



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 04:53 pm BST

PDB ID : 8PE1
Title : Crystal structure of Gel4 in complex with Nanobody 4
Authors : Macias-Leon, J.; Redrado-Hernandez, S.; Castro-Lopez, J.; Sanz, A.B.; Arias, M.; Farkas, V.; Vincke, C.; Muyldermans, S.; Pardo, J.; Arroyo, J.; Galvez, E.; Hurtado-Guerrero, R.
Deposited on : 2023-06-13
Resolution : 1.90 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

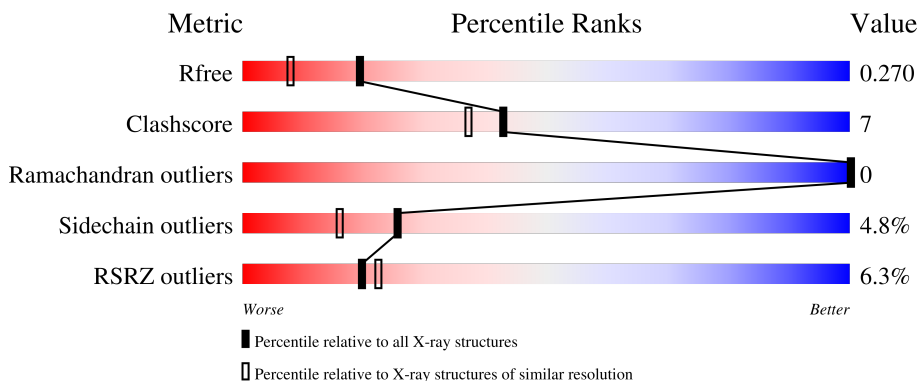
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	458	 4% (poor fit), 84% (0-1 outliers), 10% (2-3 outliers), 6% (4+ outliers), 0% (not modelled)
1	B	458	 5% (poor fit), 89% (0-1 outliers), 8% (2-3 outliers), 2% (4+ outliers), 0% (not modelled)
2	C	124	 9% (poor fit), 81% (0-1 outliers), 17% (2-3 outliers), 3% (4+ outliers), 0% (not modelled)
2	D	124	 15% (poor fit), 79% (0-1 outliers), 18% (2-3 outliers), 0% (4+ outliers), 0% (not modelled)

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
4	MAN	B	508	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9781 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.

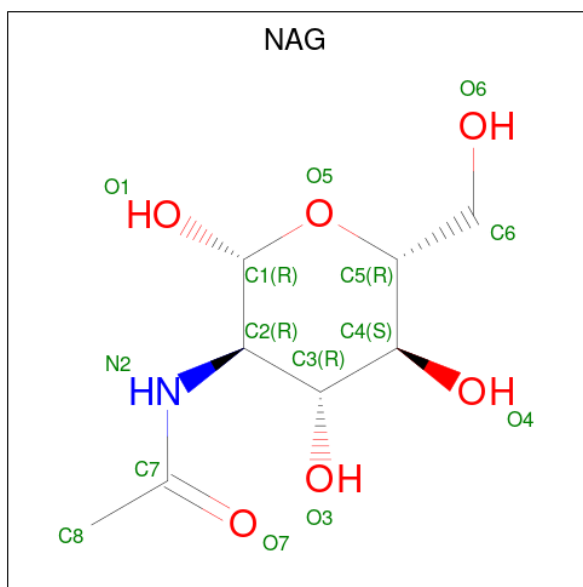
- Molecule 1 is a protein called 1,3-beta-glucanosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	451	Total 3486	C 2187	N 565	O 711	S 23	0	2	0
1	A	442	Total 3435	C 2162	N 555	O 695	S 23	0	3	0

- Molecule 2 is a protein called Nanobody 4.

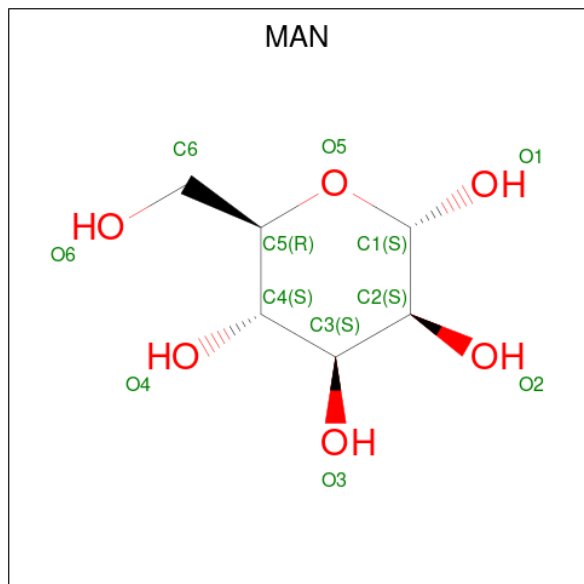
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	124	Total 969	C 591	N 177	O 195	S 6	0	1	0
2	D	124	Total 964	C 588	N 176	O 194	S 6	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



