



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 11:14 pm GMT

PDB ID : 4AX7
Title : Hypocrea jecorina Cel6A D221A mutant soaked with 4-Methylumbelliferyl-beta-D-cellobioside
Authors : Wu, M.; Nerinckx, W.; Piens, K.; Ishida, T.; Hansson, H.; Stahlberg, J.; Sandgren, M.
Deposited on : 2012-06-11
Resolution : 1.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

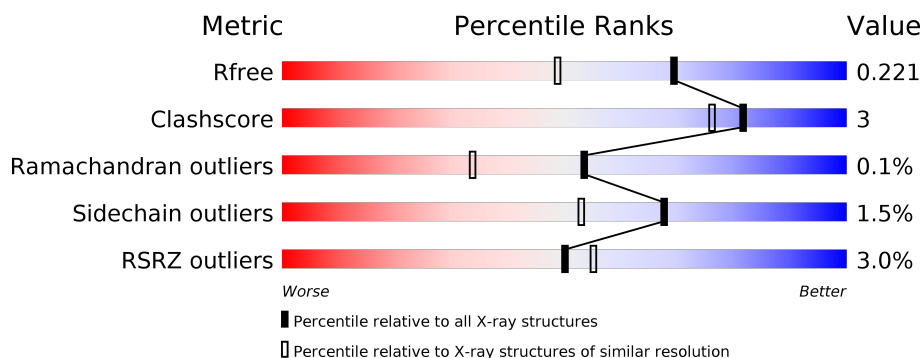
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	3793 (1.70-1.70)
Clashscore	122126	4167 (1.70-1.70)
Ramachandran outliers	120053	4100 (1.70-1.70)
Sidechain outliers	120020	4100 (1.70-1.70)
RSRZ outliers	108989	3718 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	363	<div> <div>2%</div> <div> <div></div> <div>94%</div> <div>5% •</div> </div> </div>
1	B	363	<div> <div>4%</div> <div> <div></div> <div>93%</div> <div>6% •</div> </div> </div>
1	C	363	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>7%</div> </div> </div>
1	D	363	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>9% ••</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	D	502	X	-	-	-
5	BGC	C	603	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12750 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.

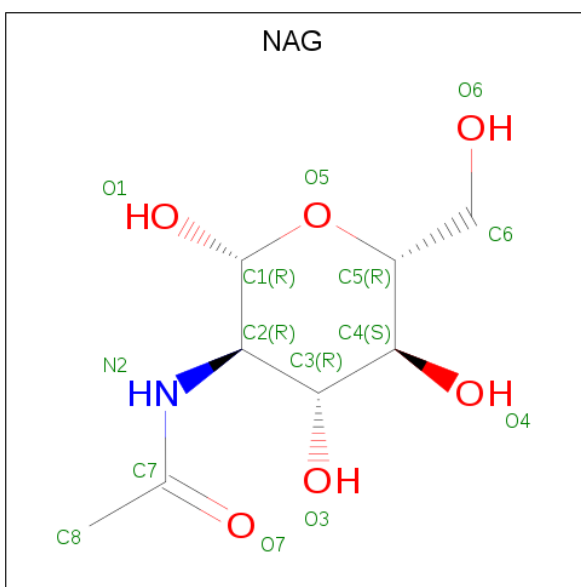
- Molecule 1 is a protein called EXOGLUCANASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	2	0
			2758	1750	466	532	10			
1	B	360	Total	C	N	O	S	0	3	0
			2740	1740	462	528	10			
1	C	363	Total	C	N	O	S	0	3	0
			2764	1755	466	533	10			
1	D	360	Total	C	N	O	S	0	3	0
			2737	1738	461	528	10			

There are 4 discrepancies between the modelled and reference sequences:

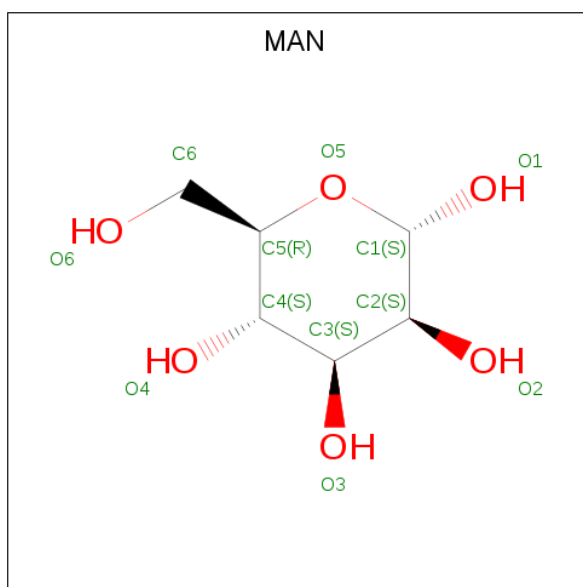
Chain	Residue	Modelled	Actual	Comment	Reference
A	221	ALA	ASP	engineered mutation	UNP P07987
B	221	ALA	ASP	engineered mutation	UNP P07987
C	221	ALA	ASP	engineered mutation	UNP P07987
D	221	ALA	ASP	engineered mutation	UNP P07987

