



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:23 PM GMT

PDB ID : 4OQO
Title : Crystal structure of the tryptic generated iron-free C-lobe of bovine Lactoferrin at 2.42 Angstrom resolution
Authors : Singh, A.; Rastogi, N.; Pandey, S.; Bhushan, A.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2014-02-10
Resolution : 2.42 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

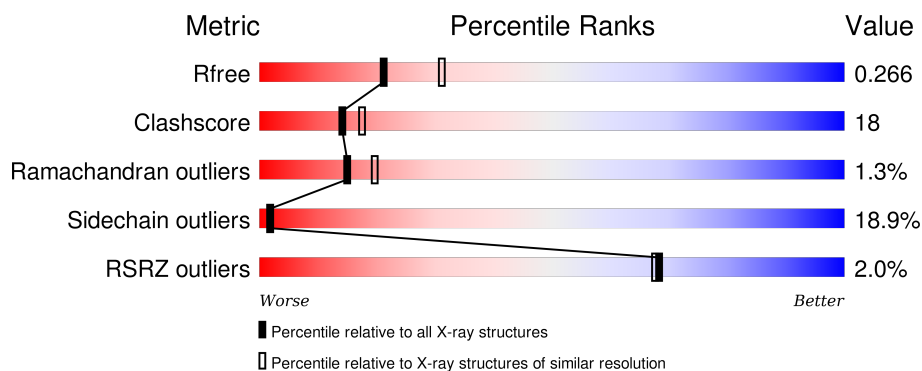
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


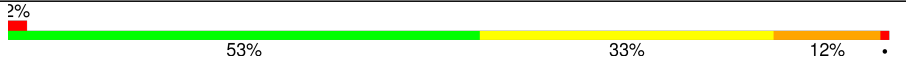
The reported resolution of this entry is 2.42 Å.

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))
R_{free}	91344	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (2.44-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. 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	348	 2% 71% 24% 5%
1	B	348	 2% 53% 33% 12%

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	NAG	A	701	-	-	-	X
2	NAG	B	703	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5696 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
1	A	348	Total	C	N	O	S	0	0	0
			2658	1656	464	517	21			
1	B	348	Total	C	N	O	S	0	0	0
			2658	1656	464	517	21			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	565	LYS	ASN	SEE REMARK 999	UNP P24627
A	608	GLU	LYS	SEE REMARK 999	UNP P24627
B	565	LYS	ASN	SEE REMARK 999	UNP P24627
B	608	GLU	LYS	SEE REMARK 999	UNP P24627

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	2	Total	C	N	O	0	0
			28	16	2	10		

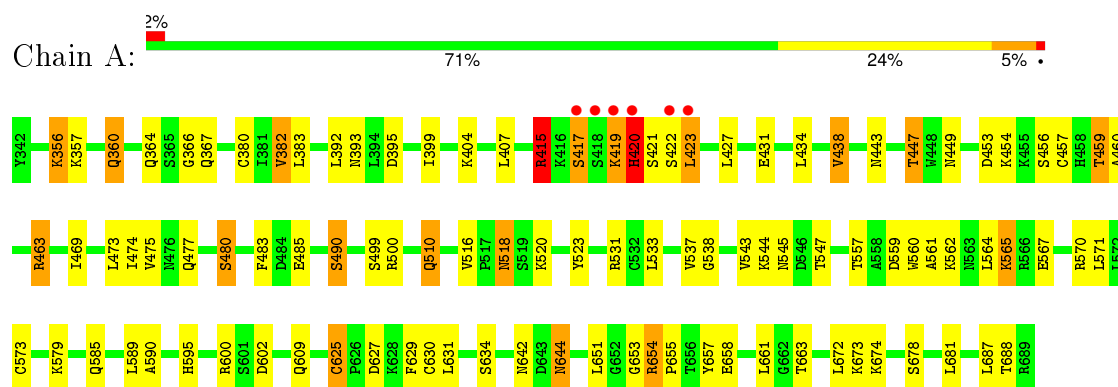
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	168	Total	O	0	0
			168	168		
4	B	142	Total	O	0	0
			142	142		