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

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

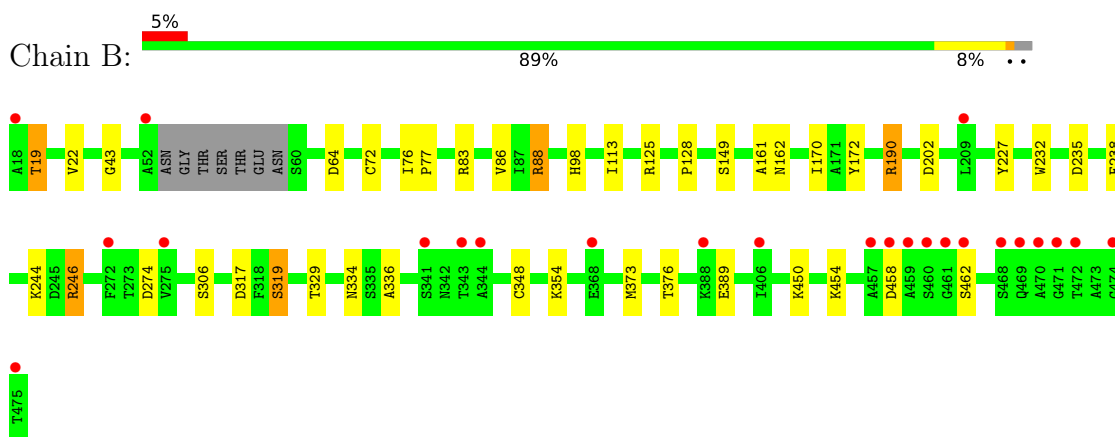
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	284	Total O 284 284	0	0
5	A	298	Total O 298 298	0	0
5	C	58	Total O 58 58	0	0
5	D	49	Total O 49 49	0	0

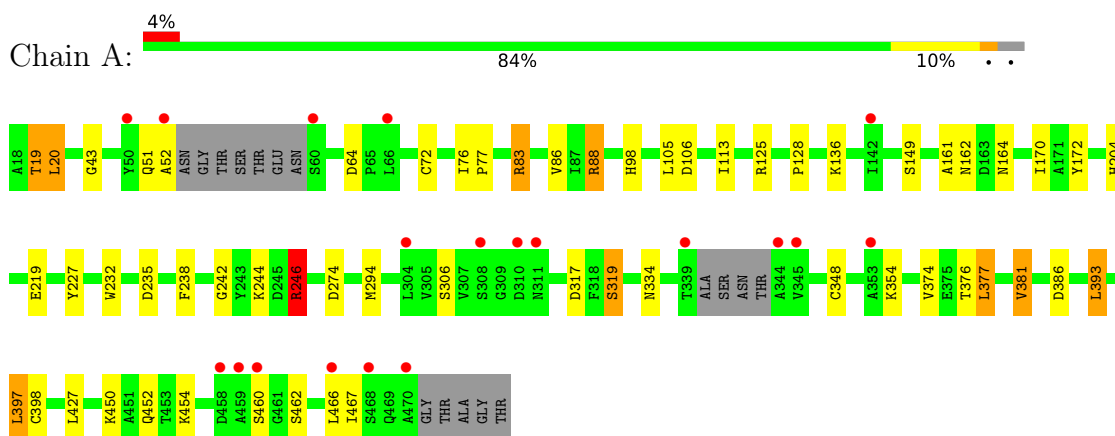
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

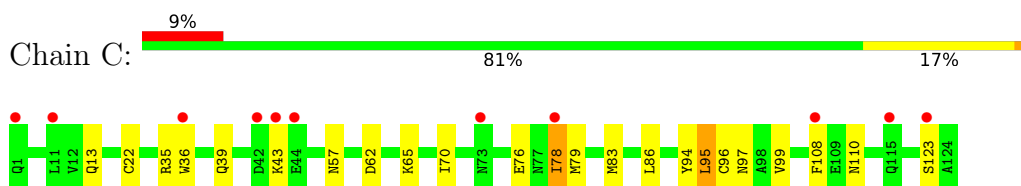
- Molecule 1: 1,3-beta-glucanosyltransferase



