



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 07:19 am GMT

PDB ID : 4ACQ
Title : Alpha-2 Macroglobulin
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Deposited on : 2011-12-17
Resolution : 4.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

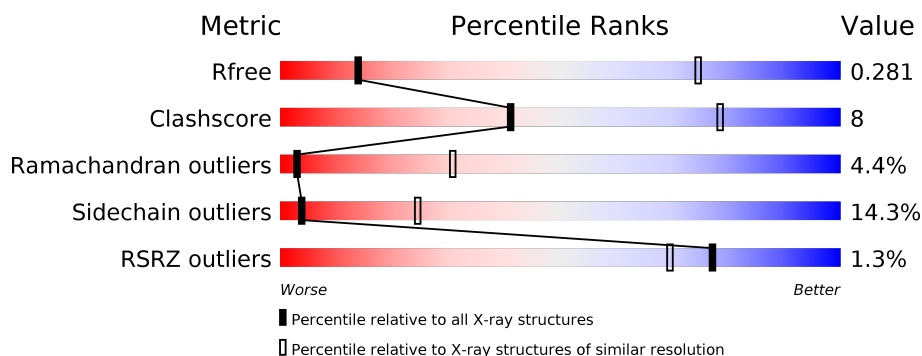
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 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}	100719	1002 (4.92-3.62)
Clashscore	112137	1001 (4.92-3.68)
Ramachandran outliers	110173	1012 (4.92-3.64)
Sidechain outliers	110143	1021 (4.92-3.62)
RSRZ outliers	101464	1009 (4.92-3.62)

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	1451	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 61%, yellow 22%, orange 5%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 61% 22% • 12% </div> </div>
1	B	1451	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 61%, yellow 22%, orange 5%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 61% 22% • 12% </div> </div>
1	C	1451	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 67%, yellow 25%, orange 5%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 67% 25% • • </div> </div>
1	D	1451	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 61%, yellow 23%, orange 5%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 61% 23% • 12% </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	A	2002	X	-	-	-
2	NAG	A	2401	-	-	-	X
2	NAG	A	2402	X	-	-	-
2	NAG	A	2502	X	-	-	-
2	NAG	B	2001	-	-	-	X
2	NAG	B	2002	X	-	-	-
2	NAG	B	2402	X	-	-	-
2	NAG	B	2502	X	-	-	-
2	NAG	C	2001	-	-	-	X
2	NAG	C	2002	X	-	-	-
2	NAG	C	2402	X	-	-	-
2	NAG	C	2502	X	-	-	-
2	NAG	D	2001	-	-	-	X
2	NAG	D	2002	X	-	-	-
2	NAG	D	2402	X	-	-	-
2	NAG	D	2502	X	-	-	-
4	NAG	A	2602	X	-	-	-
4	NAG	B	2602	X	-	-	-
4	MAN	B	2603	-	X	-	-
4	NAG	C	2602	X	-	-	-
4	MAN	C	2603	-	X	-	-
4	NAG	D	2602	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 39900 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 ALPHA-2-MACROGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1270	Total	C	N	O	S	0	0	0
			9548	6067	1606	1833	42			
1	B	1270	Total	C	N	O	S	0	0	0
			9548	6067	1606	1833	42			
1	C	1403	Total	C	N	O	S	0	0	0
			10582	6729	1774	2032	47			
1	D	1270	Total	C	N	O	S	0	0	0
			9548	6067	1606	1833	42			

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

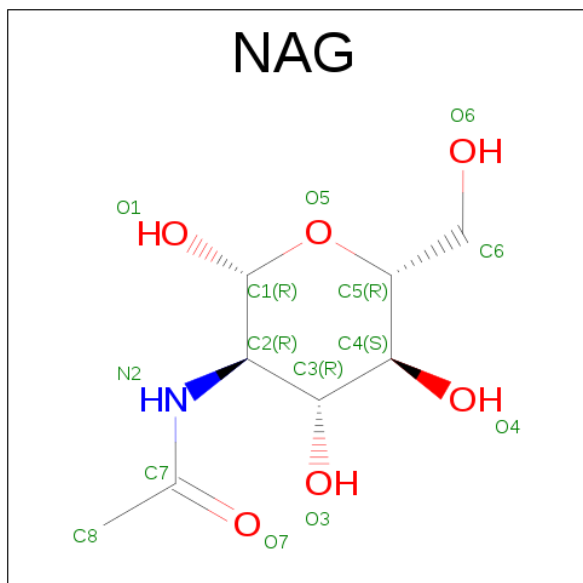
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	C	2	Total	C	N	O	0	0
			28	16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