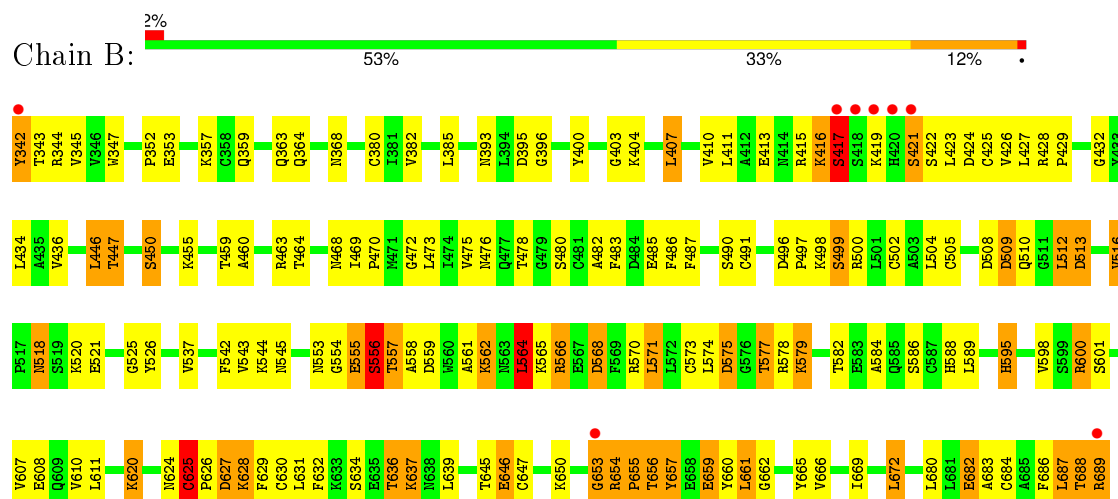
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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



• Molecule 1: Lactotransferrin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.81Å 49.44Å 97.86Å 90.00° 94.33° 90.00°	Depositor
Resolution (Å)	38.67 – 2.42 38.67 – 2.42	Depositor EDS
% Data completeness (in resolution range)	98.7 (38.67-2.42) 98.8 (38.67-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.223 , 0.260 0.226 , 0.266	Depositor DCC
R_{free} test set	1386 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 30.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 27678 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5696	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: NAG

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	0.94	0/2708	0.97	2/3670 (0.1%)
1	B	0.86	0/2708	0.93	5/3670 (0.1%)
All	All	0.90	0/5416	0.95	7/7340 (0.1%)

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
1	B	0	5
All	All	0	6

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	625	CYS	C-N-CD	5.83	140.65	128.40
1	A	415	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	B	395	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	600	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	564	LEU	CA-CB-CG	5.37	127.65	115.30
1	B	556	SER	N-CA-C	5.21	125.07	111.00
1	B	417	SER	CB-CA-C	5.00	119.61	110.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	420	HIS	Peptide
1	B	416	LYS	Peptide
1	B	555	GLU	Peptide
1	B	556	SER	Peptide
1	B	653	GLY	Peptide
1	B	688	THR	Peptide

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	2658	0	2584	63	0
1	B	2658	0	2584	131	0
2	A	28	0	26	2	0
2	B	14	0	13	0	0
3	B	28	0	25	2	0
4	A	168	0	0	2	0
4	B	142	0	0	3	0
All	All	5696	0	5232	193	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 18.

