ALA:O	2.21	0.58
1:A:357:LYS:HE2	1:A:640:LEU:HB2	1.84	0.58
1:A:341:ARG:HH12	1:A:603:ARG:HH21	1.51	0.57
1:A:448:TRP:CE3	1:A:451:LEU:HD11	2.40	0.57
1:A:12:SER:HA	1:A:38:ARG:NH2	2.20	0.57
1:A:82:TYR:CE2	1:A:252:SER:HB3	2.40	0.56
1:A:577:THR:HG22	1:A:578:ARG:H	1.70	0.56
1:A:414:ASN:ND2	1:A:649:ALA:CB	2.68	0.56
1:A:6:VAL:HG21	1:A:270:LEU:HD23	1.88	0.56
1:A:112:VAL:CG1	1:A:205:ASP:HB2	2.36	0.56
1:A:136:LEU:HD23	1:A:152:PHE:CD2	2.34	0.56
1:A:109:LEU:O	1:A:112:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:GLN:O	1:A:417:SER:N	2.39	0.55
1:A:65:TYR:HD1	1:A:65:TYR:O	1.87	0.55
1:A:428:ARG:HH22	1:A:646:GLU:CD	2.09	0.55
1:A:348:CYS:HA	1:A:372:ALA:O	2.06	0.55
1:A:263:ARG:HB3	1:A:266:LEU:HD13	1.88	0.55
1:A:107:ASN:OD1	1:A:234:ASN:OD1	2.24	0.55
1:A:625:CYS:C	1:A:630:CYS:SG	2.85	0.55
1:A:399:ILE:CD1	1:A:596:ALA:HB3	2.37	0.54
1:A:176:THR:OG1	1:A:179:ASP:HB2	2.07	0.54
1:A:133:ARG:HB3	1:A:134:PRO:HD3	1.90	0.54
1:A:399:ILE:HD13	1:A:596:ALA:HB3	1.89	0.54
1:A:417:SER:O	1:A:418:GLN:CD	2.47	0.53
1:A:415:GLN:HE22	1:A:594:ASN:HD21	1.54	0.53
1:A:417:SER:HA	1:A:428:ARG:NH1	2.23	0.53
1:A:571:LEU:CD2	1:A:581:VAL:HA	2.36	0.53
1:A:136:LEU:HD22	1:A:148:ALA:HB1	1.91	0.53
1:A:170:CYS:O	1:A:173:CYS:HB2	2.09	0.53
1:A:428:ARG:NH2	1:A:646:GLU:OE1	2.41	0.52
1:A:258:ARG:HH11	1:A:262:GLY:HA2	1.70	0.52
1:A:686:PHE:O	1:A:689:ALA:HB3	2.09	0.52
1:A:87:LYS:O	1:A:88:PRO:C	2.47	0.52
1:A:390:ASP:O	1:A:391:ALA:HB2	2.07	0.52
1:A:298:LEU:O	1:A:299:LEU:HB2	2.10	0.52
1:A:615:GLN:O	1:A:619:GLY:HA3	2.10	0.51
1:A:414:ASN:ND2	1:A:425:CYS:O	2.43	0.51
1:A:508:ASN:ND2	1:A:520:GLU:HG3	2.25	0.51
1:A:81:VAL:CG2	1:A:308:VAL:HG13	2.40	0.51
1:A:138:TRP:NE1	1:A:140:GLY:O	2.43	0.51
1:A:181:CYS:N	1:A:187:GLU:OE1	2.44	0.51
1:A:271:LEU:HD22	1:A:307:PHE:CE1	2.46	0.51
1:A:450:SER:O	1:A:450:SER:OG	2.28	0.51
1:A:569:PHE:O	1:A:581:VAL:HG23	2.10	0.51
1:A:301:LYS:HG3	1:A:302:ASP:O	2.10	0.51
1:A:322:ALA:O	1:A:326:THR:HG23	2.10	0.51
1:A:577:THR:HG22	1:A:578:ARG:N	2.26	0.51