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

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

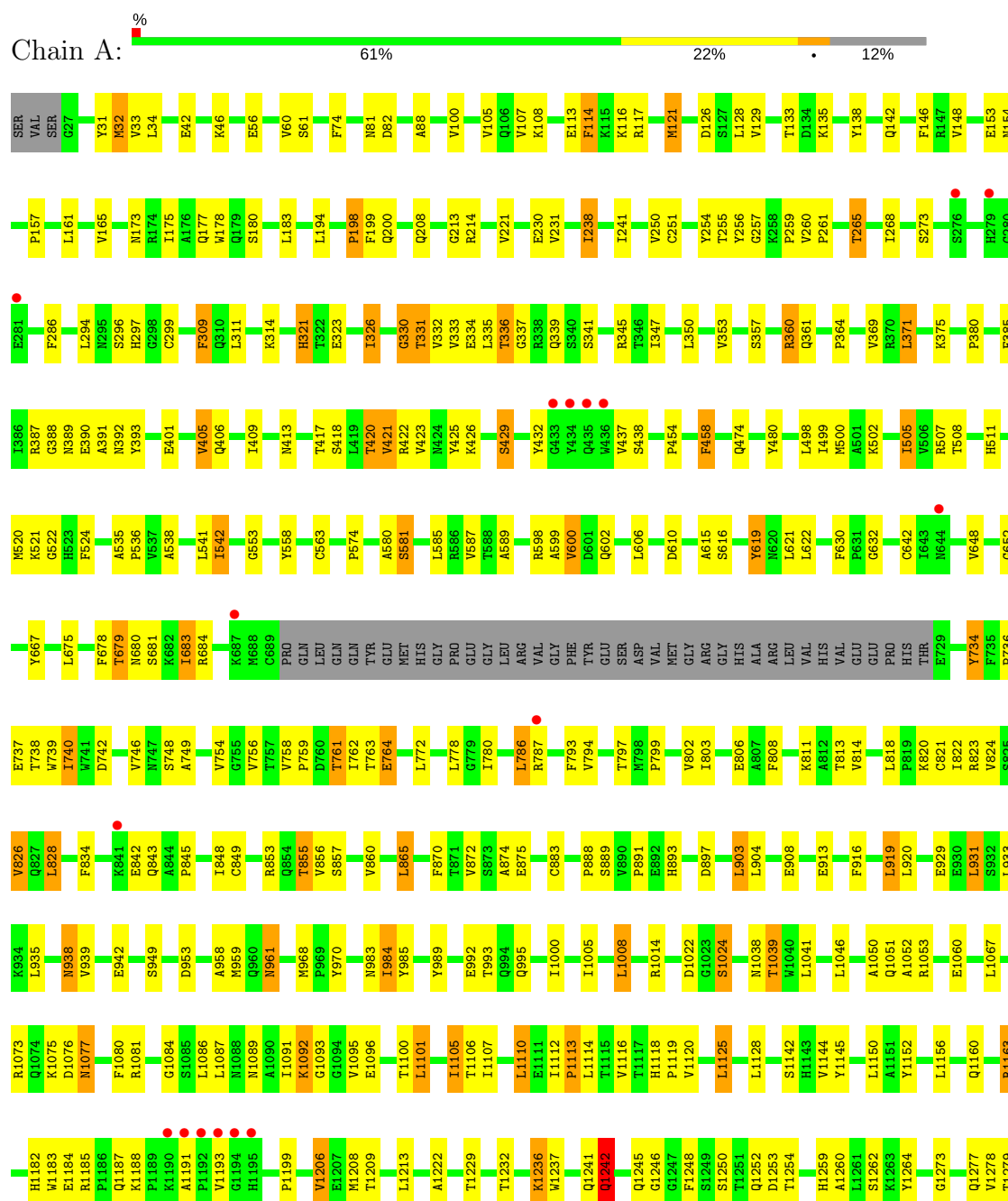
- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			39	22	2	15		
4	B	3	Total	C	N	O	0	0
			39	22	2	15		
4	C	3	Total	C	N	O	0	0
			39	22	2	15		
4	D	3	Total	C	N	O	0	0
			39	22	2	15		