All (193) 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:475:VAL:HG21	1:A:483:PHE:HD2	1.16	1.09
1:B:416:LYS:HG2	1:B:646:GLU:HG2	1.04	1.00
1:B:416:LYS:CG	1:B:646:GLU:HG2	1.92	0.98
1:B:689:ARG:HG3	1:B:689:ARG:HH11	1.33	0.94
1:B:416:LYS:HG2	1:B:646:GLU:CG	1.96	0.93
1:B:575:ASP:CB	1:B:577:THR:HG22	1.98	0.93
1:B:577:THR:OG1	1:B:578:ARG:N	1.96	0.91
1:B:636:THR:HG23	1:B:637:LYS:H	1.35	0.89
1:A:475:VAL:HG21	1:A:483:PHE:CD2	2.08	0.85
1:B:393:ASN:HD21	1:B:595:HIS:HB3	1.42	0.83
1:B:575:ASP:HB3	1:B:577:THR:HG22	1.58	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:LYS:HD2	1:A:567:GLU:HB2	1.60	0.82
1:B:416:LYS:O	1:B:421:SER:HB3	1.79	0.81
1:B:575:ASP:HB2	1:B:577:THR:HG22	1.64	0.79
1:B:573:CYS:HB2	1:B:577:THR:HG23	1.66	0.78
1:B:416:LYS:HA	1:B:646:GLU:HG3	1.68	0.75
1:B:575:ASP:HB2	1:B:577:THR:CG2	2.17	0.75
1:B:496:ASP:OD1	1:B:498:LYS:HG2	1.87	0.75
1:B:684:CYS:O	1:B:688:THR:HB	1.87	0.74
1:B:429:PRO:HD3	1:B:650:LYS:O	1.87	0.74
1:A:475:VAL:CG2	1:A:483:PHE:HD2	1.99	0.74
1:A:654:ARG:N	1:A:655:PRO:HD3	2.02	0.74
1:B:636:THR:HG23	1:B:637:LYS:N	2.04	0.72
1:B:565:LYS:O	1:B:568:ASP:HB2	1.90	0.71
1:B:416:LYS:HD2	1:B:620:LYS:HE3	1.73	0.70
1:B:557:THR:HG22	1:B:558:ALA:N	2.07	0.70
1:A:357:LYS:HA	1:A:360:GLN:HE21	1.58	0.69
1:A:422:SER:O	1:A:423:LEU:HG	1.92	0.69
1:B:475:VAL:HA	1:B:478:THR:OG1	1.92	0.69
1:B:627:ASP:OD1	1:B:627:ASP:N	2.26	0.68
1:B:689:ARG:HG3	1:B:689:ARG:NH1	2.03	0.68
1:A:415:ARG:HG3	1:A:415:ARG:HH11	1.59	0.67
1:A:463:ARG:HH11	1:A:463:ARG:HB3	1.60	0.66
1:B:626:PRO:HD2	1:B:627:ASP:OD1	1.95	0.66
1:A:559:ASP:HA	1:A:562:LYS:HD3	1.78	0.66
1:B:459:THR:HG23	1:B:525:GLY:HA2	1.78	0.66
1:A:561:ALA:O	1:A:564:LEU:HB2	1.96	0.65
1:B:625:CYS:HA	1:B:629:PHE:O	1.99	0.63
1:B:436:VAL:HG22	1:B:543:VAL:O	1.99	0.63
1:A:393:ASN:HD21	1:A:595:HIS:HB3	1.65	0.62
1:B:459:THR:HG23	1:B:525:GLY:C	2.19	0.61
1:B:516:VAL:HG12	1:B:518:ASN:HB2	1.81	0.61
1:B:625:CYS:C	1:B:630:CYS:SG	2.79	0.61
1:B:459:THR:HG23	1:B:525:GLY:CA	2.31	0.61
1:B:473:LEU:O	1:B:476:ASN:HB3	2.02	0.60
1:A:625:CYS:HA	1:A:629:PHE:O	2.01	0.60
1:A:469:ILE:O	1:A:473:LEU:HG	2.02	0.60
1:B:475:VAL:HG21	1:B:483:PHE:HE1	1.68	0.58
1:B:654:ARG:N	1:B:655:PRO:CD	2.68	0.57
1:B:557:THR:HG22	1:B:558:ALA:H	1.70	0.57
1:A:544:LYS:HG3	1:A:547:THR:OG1	2.05	0.57
1:A:434:LEU:O	1:A:544:LYS:HA	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:GLN:HB2	2:A:701:NAG:H81	1.86	0.56
1:B:447:THR:HG23	1:B:450:SER:HB3	1.87	0.56
1:B:416:LYS:CG	1:B:646:GLU:CG	2.72	0.56
1:B:459:THR:HG21	1:B:463:ARG:HH21	1.71	0.56
1:B:424:ASP:OD1	1:B:424:ASP:N	2.36	0.55
1:B:400:TYR:OH	1:B:404:LYS:HD2	2.06	0.55
1:B:654:ARG:N	1:B:655:PRO:HD3	2.21	0.55
1:A:382:VAL:HG12	1:A:383:LEU:N	2.20	0.55
1:B:556:SER:HB3	1:B:562:LYS:HA	1.89	0.55
1:B:575:ASP:CB	1:B:577:THR:CG2	2.75	0.54
1:B:557:THR:CG2	1:B:558:ALA:N	2.71	0.54
1:B:342:TYR:N	1:B:342:TYR:CD1	2.75	0.54