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



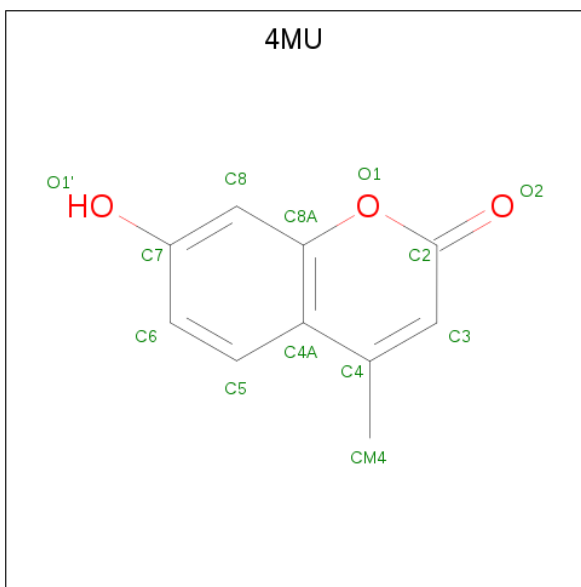
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

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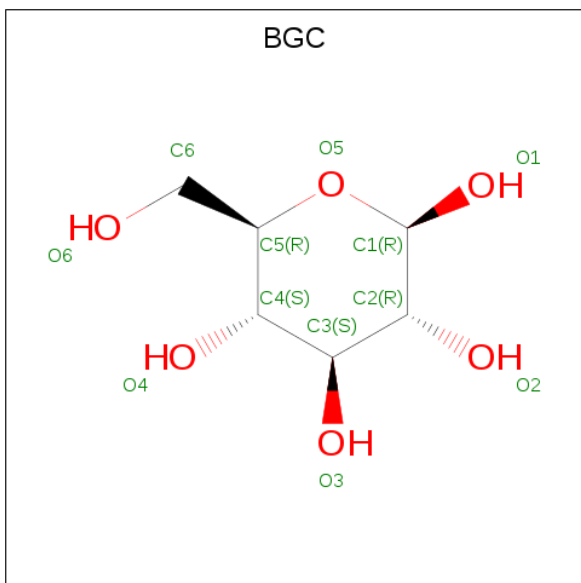
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			11	6	5		
3	C	1	Total	C	O	0	0
			11	6	5		
3	C	1	Total	C	O	0	0
			11	6	5		
3	C	1	Total	C	O	0	0
			11	6	5		
3	C	1	Total	C	O	0	0
			11	6	5		
3	D	1	Total	C	O	0	0
			11	6	5		
3	D	1	Total	C	O	0	0
			11	6	5		
3	D	1	Total	C	O	0	0
			11	6	5		
3	D	1	Total	C	O	0	0
			11	6	5		
3	D	1	Total	C	O	0	0
			11	6	5		
3	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is 7-hydroxy-4-methyl-2H-chromen-2-one (three-letter code: 4MU) (formula: C₁₀H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	10	3		
4	B	1	Total	C	O	0	0
			13	10	3		
4	C	1	Total	C	O	0	0
			13	10	3		
4	D	1	Total	C	O	0	0
			13	10	3		

- Molecule 5 is BETA-D-GLUCOSE (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	C	1	Total C O 11 6 5	0	0
5	C	1	Total C O 11 6 5	0	0
5	C	1	Total C O 11 6 5	0	0
5	C	1	Total C O 11 6 5	0	0
5	D	1	Total C O 11 6 5	0	0
5	D	1	Total C O 11 6 5	0	0

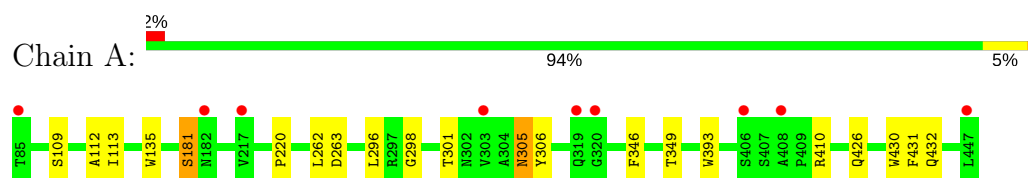
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	329	Total O 329 329	0	0
6	B	287	Total O 287 287	0	0
6	C	285	Total O 285 285	0	0
6	D	257	Total O 257 257	0	0

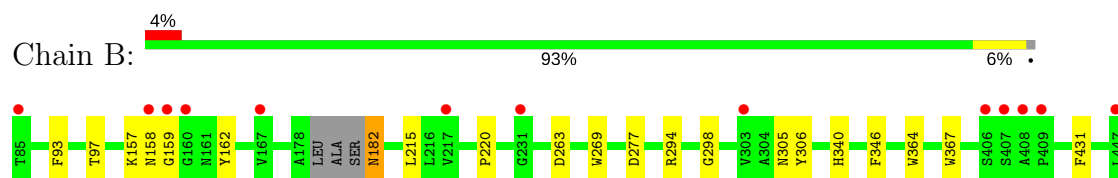
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

