



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:45 AM UTC

PDB ID : 3QNF / pdb_00003qnf
Title : Crystal structure of the open state of human endoplasmic reticulum aminopeptidase 1 ERAP1
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Deposited on : 2011-02-08
Resolution : 3.00 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

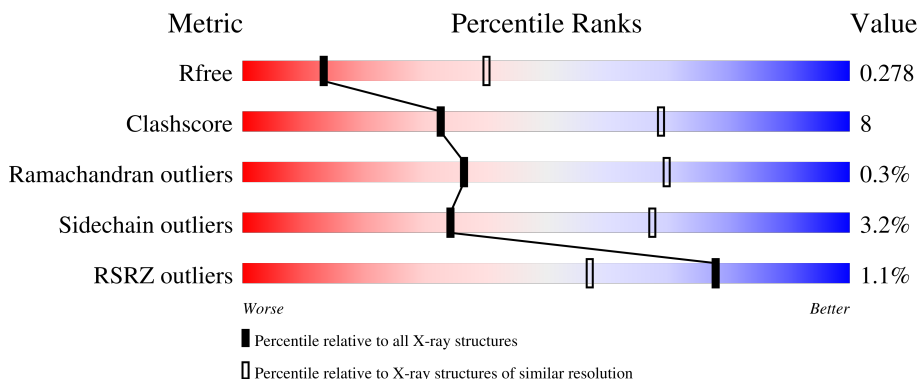
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. 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	954	% 62% 10% 27%
1	B	954	% 69% 14% 16%
1	C	954	% 69% 14% 16%
2	D	4	50% 50%

Validation Pipeline (wwPDB-VP) : 2.49

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	MAN	D	4	X	-	-	-
4	NAG	B	1154	X	-	-	-
4	NAG	C	1154	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17682 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 Endoplasmic reticulum aminopeptidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	696	Total	C	N	O	S	0	1	0
			5284	3422	863	975	24			
1	B	802	Total	C	N	O	S	0	2	0
			6178	4011	1005	1133	29			
1	C	800	Total	C	N	O	S	0	2	0
			6072	3936	998	1109	29			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	LEU	-	expression tag	UNP Q9NZ08
A	-4	ARG	-	expression tag	UNP Q9NZ08
A	-3	ARG	-	expression tag	UNP Q9NZ08
A	-2	ARG	-	expression tag	UNP Q9NZ08
A	-1	TYR	-	expression tag	UNP Q9NZ08
A	0	THR	-	expression tag	UNP Q9NZ08
A	942	ALA	-	expression tag	UNP Q9NZ08
A	943	GLU	-	expression tag	UNP Q9NZ08
A	944	ASN	-	expression tag	UNP Q9NZ08
A	945	LEU	-	expression tag	UNP Q9NZ08
A	946	TYR	-	expression tag	UNP Q9NZ08
A	947	PHE	-	expression tag	UNP Q9NZ08
A	948	GLN	-	expression tag	UNP Q9NZ08
B	-5	LEU	-	expression tag	UNP Q9NZ08
B	-4	ARG	-	expression tag	UNP Q9NZ08
B	-3	ARG	-	expression tag	UNP Q9NZ08
B	-2	ARG	-	expression tag	UNP Q9NZ08
B	-1	TYR	-	expression tag	UNP Q9NZ08
B	0	THR	-	expression tag	UNP Q9NZ08
B	942	ALA	-	expression tag	UNP Q9NZ08
B	943	GLU	-	expression tag	UNP Q9NZ08
B	944	ASN	-	expression tag	UNP Q9NZ08
B	945	LEU	-	expression tag	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
B	946	TYR	-	expression tag	UNP Q9NZ08
B	947	PHE	-	expression tag	UNP Q9NZ08
B	948	GLN	-	expression tag	UNP Q9NZ08
C	-5	LEU	-	expression tag	UNP Q9NZ08
C	-4	ARG	-	expression tag	UNP Q9NZ08
C	-3	ARG	-	expression tag	UNP Q9NZ08
C	-2	ARG	-	expression tag	UNP Q9NZ08
C	-1	TYR	-	expression tag	UNP Q9NZ08
C	0	THR	-	expression tag	UNP Q9NZ08
C	942	ALA	-	expression tag	UNP Q9NZ08
C	943	GLU	-	expression tag	UNP Q9NZ08
C	944	ASN	-	expression tag	UNP Q9NZ08
C	945	LEU	-	expression tag	UNP Q9NZ08
C	946	TYR	-	expression tag	UNP Q9NZ08
C	947	PHE	-	expression tag	UNP Q9NZ08
C	948	GLN	-	expression tag	UNP Q9NZ08

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

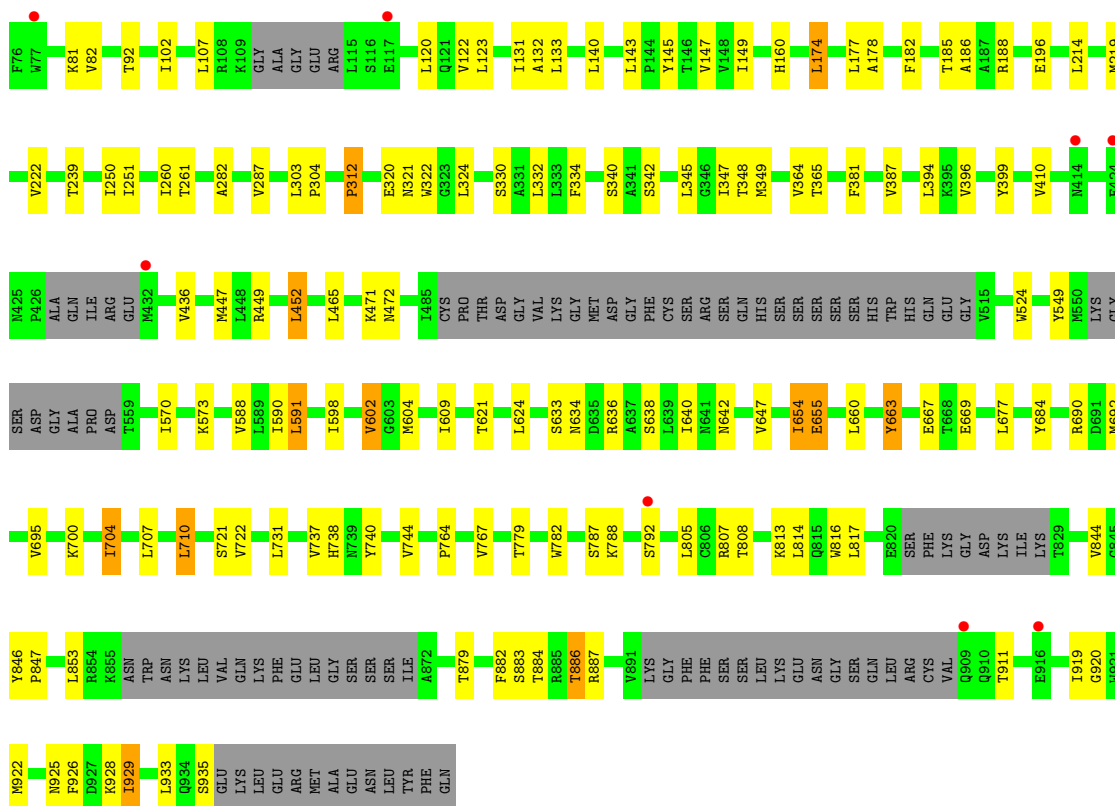
- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