1:B:584:ALA:O	1:B:588:HIS:HD2	1.91	0.54
1:B:608:GLU:OE2	1:B:654:ARG:HD2	2.07	0.54
1:B:403:GLY:HA3	1:B:657:TYR:CG	2.43	0.54
1:B:508:ASP:OD1	1:B:510:GLN:HB2	2.07	0.54
1:B:636:THR:CG2	1:B:637:LYS:N	2.72	0.53
1:B:557:THR:HB	1:B:561:ALA:HB3	1.91	0.53
1:A:475:VAL:HG13	1:A:480:SER:O	2.09	0.53
1:B:504:LEU:HD13	1:B:537:VAL:HG12	1.90	0.53
1:B:382:VAL:HG23	1:B:680:LEU:HD13	1.91	0.52
1:A:654:ARG:N	1:A:654:ARG:CD	2.71	0.52
1:A:395:ASP:O	1:A:399:ILE:HG12	2.09	0.52
1:A:531:ARG:HG3	1:A:560:TRP:CD2	2.44	0.52
1:B:475:VAL:HG21	1:B:483:PHE:CE1	2.44	0.52
1:B:554:GLY:CA	1:B:556:SER:HB2	2.40	0.52
1:A:457:CYS:SG	1:A:538:GLY:HA3	2.50	0.51
1:B:400:TYR:CZ	1:B:404:LYS:HD2	2.45	0.51
1:A:654:ARG:HD2	1:A:654:ARG:N	2.25	0.51
1:A:523:TYR:CE1	1:A:531:ARG:HD2	2.46	0.51
1:B:682:GLU:HG3	1:B:683:ALA:N	2.25	0.51
1:A:518:ASN:OD1	1:A:520:LYS:HE3	2.12	0.50
1:A:463:ARG:HB3	1:A:463:ARG:NH1	2.25	0.50
1:B:343:THR:O	1:B:343:THR:HG22	2.11	0.50
1:A:422:SER:HB3	4:A:937:HOH:O	2.11	0.50
1:B:654:ARG:H	1:B:655:PRO:HD3	1.76	0.50
1:B:657:TYR:O	1:B:661:LEU:HD22	2.11	0.50
1:B:600:ARG:CZ	1:B:600:ARG:HB2	2.40	0.50
1:A:654:ARG:N	1:A:655:PRO:CD	2.74	0.50
1:B:345:VAL:HG23	1:B:610:VAL:HG21	1.94	0.50
1:A:419:LYS:O	1:A:420:HIS:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:553:ASN:N	1:B:553:ASN:OD1	2.44	0.49
1:B:382:VAL:O	1:B:385:LEU:HB2	2.12	0.49
1:A:475:VAL:HG22	1:A:480:SER:O	2.12	0.49
1:B:654:ARG:H	1:B:655:PRO:CD	2.25	0.49
1:B:422:SER:HB2	4:B:822:HOH:O	2.12	0.49
1:A:657:TYR:O	1:A:661:LEU:HD22	2.13	0.49
1:A:456:SER:OG	1:A:490:SER:HB3	2.13	0.49
1:B:497:PRO:HA	1:B:502:CYS:SG	2.53	0.49
1:B:434:LEU:O	1:B:544:LYS:HA	2.13	0.49
1:B:526:TYR:CZ	1:B:544:LYS:HE3	2.48	0.49
1:B:624:ASN:HB3	1:B:628:LYS:HG3	1.94	0.49
1:B:347:TRP:CH2	1:B:611:LEU:HD11	2.48	0.48
1:A:460:ALA:HB3	1:A:463:ARG:HG3	1.95	0.48
1:B:512:LEU:O	1:B:513:ASP:HB2	2.11	0.48
1:A:469:ILE:HD13	1:A:590:ALA:HB3	1.95	0.48
1:A:356:LYS:HD3	1:A:356:LYS:HA	1.55	0.48
1:B:482:ALA:HB1	1:B:485:GLU:HG3	1.94	0.48
1:B:416:LYS:HB2	1:B:417:SER:O	2.14	0.48
1:B:557:THR:CG2	1:B:558:ALA:H	2.25	0.48
1:B:655:PRO:HG2	1:B:656:THR:H	1.79	0.48
1:B:555:GLU:OE2	3:B:702:NAG:H81	2.14	0.48
1:A:642:ASN:HD22	1:A:644:ASN:H	1.62	0.48
1:A:447:THR:HG23	1:A:449:ASN:H	1.79	0.47
1:B:470:PRO:HB3	1:B:542:PHE:CD1	2.49	0.47
1:B:396:GLY:HA3	1:B:665:TYR:OH	2.15	0.47
1:A:415:ARG:NH1	1:A:415:ARG:HG3	2.23	0.47
1:B:660:TYR:HD2	1:B:661:LEU:HD13	1.79	0.47
1:A:523:TYR:HE1	1:A:531:ARG:HD2	1.79	0.47
1:A:678:SER:HB3	1:A:681:LEU:HB2	1.97	0.46
1:B:620:LYS:HE2	1:B:632:PHE:HB2	1.98	0.46
1:B:347:TRP:CZ3	1:B:611:LEU:HD11	2.50	0.46
1:A:654:ARG:HD2	1:A:654:ARG:H	1.80	0.46
1:A:557:THR:HG22	1:A:557:THR:O	2.15	0.46
1:B:653:GLY:HA3	1:B:655:PRO:HD3	1.98	0.46
1:B:687:LEU:HA	1:B:689:ARG:HB2	1.98	0.46
1:B:554:GLY:C	1:B:556:SER:HB2	2.36	0.46
1:B:553:ASN:OD1	1:B:565:LYS:HA	2.16	0.45
1:B:410:VAL:HG11	1:B:607:VAL:HG13	1.96	0.45
1:A:625:CYS:C	1:A:630:CYS:SG	2.95	0.45