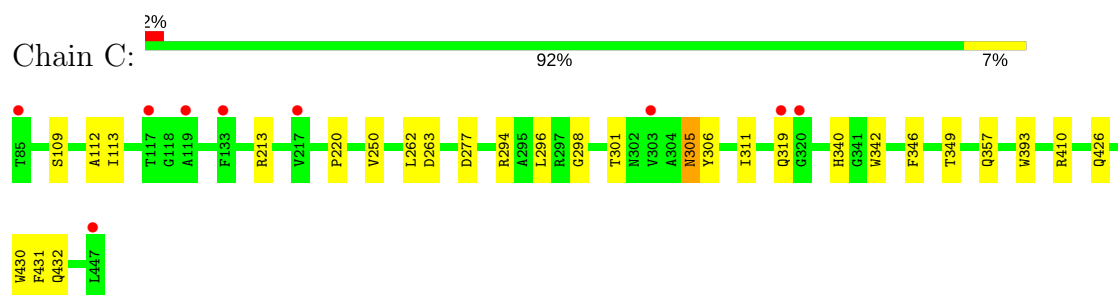
• Molecule 1: EXOGLUCANASE 2



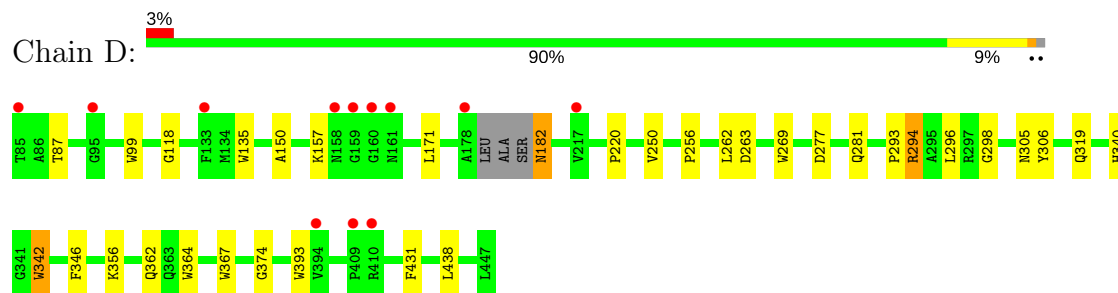
• Molecule 1: EXOGLUCANASE 2



• Molecule 1: EXOGLUCANASE 2



• Molecule 1: EXOGLUCANASE 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	48.82Å 74.68Å 93.30Å 103.97° 103.43° 90.00°	Depositor
Resolution (Å)	87.90 – 1.70 29.86 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.4 (87.90-1.70) 96.4 (29.86-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.61 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.189 , 0.221 0.188 , 0.221	Depositor DCC
R_{free} test set	6627 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	15.0	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12750	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.07 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4432e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 4MU, BGC, NAG, MAN

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	1/2834 (0.0%)	0.55	0/3887
1	B	0.52	3/2821 (0.1%)	0.54	0/3866
1	C	0.52	2/2840 (0.1%)	0.54	0/3894
1	D	0.53	7/2818 (0.2%)	0.54	0/3862
All	All	0.52	13/11313 (0.1%)	0.55	0/15509

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	364	TRP	CD2-CE2	5.24	1.47	1.41
1	B	269	TRP	CD2-CE2	5.22	1.47	1.41
1	D	269	TRP	CD2-CE2	5.17	1.47	1.41
1	D	364	TRP	CD2-CE2	5.16	1.47	1.41
1	D	135	TRP	CD2-CE2	5.11	1.47	1.41
1	C	393	TRP	CD2-CE2	5.10	1.47	1.41
1	A	393	TRP	CD2-CE2	5.10	1.47	1.41
1	C	342	TRP	CD2-CE2	5.08	1.47	1.41
1	D	342	TRP	CD2-CE2	5.07	1.47	1.41
1	B	367	TRP	CD2-CE2	5.06	1.47	1.41
1	D	99	TRP	CD2-CE2	5.06	1.47	1.41
1	D	367	TRP	CD2-CE2	5.05	1.47	1.41
1	D	393	TRP	CD2-CE2	5.05	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2758	0	2618	14	0
1	B	2740	0	2604	10	0
1	C	2764	0	2628	15	0
1	D	2737	0	2601	19	0
2	A	28	0	26	0	0
2	B	28	0	26	0	0
2	C	28	0	26	0	0
2	D	28	0	26	0	0
3	A	77	0	70	1	0
3	B	77	0	70	0	0
3	C	66	0	60	0	0
3	D	77	0	70	1	0
4	A	13	0	7	1	0
4	B	13	0	7	1	0
4	C	13	0	7	0	0
4	D	13	0	7	0	0
5	A	44	0	37	3	0
5	B	22	0	19	0	0
5	C	44	0	37	1	0
5	D	22	0	19	0	0
6	A	329	0	0	1	0
6	B	287	0	0	1	0
6	C	285	0	0	1	0
6	D	257	0	0	4	0
All	All	12750	0	10965	62	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 3.