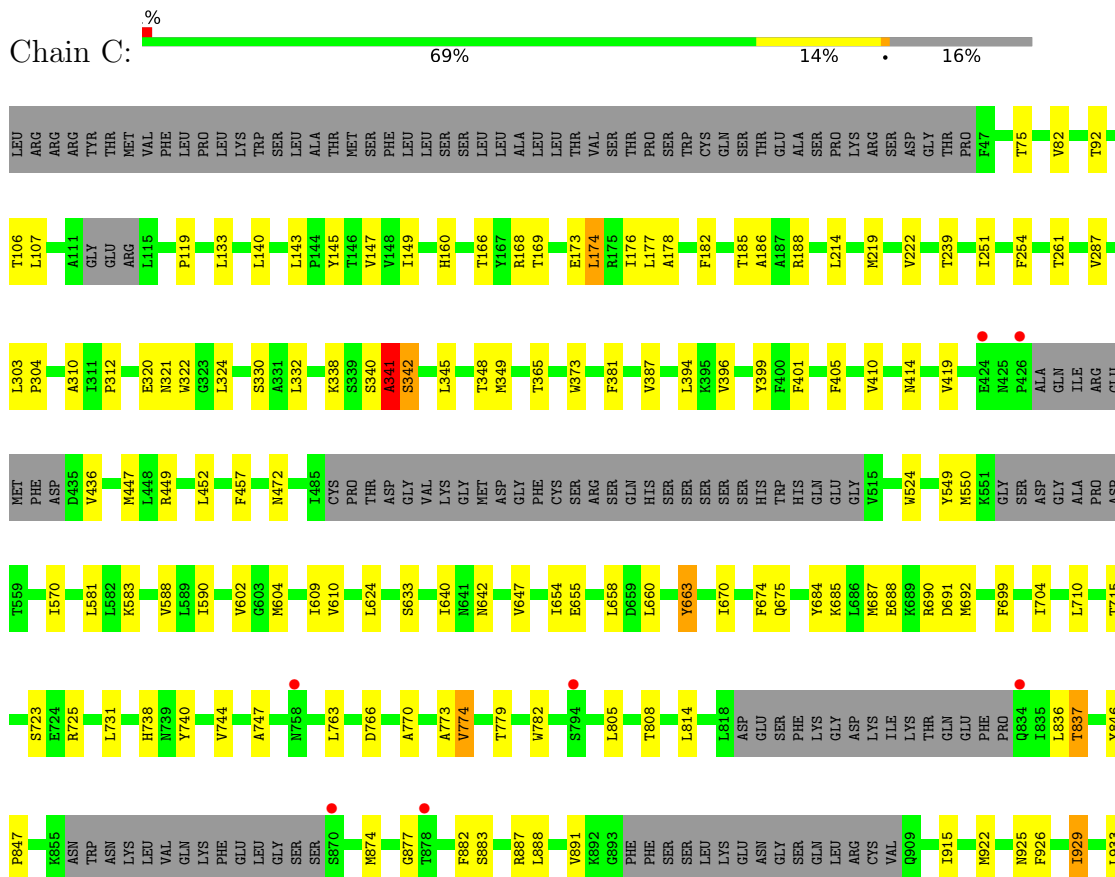
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	8	Total	O	0	0
			8	8		
5	B	19	Total	O	0	0
			19	19		
5	C	12	Total	O	0	0
			12	12		



- Molecule 1: Endoplasmic reticulum aminopeptidase 1



K9S7
LEU
GLU
ARG
MET
ALA
GLU
ASN
LEU
TYR
PHE
GLN

- Molecule 2: α -D-mannopyranose-(1-6)- α -D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  50% 50%

MAG1
MAG2
MAN3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.25Å 132.82Å 233.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.00 19.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.6 (19.99-3.00) 97.2 (19.99-3.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.229 , 0.283 0.228 , 0.278	Depositor DCC
R_{free} test set	3019 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	55.1	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	17682	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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, 0.333 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: MAN, ZN, 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	0.53	0/5419	0.75	2/7396 (0.0%)
1	B	0.53	0/6343	0.77	3/8661 (0.0%)
1	C	0.53	0/6229	0.77	2/8502 (0.0%)
All	All	0.53	0/17991	0.77	7/24559 (0.0%)

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	C	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	452	LEU	N-CA-C	-6.85	101.49	110.53
1	C	342	SER	N-CA-C	-6.36	102.75	110.88
1	A	452	LEU	N-CA-C	-5.78	103.30	110.41
1	B	591	LEU	CA-C-N	5.74	125.21	119.24
1	B	591	LEU	C-N-CA	5.74	125.21	119.24
1	A	743	CYS	N-CA-C	-5.56	104.86	111.03
1	C	452	LEU	N-CA-C	-5.43	103.73	110.41

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	736	CYS	Peptide
1	C	341	ALA	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	5284	0	4868	59	0
1	B	6178	0	5791	107	0
1	C	6072	0	5618	101	0
2	D	50	0	43	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	B	28	0	26	0	0
4	C	28	0	26	0	0
5	A	8	0	0	0	0
5	B	19	0	0	1	0
5	C	12	0	0	0	0
All	All	17682	0	16372	268	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 8.