1:B:656:THR:OG1	1:B:659:GLU:HB2	2.16	0.45
1:B:464:THR:HG22	1:B:469:ILE:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:LYS:HE3	1:B:498:LYS:HB2	1.78	0.45
1:B:411:LEU:HD21	1:B:608:GLU:HG3	1.99	0.45
1:A:585:GLN:HB2	2:A:701:NAG:C8	2.46	0.45
1:A:459:THR:HG22	1:A:460:ALA:N	2.32	0.44
1:A:537:VAL:CG2	1:B:352:PRO:HG3	2.47	0.44
1:B:665:TYR:CE2	1:B:669:ILE:HG13	2.52	0.44
1:B:491:CYS:HB2	1:B:504:LEU:HB2	2.00	0.44
1:B:662:GLY:O	1:B:666:VAL:HG23	2.18	0.44
1:A:438:VAL:HG22	1:A:533:LEU:HD21	2.00	0.44
1:B:416:LYS:O	1:B:417:SER:HB3	2.18	0.44
1:B:468:ASN:HA	1:B:672:LEU:HD21	2.00	0.43
1:A:688:THR:HG22	1:A:688:THR:O	2.18	0.43
1:B:426:VAL:HG12	1:B:426:VAL:O	2.18	0.43
1:B:559:ASP:O	1:B:562:LYS:HG2	2.18	0.43
1:A:657:TYR:O	1:A:661:LEU:CD2	2.67	0.43
1:B:357:LYS:HD3	1:B:639:LEU:HB2	2.01	0.43
1:A:366:GLY:C	1:A:367:GLN:HG2	2.39	0.43
1:B:459:THR:CG2	1:B:525:GLY:HA2	2.47	0.43
1:B:486:PHE:O	1:B:487:PHE:HB2	2.19	0.43
1:A:417:SER:HB3	1:A:419:LYS:O	2.18	0.43
1:B:428:ARG:HA	1:B:429:PRO:HD2	1.91	0.42
1:B:382:VAL:CG2	1:B:680:LEU:HD13	2.49	0.42
1:B:555:GLU:OE2	3:B:702:NAG:C8	2.67	0.42
1:A:510:GLN:HB2	1:A:510:GLN:HE21	1.65	0.42
1:B:353:GLU:OE1	1:B:636:THR:HG21	2.19	0.42
1:B:460:ALA:HB3	1:B:463:ARG:HG3	2.02	0.42
1:B:410:VAL:CG1	1:B:608:GLU:HB2	2.50	0.42
1:B:509:ASP:OD1	1:B:510:GLN:N	2.52	0.42
1:B:566:ARG:C	1:B:568:ASP:N	2.71	0.42
1:B:573:CYS:SG	1:B:579:LYS:HG2	2.60	0.42
1:A:653:GLY:C	1:A:655:PRO:HD3	2.40	0.42
1:A:564:LEU:HA	1:A:564:LEU:HD23	1.76	0.42
1:B:455:LYS:HB3	1:B:504:LEU:HD11	2.02	0.42
1:B:475:VAL:CG2	1:B:483:PHE:HE1	2.31	0.41
1:B:472:GLY:HA2	1:B:672:LEU:HD13	2.01	0.41
1:B:499:SER:OG	1:B:500:ARG:N	2.51	0.41
1:B:446:LEU:HD12	1:B:446:LEU:HA	1.87	0.41
1:A:475:VAL:CG2	1:A:480:SER:O	2.68	0.41
1:B:661:LEU:HG	1:B:665:TYR:HD2	1.85	0.41
1:A:419:LYS:O	1:A:420:HIS:CB	2.69	0.41
1:B:410:VAL:HG12	1:B:411:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:CYS:HB3	1:B:521:GLU:OE2	2.20	0.41
1:A:475:VAL:HG23	1:A:483:PHE:HB3	2.02	0.41
1:A:438:VAL:HG22	1:A:533:LEU:CD2	2.50	0.41
1:A:380:CYS:HB3	1:A:392:LEU:HD13	2.03	0.41
1:B:496:ASP:HA	1:B:497:PRO:HD3	1.94	0.41
1:B:686:PHE:O	1:B:689:ARG:NH1	2.53	0.41
1:A:474:ILE:O	1:A:477:GLN:HB3	2.20	0.41
1:B:407:LEU:HD12	1:B:407:LEU:HA	1.83	0.41
1:B:364:GLN:NE2	1:B:364:GLN:HA	2.34	0.41
1:B:432:GLY:HA2	4:B:842:HOH:O	2.21	0.41
1:B:393:ASN:ND2	1:B:413:GLU:OE1	2.54	0.40
1:B:561:ALA:HA	1:B:564:LEU:HD22	2.02	0.40
1:B:568:ASP:HA	4:B:900:HOH:O	2.20	0.40
1:B:661:LEU:HG	1:B:665:TYR:CD2	2.56	0.40
1:A:673:LYS:HE3	4:A:875:HOH:O	2.21	0.40
1:A:475:VAL:CG1	1:A:480:SER:O	2.69	0.40
1:B:571:LEU:O	1:B:578:ARG:HA	2.21	0.40
1:B:447:THR:CG2	1:B:450:SER:HB3	2.49	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	346/348 (99%)	321 (93%)	21 (6%)	4 (1%)	16	22
1	B	346/348 (99%)	323 (93%)	18 (5%)	5 (1%)	14	18
All	All	692/696 (99%)	644 (93%)	39 (6%)	9 (1%)	15	20