3 Residue-property plots

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

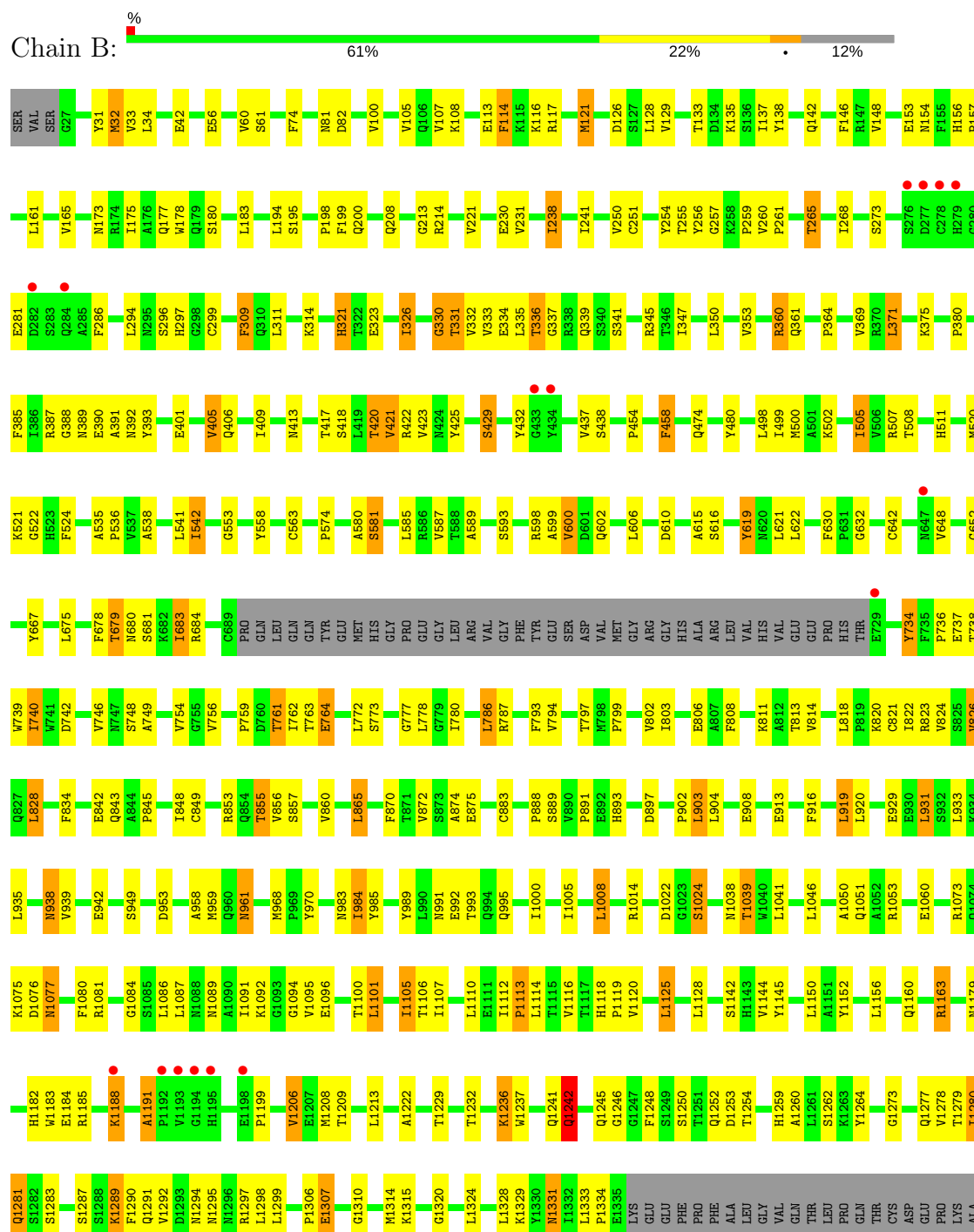
• Molecule 1: ALPHA-2-MACROGLOBULIN



L1280	THR
Q1281	SER
S1282	PHE
S1283	GLN
K1289	SER
F1290	LEU
Q1291	SER
V1292	VAL
D1293	SER
N1294	TYR
M1295	THR
L1298	GLY
L1299	SER
L1305	ARG
P1306	ALA
E1307	ASP
G1310	VAL
E1311	ILE
Y1312	VAL
S1313	ASP
M1314	VAL
K1315	LYS
L1324	MET
L1328	SER
K1329	GLY
Y1330	PHE
M1331	ILE
L1332	PRO
L1333	LEU
P1334	LYS
F1335	THR
L1335	THR
LYS	VAL
GLU	ASP
GLU	GLY
PHE	MET
LEU	LEU
PRO	ILE
PHE	GLU
ALA	ARG
LEU	SER
GLY	ASN
VAL	ASN
GLN	VAL
THR	SER
LEU	THR
PRO	GLY
GLN	VAL
THR	SER
CYS	GLY
ASP	ASN
GLU	HIS
PRO	VAL
LYS	LEU
ALA	ILE
HIS	TYR

LEU	ASP
LYS	VAL
VAL	GLN
SER	ASN
ILE	GLN
THR	THR
LEU	VAL
SER	SER
LEU	LEU
TYR	TYR
THR	THR
GLY	PHE
SER	THR
ARG	VAL
SER	LEU
ALA	GLN
ASP	ASP
VAL	VAL
PRO	PRO
VAL	VAL
VAL	VAL
GLY	LYS
LYS	TYR
PHE	ILE
ILE	PRO
VAL	ASP
GLY	TYR
THR	TYR
VAL	GLU
ASP	THR
GLY	ASP
MET	PHE
LEU	ALA
GLN	ILE
ASN	GLU
ALA	THR