All (268) 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:410:VAL:HG11	1:A:436:VAL:HG21	1.50	0.94
1:B:624:LEU:CD1	1:B:660:LEU:HD21	1.98	0.93
1:C:692:MET:HE1	1:C:922:MET:HE2	1.57	0.86
1:C:341:ALA:HB3	1:C:725:ARG:CZ	2.09	0.82
1:C:107:LEU:HD11	1:C:145:TYR:HB3	1.62	0.80
1:C:410:VAL:HG11	1:C:436:VAL:HG21	1.63	0.79
1:B:624:LEU:HD13	1:B:660:LEU:HD21	1.64	0.78
1:B:609:ILE:HG23	1:B:642:ASN:OD1	1.86	0.75
1:A:609:ILE:HG23	1:A:642:ASN:OD1	1.88	0.74
1:C:770:ALA:O	1:C:773:ALA:HB3	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:ILE:HD11	1:A:663:TYR:HE2	1.52	0.73
1:B:261:THR:HG22	1:B:287:VAL:HG13	1.71	0.72
1:B:677:LEU:HD21	1:B:707:LEU:CD1	2.19	0.72
1:B:345:LEU:HA	1:B:394:LEU:HD13	1.71	0.72
1:A:410:VAL:CG1	1:A:436:VAL:HG21	2.20	0.72
1:B:853:LEU:HD23	1:B:853:LEU:O	1.90	0.71
1:B:410:VAL:HG11	1:B:436:VAL:HG21	1.72	0.70
1:C:405:PHE:CD2	1:C:675:GLN:NE2	2.60	0.70
1:B:604:MET:HE3	1:B:634:ASN:HB3	1.75	0.69
1:C:447:MET:HE1	1:C:524:TRP:CE2	2.26	0.69
1:B:196:GLU:OE1	5:B:960:HOH:O	2.09	0.68
1:A:140:LEU:HD12	1:A:143:LEU:HD22	1.75	0.68
1:B:345:LEU:HD11	1:B:396:VAL:HG12	1.76	0.68
1:C:624:LEU:CD1	1:C:660:LEU:HD21	2.23	0.67
1:A:261:THR:HG22	1:A:287:VAL:HG13	1.75	0.67
1:B:704:ILE:HD11	1:B:738:HIS:HB2	1.77	0.67
1:A:609:ILE:HG23	1:A:642:ASN:CG	2.22	0.65
1:C:414:ASN:CB	1:C:550:MET:HE1	2.27	0.65
1:B:640:ILE:HD11	1:B:663:TYR:HE2	1.60	0.65
1:C:692:MET:HE1	1:C:922:MET:CE	2.25	0.64
1:B:447:MET:HE1	1:B:524:TRP:CE2	2.32	0.64
1:C:410:VAL:CG1	1:C:436:VAL:HG21	2.28	0.64
1:C:401:PHE:CG	1:C:604:MET:HE3	2.33	0.63
1:B:219:MET:HG2	1:B:239:THR:HG22	1.81	0.63
1:B:853:LEU:HD23	1:B:853:LEU:C	2.24	0.63
1:B:677:LEU:HD21	1:B:707:LEU:HD11	1.80	0.62
1:A:716:TRP:CZ3	1:A:732:LEU:HD13	2.34	0.62
1:B:182:PHE:HA	1:B:186:ALA:HB3	1.82	0.62
1:C:782:TRP:CE2	1:C:805:LEU:HD22	2.35	0.62
1:C:725:ARG:HG3	1:C:766:ASP:OD2	2.00	0.61
1:B:102:ILE:HD11	1:B:131:ILE:HD13	1.81	0.61
1:B:570:ILE:HG23	1:B:602:VAL:HG21	1.81	0.61
1:A:640:ILE:HD11	1:A:663:TYR:CE2	2.34	0.60
1:B:604:MET:HG3	1:B:638:SER:HB2	1.82	0.60
1:B:737:VAL:HG11	1:B:807:ARG:NH2	2.16	0.60
1:B:140:LEU:HD12	1:B:143:LEU:HD22	1.83	0.60
1:A:219:MET:HG2	1:A:239:THR:HG22	1.82	0.60
1:C:182:PHE:HA	1:C:186:ALA:HB3	1.84	0.59
1:C:261:THR:HG22	1:C:287:VAL:HG13	1.83	0.59
1:A:743:CYS:O	1:A:747:ALA:CB	2.50	0.59
1:C:624:LEU:HD13	1:C:660:LEU:HD21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:692:MET:SD	1:B:922:MET:HE1	2.43	0.58
1:A:461:ILE:HD13	1:A:478:LEU:HD11	1.86	0.57
1:C:140:LEU:HD12	1:C:143:LEU:HD22	1.85	0.57
1:C:740:TYR:O	1:C:744:VAL:HG23	2.04	0.57
1:A:447:MET:HE1	1:A:524:TRP:CE2	2.40	0.57
1:B:321:ASN:HB2	1:B:324:LEU:O	2.04	0.57
1:B:590:ILE:N	1:B:590:ILE:HD12	2.20	0.57
1:C:888:LEU:HD21	1:C:915:ILE:HG22	1.86	0.56
1:C:341:ALA:HB3	1:C:725:ARG:NH2	2.21	0.56
1:C:647:VAL:HG11	1:C:654:ILE:HD13	1.86	0.56
1:C:405:PHE:CE2	1:C:675:GLN:NE2	2.73	0.56
1:A:549:TYR:CE2	1:A:649:ILE:HD13	2.41	0.56
1:A:573:LYS:HD3	1:A:595:VAL:HG12	1.87	0.56
1:C:888:LEU:HD21	1:C:915:ILE:CG2	2.37	0.55
1:B:107:LEU:HB2	1:B:120:LEU:HD21	1.87	0.55
1:B:604:MET:HE3	1:B:634:ASN:CB	2.37	0.55
1:B:883:SER:OG	1:B:922:MET:HG3	2.06	0.55
1:A:182:PHE:HA	1:A:186:ALA:HB3	1.89	0.55
1:A:624:LEU:CD1	1:A:660:LEU:HD21	2.36	0.55
1:B:879:THR:HG22	1:B:882:PHE:HE2	1.71	0.55
1:C:782:TRP:CD2	1:C:805:LEU:HD22	2.41	0.55
1:C:219:MET:HG2	1:C:239:THR:HG22	1.87	0.55
1:A:178:ALA:HB3	1:A:251:ILE:HB	1.89	0.55
1:A:107:LEU:HD11	1:A:145:TYR:HB3	1.88	0.54
1:C:349:MET:SD	1:C:396:VAL:HG23	2.46	0.54
1:B:624:LEU:HD12	1:B:660:LEU:HD21	1.86	0.53
1:C:710:LEU:HG	1:C:731:LEU:HD11	1.91	0.53
1:B:604:MET:HE2	1:B:634:ASN:O	2.08	0.53
1:C:704:ILE:HD11	1:C:738:HIS:ND1	2.24	0.53
1:C:106:THR:HG22	1:C:119:PRO:HA	1.91	0.53
1:B:349:MET:HE1	1:B:399:TYR:CD2	2.43	0.52
1:C:883:SER:CB	1:C:922:MET:HG3	2.39	0.52
1:C:692:MET:SD	1:C:926:PHE:CE1	3.03	0.52
1:C:808:THR:O	1:C:814:LEU:HD11	2.09	0.52
1:B:133:LEU:HD11	1:B:149:ILE:HD11	1.91	0.52
1:C:685:LYS:NZ	1:C:688:GLU:OE1	2.36	0.52
1:B:609:ILE:HG23	1:B:642:ASN:CG	2.34	0.52
1:B:647:VAL:HG11	1:B:654:ILE:HD12	1.92	0.52