All (62) 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:305:ASN:HD22	1:A:306:TYR:H	1.21	0.87
1:B:305:ASN:HD22	1:B:306:TYR:H	1.25	0.83
1:D:305:ASN:HD22	1:D:306:TYR:H	1.25	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:ASN:HD22	1:C:306:TYR:H	1.29	0.81
1:B:305:ASN:ND2	1:B:306:TYR:H	1.84	0.76
1:C:301:THR:OG1	1:C:349[B]:THR:HG22	1.88	0.74
5:A:603:BGC:H3	6:A:2112:HOH:O	1.89	0.73
1:A:301:THR:OG1	1:A:349[B]:THR:HG22	1.89	0.71
1:D:305:ASN:ND2	1:D:306:TYR:H	1.91	0.69
1:A:305:ASN:ND2	1:A:306:TYR:H	1.93	0.66
1:D:356:LYS:HE3	6:D:2192:HOH:O	1.97	0.65
1:B:277:ASP:OD1	1:B:340:HIS:HE1	1.84	0.60
3:A:509:MAN:H62	1:D:150:ALA:HB1	1.84	0.59
1:D:182:ASN:HB2	6:D:2071:HOH:O	2.03	0.57
1:C:298:GLY:HA3	1:C:346:PHE:O	2.06	0.56
1:C:410:ARG:HH21	1:C:426:GLN:HE21	1.55	0.55
1:C:305:ASN:ND2	1:C:306:TYR:H	2.02	0.54
1:D:118:GLY:O	3:D:509:MAN:H2	2.07	0.54
1:A:410:ARG:HH21	1:A:426:GLN:HE21	1.55	0.53
1:C:277:ASP:OD1	1:C:340:HIS:HE1	1.92	0.53
1:A:109:SER:HA	1:A:113:ILE:HD12	1.91	0.52
1:C:430:TRP:HE1	1:C:432:GLN:HE21	1.58	0.50
1:D:277:ASP:OD1	1:D:340:HIS:HE1	1.95	0.50
1:B:220:PRO:HA	1:B:263:ASP:CG	2.33	0.49
1:C:430:TRP:HE1	1:C:432:GLN:NE2	2.11	0.49
1:C:262:LEU:HG	1:C:296:LEU:HD11	1.94	0.49
1:B:182:ASN:HB2	6:B:2086:HOH:O	2.13	0.48
1:D:157:LYS:HG3	6:D:2060:HOH:O	2.14	0.47
1:C:250:VAL:HG11	1:C:296:LEU:HD22	1.95	0.47
5:C:603:BGC:H3	6:C:2084:HOH:O	2.15	0.47
1:C:220:PRO:HA	1:C:263:ASP:CG	2.35	0.47
1:A:220:PRO:HA	1:A:263:ASP:CG	2.36	0.46
1:A:430:TRP:HE1	1:A:432:GLN:HE21	1.62	0.46
1:A:430:TRP:HE1	1:A:432:GLN:NE2	2.14	0.45
1:B:93:PHE:CE2	1:B:215:LEU:HD13	2.52	0.45
1:D:220:PRO:HA	1:D:263:ASP:CG	2.38	0.44
1:B:220:PRO:HA	1:B:263:ASP:CB	2.48	0.44
1:D:277:ASP:O	1:D:281:GLN:HG3	2.17	0.44
1:A:262:LEU:HG	1:A:296:LEU:HD11	1.99	0.44
1:D:298:GLY:HA3	1:D:346:PHE:O	2.17	0.44
1:A:112:ALA:HA	1:A:432:GLN:HE22	1.83	0.44
1:C:109:SER:HA	1:C:113:ILE:HD12	2.00	0.43
1:D:250:VAL:CG1	1:D:293:PRO:HG2	2.48	0.43
1:D:294:ARG:HD2	6:D:2136:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:THR:O	1:B:162:TYR:HA	2.18	0.43
1:A:298:GLY:HA3	1:A:346:PHE:O	2.19	0.43
4:A:600:4MU:HM4	4:A:600:4MU:H5	1.81	0.42
1:C:311:ILE:HG21	1:C:357:GLN:HG3	2.01	0.42
1:C:220:PRO:HA	1:C:263:ASP:CB	2.49	0.42
1:A:135:TRP:CE3	5:A:604:BGC:H5	2.55	0.42
1:D:220:PRO:HA	1:D:263:ASP:CB	2.50	0.42
1:B:157:LYS:C	1:B:159:GLY:H	2.23	0.41
1:C:112:ALA:HA	1:C:432:GLN:HE22	1.84	0.41
4:B:600:4MU:H5	4:B:600:4MU:HM4	1.92	0.41
1:B:298:GLY:HA3	1:B:346:PHE:O	2.20	0.41
1:A:220:PRO:HA	1:A:263:ASP:CB	2.50	0.41
1:D:250:VAL:HG12	1:D:293:PRO:HG2	2.04	0.41
1:D:87:THR:HG22	1:D:256:PRO:HB2	2.03	0.40
1:D:262:LEU:HG	1:D:296:LEU:HD11	2.02	0.40
1:A:181:SER:OG	5:A:604:BGC:O2	2.21	0.40
1:D:298:GLY:HA2	1:D:342:TRP:CZ2	2.57	0.40
1:D:374:GLY:HA2	1:D:438:LEU:HA	2.02	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	363/363 (100%)	353 (97%)	10 (3%)	0	100	100
1	B	359/363 (99%)	343 (96%)	15 (4%)	1 (0%)	43	25
1	C	364/363 (100%)	351 (96%)	13 (4%)	0	100	100
1	D	359/363 (99%)	345 (96%)	14 (4%)	0	100	100
All	All	1445/1452 (100%)	1392 (96%)	52 (4%)	1 (0%)	53	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	158	ASN

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	285/283 (101%)	282 (99%)	3 (1%)	76	65
1	B	283/283 (100%)	280 (99%)	3 (1%)	76	65
1	C	285/283 (101%)	280 (98%)	5 (2%)	62	45
1	D	283/283 (100%)	277 (98%)	6 (2%)	56	38
All	All	1136/1132 (100%)	1119 (98%)	17 (2%)	67	53