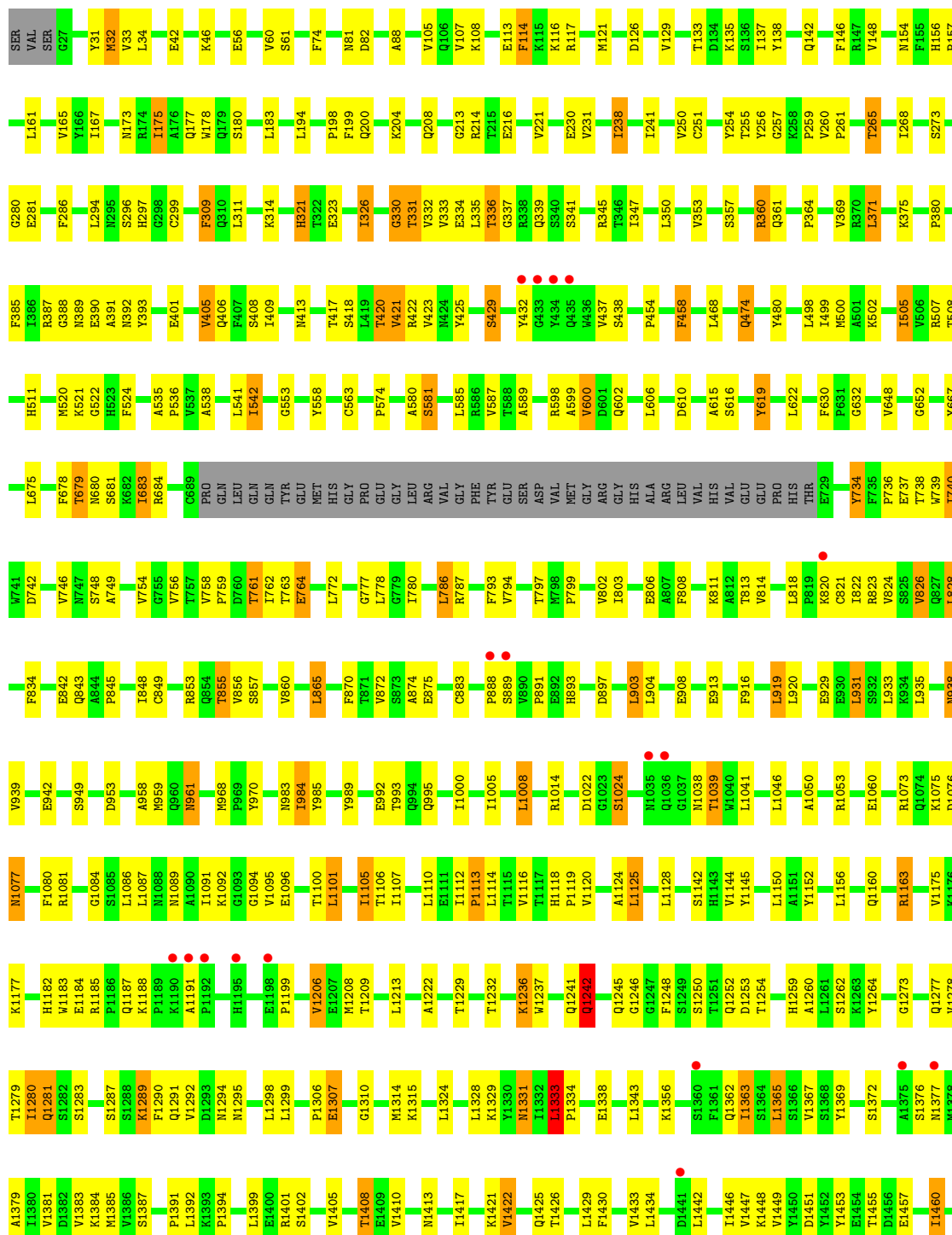
● Molecule 1: ALPHA-2-MACROGLOBULIN



HIS THR SER PHE ILE SER LEU VAL SER THR TYR PHE GLY SER ARG SER ALA SER ASN MET ALA ILE ASP VAL LYS MET VAL LYS VAL SER GLY PHE ILE PRO LEU LYS PRO THR VAL LYS MET PHE LEU ILE ARG GLU SER ASN HIS VAL PRO CYS ARG THR GLU VAL ASP LEU LEU ILE ALA ARG SER ASN TYR HIS ALA VAL PRO CYS SER LYS VAL ASP LEU GLY SER ASN HIS VAL LEU ILE

TYR LEU ASP LYS VAL SER ASN GLN THR SER LEU LEU PHE PHE THR VAL LEU GLN ASP VAL PRO MET VAL ARG ASP LEU LYS PRO MET VAL ILE VAL LYS VAL LYS VAL TYR ASP TYR TYR GLU THR ASP GLU PHE ILE ALA LEU ARG GLU TYR ASN HIS VAL PRO CYS SER LYS VAL ASP LEU GLY SER ASN HIS VAL LEU ILE

• Molecule 1: ALPHA-2-MACROGLOBULIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	130.69Å 260.30Å 281.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 4.30 24.95 – 4.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (25.00-4.30) 99.0 (24.95-4.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 4.24Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.238 , 0.260 0.263 , 0.281	Depositor DCC
R_{free} test set	3303 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	205.8	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 157.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	39900	wwPDB-VP
Average B, all atoms (Å ²)	175.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MEQ, 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	0.42	0/9743	0.72	0/13275
1	B	0.42	0/9743	0.72	0/13275
1	C	0.44	0/10801	0.73	0/14718
1	D	0.41	0/9743	0.72	0/13275
All	All	0.43	0/40030	0.72	0/54543

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	2
1	B	0	2
1	C	0	2
1	D	0	2
2	A	3	0
2	B	3	0
2	C	3	0
2	D	3	0
4	A	1	0
4	B	1	0
4	C	4	0
4	D	1	0
All	All	19	8

There are no bond length outliers.