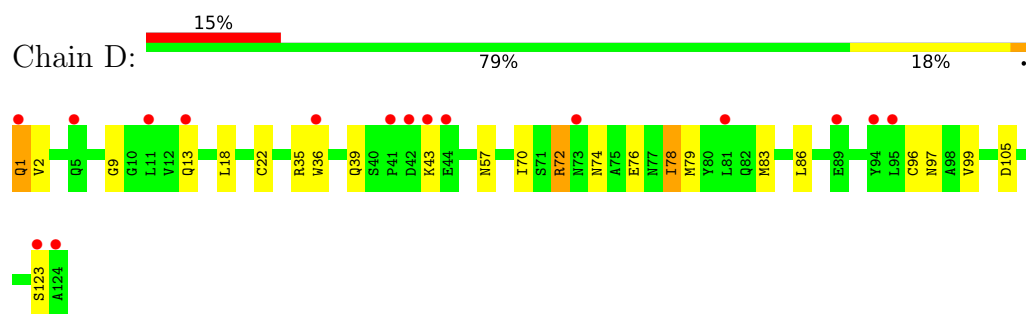
- Molecule 1: 1,3-beta-glucanosyltransferase



- Molecule 2: Nanobody 4



- Molecule 2: Nanobody 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.39Å 86.33Å 178.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.01 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (20.01-1.90) 99.6 (20.00-1.90)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 1.90Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.215 , 0.264 0.223 , 0.270	Depositor DCC
R_{free} test set	4072 reflections (3.92%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtrriage
Anisotropy	0.606	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtrriage
Estimated twinning fraction	0.000 for k,h,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9781	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.03 % 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 1.4015e-04. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, 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	0.69	0/3517	0.80	2/4765 (0.0%)
1	B	0.69	0/3566	0.81	3/4834 (0.1%)
2	C	0.66	0/988	0.86	0/1335
2	D	0.69	0/980	0.87	1/1324 (0.1%)
All	All	0.69	0/9051	0.82	6/12258 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	72	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	B	83	ARG	CG-CD-NE	6.01	124.41	111.80
1	A	246	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	B	190	ARG	N-CA-CB	-5.19	101.25	110.60
1	A	83	ARG	CG-CD-NE	5.12	122.54	111.80
1	B	246	ARG	NE-CZ-NH2	-5.09	117.75	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3435	0	3246	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3486	0	3285	26	0
2	C	969	0	920	23	0
2	D	964	0	914	24	0
3	A	42	0	39	0	0
3	B	42	0	39	1	0
4	A	77	0	70	7	0
4	B	77	0	70	15	0
5	A	298	0	0	6	0
5	B	284	0	0	4	0
5	C	58	0	0	1	0
5	D	49	0	0	0	0
All	All	9781	0	8583	118	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 7.