1:C:345:LEU:HA	1:C:394:LEU:HD13	1.92	0.51
1:C:590:ILE:HD12	1:C:590:ILE:N	2.25	0.51
1:A:321:ASN:HB2	1:A:324:LEU:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:THR:HG22	1:A:598:ILE:HG13	1.91	0.51
1:C:699:PHE:HA	1:C:933:LEU:HD21	1.92	0.51
1:B:640:ILE:HD11	1:B:663:TYR:CE2	2.44	0.51
1:C:405:PHE:CE2	1:C:604:MET:SD	3.03	0.51
1:B:886:THR:HG22	1:B:887:ARG:N	2.25	0.51
1:B:884:THR:O	1:B:919:ILE:HD11	2.10	0.51
1:C:710:LEU:HG	1:C:731:LEU:CD1	2.41	0.51
1:A:381:PHE:HZ	1:A:449:ARG:HD3	1.76	0.50
1:A:741:GLN:HB3	1:A:742:PRO:HD3	1.92	0.50
1:C:303:LEU:HD11	1:C:322:TRP:CG	2.46	0.50
1:C:888:LEU:CD2	1:C:915:ILE:CG2	2.89	0.50
1:C:133:LEU:HD11	1:C:149:ILE:HD11	1.93	0.50
1:B:410:VAL:CG1	1:B:436:VAL:HG21	2.39	0.50
1:C:447:MET:HE1	1:C:524:TRP:CD2	2.46	0.50
1:C:581:LEU:HD23	1:C:583:LYS:HE3	1.93	0.50
1:C:640:ILE:HD11	1:C:663:TYR:HE2	1.76	0.50
1:A:590:ILE:N	1:A:590:ILE:HD12	2.26	0.50
1:A:743:CYS:O	1:A:747:ALA:HB2	2.10	0.50
1:B:345:LEU:CD1	1:B:396:VAL:HG12	2.40	0.50
1:A:250:ILE:HD12	1:A:324:LEU:HD11	1.93	0.50
1:A:448:LEU:HD21	1:A:482:MET:HG2	1.93	0.50
1:B:624:LEU:CD1	1:B:660:LEU:CD2	2.81	0.49
1:B:808:THR:HG23	1:B:814:LEU:HG	1.93	0.49
1:C:887:ARG:O	1:C:891:VAL:HG23	2.12	0.49
1:C:925:ASN:O	1:C:926:PHE:C	2.56	0.49
1:B:387:VAL:HB	1:B:396:VAL:HG11	1.95	0.49
1:B:667:GLU:OE2	1:B:669:GLU:N	2.41	0.49
1:B:919:ILE:HG22	1:B:920:GLY:N	2.27	0.49
1:A:347:ILE:O	1:A:351:VAL:HG23	2.13	0.49
1:B:782:TRP:HZ2	1:B:817:LEU:HD11	1.78	0.49
1:A:447:MET:HE1	1:A:524:TRP:CD2	2.48	0.49
1:B:846:TYR:N	1:B:847:PRO:CD	2.76	0.48
1:B:879:THR:OG1	1:B:911:THR:HG21	2.13	0.48
1:C:837:THR:HG23	1:C:877:GLY:HA3	1.95	0.48
1:B:690:ARG:CD	1:B:884:THR:HG22	2.44	0.48
1:C:321:ASN:HB2	1:C:324:LEU:O	2.13	0.48
1:B:740:TYR:O	1:B:744:VAL:HG23	2.14	0.47
1:C:349:MET:HE1	1:C:399:TYR:CE2	2.50	0.47
1:B:710:LEU:HD12	1:B:731:LEU:CD1	2.45	0.47
1:C:658:LEU:HD11	1:C:929:ILE:HD13	1.97	0.47
1:A:419:VAL:HG23	1:A:440:LYS:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:THR:HG22	1:B:387:VAL:HG22	1.95	0.47
1:A:183:GLU:OE1	1:A:319:MET:SD	2.73	0.47
1:B:177:LEU:HD21	1:B:312:PRO:HG2	1.97	0.47
1:C:882:PHE:O	1:C:915:ILE:HG23	2.15	0.47
1:A:624:LEU:HD13	1:A:660:LEU:HD21	1.96	0.46
1:B:381:PHE:HZ	1:B:449:ARG:HD3	1.79	0.46
1:B:764:PRO:O	1:B:767:VAL:HG22	2.15	0.46
1:C:166:THR:HG22	1:C:176:ILE:HG12	1.97	0.46
1:C:549:TYR:CD2	1:C:609:ILE:HD12	2.50	0.46
1:B:879:THR:HG22	1:B:882:PHE:CE2	2.50	0.46
1:B:122:VAL:HG22	1:B:133:LEU:HD22	1.96	0.46
1:B:621:THR:HG23	1:B:660:LEU:HA	1.98	0.46
1:B:660:LEU:O	1:B:660:LEU:HD23	2.14	0.46
1:C:690:ARG:HG3	1:C:692:MET:CE	2.45	0.46
1:A:263:SER:OG	1:A:294:GLU:OE1	2.27	0.46
1:B:604:MET:CE	1:B:634:ASN:HB3	2.45	0.46
1:C:381:PHE:HZ	1:C:449:ARG:HD3	1.81	0.46
1:B:107:LEU:HD11	1:B:145:TYR:HB3	1.97	0.45
1:B:788:LYS:O	1:B:792:SER:CB	2.64	0.45
1:B:177:LEU:HD21	1:B:312:PRO:HD2	1.98	0.45
1:C:609:ILE:HG22	1:C:610:VAL:N	2.31	0.45
1:A:102:ILE:HD11	1:A:131:ILE:HD13	1.99	0.45
1:B:782:TRP:CE2	1:B:805:LEU:HD22	2.51	0.45
1:C:836:LEU:HD23	1:C:874:MET:CB	2.46	0.45
1:B:695:VAL:HG21	1:B:926:PHE:CE1	2.52	0.45
1:C:401:PHE:CB	1:C:604:MET:HE3	2.46	0.45
1:B:677:LEU:CD2	1:B:707:LEU:HD11	2.47	0.45
1:C:365:THR:HB	1:C:472:ASN:ND2	2.31	0.45
1:B:549:TYR:CD2	1:B:609:ILE:HD12	2.50	0.45
1:C:684:TYR:HA	1:C:687:MET:HE3	1.98	0.45
1:B:250:ILE:HD12	1:B:324:LEU:HD11	1.97	0.45
1:B:704:ILE:HD11	1:B:738:HIS:CB	2.46	0.45
1:B:690:ARG:HG3	1:B:922:MET:HE2	1.99	0.45
1:A:535:ILE:HD12	1:A:600:PHE:CE1	2.52	0.44
1:A:683:MET:C	1:A:687:MET:HE3	2.42	0.44
1:C:654:ILE:HG12	1:C:929:ILE:HD11	1.99	0.44
1:A:716:TRP:CE3	1:A:732:LEU:HD13	2.52	0.44
1:C:373:TRP:CE3	1:C:419:VAL:HG11	2.52	0.44
1:B:174:LEU:C	1:B:174:LEU:HD23	2.43	0.44
1:B:636:ARG:NH1	1:B:667:GLU:OE1	2.50	0.44
1:A:185:THR:HB	1:A:188:ARG:CZ	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:THR:HG22	1:C:173:GLU:O	2.17	0.44
1:B:365:THR:O	1:B:472:ASN:HA	2.17	0.44
1:C:846:TYR:CD1	1:C:847:PRO:HD3	2.52	0.44
1:B:260:ILE:HG22	1:B:261:THR:O	2.18	0.44
1:C:888:LEU:CD2	1:C:915:ILE:HG21	2.48	0.43
1:C:168:ARG:CZ	1:C:174:LEU:HB2	2.48	0.43
1:B:655:GLU:OE2	1:B:928:LYS:HD3	2.18	0.43