There are no bond angle outliers.

5 of 19 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2002	NAG	C1
2	A	2402	NAG	C1
2	A	2502	NAG	C1
4	A	2602	NAG	C1
2	B	2002	NAG	C1

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	429	SER	Mainchain,Peptide
1	B	429	SER	Mainchain,Peptide
1	C	429	SER	Mainchain,Peptide
1	D	429	SER	Mainchain,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	9548	0	9181	153	0
1	B	9548	0	9181	152	0
1	C	10582	0	10201	174	0
1	D	9548	0	9181	153	0
2	A	84	0	75	3	0
2	B	84	0	75	3	0
2	C	84	0	75	3	0
2	D	84	0	75	2	0
3	A	42	0	39	0	0
3	B	42	0	39	0	0
3	C	56	0	52	0	0
3	D	42	0	39	0	0
4	A	39	0	34	1	0
4	B	39	0	34	2	0
4	C	39	0	32	1	0
4	D	39	0	34	1	0
All	All	39900	0	38347	633	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.

The worst 5 of 633 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)
2:D:2501:NAG:H83	2:D:2502:NAG:H82	1.65	0.79
2:C:2501:NAG:H83	2:C:2502:NAG:H82	1.65	0.78
2:B:2501:NAG:H83	2:B:2502:NAG:H82	1.65	0.78
1:C:280:GLY:HA3	1:D:429:SER:HA	1.65	0.77
1:C:535:ALA:HB1	1:C:536:PRO:HD2	1.65	0.76

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	1265/1451 (87%)	1061 (84%)	147 (12%)	57 (4%)	3	30
1	B	1265/1451 (87%)	1058 (84%)	149 (12%)	58 (5%)	3	30
1	C	1398/1451 (96%)	1162 (83%)	177 (13%)	59 (4%)	3	31
1	D	1265/1451 (87%)	1059 (84%)	149 (12%)	57 (4%)	3	30
All	All	5193/5804 (90%)	4340 (84%)	622 (12%)	231 (4%)	3	31

5 of 231 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	PRO
1	A	425	TYR
1	A	429	SER
1	A	580	ALA
1	A	736	PRO

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	1013/1268 (80%)	868 (86%)	145 (14%)	4	24
1	B	1013/1268 (80%)	869 (86%)	144 (14%)	4	25
1	C	1132/1268 (89%)	970 (86%)	162 (14%)	4	24
1	D	1013/1268 (80%)	868 (86%)	145 (14%)	4	24
All	All	4171/5072 (82%)	3575 (86%)	596 (14%)	4	24

5 of 596 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1163	ARG
1	C	474	GLN
1	D	968	MET
1	B	1277	GLN
1	C	175	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1242	GLN
1	C	406	GLN
1	D	1118	HIS
1	B	1325	GLN
1	C	106	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	MEQ	A	975	1	9,9,10	0.92	1 (11%)	7,10,12	1.01	1 (14%)
1	MEQ	B	975	1	9,9,10	0.91	1 (11%)	7,10,12	0.99	1 (14%)
1	MEQ	C	975	1	9,9,10	0.90	1 (11%)	7,10,12	1.02	1 (14%)
1	MEQ	D	975	1	9,9,10	0.88	1 (11%)	7,10,12	1.03	1 (14%)

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
1	MEQ	A	975	1	-	0/7/9/11	0/0/0/0
1	MEQ	B	975	1	-	0/7/9/11	0/0/0/0
1	MEQ	C	975	1	-	0/7/9/11	0/0/0/0
1	MEQ	D	975	1	-	0/7/9/11	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	975	MEQ	CA-C	2.02	1.52	1.50
1	D	975	MEQ	CA-C	2.11	1.53	1.50
1	B	975	MEQ	CA-C	2.15	1.53	1.50
1	A	975	MEQ	CA-C	2.21	1.53	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	975	MEQ	O-C-CA	-2.46	118.21	125.02
1	C	975	MEQ	O-C-CA	-2.44	118.28	125.02
1	A	975	MEQ	O-C-CA	-2.42	118.34	125.02
1	B	975	MEQ	O-C-CA	-2.39	118.41	125.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