All (118) 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:B:373:MET:O	1:B:376:THR:HG22	1.68	0.93
1:B:19[A]:THR:HG23	1:B:149:SER:OG	1.76	0.86
2:D:22:CYS:HG	2:D:96:CYS:HG	1.14	0.84
2:C:22:CYS:HG	2:C:96:CYS:HG	1.12	0.82
1:A:19:THR:HG23	1:A:149:SER:OG	1.82	0.80
1:A:319:SER:HB3	4:A:1005:MAN:H5	1.66	0.77
1:B:319:SER:HB3	4:B:504:MAN:H5	1.66	0.74
4:B:509:MAN:O2	4:A:1001:MAN:O2	2.08	0.71
4:B:508:MAN:H4	4:A:1010:MAN:O6	1.92	0.70
1:A:386:ASP:CB	5:A:1286:HOH:O	2.41	0.69
1:B:72:CYS:O	1:B:76:ILE:HG12	1.94	0.67
2:C:95:LEU:HD12	2:C:95:LEU:N	2.08	0.67
1:A:232:TRP:CD2	1:A:274:ASP:HB3	2.30	0.66
2:C:22:CYS:HG	2:C:96:CYS:CB	2.08	0.66
1:A:98:HIS:HD2	5:A:1149:HOH:O	1.78	0.66
1:B:125:ARG:NH1	1:B:162:ASN:ND2	2.43	0.66
1:A:72:CYS:O	1:A:76:ILE:HG12	1.95	0.66
1:A:125:ARG:NH1	1:A:162:ASN:ND2	2.44	0.66
2:C:94:TYR:C	2:C:95:LEU:HD12	2.17	0.66
1:B:232:TRP:CD2	1:B:274:ASP:HB3	2.31	0.65
1:B:319:SER:HB3	4:B:504:MAN:C5	2.28	0.64
4:B:508:MAN:H62	1:A:334:ASN:CB	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:36:TRP:HE1	2:D:79:MET:CE	2.12	0.62
2:C:35:ARG:HH21	2:C:97:ASN:HD21	1.47	0.61
2:D:22:CYS:HG	2:D:96:CYS:CB	2.11	0.61
2:D:110:ASN:HD22	2:D:110:ASN:N	1.97	0.61
2:C:36:TRP:HE1	2:C:79:MET:CE	2.14	0.60
1:A:64:ASP:OD2	1:A:98:HIS:HE1	1.85	0.60
1:B:161:ALA:HB3	1:B:170:ILE:HD11	1.83	0.60
1:B:64:ASP:OD2	1:B:98:HIS:HE1	1.85	0.59
1:A:374:VAL:HA	1:A:377:LEU:HD22	1.85	0.59
2:D:83:MET:HE2	2:D:86:LEU:HD21	1.86	0.58
1:B:348:CYS:O	4:B:506:MAN:H2	2.05	0.57
4:B:508:MAN:H62	1:A:334:ASN:HB3	1.86	0.56
2:C:83:MET:HE2	2:C:86:LEU:HD21	1.89	0.55
2:C:95:LEU:N	2:C:95:LEU:CD1	2.69	0.55
1:A:161:ALA:CB	1:A:170:ILE:HD11	2.37	0.55
1:A:161:ALA:HB3	1:A:170:ILE:HD11	1.89	0.54
1:B:161:ALA:CB	1:B:170:ILE:HD11	2.37	0.54
2:D:9:GLY:HA2	2:D:18:LEU:HD13	1.89	0.54
2:D:36:TRP:NE1	2:D:79:MET:CE	2.70	0.54
2:D:36:TRP:HE1	2:D:79:MET:HE3	1.72	0.54
1:B:19[A]:THR:CG2	1:B:149:SER:OG	2.54	0.53
1:B:232:TRP:CG	1:B:274:ASP:HB3	2.43	0.53
4:B:508:MAN:H61	5:B:646:HOH:O	2.07	0.53
1:A:232:TRP:CG	1:A:274:ASP:HB3	2.44	0.53
2:C:36:TRP:NE1	2:C:79:MET:CE	2.71	0.53
2:D:35:ARG:HH21	2:D:97:ASN:HD21	1.55	0.53
1:B:98:HIS:HD2	5:B:625:HOH:O	1.90	0.52
1:A:452:GLN:NE2	5:A:1107:HOH:O	2.40	0.52
1:A:381:VAL:HG21	1:A:427:LEU:HD23	1.92	0.52
2:D:70:ILE:HG13	2:D:79:MET:HE1	1.92	0.51
2:C:70:ILE:HD11	2:C:79:MET:HE2	1.92	0.51
1:A:393[A]:LEU:CD1	5:A:1368:HOH:O	2.58	0.51
4:B:509:MAN:HO4	4:A:1010:MAN:HO4	1.56	0.50
2:C:76:GLU:O	2:C:78:ILE:CG1	2.59	0.50
2:D:35:ARG:HE	2:D:97:ASN:HD22	1.59	0.50
1:A:319:SER:HB3	4:A:1005:MAN:C5	2.38	0.50
2:D:76:GLU:O	2:D:78:ILE:CG1	2.60	0.50
2:D:76:GLU:O	2:D:78:ILE:HG13	2.12	0.49
1:A:393[B]:LEU:HD11	1:A:450:LYS:HD3	1.94	0.49
4:B:508:MAN:O6	4:B:509:MAN:H5	2.12	0.49
1:A:393[A]:LEU:HD23	1:A:427:LEU:HD21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:CYS:HB3	5:C:244:HOH:O	2.12	0.49