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	181	SER
1	A	305	ASN
1	A	431	PHE
1	B	182	ASN
1	B	294	ARG
1	B	431	PHE
1	C	213	ARG
1	C	294	ARG
1	C	305	ASN
1	C	319	GLN
1	C	431	PHE
1	D	171	LEU
1	D	182	ASN
1	D	294	ARG
1	D	319	GLN
1	D	362	GLN
1	D	431	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	ASN
1	A	281	GLN
1	A	305	ASN
1	A	426	GLN
1	A	432	GLN
1	A	441	ASN
1	B	158	ASN
1	B	285	ASN
1	B	305	ASN
1	B	340	HIS
1	B	382	ASN
1	C	161	ASN
1	C	182	ASN
1	C	204	GLN
1	C	285	ASN
1	C	305	ASN
1	C	319	GLN
1	C	363	GLN
1	C	426	GLN
1	C	432	GLN
1	C	441	ASN
1	D	158	ASN
1	D	285	ASN
1	D	305	ASN
1	D	319	GLN
1	D	340	HIS
1	D	426	GLN
1	D	441	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

51 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	501	1	14,14,15	0.54	0	17,19,21	0.80	0
2	NAG	A	502	1	14,14,15	0.48	0	17,19,21	0.80	1 (5%)
3	MAN	A	503	1	11,11,12	0.63	0	15,15,17	1.16	2 (13%)
3	MAN	A	504	1	11,11,12	0.58	0	15,15,17	1.10	2 (13%)
3	MAN	A	505	1	11,11,12	0.61	0	15,15,17	0.92	1 (6%)
3	MAN	A	506	1	11,11,12	0.62	0	15,15,17	0.67	0
3	MAN	A	507	1	11,11,12	0.51	0	15,15,17	1.06	1 (6%)
3	MAN	A	508	1	11,11,12	0.54	0	15,15,17	0.75	1 (6%)
3	MAN	A	509	1	11,11,12	0.69	0	15,15,17	1.44	3 (20%)
4	4MU	A	600	5	13,14,14	1.81	1 (7%)	15,20,20	1.49	2 (13%)
5	BGC	A	601	5,4	11,11,12	0.60	0	15,15,17	0.70	0
5	BGC	A	602	5	11,11,12	1.13	1 (9%)	15,15,17	0.66	0
5	BGC	A	603	5	11,11,12	1.01	0	15,15,17	1.67	3 (20%)
5	BGC	A	604	5	11,11,12	1.02	1 (9%)	15,15,17	1.29	3 (20%)
2	NAG	B	501	1	14,14,15	0.50	0	17,19,21	0.90	0
2	NAG	B	502	1	14,14,15	0.53	0	17,19,21	0.93	2 (11%)
3	MAN	B	503	1	11,11,12	0.52	0	15,15,17	0.93	1 (6%)
3	MAN	B	504	1	11,11,12	0.62	0	15,15,17	1.02	2 (13%)
3	MAN	B	505	1	11,11,12	0.67	0	15,15,17	1.17	2 (13%)
3	MAN	B	506	1	11,11,12	0.57	0	15,15,17	0.96	1 (6%)
3	MAN	B	507	1	11,11,12	0.54	0	15,15,17	0.96	2 (13%)
3	MAN	B	508	1	11,11,12	0.54	0	15,15,17	1.10	2 (13%)
3	MAN	B	509	1	11,11,12	0.49	0	15,15,17	1.03	1 (6%)
4	4MU	B	600	5	13,14,14	1.02	0	15,20,20	1.39	3 (20%)
5	BGC	B	601	5,4	11,11,12	0.42	0	15,15,17	0.85	0
5	BGC	B	602	5	11,11,12	0.62	0	15,15,17	0.50	0
2	NAG	C	501	1	14,14,15	0.61	0	17,19,21	1.38	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	502	1	14,14,15	0.55	0	17,19,21	0.81	0
3	MAN	C	504	1	11,11,12	0.60	0	15,15,17	0.96	1 (6%)
3	MAN	C	505	1	11,11,12	0.62	0	15,15,17	1.09	1 (6%)
3	MAN	C	506	1	11,11,12	0.65	0	15,15,17	1.10	0
3	MAN	C	507	1	11,11,12	0.57	0	15,15,17	1.05	1 (6%)
3	MAN	C	508	1	11,11,12	0.67	0	15,15,17	1.40	3 (20%)
3	MAN	C	509	1	11,11,12	0.61	0	15,15,17	1.05	1 (6%)
4	4MU	C	600	5	13,14,14	1.86	1 (7%)	15,20,20	1.76	3 (20%)
5	BGC	C	601	5,4	11,11,12	0.60	0	15,15,17	0.79	0
5	BGC	C	602	5	11,11,12	1.34	2 (18%)	15,15,17	0.75	0
5	BGC	C	603	5	11,11,12	0.80	0	15,15,17	1.76	4 (26%)
5	BGC	C	604	5	11,11,12	0.52	0	15,15,17	0.89	0