1:C:405:PHE:CZ	1:C:604:MET:SD	3.12	0.43
1:C:178:ALA:HB3	1:C:251:ILE:HB	2.00	0.43
1:C:888:LEU:HD23	1:C:915:ILE:HG21	2.00	0.43
1:A:536:THR:O	1:A:543[B]:HIS:HB2	2.18	0.43
1:B:604:MET:CE	1:B:634:ASN:CB	2.97	0.43
1:C:449:ARG:HD2	1:C:457:PHE:CD2	2.53	0.43
1:B:387:VAL:CG1	1:B:396:VAL:HG11	2.48	0.43
1:C:687:MET:HE1	1:C:699:PHE:CD1	2.54	0.43
1:C:185:THR:HB	1:C:188:ARG:CZ	2.48	0.43
1:B:102:ILE:HG23	1:B:149:ILE:HG23	2.01	0.43
1:A:177:LEU:HD21	1:A:312:PRO:HG2	2.01	0.42
1:B:320:GLU:O	1:B:321:ASN:C	2.61	0.42
1:B:624:LEU:HD12	1:B:660:LEU:CD2	2.47	0.42
1:B:684:TYR:CD1	1:B:700:LYS:HE2	2.54	0.42
1:B:925:ASN:O	1:B:929:ILE:HG13	2.18	0.42
1:C:690:ARG:HG3	1:C:692:MET:HE2	2.00	0.42
1:A:133:LEU:HD11	1:A:149:ILE:HD11	2.00	0.42
1:C:348:THR:HG22	1:C:387:VAL:HG22	2.01	0.42
1:A:687:MET:HE1	1:A:699:PHE:CD1	2.54	0.42
1:B:82:VAL:HG13	1:B:147:VAL:HB	2.02	0.42
1:B:303:LEU:HD11	1:B:322:TRP:CG	2.54	0.42
1:B:591:LEU:HD11	1:B:598:ILE:HD12	2.01	0.42
1:B:813:LYS:O	1:B:816:TRP:HB3	2.18	0.42
1:C:570:ILE:HG23	1:C:602:VAL:HG21	2.01	0.42
1:C:690:ARG:O	1:C:692:MET:N	2.52	0.42
1:A:140:LEU:HD12	1:A:143:LEU:CD2	2.46	0.42
1:B:334:PHE:HB2	1:B:347:ILE:CD1	2.49	0.42
1:C:373:TRP:CD2	1:C:419:VAL:CG1	3.02	0.42
1:C:82:VAL:HG13	1:C:147:VAL:HB	2.01	0.42
1:C:310:ALA:HB2	1:C:332:LEU:HD23	2.00	0.42
1:A:320:GLU:O	1:A:321:ASN:C	2.61	0.42
1:C:609:ILE:HG23	1:C:642:ASN:CG	2.45	0.42
1:C:747:ALA:HB1	1:C:774:VAL:HB	2.01	0.42
2:D:3:MAN:H61	2:D:4:MAN:H2	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:GLU:O	1:C:321:ASN:C	2.60	0.42
1:C:624:LEU:HD12	1:C:660:LEU:HD21	1.98	0.42
1:C:723:SER:C	1:C:725:ARG:N	2.76	0.42
1:B:844:VAL:O	1:B:844:VAL:HG23	2.21	0.41
1:C:340:SER:O	1:C:342:SER:N	2.48	0.41
1:A:61:VAL:HG12	1:A:83:GLU:O	2.19	0.41
1:A:107:LEU:HB2	1:A:120:LEU:HD21	2.01	0.41
1:B:185:THR:HB	1:B:188:ARG:CZ	2.50	0.41
1:B:364:VAL:HG21	1:B:465:LEU:HA	2.01	0.41
1:B:933:LEU:O	1:B:935:SER:N	2.54	0.41
1:C:303:LEU:HB3	1:C:304:PRO:HD2	2.02	0.41
1:C:731:LEU:HD23	1:C:731:LEU:HA	1.92	0.41
1:A:647:VAL:HG21	1:A:657:ALA:CB	2.51	0.41
1:B:282:ALA:HB1	1:B:332:LEU:CD1	2.50	0.41
1:C:177:LEU:HD22	1:C:254:PHE:CZ	2.55	0.41
1:C:763:LEU:HD23	1:C:763:LEU:HA	1.88	0.41
1:A:345:LEU:HG	1:A:349:MET:HE2	2.03	0.41
1:A:589:LEU:C	1:A:589:LEU:HD12	2.45	0.41
1:B:282:ALA:HB1	1:B:332:LEU:HD11	2.02	0.41
1:C:341:ALA:HB3	1:C:725:ARG:NH1	2.35	0.41
1:C:670:ILE:CG1	1:C:674:PHE:CE2	3.03	0.41
1:B:925:ASN:O	1:B:926:PHE:C	2.63	0.41
1:A:421:THR:HG22	1:A:422:PRO:O	2.21	0.41
1:B:123:LEU:HB2	1:B:132:ALA:HB3	2.02	0.41
1:B:449:ARG:O	1:B:452:LEU:O	2.38	0.41
1:C:177:LEU:HD22	1:C:254:PHE:CE1	2.56	0.41
1:C:349:MET:HE1	1:C:399:TYR:CD2	2.56	0.41
1:B:342:SER:HB3	1:B:722:VAL:HG22	2.03	0.41
1:C:401:PHE:HB3	1:C:604:MET:HE3	2.02	0.41
1:A:169:THR:HG22	1:A:173:GLU:O	2.21	0.41
1:A:260:ILE:HG22	1:A:261:THR:O	2.20	0.41
1:B:64:ASP:HB3	1:B:81:LYS:HB2	2.03	0.41
1:B:178:ALA:HB3	1:B:251:ILE:HB	2.03	0.41
1:B:447:MET:HE1	1:B:524:TRP:CD2	2.55	0.41
1:B:660:LEU:HD23	1:B:660:LEU:C	2.46	0.41
1:A:95:LEU:HD11	1:A:131:ILE:HD11	2.03	0.41
1:A:162:PHE:CE1	1:A:178:ALA:HB1	2.55	0.41
1:A:717:THR:O	1:A:728:ARG:NE	2.54	0.41
1:B:303:LEU:HB3	1:B:304:PRO:HD2	2.03	0.41
1:C:670:ILE:HG12	1:C:674:PHE:CD2	2.56	0.41
1:A:140:LEU:HB2	1:A:143:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:624:LEU:HD13	1:B:660:LEU:CD2	2.43	0.40
1:B:549:TYR:CE2	1:B:609:ILE:HD12	2.57	0.40
1:C:710:LEU:CD2	1:C:731:LEU:HD11	2.51	0.40
1:A:647:VAL:HG21	1:A:657:ALA:HB2	2.01	0.40
1:C:609:ILE:HG23	1:C:642:ASN:OD1	2.21	0.40
1:C:640:ILE:HD11	1:C:663:TYR:CE2	2.56	0.40
1:B:731:LEU:HD23	1:B:731:LEU:HA	1.94	0.40
1:C:670:ILE:HD11	1:C:674:PHE:CE2	2.57	0.40
1:A:259:LYS:HD3	1:A:287:VAL:HG21	2.03	0.40
1:A:660:LEU:HD23	1:A:660:LEU:O	2.21	0.40
1:B:853:LEU:C	1:B:853:LEU:CD2	2.94	0.40
1:C:723:SER:C	1:C:725:ARG:H	2.29	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	683/954 (72%)	642 (94%)	40 (6%)	1 (0%)	48	80
1	B	788/954 (83%)	741 (94%)	46 (6%)	1 (0%)	48	80
1	C	786/954 (82%)	736 (94%)	46 (6%)	4 (0%)	24	60
All	All	2257/2862 (79%)	2119 (94%)	132 (6%)	6 (0%)	36	70