36 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	2001	1,2	14,14,15	1.64	2 (14%)	15,19,21	1.16	1 (6%)
2	NAG	A	2002	2	14,14,15	1.53	1 (7%)	15,19,21	1.65	2 (13%)
2	NAG	A	2401	1,2	14,14,15	1.57	1 (7%)	15,19,21	1.98	3 (20%)
2	NAG	A	2402	2	14,14,15	1.70	1 (7%)	15,19,21	1.77	4 (26%)
2	NAG	A	2501	1,2	14,14,15	1.90	2 (14%)	15,19,21	2.15	4 (26%)
2	NAG	A	2502	2	14,14,15	1.40	1 (7%)	15,19,21	1.87	4 (26%)
4	NAG	A	2601	1,4	14,14,15	2.10	6 (42%)	15,19,21	2.84	7 (46%)
4	NAG	A	2602	4	14,14,15	2.62	5 (35%)	15,19,21	2.58	4 (26%)
4	MAN	A	2603	4	11,11,12	3.97	10 (90%)	13,15,17	3.07	7 (53%)
2	NAG	B	2001	1,2	14,14,15	1.68	2 (14%)	15,19,21	1.17	1 (6%)
2	NAG	B	2002	2	14,14,15	1.55	1 (7%)	15,19,21	1.66	2 (13%)
2	NAG	B	2401	1,2	14,14,15	1.56	1 (7%)	15,19,21	1.98	3 (20%)
2	NAG	B	2402	2	14,14,15	1.75	2 (14%)	15,19,21	1.84	4 (26%)
2	NAG	B	2501	1,2	14,14,15	1.92	3 (21%)	15,19,21	2.07	5 (33%)
2	NAG	B	2502	2	14,14,15	1.71	2 (14%)	15,19,21	1.80	4 (26%)
4	NAG	B	2601	1,4	14,14,15	2.07	7 (50%)	15,19,21	2.90	6 (40%)
4	NAG	B	2602	4	14,14,15	2.57	5 (35%)	15,19,21	2.64	4 (26%)
4	MAN	B	2603	4	11,11,12	4.45	10 (90%)	13,15,17	3.13	9 (69%)
2	NAG	C	2001	1,2	14,14,15	1.86	2 (14%)	15,19,21	1.16	1 (6%)
2	NAG	C	2002	2	14,14,15	1.56	1 (7%)	15,19,21	1.63	2 (13%)
2	NAG	C	2401	1,2	14,14,15	1.66	1 (7%)	15,19,21	2.02	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	2402	2	14,14,15	1.79	4 (28%)	15,19,21	1.68	4 (26%)
2	NAG	C	2501	1,2	14,14,15	1.96	3 (21%)	15,19,21	2.10	5 (33%)
2	NAG	C	2502	2	14,14,15	1.41	1 (7%)	15,19,21	1.89	4 (26%)
4	NAG	C	2601	1	14,14,15	2.28	9 (64%)	15,19,21	2.81	7 (46%)
4	NAG	C	2602	4	14,14,15	34.48	6 (42%)	16,19,21	18.67	9 (56%)
4	MAN	C	2603	4	11,11,12	2.91	10 (90%)	13,15,17	3.25	9 (69%)
2	NAG	D	2001	1,2	14,14,15	1.72	2 (14%)	15,19,21	1.16	1 (6%)
2	NAG	D	2002	2	14,14,15	1.52	1 (7%)	15,19,21	1.62	2 (13%)
2	NAG	D	2401	1,2	14,14,15	1.59	1 (7%)	15,19,21	2.01	4 (26%)
2	NAG	D	2402	2	14,14,15	1.79	2 (14%)	15,19,21	1.67	4 (26%)
2	NAG	D	2501	1,2	14,14,15	2.05	3 (21%)	15,19,21	1.98	3 (20%)
2	NAG	D	2502	2	14,14,15	1.43	1 (7%)	15,19,21	1.88	3 (20%)
4	NAG	D	2601	1,4	14,14,15	1.94	6 (42%)	15,19,21	2.80	7 (46%)
4	NAG	D	2602	4	14,14,15	2.40	6 (42%)	15,19,21	2.65	4 (26%)
4	MAN	D	2603	4	11,11,12	2.78	8 (72%)	13,15,17	3.25	6 (46%)

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	2001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2002	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	2401	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2402	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	2501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2502	2	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	2601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2602	4	1/1/5/7	0/6/23/26	0/1/1/1
4	MAN	A	2603	4	-	0/2/19/22	0/1/1/1
2	NAG	B	2001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2002	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	2401	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2402	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	2501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2502	2	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	B	2601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	2602	4	1/1/5/7	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	B	2603	4	-	0/2/19/22	0/1/1/1
2	NAG	C	2001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2002	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	C	2401	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2402	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	C	2501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2502	2	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	C	2601	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2602	4	4/4/5/7	0/6/22/26	1/1/1/1
4	MAN	C	2603	4	-	0/2/19/22	0/1/1/1
2	NAG	D	2001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2002	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	D	2401	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2402	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	D	2501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2502	2	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	D	2601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2602	4	1/1/5/7	0/6/23/26	0/1/1/1
4	MAN	D	2603	4	-	0/2/19/22	0/1/1/1

The worst 5 of 129 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2602	NAG	C2-N2	2.01	1.49	1.46
2	C	2402	NAG	C3-C2	2.02	1.56	1.52
2	B	2501	NAG	C2-N2	2.02	1.49	1.46
4	C	2601	NAG	O3-C3	2.04	1.47	1.43
2	C	2501	NAG	O5-C5	2.04	1.47	1.43