1:A:104:PHE:HZ	1:A:205:ASP:CB	2.10	0.51
1:A:192:TYR:HB3	1:A:213:THR:OG1	2.10	0.50
1:A:615:GLN:HE22	1:A:648:LEU:N	2.05	0.50
1:A:317:GLY:HA2	1:A:325:LEU:HD11	1.94	0.50
1:A:506:VAL:HG12	1:A:506:VAL:O	2.10	0.50
1:A:60:ASP:HA	1:A:253:HIS:CG	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:VAL:CG2	1:A:270:LEU:HD23	2.41	0.50
1:A:508:ASN:HD22	1:A:520:GLU:HG3	1.76	0.49
1:A:186:GLN:O	1:A:188:PRO:HD3	2.12	0.49
1:A:104:PHE:CZ	1:A:112:VAL:HG11	2.46	0.49
1:A:112:VAL:HG12	1:A:113:LYS:N	2.28	0.49
1:A:302:ASP:O	1:A:303:SER:HB2	2.12	0.49
1:A:87:LYS:O	1:A:89:GLN:HG3	2.12	0.49
1:A:32:PRO:HD2	1:A:273:ARG:HG3	1.95	0.49
1:A:173:CYS:HB3	1:A:187:GLU:OE2	2.13	0.48
1:A:173:CYS:O	1:A:180:LYS:HE3	2.12	0.48
1:A:416:LYS:HA	1:A:646:GLU:HB2	1.94	0.48
1:A:7:ARG:HH22	1:A:52:ASN:HD21	1.59	0.48
1:A:466:ALA:O	1:A:470:PRO:CD	2.50	0.48
1:A:128:PRO:HG2	1:A:129:ILE:H	1.77	0.48
1:A:593:PRO:HA	2:A:692:GLC:H2	1.94	0.48
1:A:548:VAL:HG12	1:A:552:THR:HG21	1.95	0.48
1:A:625:CYS:HB3	1:A:626:PRO:HD3	1.96	0.48
1:A:665:TYR:O	1:A:669:ILE:HG13	2.13	0.48
1:A:524:TYR:O	1:A:528:GLY:HA3	2.14	0.47
1:A:278:PHE:O	1:A:279:GLY:O	2.32	0.47
1:A:192:TYR:CD1	1:A:210:LYS:HB2	2.49	0.47
1:A:34:VAL:HG12	1:A:35:SER:H	1.79	0.47
1:A:65:TYR:CE1	1:A:69:LEU:HD21	2.49	0.47
1:A:196:PHE:CZ	1:A:218:LEU:HD11	2.44	0.47
1:A:448:TRP:CZ3	1:A:542:PHE:HE1	2.33	0.47
1:A:533:LEU:HD22	1:A:541:ALA:HB3	1.96	0.47
1:A:416:LYS:O	1:A:417:SER:HB3	2.14	0.47
1:A:448:TRP:CZ3	1:A:451:LEU:HD11	2.50	0.47
1:A:419:ASN:O	1:A:420:SER:HB3	2.15	0.47
1:A:671:ASN:O	1:A:674:ARG:HB3	2.15	0.47
1:A:166:TYR:HB2	1:A:169:LEU:HD12	1.97	0.46
1:A:10:THR:HB	1:A:15:GLU:HB3	1.96	0.46
1:A:625:CYS:O	1:A:630:CYS:SG	2.73	0.46
1:A:341:ARG:NH1	1:A:603:ARG:HH21	2.14	0.46
1:A:233:ASP:O	1:A:235:THR:HG22	2.15	0.46
1:A:678:SER:N	1:A:681:LEU:HD23	2.27	0.46
1:A:184:SER:C	1:A:186:GLN:H	2.18	0.46
1:A:231:CYS:SG	1:A:237:LYS:HD2	2.55	0.46
1:A:6:VAL:HB	1:A:270:LEU:HD23	1.97	0.46
1:A:128:PRO:HB2	1:A:208:PHE:CE2	2.51	0.46