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	338	LYS
1	C	691	ASP
1	C	341	ALA
1	C	312	PRO
1	A	312	PRO

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Mol	Chain	Res	Type
1	B	312	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	515/851 (60%)	500 (97%)	15 (3%)	37	70
1	B	623/851 (73%)	598 (96%)	25 (4%)	28	62
1	C	591/851 (69%)	575 (97%)	16 (3%)	39	71
All	All	1729/2553 (68%)	1673 (97%)	56 (3%)	34	67

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	THR
1	A	92	THR
1	A	160	HIS
1	A	214	LEU
1	A	222	VAL
1	A	263	SER
1	A	330	SER
1	A	342	SER
1	A	374	LEU
1	A	588	VAL
1	A	593	GLU
1	A	633	SER
1	A	655	GLU
1	A	663	TYR
1	A	707	LEU
1	B	59	ILE
1	B	71	LEU
1	B	75	THR
1	B	92	THR
1	B	160	HIS
1	B	174	LEU

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Mol	Chain	Res	Type
1	B	214	LEU
1	B	222	VAL
1	B	330	SER
1	B	340	SER
1	B	471	LYS
1	B	573	LYS
1	B	588	VAL
1	B	602	VAL
1	B	633	SER
1	B	654	ILE
1	B	655	GLU
1	B	663	TYR
1	B	704	ILE
1	B	710	LEU
1	B	721	SER
1	B	779	THR
1	B	787	SER
1	B	886	THR
1	B	929	ILE
1	C	75	THR
1	C	92	THR
1	C	160	HIS
1	C	174	LEU
1	C	214	LEU
1	C	222	VAL
1	C	330	SER
1	C	588	VAL
1	C	633	SER
1	C	655	GLU
1	C	663	TYR
1	C	715	THR
1	C	774	VAL
1	C	779	THR
1	C	837	THR
1	C	929	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	306	GLN
1	A	375	ASN
1	A	446	ASN