The worst 5 of 153 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2602	NAG	O5-C1-C2	-49.28	59.99	109.52
4	C	2602	NAG	C3-C4-C5	-45.92	50.56	110.82
4	C	2602	NAG	C1-O5-C5	-26.90	64.87	113.39
4	C	2602	NAG	O4-C4-C3	-11.20	82.91	110.02
2	C	2401	NAG	C8-C7-N2	-2.63	111.35	116.11

5 of 19 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	2002	NAG	C1

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Mol	Chain	Res	Type	Atom
2	B	2402	NAG	C1
2	A	2402	NAG	C1
2	A	2502	NAG	C1
2	D	2502	NAG	C1

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2602	NAG	C1-C2-C3-C4-C5-O5

20 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2401	NAG	1	0
2	A	2501	NAG	2	0
2	A	2502	NAG	2	0
4	A	2601	NAG	1	0
4	A	2602	NAG	1	0
2	B	2401	NAG	1	0
2	B	2501	NAG	2	0
2	B	2502	NAG	2	0
4	B	2601	NAG	2	0
4	B	2602	NAG	1	0
2	C	2401	NAG	1	0
2	C	2501	NAG	2	0
2	C	2502	NAG	2	0
4	C	2601	NAG	1	0
4	C	2602	NAG	1	0
2	D	2401	NAG	1	0
2	D	2501	NAG	1	0
2	D	2502	NAG	1	0
4	D	2601	NAG	1	0
4	D	2602	NAG	1	0

5.6 Ligand geometry

13 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
3	NAG	A	2101	1	14,14,15	1.85	3 (21%)	15,19,21	2.43	5 (33%)
3	NAG	A	2201	1	14,14,15	1.81	3 (21%)	15,19,21	1.44	2 (13%)
3	NAG	A	2301	1	14,14,15	1.78	3 (21%)	15,19,21	2.41	4 (26%)
3	NAG	B	2101	1	14,14,15	1.98	3 (21%)	15,19,21	2.39	5 (33%)
3	NAG	B	2201	1	14,14,15	1.72	2 (14%)	15,19,21	1.61	2 (13%)
3	NAG	B	2301	1	14,14,15	1.83	3 (21%)	15,19,21	2.37	5 (33%)
3	NAG	C	2101	1	14,14,15	2.30	3 (21%)	15,19,21	2.42	7 (46%)
3	NAG	C	2201	1	14,14,15	1.84	1 (7%)	15,19,21	2.00	3 (20%)
3	NAG	C	2301	1	14,14,15	2.18	5 (35%)	15,19,21	2.40	5 (33%)
3	NAG	C	2701	1	14,14,15	1.56	2 (14%)	15,19,21	1.29	2 (13%)
3	NAG	D	2101	1	14,14,15	1.76	3 (21%)	15,19,21	2.44	5 (33%)
3	NAG	D	2201	1	14,14,15	1.71	2 (14%)	15,19,21	1.42	2 (13%)
3	NAG	D	2301	1	14,14,15	1.72	2 (14%)	15,19,21	2.41	5 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	2101	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2201	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2301	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2101	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2201	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2301	1	-	0/6/23/26	0/1/1/1
3	NAG	C	2101	1	-	0/6/23/26	0/1/1/1
3	NAG	C	2201	1	-	0/6/23/26	0/1/1/1
3	NAG	C	2301	1	-	0/6/23/26	0/1/1/1
3	NAG	C	2701	1	-	0/6/23/26	0/1/1/1
3	NAG	D	2101	1	-	0/6/23/26	0/1/1/1
3	NAG	D	2201	1	-	0/6/23/26	0/1/1/1
3	NAG	D	2301	1	-	0/6/23/26	0/1/1/1

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2301	NAG	C3-C2	2.03	1.56	1.52
3	D	2301	NAG	C3-C2	2.04	1.57	1.52
3	A	2201	NAG	O5-C5	2.05	1.47	1.43
3	A	2301	NAG	C3-C2	2.07	1.57	1.52
3	D	2201	NAG	C3-C2	2.08	1.57	1.52

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2301	NAG	C8-C7-N2	-2.55	111.51	116.11
3	C	2301	NAG	C8-C7-N2	-2.31	111.94	116.11
3	B	2301	NAG	C8-C7-N2	-2.16	112.20	116.11
3	C	2101	NAG	C6-C5-C4	-2.13	108.02	113.00
3	C	2101	NAG	C8-C7-N2	-2.00	112.49	116.11

There are no chirality outliers.