2	NAG	D	501	1	14,14,15	0.52	0	17,19,21	0.64	0
2	NAG	D	502	1	14,14,15	1.04	1 (7%)	17,19,21	2.58	3 (17%)
3	MAN	D	503	1	11,11,12	0.59	0	15,15,17	0.74	0
3	MAN	D	504	1	11,11,12	0.54	0	15,15,17	0.75	1 (6%)
3	MAN	D	505	1	11,11,12	0.60	0	15,15,17	1.10	1 (6%)
3	MAN	D	506	1	11,11,12	0.61	0	15,15,17	0.94	2 (13%)
3	MAN	D	507	1	11,11,12	0.59	0	15,15,17	1.18	2 (13%)
3	MAN	D	508	1	11,11,12	0.51	0	15,15,17	1.09	1 (6%)
3	MAN	D	509	1	11,11,12	0.53	0	15,15,17	1.05	1 (6%)
4	4MU	D	600	5	13,14,14	0.96	0	15,20,20	1.52	4 (26%)
5	BGC	D	601	5,4	11,11,12	0.62	0	15,15,17	0.70	0
5	BGC	D	602	5	11,11,12	0.69	0	15,15,17	0.64	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	NAG	A	501	1	-	0/6/23/26	0/1/1/1
2	NAG	A	502	1	-	0/6/23/26	0/1/1/1
3	MAN	A	503	1	-	0/2/19/22	0/1/1/1
3	MAN	A	504	1	-	0/2/19/22	0/1/1/1
3	MAN	A	505	1	-	0/2/19/22	0/1/1/1
3	MAN	A	506	1	-	0/2/19/22	0/1/1/1
3	MAN	A	507	1	-	0/2/19/22	0/1/1/1
3	MAN	A	508	1	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	A	509	1	-	0/2/19/22	0/1/1/1
4	4MU	A	600	5	-	0/0/0/0	0/2/2/2
5	BGC	A	601	5,4	-	0/2/19/22	0/1/1/1
5	BGC	A	602	5	-	0/2/19/22	0/1/1/1
5	BGC	A	603	5	-	0/2/19/22	0/1/1/1
5	BGC	A	604	5	-	0/2/19/22	0/1/1/1
2	NAG	B	501	1	-	0/6/23/26	0/1/1/1
2	NAG	B	502	1	-	0/6/23/26	0/1/1/1
3	MAN	B	503	1	-	0/2/19/22	0/1/1/1
3	MAN	B	504	1	-	0/2/19/22	0/1/1/1
3	MAN	B	505	1	-	0/2/19/22	0/1/1/1
3	MAN	B	506	1	-	0/2/19/22	0/1/1/1
3	MAN	B	507	1	-	0/2/19/22	0/1/1/1
3	MAN	B	508	1	-	0/2/19/22	0/1/1/1
3	MAN	B	509	1	-	0/2/19/22	0/1/1/1
4	4MU	B	600	5	-	0/0/0/0	0/2/2/2
5	BGC	B	601	5,4	-	0/2/19/22	0/1/1/1
5	BGC	B	602	5	-	0/2/19/22	0/1/1/1
2	NAG	C	501	1	-	0/6/23/26	0/1/1/1
2	NAG	C	502	1	-	0/6/23/26	0/1/1/1
3	MAN	C	504	1	-	0/2/19/22	0/1/1/1
3	MAN	C	505	1	-	0/2/19/22	0/1/1/1
3	MAN	C	506	1	-	0/2/19/22	0/1/1/1
3	MAN	C	507	1	-	0/2/19/22	0/1/1/1
3	MAN	C	508	1	-	0/2/19/22	0/1/1/1
3	MAN	C	509	1	-	0/2/19/22	0/1/1/1
4	4MU	C	600	5	-	0/0/0/0	0/2/2/2
5	BGC	C	601	5,4	-	0/2/19/22	0/1/1/1
5	BGC	C	602	5	-	0/2/19/22	0/1/1/1
5	BGC	C	603	5	-	0/2/19/22	0/1/1/1
5	BGC	C	604	5	-	0/2/19/22	0/1/1/1
2	NAG	D	501	1	-	0/6/23/26	0/1/1/1
2	NAG	D	502	1	1/1/5/7	0/6/23/26	0/1/1/1
3	MAN	D	503	1	-	0/2/19/22	0/1/1/1
3	MAN	D	504	1	-	0/2/19/22	0/1/1/1
3	MAN	D	505	1	-	0/2/19/22	0/1/1/1
3	MAN	D	506	1	-	0/2/19/22	0/1/1/1
3	MAN	D	507	1	-	0/2/19/22	0/1/1/1
3	MAN	D	508	1	-	0/2/19/22	0/1/1/1
3	MAN	D	509	1	-	0/2/19/22	0/1/1/1
4	4MU	D	600	5	-	0/0/0/0	0/2/2/2
5	BGC	D	601	5,4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BGC	D	602	5	-	0/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	600	4MU	CM4-C4	-5.86	1.40	1.51
4	A	600	4MU	CM4-C4	-5.76	1.40	1.51
5	A	604	BGC	O5-C5	2.10	1.47	1.43
5	C	602	BGC	C2-C3	2.18	1.55	1.52
5	C	602	BGC	O4-C4	2.34	1.48	1.43
5	A	602	BGC	O4-C4	2.46	1.49	1.43
2	D	502	NAG	C1-C2	3.55	1.57	1.52