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	654	ARG
1	B	655	PRO
1	A	417	SER
1	A	420	HIS
1	B	417	SER
1	B	556	SER
1	B	557	THR
1	A	625	CYS
1	A	543	VAL

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	289/289 (100%)	242 (84%)	47 (16%)	3	3
1	B	289/289 (100%)	227 (78%)	62 (22%)	1	1
All	All	578/578 (100%)	469 (81%)	109 (19%)	2	2

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	356	LYS
1	A	360	GLN
1	A	364	GLN
1	A	382	VAL
1	A	404	LYS
1	A	407	LEU
1	A	415	ARG
1	A	419	LYS
1	A	421	SER
1	A	423	LEU
1	A	427	LEU
1	A	431	GLU
1	A	438	VAL
1	A	443	ASN
1	A	447	THR

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Mol	Chain	Res	Type
1	A	453	ASP
1	A	454	LYS
1	A	459	THR
1	A	463	ARG
1	A	480	SER
1	A	485	GLU
1	A	490	SER
1	A	499	SER
1	A	500	ARG
1	A	510	GLN
1	A	516	VAL
1	A	518	ASN
1	A	545	ASN
1	A	565	LYS
1	A	570	ARG
1	A	571	LEU
1	A	573	CYS
1	A	579	LYS
1	A	589	LEU
1	A	602	ASP
1	A	609	GLN
1	A	627	ASP
1	A	631	LEU
1	A	634	SER
1	A	644	ASN
1	A	651	LEU
1	A	654	ARG
1	A	658	GLU
1	A	663	THR
1	A	672	LEU
1	A	674	LYS
1	A	687	LEU
1	B	342	TYR
1	B	344	ARG
1	B	359	GLN
1	B	363	GLN
1	B	368	ASN
1	B	380	CYS
1	B	407	LEU
1	B	415	ARG
1	B	419	LYS
1	B	421	SER