2:C:76:GLU:O	2:C:78:ILE:HG13	2.13	0.48
1:A:20:LEU:HD22	1:A:106:ASP:HA	1.96	0.48
1:A:51:GLN:O	1:A:52:ALA:HB3	2.14	0.47
2:C:35:ARG:HE	2:C:97:ASN:HD22	1.63	0.47
1:B:88:ARG:HA	1:B:113:ILE:O	2.15	0.47
1:A:242:GLY:HA2	5:A:1201:HOH:O	2.15	0.47
1:A:43:GLY:HA2	1:A:86:VAL:O	2.15	0.46
4:B:508:MAN:H62	1:A:334:ASN:HB2	1.98	0.46
2:C:62:ASP:OD1	2:C:65:LYS:NZ	2.49	0.46
1:A:164:ASN:HD21	1:A:204:HIS:HB2	1.81	0.46
4:B:508:MAN:C4	4:A:1010:MAN:O6	2.61	0.46
1:A:128:PRO:HB2	1:A:172:TYR:CD1	2.51	0.46
1:B:43:GLY:HA2	1:B:86:VAL:O	2.16	0.45
1:A:88:ARG:HA	1:A:113:ILE:O	2.16	0.45
1:A:376[B]:THR:HG21	1:A:467:ILE:HD13	1.98	0.45
2:C:39:GLN:NE2	2:C:43:LYS:O	2.50	0.45
1:B:319:SER:CB	4:B:504:MAN:H5	2.42	0.45
1:B:128:PRO:HB2	1:B:172:TYR:CD1	2.51	0.45
1:B:389:GLU:OE1	1:B:450:LYS:HE3	2.17	0.45
1:A:348:CYS:O	4:A:1007:MAN:H2	2.17	0.44
2:C:99:VAL:HA	2:C:110:ASN:O	2.16	0.44
2:D:110:ASN:N	2:D:110:ASN:ND2	2.65	0.44
2:D:1:GLN:CD	2:D:2:VAL:H	2.20	0.44
1:B:334:ASN:HD22	1:B:336:ALA:H	1.66	0.44
2:C:36:TRP:HE1	2:C:79:MET:HE3	1.82	0.44
2:D:39:GLN:NE2	2:D:43:LYS:O	2.50	0.44
1:B:348:CYS:O	4:B:506:MAN:C2	2.66	0.44
1:B:238:PHE:CZ	1:B:244:LYS:HA	2.53	0.44
2:D:99:VAL:HA	2:D:110:ASN:O	2.18	0.44
2:D:36:TRP:NE1	2:D:79:MET:HE3	2.33	0.43
3:B:507:NAG:H82	2:D:105:ASP:O	2.18	0.43
2:D:72:ARG:HD3	2:D:74:ASN:OD1	2.18	0.43
5:B:735:HOH:O	1:A:83:ARG:HD2	2.19	0.43
2:C:22:CYS:SG	2:C:96:CYS:CB	3.07	0.43
1:B:76:ILE:N	1:B:77:PRO:CD	2.81	0.43
1:B:22:VAL:HG11	1:B:190:ARG:HD2	2.01	0.43
1:A:76:ILE:N	1:A:77:PRO:CD	2.82	0.43
1:A:219:GLU:CG	5:A:1284:HOH:O	2.66	0.43
1:A:19:THR:HG23	1:A:149:SER:HG	1.84	0.42
1:A:238:PHE:CZ	1:A:244:LYS:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:36:TRP:NE1	2:C:79:MET:HE3	2.34	0.42
2:D:72:ARG:CD	2:D:74:ASN:OD1	2.67	0.42
1:B:202:ASP:OD1	5:B:601:HOH:O	2.21	0.42
2:C:22:CYS:O	2:C:78:ILE:HG23	2.20	0.42
1:B:329:THR:HB	4:B:508:MAN:C5	2.48	0.41
1:A:19:THR:CG2	1:A:149:SER:OG	2.63	0.41
2:C:79:MET:HE3	2:C:79:MET:HB3	1.79	0.41
2:D:35:ARG:HE	2:D:97:ASN:ND2	2.17	0.41
2:D:22:CYS:O	2:D:78:ILE:HG23	2.20	0.41
2:C:76:GLU:O	2:C:78:ILE:HG12	2.21	0.40
2:D:79:MET:HE3	2:D:79:MET:HB3	1.78	0.40
2:C:35:ARG:HE	2:C:97:ASN:ND2	2.18	0.40
1:A:246:ARG:HA	1:A:246:ARG:HD3	1.98	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	439/458 (96%)	432 (98%)	7 (2%)	0	100	100
1	B	449/458 (98%)	441 (98%)	8 (2%)	0	100	100
2	C	123/124 (99%)	121 (98%)	2 (2%)	0	100	100
2	D	122/124 (98%)	120 (98%)	2 (2%)	0	100	100
All	All	1133/1164 (97%)	1114 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	374/383 (98%)	351 (94%)	23 (6%)	18	9
1	B	379/383 (99%)	366 (97%)	13 (3%)	37	28
2	C	106/105 (101%)	100 (94%)	6 (6%)	20	11
2	D	105/105 (100%)	98 (93%)	7 (7%)	16	7
All	All	964/976 (99%)	915 (95%)	49 (5%)	25	14