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	502	NAG	O5-C1-C2	-6.94	101.94	111.52
5	A	604	BGC	O5-C1-C2	-2.95	106.19	110.78
3	C	508	MAN	C1-O5-C5	-2.67	108.51	112.19
5	C	603	BGC	O4-C4-C3	-2.49	104.53	110.34
5	A	603	BGC	O2-C2-C3	-2.33	105.64	110.19
4	C	600	4MU	C8-C8A-C4A	-2.29	120.52	123.05
4	B	600	4MU	C8-C8A-C4A	-2.23	120.58	123.05
5	C	603	BGC	O2-C2-C3	-2.21	105.88	110.19
4	D	600	4MU	C8-C8A-C4A	-2.10	120.72	123.05
2	B	502	NAG	C2-N2-C7	-2.08	119.91	122.94
3	D	506	MAN	O5-C1-C2	-2.07	107.56	110.78
3	C	508	MAN	C1-C2-C3	-2.05	107.06	109.66
2	B	502	NAG	C1-C2-N2	-2.03	107.02	110.49
5	A	604	BGC	C1-O5-C5	-2.01	109.43	112.19
4	D	600	4MU	C4-C4A-C8A	2.03	119.30	118.06
3	D	507	MAN	C1-C2-C3	2.04	112.23	109.66
3	A	504	MAN	C3-C4-C5	2.05	113.91	110.24
3	B	508	MAN	C1-C2-C3	2.05	112.25	109.66
3	D	504	MAN	C1-O5-C5	2.07	115.03	112.19
3	B	507	MAN	O5-C5-C6	2.10	110.48	107.15
2	A	502	NAG	C1-O5-C5	2.10	115.08	112.19
3	B	504	MAN	C1-C2-C3	2.12	112.34	109.66
3	B	504	MAN	C1-O5-C5	2.12	115.11	112.19
3	A	508	MAN	C1-O5-C5	2.13	115.12	112.19
3	B	505	MAN	C1-C2-C3	2.15	112.38	109.66
3	A	509	MAN	O5-C5-C6	2.17	110.59	107.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	MAN	O5-C5-C6	2.19	110.61	107.15
3	D	509	MAN	O5-C5-C6	2.22	110.65	107.15
5	A	604	BGC	O5-C5-C6	2.22	110.66	107.15
4	B	600	4MU	C5-C4A-C8A	2.22	119.07	116.50
4	A	600	4MU	O1-C8A-C8	2.24	118.68	116.03
4	B	600	4MU	O1-C2-C3	2.24	122.18	119.28
2	D	502	NAG	O5-C5-C6	2.27	110.75	107.15
3	D	506	MAN	C1-O5-C5	2.29	115.34	112.19
3	A	504	MAN	C1-O5-C5	2.37	115.44	112.19
3	B	507	MAN	C1-O5-C5	2.41	115.51	112.19
3	C	509	MAN	C1-C2-C3	2.44	112.75	109.66
3	C	504	MAN	O5-C5-C6	2.51	111.12	107.15
3	A	505	MAN	C1-O5-C5	2.56	115.70	112.19
5	A	603	BGC	O5-C5-C6	2.57	111.21	107.15
3	B	509	MAN	C1-O5-C5	2.62	115.79	112.19
4	D	600	4MU	C5-C4A-C8A	2.67	119.59	116.50
4	D	600	4MU	O1-C2-C3	2.72	122.80	119.28
3	A	509	MAN	C2-C3-C4	2.75	115.64	110.87
3	A	503	MAN	C1-C2-C3	2.78	113.18	109.66
2	C	501	NAG	C4-C3-C2	2.82	115.16	111.02
4	A	600	4MU	C4-C4A-C8A	2.85	119.81	118.06
3	B	503	MAN	C1-O5-C5	2.87	116.13	112.19
5	C	603	BGC	O5-C5-C6	2.88	111.71	107.15
2	C	501	NAG	C2-N2-C7	2.97	127.27	122.94
3	B	505	MAN	C1-O5-C5	3.04	116.37	112.19
3	B	506	MAN	C1-O5-C5	3.05	116.38	112.19
3	B	508	MAN	C1-O5-C5	3.10	116.45	112.19
4	C	600	4MU	O1-C8A-C8	3.10	119.71	116.03
3	D	505	MAN	C1-O5-C5	3.12	116.48	112.19
3	C	507	MAN	C1-O5-C5	3.15	116.52	112.19
3	D	508	MAN	C1-O5-C5	3.20	116.59	112.19
3	D	507	MAN	C1-O5-C5	3.20	116.59	112.19
3	C	505	MAN	C1-O5-C5	3.30	116.73	112.19
3	A	507	MAN	C1-O5-C5	3.39	116.86	112.19
3	C	508	MAN	O5-C5-C6	3.49	112.68	107.15
4	C	600	4MU	C4-C4A-C8A	3.60	120.27	118.06
3	A	509	MAN	C1-C2-C3	3.88	114.57	109.66
5	A	603	BGC	C1-O5-C5	4.02	117.72	112.19
5	C	603	BGC	C1-O5-C5	4.64	118.57	112.19
2	D	502	NAG	C1-O5-C5	7.05	121.88	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	502	NAG	C1