There are no torsion outliers.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1269/1451 (87%)	-0.31	18 (1%) 75 67	81, 159, 293, 300	0
1	B	1269/1451 (87%)	-0.29	16 (1%) 77 69	65, 153, 297, 300	0
1	C	1402/1451 (96%)	-0.31	18 (1%) 77 69	60, 148, 292, 300	0
1	D	1269/1451 (87%)	-0.21	17 (1%) 77 69	91, 182, 300, 300	0
All	All	5209/5804 (89%)	-0.28	69 (1%) 77 69	60, 161, 299, 300	0

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1192	PRO	7.0
1	C	433	GLY	6.0
1	A	1191	ALA	4.7
1	D	633	PRO	4.5
1	B	277	ASP	4.4

6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	MEQ	B	975	10/11	0.90	0.20	-	164,187,254,273	0
1	MEQ	A	975	10/11	0.89	0.44	-	156,174,185,253	0
1	MEQ	D	975	10/11	0.85	0.35	-	190,274,288,289	0
1	MEQ	C	975	10/11	0.76	0.30	-	136,153,165,173	0

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	A	2401	14/15	0.72	0.32	2.78	208,291,293,294	0
2	NAG	C	2001	14/15	0.69	0.64	1.89	200,206,300,300	0
2	NAG	D	2001	14/15	0.77	0.69	1.62	287,288,290,291	0
2	NAG	B	2001	14/15	0.78	0.45	0.76	299,300,300,300	0
2	NAG	C	2401	14/15	0.76	0.26	0.53	156,171,244,254	0
2	NAG	A	2001	14/15	0.81	0.28	-0.16	292,292,294,295	0
4	MAN	C	2603	11/12	0.46	0.58	-	186,200,293,296	0
2	NAG	B	2002	14/15	0.77	0.65	-	296,298,300,300	0
2	NAG	D	2502	14/15	0.72	0.64	-	300,300,300,300	0
2	NAG	C	2002	14/15	0.72	0.68	-	194,299,300,300	0
2	NAG	D	2402	14/15	0.71	0.71	-	300,300,300,300	0
2	NAG	D	2501	14/15	0.78	0.56	-	193,295,300,300	0
2	NAG	C	2402	14/15	0.76	0.41	-	259,262,266,267	0
4	NAG	B	2601	14/15	0.96	0.24	-	143,166,224,228	0
4	MAN	D	2603	11/12	0.66	0.55	-	295,297,299,300	0
2	NAG	C	2501	14/15	0.89	0.41	-	186,209,298,300	0
2	NAG	B	2501	14/15	0.92	0.39	-	126,141,148,151	0
2	NAG	A	2002	14/15	0.72	0.42	-	292,293,295,295	0
2	NAG	C	2502	14/15	0.93	0.38	-	267,300,300,300	0
4	MAN	B	2603	11/12	0.82	0.48	-	100,100,100,100	0
4	NAG	C	2602	14/15	0.87	0.50	-	139,163,178,180	0
2	NAG	A	2501	14/15	0.90	0.51	-	180,196,251,259	0
4	NAG	B	2602	14/15	0.82	0.36	-	154,221,227,228	0
4	NAG	D	2601	14/15	0.77	0.38	-	167,210,263,270	0
2	NAG	D	2401	14/15	0.64	0.44	-	300,300,300,300	0
2	NAG	B	2401	14/15	0.57	0.39	-	300,300,300,300	0
4	NAG	D	2602	14/15	0.73	0.59	-	181,277,288,294	0
2	NAG	B	2402	14/15	0.80	0.79	-	300,300,300,300	0
2	NAG	B	2502	14/15	0.89	0.40	-	154,162,183,190	0
4	NAG	C	2601	14/15	0.90	0.36	-	119,140,154,161	0
4	NAG	A	2601	14/15	0.91	0.31	-	128,148,165,169	0
4	MAN	A	2603	11/12	0.60	0.62	-	100,100,100,100	0
4	NAG	A	2602	14/15	0.79	0.57	-	140,166,182,185	0
2	NAG	D	2002	14/15	0.64	0.52	-	286,288,291,291	0
2	NAG	A	2402	14/15	0.80	0.50	-	289,292,295,296	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	A	2502	14/15	0.77	0.56	-	211,286,300,300	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	A	2101	14/15	0.57	0.65	-	198,290,291,291	0
3	NAG	B	2201	14/15	0.74	0.59	-	190,197,262,265	0
3	NAG	D	2201	14/15	0.60	0.39	-	215,300,300,300	0
3	NAG	C	2201	14/15	0.32	0.65	-	202,298,300,300	0
3	NAG	C	2701	14/15	0.72	0.55	-	300,300,300,300	0
3	NAG	B	2101	14/15	0.80	0.41	-	180,203,294,295	0
3	NAG	C	2301	14/15	0.81	0.25	-	158,176,251,258	0
3	NAG	A	2201	14/15	0.69	0.30	-	183,192,270,280	0
3	NAG	D	2101	14/15	0.62	0.65	-	287,297,300,300	0
3	NAG	C	2101	14/15	0.70	0.49	-	129,154,175,189	0
3	NAG	B	2301	14/15	0.74	0.23	-	300,300,300,300	0
3	NAG	A	2301	14/15	0.87	0.15	-	278,290,292,292	0
3	NAG	D	2301	14/15	0.82	0.28	-	300,300,300,300	0

6.5 Other polymers [i](#)

There are no such residues in this entry.