1:A:133:ARG:N	1:A:134:PRO:CD	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ARG:HD3	1:A:266:LEU:HD22	1.98	0.46
1:A:14:ALA:HB2	1:A:295:GLU:OE2	2.16	0.45
1:A:75:ARG:NE	1:A:264:GLU:OE2	2.48	0.45
1:A:102:SER:OG	1:A:236:ARG:NH2	2.47	0.45
1:A:147:LYS:HE3	1:A:166:TYR:OH	2.16	0.45
1:A:417:SER:O	1:A:418:GLN:OE1	2.34	0.45
1:A:22:PHE:CZ	1:A:270:LEU:HD11	2.51	0.45
1:A:65:TYR:CD2	1:A:328:THR:CG2	2.98	0.45
1:A:464:THR:HG23	1:A:665:TYR:CZ	2.52	0.45
1:A:651:LEU:HB3	1:A:654:LYS:O	2.16	0.45
1:A:98:VAL:HG21	1:A:236:ARG:CZ	2.47	0.45
1:A:192:TYR:CE1	1:A:210:LYS:HB2	2.51	0.45
1:A:260:VAL:O	1:A:261:ASP:HB2	2.16	0.45
1:A:18:LYS:CD	1:A:298:LEU:HB2	2.47	0.44
1:A:574:LEU:HA	1:A:574:LEU:HD23	1.67	0.44
1:A:6:VAL:CB	1:A:270:LEU:HD23	2.46	0.44
1:A:425:CYS:HB2	1:A:428:ARG:NH2	2.32	0.44
1:A:591:ARG:HG3	2:A:692:GLC:C6	2.47	0.44
1:A:133:ARG:NH1	1:A:330:ASN:O	2.50	0.44
1:A:436:VAL:HB	1:A:571:LEU:HD13	2.00	0.44
1:A:55:ASP:OD1	1:A:258:ARG:NH2	2.51	0.44
1:A:98:VAL:HG12	1:A:206:VAL:HG23	2.00	0.44
1:A:493:PRO:HA	1:A:515:CYS:O	2.18	0.44
1:A:526:TYR:HH	1:A:595:HIS:HE2	1.66	0.44
1:A:506:VAL:O	1:A:506:VAL:CG1	2.66	0.43
1:A:683:ALA:O	1:A:687:LEU:HG	2.18	0.43
1:A:6:VAL:HB	1:A:270:LEU:CD2	2.49	0.43
1:A:615:GLN:NE2	1:A:648:LEU:H	2.08	0.43
1:A:12:SER:C	1:A:38:ARG:HH21	2.21	0.43
1:A:65:TYR:CE1	1:A:69:LEU:CD2	3.01	0.43
1:A:377:THR:O	1:A:381:ILE:HD12	2.19	0.43
1:A:438:VAL:CG1	1:A:533:LEU:HD21	2.49	0.43
1:A:141:PRO:C	1:A:143:GLU:N	2.69	0.43
1:A:403:GLY:HA3	1:A:657:TYR:CD2	2.54	0.43
1:A:138:TRP:NE1	1:A:143:GLU:O	2.52	0.42
1:A:350:VAL:HG21	1:A:377:THR:HG23	2.00	0.42
1:A:434:LEU:HD13	1:A:588:HIS:HB3	2.01	0.42
1:A:657:TYR:CE1	1:A:658:GLU:HG3	2.54	0.42
1:A:82:TYR:O	1:A:88:PRO:HA	2.20	0.42
1:A:459:THR:H	1:A:466:ALA:CB	2.33	0.42
1:A:221:GLU:N	1:A:224:ARG:NH1	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:VAL:CG1	1:A:550:GLN:NE2	2.79	0.42
1:A:18:LYS:HD3	1:A:298:LEU:HB2	2.02	0.42
1:A:47:GLN:HG2	1:A:72:TYR:CE1	2.54	0.42
1:A:148:ALA:O	1:A:149:VAL:C	2.58	0.42
1:A:374:ALA:HB1	1:A:379:GLU:HB2	2.02	0.42