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	509	MAN	1	0
4	A	600	4MU	1	0
5	A	603	BGC	1	0
5	A	604	BGC	2	0
4	B	600	4MU	1	0
5	C	603	BGC	1	0
3	D	509	MAN	1	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	363/363 (100%)	-0.06	9 (2%) 57 62	7, 14, 23, 29	1 (0%)
1	B	360/363 (99%)	0.05	13 (3%) 42 48	7, 15, 27, 43	0
1	C	363/363 (100%)	0.01	9 (2%) 57 62	9, 16, 24, 37	0
1	D	360/363 (99%)	0.14	12 (3%) 46 51	10, 18, 27, 44	1 (0%)
All	All	1446/1452 (99%)	0.04	43 (2%) 50 55	7, 15, 26, 44	2 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	159	GLY	7.2
1	C	85	THR	5.6
1	D	160	GLY	5.0
1	D	158	ASN	4.8
1	B	447	LEU	4.8
1	D	409	PRO	4.6
1	D	85	THR	4.5
1	D	178	ALA	3.9
1	B	408	ALA	3.4
1	B	160	GLY	3.2
1	B	158	ASN	3.0
1	C	447	LEU	2.8
1	C	303	VAL	2.8
1	A	320	GLY	2.7
1	D	161	ASN	2.7
1	D	133	PHE	2.6
1	C	117	THR	2.6
1	A	303	VAL	2.4
1	B	159	GLY	2.4
1	A	217	VAL	2.4
1	B	407	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	319	GLN	2.4
1	C	119	ALA	2.3
1	B	406	SER	2.3
1	C	319	GLN	2.3
1	D	95	GLY	2.3
1	A	406	SER	2.3
1	D	410	ARG	2.3
1	B	231	GLY	2.2
1	C	133	PHE	2.2
1	D	217	VAL	2.2
1	A	182	ASN	2.2
1	A	85	THR	2.2
1	C	320	GLY	2.1
1	B	217	VAL	2.1
1	D	394	VAL	2.1
1	A	408	ALA	2.1
1	B	409	PRO	2.1
1	B	303	VAL	2.1
1	B	85	THR	2.1
1	C	217	VAL	2.1
1	A	447	LEU	2.1
1	B	167	VAL	2.0

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](#)

There are no carbohydrates in this entry.

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(Å ²)	Q<0.9
2	NAG	C	501	14/15	0.60	0.31	33,36,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	B	501	14/15	0.63	0.30	39,42,43,44	0
5	BGC	A	603	11/12	0.69	0.35	17,18,19,21	10
3	MAN	B	503	11/12	0.70	0.28	33,38,39,41	0
3	MAN	A	503	11/12	0.72	0.25	31,35,38,39	0
3	MAN	B	509	11/12	0.73	0.29	37,39,41,42	0
5	BGC	C	603	11/12	0.74	0.41	18,19,20,20	10
3	MAN	A	509	11/12	0.74	0.24	30,32,33,33	0
2	NAG	D	501	14/15	0.74	0.24	38,40,41,43	0
3	MAN	D	503	11/12	0.75	0.27	36,39,40,41	0
3	MAN	C	509	11/12	0.76	0.18	33,34,36,36	0
5	BGC	A	604	11/12	0.77	0.15	17,21,22,22	0
3	MAN	D	504	11/12	0.78	0.24	32,35,37,37	0
3	MAN	D	507	11/12	0.80	0.18	26,30,31,32	0
3	MAN	D	509	11/12	0.81	0.21	26,30,32,33	0
3	MAN	B	504	11/12	0.82	0.22	26,29,32,32	0
3	MAN	C	506	11/12	0.83	0.12	22,23,24,27	0
4	4MU	B	600	13/13	0.83	0.17	18,22,25,26	0
4	4MU	C	600	13/13	0.84	0.24	24,29,31,32	0
3	MAN	B	508	11/12	0.84	0.10	29,31,32,32	0
3	MAN	C	507	11/12	0.85	0.12	25,27,29,29	0
3	MAN	A	505	11/12	0.85	0.14	22,24,27,27	0
3	MAN	B	507	11/12	0.86	0.17	27,29,30,32	0
3	MAN	A	504	11/12	0.86	0.16	22,26,29,30	0
3	MAN	D	505	11/12	0.87	0.12	23,26,27,28	0
3	MAN	C	504	11/12	0.87	0.21	28,31,32,34	0
3	MAN	A	507	11/12	0.87	0.14	25,28,30,30	0
3	MAN	C	505	11/12	0.88	0.11	21,23,24,25	0
5	BGC	C	604	11/12	0.88	0.13	16,20,21,21	0
3	MAN	A	506	11/12	0.88	0.12	20,22,24,24	0
2	NAG	D	502	14/15	0.88	0.10	18,20,22,24	0
3	MAN	A	508	11/12	0.88	0.10	24,25,27,28	0
2	NAG	C	502	14/15	0.89	0.10	19,21,22,24	0
3	MAN	B	505	11/12	0.89	0.12	22,23,24,25	0
2	NAG	A	501	14/15	0.89	0.12	28,29,32,33	0
4	4MU	D	600	13/13	0.89	0.13	19,22,24,24	0
5	BGC	C	602	11/12	0.90	0.12	19,20,21,21	0
3	MAN	B	506	11/12	0.90	0.11	21,22,23,25	0
2	NAG	A	502	14/15	0.91	0.11	18,19,21,21	0
4	4MU	A	600	13/13	0.92	0.15	17,21,22,23	0
3	MAN	C	508	11/12	0.93	0.08	21,21,22,23	0
2	NAG	B	502	14/15	0.93	0.09	16,18,19,20	0
5	BGC	D	602	11/12	0.93	0.08	13,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MAN	D	506	11/12	0.94	0.09	18,20,21,23	0
5	BGC	B	601	11/12	0.94	0.08	14,14,16,16	0
3	MAN	D	508	11/12	0.94	0.07	18,19,20,20	0
5	BGC	C	601	11/12	0.94	0.08	17,19,20,21	0
5	BGC	D	601	11/12	0.94	0.08	15,16,18,20	0
5	BGC	A	602	11/12	0.95	0.12	14,15,16,17	0
5	BGC	A	601	11/12	0.96	0.08	14,15,16,17	0
5	BGC	B	602	11/12	0.97	0.08	12,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.