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Mol	Chain	Res	Type
1	A	645	GLN
1	B	278	GLN
1	B	446	ASN
1	B	472	ASN
1	B	548	HIS
1	B	628	HIS
1	B	645	GLN
1	B	790	GLN
1	C	128	GLN
1	C	446	ASN
1	C	548	HIS
1	C	628	HIS
1	C	645	GLN

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 ⓘ

4 monosaccharides 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	D	1	1,2	14,14,15	0.54	0	17,19,21	1.15	1 (5%)
2	NAG	D	2	2	14,14,15	0.52	0	17,19,21	1.38	2 (11%)
2	MAN	D	3	2	11,11,12	0.71	0	15,15,17	1.15	1 (6%)
2	MAN	D	4	2	11,11,12	0.63	0	15,15,17	1.94	3 (20%)

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	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	MAN	D	3	2	-	1/2/19/22	1/1/1/1
2	MAN	D	4	2	1/1/4/5	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4	MAN	C1-O5-C5	5.67	119.78	112.19
2	D	2	NAG	C1-O5-C5	3.77	117.24	112.19
2	D	4	MAN	C3-C4-C5	3.01	115.69	110.23
2	D	2	NAG	O4-C4-C3	-2.77	103.85	110.38
2	D	4	MAN	O5-C5-C6	2.74	113.00	107.66
2	D	1	NAG	O5-C1-C2	-2.46	107.49	111.29
2	D	3	MAN	O6-C6-C5	-2.13	104.09	111.33

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	4	MAN	C1

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	D	4	MAN	O5-C5-C6-O6
2	D	3	MAN	O5-C5-C6-O6
2	D	4	MAN	C4-C5-C6-O6

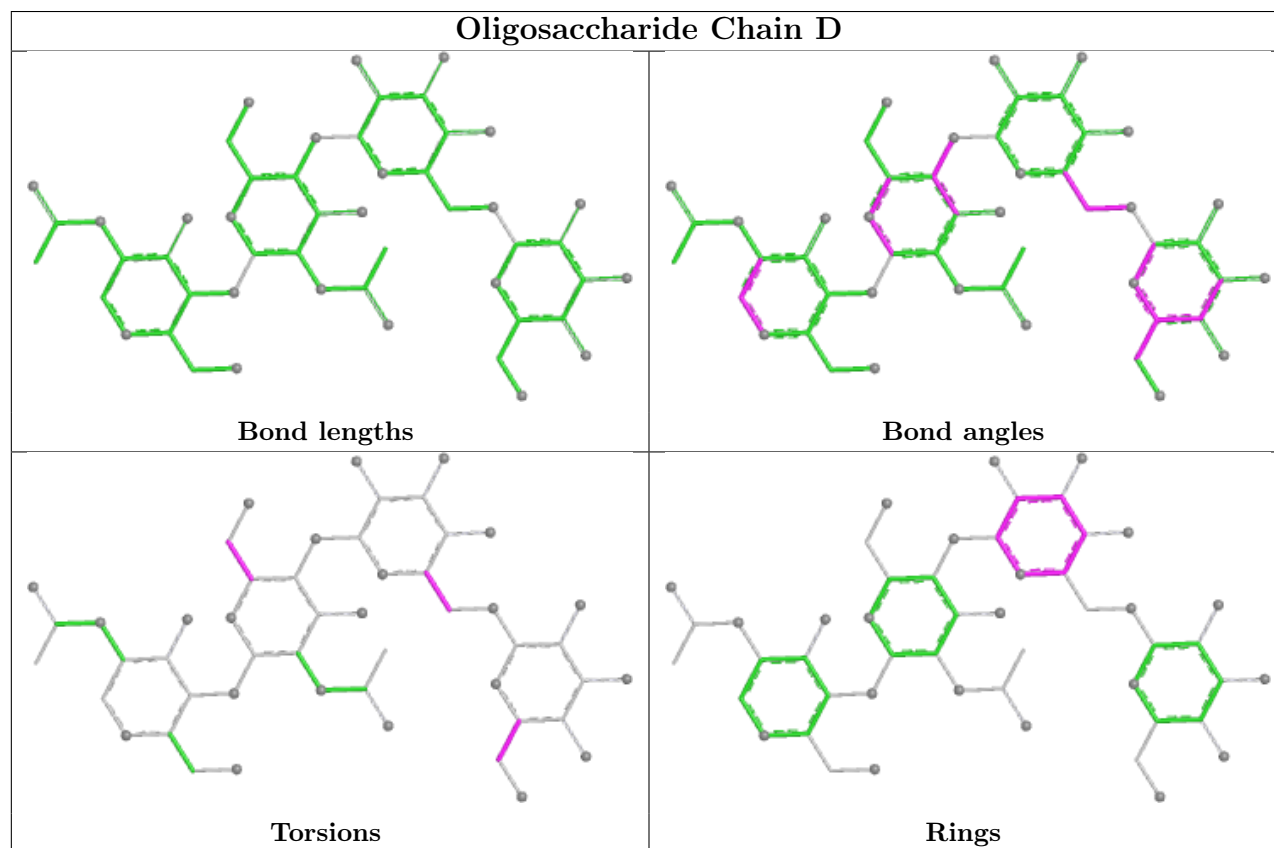
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	4	MAN	1	0
2	D	3	MAN	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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$
4	NAG	C	1154	1	14,14,15	0.85	1 (7%)	17,19,21	1.92	5 (29%)
4	NAG	C	1070	1	14,14,15	0.46	0	17,19,21	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	1154	1	14,14,15	0.68	1 (7%)	17,19,21	1.03	1 (5%)
4	NAG	B	1070	1	14,14,15	0.41	0	17,19,21	0.86	1 (5%)

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
4	NAG	C	1154	1	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	C	1070	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1154	1	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	B	1070	1	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1154	NAG	C1-C2	2.26	1.55	1.52
4	B	1154	NAG	C1-C2	2.03	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1154	NAG	C1-O5-C5	4.83	118.67	112.19
4	C	1154	NAG	C2-N2-C7	3.72	127.88	122.90
4	C	1154	NAG	C4-C3-C2	2.39	114.52	111.02
4	B	1154	NAG	C1-O5-C5	2.30	115.27	112.19
4	C	1154	NAG	O7-C7-N2	2.25	125.95	121.98
4	C	1154	NAG	O7-C7-C8	-2.24	118.07	122.05
4	B	1070	NAG	O5-C1-C2	-2.02	108.17	111.29