1:A:83:GLN:HG3	1:A:305:LEU:HG	2.02	0.42
1:A:417:SER:C	1:A:418:GLN:HG3	2.39	0.42
1:A:550:GLN:NE2	1:A:644:ASN:HD22	2.00	0.42
1:A:570:GLU:HG3	1:A:578:ARG:HH21	1.85	0.42
1:A:82:TYR:O	1:A:89:GLN:N	2.45	0.42
1:A:147:LYS:CG	1:A:166:TYR:CE1	3.03	0.42
1:A:136:LEU:HD22	1:A:148:ALA:CB	2.50	0.42
1:A:297:ASP:OD1	1:A:301:LYS:HE3	2.20	0.42
1:A:22:PHE:HZ	1:A:270:LEU:HD11	1.85	0.42
1:A:565:LYS:C	1:A:567:GLU:N	2.71	0.42
1:A:273:ARG:NH2	1:A:277:GLU:OE1	2.53	0.41
1:A:365:SER:O	1:A:368:LYS:HG3	2.20	0.41
1:A:317:GLY:CA	1:A:325:LEU:HD11	2.51	0.41
1:A:341:ARG:NH1	1:A:341:ARG:CG	2.77	0.41
1:A:428:ARG:NH1	1:A:646:GLU:OE1	2.52	0.41
1:A:478:THR:HG21	1:A:486:PHE:CE2	2.56	0.41
1:A:11:ILE:C	1:A:11:ILE:HD12	2.41	0.41
1:A:13:PRO:HD3	1:A:38:ARG:NH2	2.31	0.41
1:A:144:PRO:HD2	1:A:147:LYS:HD2	2.02	0.41
1:A:468:ASN:ND2	1:A:669:ILE:HG12	2.35	0.41
1:A:237:LYS:HB3	1:A:238:PRO:HD2	2.01	0.41
1:A:417:SER:O	1:A:418:GLN:CG	2.68	0.41
1:A:611:LEU:HD23	1:A:611:LEU:HA	1.85	0.41
1:A:11:ILE:HD13	1:A:184:SER:CB	2.50	0.41
1:A:87:LYS:C	1:A:88:PRO:O	2.57	0.41
1:A:91:ARG:NH1	1:A:687:LEU:O	2.54	0.41
1:A:141:PRO:O	1:A:143:GLU:N	2.54	0.41
1:A:216:GLU:OE2	1:A:301:LYS:HE2	2.20	0.41
1:A:4:LYS:CG	1:A:5:SER:N	2.77	0.41
1:A:138:TRP:CZ2	1:A:140:GLY:C	2.94	0.41
1:A:147:LYS:HG3	1:A:166:TYR:CE1	2.56	0.41
1:A:464:THR:HG22	1:A:469:ILE:HG13	2.03	0.41
1:A:467:TRP:HB3	1:A:468:ASN:H	1.79	0.41
1:A:87:LYS:H	1:A:87:LYS:HG2	0.97	0.41
1:A:104:PHE:CD1	1:A:104:PHE:N	2.88	0.41
1:A:125:TRP:O	1:A:128:PRO:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:ASN:HB2	1:A:509:ASN:H	1.14	0.41
1:A:197:LYS:HA	1:A:197:LYS:HD2	1.74	0.40
1:A:392:LEU:HD13	1:A:394:LEU:HG	2.02	0.40
1:A:424:ASP:C	1:A:424:ASP:OD2	2.59	0.40
1:A:459:THR:H	1:A:466:ALA:HB2	1.85	0.40
1:A:447:THR:O	1:A:448:TRP:C	2.59	0.40
1:A:593:PRO:HB3	2:A:692:GLC:H2	2.03	0.40
1:A:447:THR:O	1:A:450:SER:N	2.38	0.40
1:A:573:CYS:SG	1:A:579:LYS:HG2	2.61	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%)	600 (87%)	63 (9%)	24 (4%)	3 27