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	19[A]	THR
1	B	19[B]	THR
1	B	88	ARG
1	B	227	TYR
1	B	235	ASP
1	B	246	ARG
1	B	306	SER
1	B	317	ASP
1	B	319	SER
1	B	354	LYS
1	B	454	LYS
1	B	458	ASP
1	B	462	SER
1	A	19	THR
1	A	20	LEU
1	A	88	ARG
1	A	105	LEU
1	A	136	LYS
1	A	227	TYR
1	A	235	ASP
1	A	246	ARG
1	A	294[A]	MET
1	A	294[B]	MET
1	A	306	SER

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Mol	Chain	Res	Type
1	A	317	ASP
1	A	319	SER
1	A	354	LYS
1	A	377	LEU
1	A	381	VAL
1	A	393[A]	LEU
1	A	393[B]	LEU
1	A	397	LEU
1	A	454	LYS
1	A	460	SER
1	A	462	SER
1	A	466	LEU
2	C	13	GLN
2	C	57	ASN
2	C	78	ILE
2	C	95	LEU
2	C	108	PHE
2	C	123	SER
2	D	1	GLN
2	D	13	GLN
2	D	57	ASN
2	D	78	ILE
2	D	108	PHE
2	D	110	ASN
2	D	123	SER

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

Mol	Chain	Res	Type
1	B	98	HIS
1	B	164	ASN
1	B	228	ASN
1	B	311	ASN
1	B	334	ASN
1	B	342	ASN
1	A	51	GLN
1	A	98	HIS
1	A	164	ASN
1	A	228	ASN
2	C	57	ASN
2	C	97	ASN
2	D	1	GLN

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Mol	Chain	Res	Type
2	D	97	ASN
2	D	110	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 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
4	MAN	B	504	1	11,11,12	0.56	0	15,15,17	1.04	1 (6%)
4	MAN	B	510	1	11,11,12	1.09	1 (9%)	15,15,17	1.45	3 (20%)
4	MAN	A	1010	1	11,11,12	0.26	0	15,15,17	0.62	0
4	MAN	B	506	1	11,11,12	0.33	0	15,15,17	1.39	2 (13%)
4	MAN	A	1006	1	11,11,12	0.82	0	15,15,17	1.98	5 (33%)
4	MAN	B	502	1	11,11,12	0.64	0	15,15,17	1.18	1 (6%)
3	NAG	A	1008	1	14,14,15	1.05	1 (7%)	17,19,21	1.14	2 (11%)
3	NAG	B	503	1	14,14,15	0.29	0	17,19,21	0.62	0
4	MAN	B	509	1	11,11,12	1.57	3 (27%)	15,15,17	2.84	9 (60%)
3	NAG	B	507	1	14,14,15	0.80	0	17,19,21	1.63	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	A	1007	1	11,11,12	0.64	0	15,15,17	1.37	1 (6%)
3	NAG	A	1002	1	14,14,15	0.62	0	17,19,21	1.24	2 (11%)
3	NAG	B	501	1	14,14,15	0.50	0	17,19,21	1.31	2 (11%)
4	MAN	A	1005	1	11,11,12	0.35	0	15,15,17	1.22	1 (6%)
4	MAN	A	1001	1	11,11,12	0.46	0	15,15,17	0.96	0
3	NAG	A	1004	1	14,14,15	0.29	0	17,19,21	0.61	0
4	MAN	A	1009	1	11,11,12	0.58	0	15,15,17	1.22	1 (6%)
4	MAN	B	508	1	11,11,12	1.10	1 (9%)	15,15,17	2.46	4 (26%)
4	MAN	B	505	1	11,11,12	0.78	0	15,15,17	1.98	6 (40%)
4	MAN	A	1003	1	11,11,12	0.41	0	15,15,17	1.27	2 (13%)

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	MAN	B	504	1	-	2/2/19/22	0/1/1/1
4	MAN	B	510	1	-	2/2/19/22	0/1/1/1
4	MAN	A	1010	1	-	2/2/19/22	0/1/1/1
4	MAN	B	506	1	-	0/2/19/22	0/1/1/1
4	MAN	A	1006	1	-	2/2/19/22	0/1/1/1
4	MAN	B	502	1	-	1/2/19/22	0/1/1/1
3	NAG	A	1008	1	-	0/6/23/26	0/1/1/1
3	NAG	B	503	1	-	3/6/23/26	0/1/1/1
4	MAN	B	509	1	-	2/2/19/22	0/1/1/1
3	NAG	B	507	1	-	0/6/23/26	0/1/1/1
4	MAN	A	1007	1	-	2/2/19/22	0/1/1/1
3	NAG	A	1002	1	-	0/6/23/26	0/1/1/1
3	NAG	B	501	1	-	0/6/23/26	0/1/1/1
4	MAN	A	1005	1	-	1/2/19/22	0/1/1/1
4	MAN	A	1001	1	-	0/2/19/22	0/1/1/1
3	NAG	A	1004	1	-	2/6/23/26	0/1/1/1
4	MAN	A	1009	1	-	0/2/19/22	0/1/1/1
4	MAN	B	508	1	-	1/2/19/22	0/1/1/1
4	MAN	B	505	1	-	2/2/19/22	0/1/1/1
4	MAN	A	1003	1	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	509	MAN	C6-C5	3.11	1.62	1.51
4	B	510	MAN	C2-C3	2.74	1.56	1.52
4	B	509	MAN	O6-C6	2.69	1.53	1.42
4	B	509	MAN	C4-C5	2.38	1.58	1.53
3	A	1008	NAG	O7-C7	-2.22	1.18	1.23
4	B	508	MAN	O5-C1	-2.15	1.40	1.43