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Mol	Chain	Res	Type
1	B	423	LEU
1	B	425	CYS
1	B	427	LEU
1	B	446	LEU
1	B	447	THR
1	B	450	SER
1	B	480	SER
1	B	490	SER
1	B	499	SER
1	B	509	ASP
1	B	512	LEU
1	B	513	ASP
1	B	516	VAL
1	B	518	ASN
1	B	520	LYS
1	B	545	ASN
1	B	562	LYS
1	B	564	LEU
1	B	566	ARG
1	B	568	ASP
1	B	570	ARG
1	B	571	LEU
1	B	574	LEU
1	B	575	ASP
1	B	577	THR
1	B	579	LYS
1	B	582	THR
1	B	586	SER
1	B	589	LEU
1	B	595	HIS
1	B	598	VAL
1	B	600	ARG
1	B	601	SER
1	B	620	LYS
1	B	625	CYS
1	B	627	ASP
1	B	628	LYS
1	B	631	LEU
1	B	634	SER
1	B	636	THR
1	B	637	LYS
1	B	645	THR

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Mol	Chain	Res	Type
1	B	646	GLU
1	B	647	CYS
1	B	656	THR
1	B	657	TYR
1	B	659	GLU
1	B	661	LEU
1	B	672	LEU
1	B	682	GLU
1	B	687	LEU
1	B	689	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	355	GLN
1	A	360	GLN
1	A	393	ASN
1	A	510	GLN
1	A	551	ASN
1	A	585	GLN
1	A	642	ASN
1	A	644	ASN
1	B	363	GLN
1	B	364	GLN
1	B	368	ASN
1	B	393	ASN
1	B	563	ASN
1	B	588	HIS
1	B	642	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 ⓘ

2 carbohydrates are modelled in this entry.

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	NAG	B	701	1,3	14,14,15	0.63	0	15,19,21	1.41	2 (13%)
3	NAG	B	702	3	14,14,15	0.50	0	15,19,21	1.37	4 (26%)

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	NAG	B	701	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	702	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	NAG	O7-C7-C8	-2.19	118.05	122.06
3	B	702	NAG	C1-O5-C5	-2.08	109.61	112.25
3	B	702	NAG	O7-C7-N2	2.23	126.40	121.86
3	B	702	NAG	O5-C5-C6	2.25	112.23	107.35
3	B	701	NAG	O5-C5-C6	2.61	113.00	107.35
3	B	701	NAG	C4-C3-C2	4.00	117.45	111.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	NAG	2	0

5.6 Ligand geometry

3 ligands are modelled in this entry.

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	NAG	A	701	1	14,14,15	0.66	0	15,19,21	1.17	1 (6%)
2	NAG	A	702	1	14,14,15	0.63	0	15,19,21	1.55	1 (6%)
2	NAG	B	703	1	14,14,15	0.47	0	15,19,21	1.02	1 (6%)

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	NAG	A	701	1	-	0/6/23/26	0/1/1/1
2	NAG	A	702	1	-	0/6/23/26	0/1/1/1
2	NAG	B	703	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	703	NAG	C1-O5-C5	3.20	116.31	112.25
2	A	701	NAG	C1-O5-C5	3.97	117.28	112.25
2	A	702	NAG	C1-O5-C5	4.67	118.17	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	NAG	2	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 ⓘ

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	348/348 (100%)	-0.46	6 (1%) 73 72	4, 21, 49, 93	0
1	B	348/348 (100%)	-0.28	8 (2%) 64 63	8, 31, 58, 97	0
All	All	696/696 (100%)	-0.37	14 (2%) 68 67	4, 26, 55, 97	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	417	SER	5.8
1	B	417	SER	5.5
1	B	421	SER	5.2
1	A	420	HIS	4.4
1	A	423	LEU	4.1
1	B	420	HIS	3.7
1	A	418	SER	3.2
1	A	419	LYS	2.8
1	B	418	SER	2.6
1	B	342	TYR	2.5
1	B	689	ARG	2.4
1	A	422	SER	2.4
1	B	419	LYS	2.1
1	B	653	GLY	2.1

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 ⓘ

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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	B	701	14/15	0.88	0.16	-0.42	49,56,61,64	0
3	NAG	B	702	14/15	0.82	0.20	-	65,73,86,97	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	A	701	14/15	0.75	0.28	3.23	63,67,75,81	0
2	NAG	B	703	14/15	0.79	0.21	2.55	64,70,75,75	0
2	NAG	A	702	14/15	0.92	0.12	-0.33	33,39,50,52	0

6.5 Other polymers

There are no such residues in this entry.