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	GLU
1	A	416	LYS
1	A	421	ASN
1	A	422	ALA
1	A	423	PRO
1	A	425	CYS
1	A	467	TRP
1	A	562	LYS
1	A	104	PHE
1	A	176	THR
1	A	279	GLY
1	A	418	GLN

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Mol	Chain	Res	Type
1	A	664	GLU
1	A	122	SER
1	A	419	ASN
1	A	464	THR
1	A	311	PRO
1	A	508	ASN
1	A	627	GLY
1	A	663	SER
1	A	70	HIS
1	A	4	LYS
1	A	442	SER
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%)	497 (88%)	68 (12%)	5	24

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	28	LYS
1	A	38	ARG
1	A	39	LYS
1	A	52	ASN
1	A	57	VAL
1	A	65	TYR
1	A	69	LEU
1	A	83	GLN
1	A	84	THR
1	A	87	LYS
1	A	104	PHE
1	A	119	LEU
1	A	152	PHE

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Mol	Chain	Res	Type
1	A	154	SER
1	A	162	ASP
1	A	181	CYS
1	A	184	SER
1	A	185	SER
1	A	199	LEU
1	A	225	ASP
1	A	235	THR
1	A	243	LYS
1	A	250	VAL
1	A	252	SER
1	A	258	ARG
1	A	265	ASP
1	A	270	LEU
1	A	273	ARG
1	A	281	ASN
1	A	295	GLU
1	A	301	LYS
1	A	312	SER
1	A	329	GLN
1	A	332	ARG
1	A	341	ARG
1	A	356	ARG
1	A	366	ASN
1	A	377	THR
1	A	392	LEU
1	A	404	LYS
1	A	415	GLN
1	A	419	ASN
1	A	425	CYS
1	A	445	ASP
1	A	454	LYS
1	A	478	THR
1	A	488	SER
1	A	500	SER
1	A	508	ASN
1	A	515	CYS
1	A	516	MET
1	A	552	THR
1	A	556	ASN
1	A	571	LEU
1	A	615	GLN

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Mol	Chain	Res	Type
1	A	633	LYS
1	A	635	GLU
1	A	654	LYS
1	A	655	THR
1	A	663	SER
1	A	667	THR
1	A	670	THR
1	A	673	ARG
1	A	676	SER
1	A	680	LEU
1	A	681	LEU
1	A	688	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	25	ASN
1	A	52	ASN
1	A	89	GLN
1	A	108	GLN
1	A	137	ASN
1	A	168	ASN
1	A	201	ASN
1	A	330	ASN
1	A	360	GLN
1	A	414	ASN
1	A	415	GLN
1	A	419	ASN
1	A	449	ASN
1	A	468	ASN
1	A	477	GLN
1	A	508	ASN
1	A	513	ASN
1	A	550	GLN
1	A	556	ASN
1	A	615	GLN

5.3.3   RNA (i)

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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\#|Z| > 2$
2	GLC	A	692	-	12,12,12	0.40	0	17,17,17	0.48	0

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
2	GLC	A	692	-	-	2/2/22/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	692	GLC	O5-C5-C6-O6
2	A	692	GLC	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	692	GLC	3	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 ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	689/689 (100%)	-0.66	5 (0%)	87	83	4, 38, 67, 89	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	PRO	6.2
1	A	1	ALA	5.7
1	A	3	ARG	4.2
1	A	418	GLN	3.0
1	A	421	ASN	2.6

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	A	692	12/12	0.73	0.43	65,66,68,68	12
3	FE	A	691	1/1	0.94	0.13	23,23,23,23	0
3	FE	A	690	1/1	0.96	0.13	36,36,36,36	0

6.5 Other polymers ⓘ

There are no such residues in this entry.