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	1154	NAG	C1
4	C	1154	NAG	C1

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1154	NAG	C3-C2-N2-C7
4	C	1154	NAG	O5-C5-C6-O6
4	B	1070	NAG	O5-C5-C6-O6
4	B	1154	NAG	O5-C5-C6-O6
4	B	1154	NAG	C3-C2-N2-C7

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

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	696/954 (72%)	-0.12	10 (1%) 73 51	18, 39, 78, 104	1 (0%)
1	B	802/954 (84%)	-0.21	8 (0%) 79 59	18, 40, 69, 104	2 (0%)
1	C	800/954 (83%)	-0.11	7 (0%) 81 61	12, 41, 73, 103	2 (0%)
All	All	2298/2862 (80%)	-0.15	25 (1%) 78 57	12, 40, 74, 104	5 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	870	SER	3.4
1	C	834	GLN	3.4
1	C	426	PRO	3.2
1	A	757	SER	2.9
1	A	736	CYS	2.8
1	B	432	MET	2.8
1	B	792	SER	2.7
1	C	878	THR	2.7
1	B	909	GLN	2.6
1	C	794	SER	2.5
1	A	718	ASP	2.5
1	C	424	GLU	2.4
1	A	434	ASP	2.4
1	B	424	GLU	2.3
1	A	171	GLU	2.3
1	B	916	GLU	2.2
1	A	172	GLY	2.2
1	A	341	ALA	2.2
1	C	758	ASN	2.2
1	A	750	TYR	2.1
1	B	414	ASN	2.1
1	B	77[A]	TRP	2.1
1	A	721	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	46	PRO	2.1
1	B	117	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

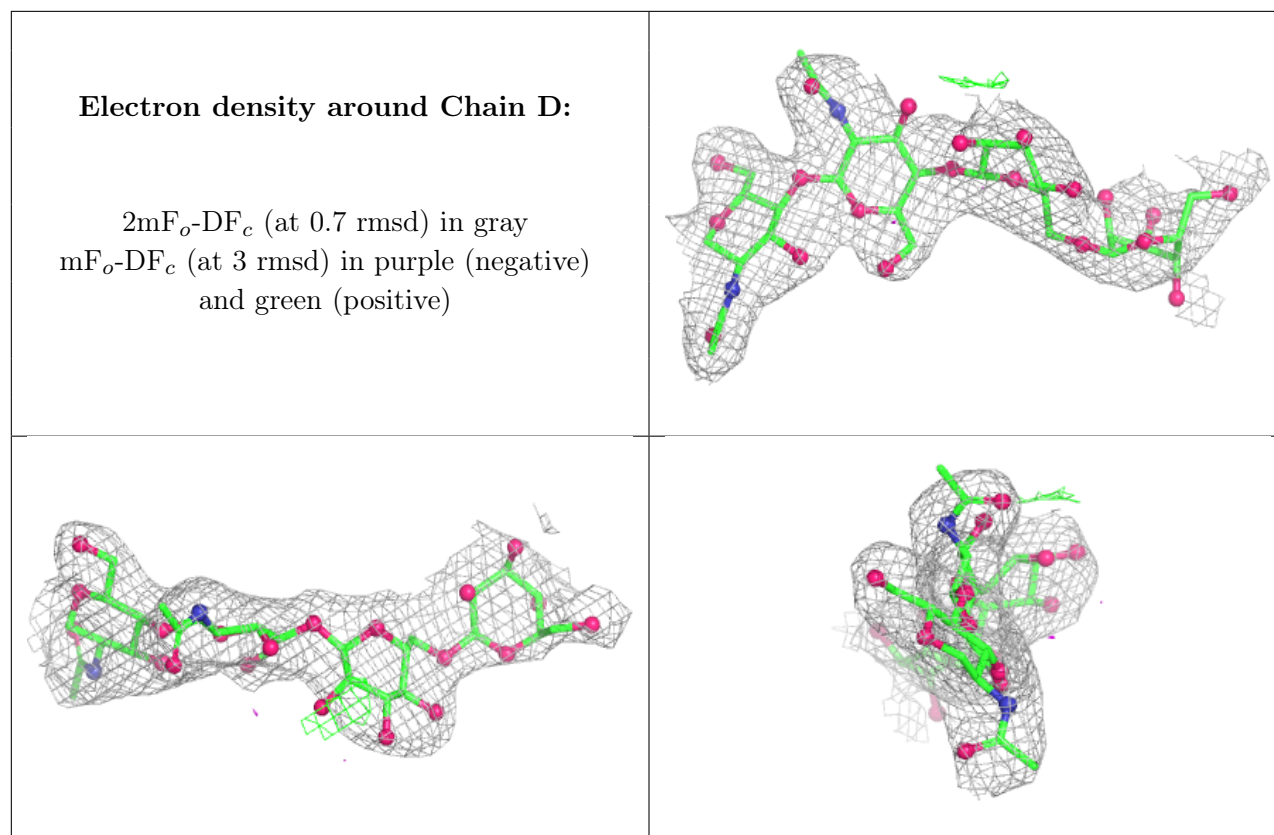
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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($\text{\AA}^2$)	Q<0.9
2	MAN	D	4	11/12	0.81	0.16	66,77,89,92	0
2	MAN	D	3	11/12	0.87	0.10	35,45,58,61	0
2	NAG	D	2	14/15	0.93	0.07	30,46,55,64	0
2	NAG	D	1	14/15	0.95	0.06	14,37,46,50	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
4	NAG	C	1154	14/15	0.49	0.14	98,107,107,110	0
4	NAG	B	1154	14/15	0.65	0.15	80,94,104,105	0
4	NAG	B	1070	14/15	0.79	0.12	37,72,96,97	0
4	NAG	C	1070	14/15	0.88	0.11	80,88,97,103	0
3	ZN	C	5000	1/1	0.99	0.01	31,31,31,31	0
3	ZN	B	5000	1/1	1.00	0.02	25,25,25,25	0
3	ZN	A	5000	1/1	1.00	0.03	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.