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	508	MAN	O5-C5-C6	-7.48	95.47	107.20
4	B	509	MAN	C6-C5-C4	6.36	127.90	113.00
4	B	509	MAN	O5-C5-C4	-5.51	97.42	110.83
4	A	1007	MAN	O5-C1-C2	-4.51	103.80	110.77
4	A	1005	MAN	O5-C1-C2	-3.79	104.93	110.77
4	A	1006	MAN	C1-O5-C5	3.74	117.25	112.19
3	B	507	NAG	O5-C5-C6	3.58	112.82	107.20
3	B	501	NAG	O5-C1-C2	-3.48	105.79	111.29
4	B	505	MAN	C6-C5-C4	-3.43	104.97	113.00
4	B	510	MAN	O5-C5-C6	3.34	112.44	107.20
3	B	507	NAG	O5-C1-C2	-3.25	106.16	111.29
4	B	504	MAN	O5-C1-C2	-3.23	105.79	110.77
4	B	506	MAN	C1-C2-C3	3.18	113.57	109.67
4	B	508	MAN	O5-C5-C4	3.16	118.52	110.83
4	A	1006	MAN	O5-C5-C4	3.04	118.22	110.83
4	A	1009	MAN	O5-C1-C2	-3.03	106.09	110.77
4	B	505	MAN	O6-C6-C5	-2.99	101.04	111.29
4	B	505	MAN	C1-O5-C5	2.94	116.18	112.19
4	B	506	MAN	O5-C1-C2	-2.82	106.41	110.77
4	B	505	MAN	O2-C2-C1	-2.81	103.39	109.15
4	B	509	MAN	O4-C4-C5	2.77	116.18	109.30
4	A	1006	MAN	O5-C5-C6	-2.76	102.88	107.20
4	B	509	MAN	O6-C6-C5	2.71	120.59	111.29
4	B	505	MAN	O3-C3-C2	2.61	114.99	109.99
4	A	1003	MAN	O5-C1-C2	-2.57	106.80	110.77
3	A	1002	NAG	O5-C1-C2	-2.56	107.24	111.29
4	B	510	MAN	O2-C2-C3	2.55	115.25	110.14
4	B	509	MAN	C1-O5-C5	2.55	115.64	112.19
3	B	501	NAG	O5-C5-C6	2.54	111.18	107.20
3	A	1008	NAG	O5-C1-C2	-2.54	107.28	111.29
4	A	1006	MAN	C1-C2-C3	2.51	112.75	109.67
4	B	508	MAN	O4-C4-C3	2.50	116.14	110.35
4	B	509	MAN	O4-C4-C3	-2.50	104.56	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	509	MAN	O3-C3-C4	2.46	116.03	110.35
4	B	502	MAN	O5-C1-C2	-2.42	107.04	110.77
4	B	508	MAN	C6-C5-C4	-2.41	107.35	113.00
4	B	509	MAN	O5-C5-C6	2.35	110.89	107.20
3	A	1002	NAG	O4-C4-C3	-2.33	104.96	110.35
3	B	507	NAG	C1-C2-N2	2.22	114.29	110.49
4	B	509	MAN	O5-C1-C2	2.18	114.13	110.77
3	B	507	NAG	C2-N2-C7	-2.17	119.81	122.90
3	A	1008	NAG	C2-N2-C7	-2.16	119.82	122.90
4	A	1006	MAN	C6-C5-C4	-2.13	108.02	113.00
4	A	1003	MAN	O4-C4-C3	-2.10	105.50	110.35
4	B	505	MAN	O2-C2-C3	2.09	114.31	110.14
4	B	510	MAN	C2-C3-C4	2.08	114.49	110.89

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	503	NAG	C8-C7-N2-C2
3	B	503	NAG	O7-C7-N2-C2
4	B	510	MAN	O5-C5-C6-O6
4	A	1007	MAN	C4-C5-C6-O6
4	B	509	MAN	O5-C5-C6-O6
4	B	510	MAN	C4-C5-C6-O6
4	B	509	MAN	C4-C5-C6-O6
4	A	1006	MAN	O5-C5-C6-O6
4	A	1007	MAN	O5-C5-C6-O6
4	A	1006	MAN	C4-C5-C6-O6
4	B	505	MAN	C4-C5-C6-O6
4	B	504	MAN	O5-C5-C6-O6
4	B	504	MAN	C4-C5-C6-O6
4	A	1010	MAN	C4-C5-C6-O6
4	A	1005	MAN	O5-C5-C6-O6
3	A	1004	NAG	C8-C7-N2-C2
4	B	505	MAN	O5-C5-C6-O6
4	A	1010	MAN	O5-C5-C6-O6
3	A	1004	NAG	O7-C7-N2-C2
4	B	502	MAN	C4-C5-C6-O6
4	B	508	MAN	O5-C5-C6-O6
3	B	503	NAG	O5-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	504	MAN	3	0
4	A	1010	MAN	3	0
4	B	506	MAN	2	0
4	B	509	MAN	3	0
3	B	507	NAG	1	0
4	A	1007	MAN	1	0
4	A	1005	MAN	2	0
4	A	1001	MAN	1	0
4	B	508	MAN	8	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	442/458 (96%)	0.23	19 (4%) 35 38	15, 27, 52, 82	0
1	B	451/458 (98%)	0.28	24 (5%) 26 29	16, 27, 55, 88	0
2	C	124/124 (100%)	0.51	11 (8%) 9 11	20, 33, 58, 73	0
2	D	124/124 (100%)	0.74	18 (14%) 2 2	23, 37, 65, 80	0
All	All	1141/1164 (98%)	0.33	72 (6%) 20 22	15, 28, 56, 88	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	459	ALA	7.2
1	B	458	ASP	7.0
1	A	458	ASP	6.7
1	A	344	ALA	6.1
1	A	60	SER	5.1
1	B	475	THR	5.0
1	B	472	THR	4.9
2	D	123	SER	4.4
2	D	11	LEU	4.3
1	A	459	ALA	4.2
1	B	52	ALA	4.2
1	B	460	SER	4.1
2	C	123	SER	4.1
2	D	42	ASP	3.8
1	A	468	SER	3.8
2	C	108	PHE	3.7
1	A	460	SER	3.6
2	D	115	GLN	3.6
2	D	44	GLU	3.6
1	B	343	THR	3.5
1	B	344	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	353	ALA	3.5
1	B	457	ALA	3.4
1	B	461	GLY	3.4
2	D	95	LEU	3.3
1	A	345	VAL	3.3
2	D	13	GLN	3.2
2	C	42	ASP	3.0
2	D	43	LYS	3.0
2	D	108	PHE	2.9
2	D	36	TRP	2.9
1	A	470	ALA	2.9
2	D	1	GLN	2.9
2	D	124	ALA	2.9
2	D	73	ASN	2.8
1	A	339	THR	2.8
2	C	73[A]	ASN	2.8
2	C	1	GLN	2.7
2	C	11	LEU	2.7
1	B	341	SER	2.5
2	D	94	TYR	2.5
1	B	468	SER	2.5
1	B	474	GLY	2.5
1	A	466	LEU	2.4
1	B	209	LEU	2.4
1	A	304	LEU	2.4
1	B	406	ILE	2.4
1	B	388	LYS	2.4
1	B	469	GLN	2.4
2	D	5	GLN	2.3
2	C	36	TRP	2.3
2	C	78	ILE	2.3
1	A	308	SER	2.3
2	C	44	GLU	2.2
1	B	470	ALA	2.2
1	B	272	PHE	2.2
2	C	115	GLN	2.2
1	A	50	TYR	2.2
2	C	43	LYS	2.2
2	D	81	LEU	2.2
1	B	18	ALA	2.2
1	A	310	ASP	2.1
1	A	142	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	368	GLU	2.1
1	B	462	SER	2.1
2	D	41	PRO	2.1
1	B	471	GLY	2.1
1	A	52	ALA	2.1
1	B	275	VAL	2.0
1	A	66	LEU	2.0
1	A	311	ASN	2.0
2	D	89	GLU	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 monosaccharides 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
4	MAN	A	1007	11/12	0.70	0.28	71,77,85,91	0
4	MAN	B	509	11/12	0.71	0.23	28,49,54,57	0
4	MAN	A	1010	11/12	0.71	0.30	41,59,65,77	0
4	MAN	B	504	11/12	0.74	0.28	40,43,45,49	0
3	NAG	B	503	14/15	0.74	0.39	57,71,76,77	0
4	MAN	B	508	11/12	0.76	0.25	43,50,59,67	0
4	MAN	A	1005	11/12	0.78	0.28	45,49,52,55	0
3	NAG	A	1004	14/15	0.81	0.32	58,65,76,85	0
4	MAN	A	1001	11/12	0.86	0.15	48,52,54,55	0
3	NAG	B	507	14/15	0.86	0.14	34,41,44,57	0
4	MAN	B	506	11/12	0.87	0.27	58,60,67,82	0
4	MAN	B	510	11/12	0.87	0.23	35,43,54,59	0
3	NAG	A	1008	14/15	0.89	0.16	40,44,48,61	0
4	MAN	B	505	11/12	0.91	0.11	25,26,30,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MAN	A	1006	11/12	0.91	0.11	29,30,40,46	0
4	MAN	A	1009	11/12	0.92	0.16	35,36,38,41	0
3	NAG	A	1002	14/15	0.93	0.09	26,30,33,34	0
4	MAN	A	1003	11/12	0.94	0.08	30,33,36,39	0
4	MAN	B	502	11/12	0.94	0.10	27,32,36,37	0
3	NAG	B	501	14/15	0.94	0.08	26,29,36,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.