



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:24 AM GMT

PDB ID : 3ALA
Title : Crystal structure of vascular adhesion protein-1 in space group C2
Authors : Ernberg, K.E.; McGrath, A.P.; Guss, J.M.
Deposited on : 2010-07-29
Resolution : 2.90 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

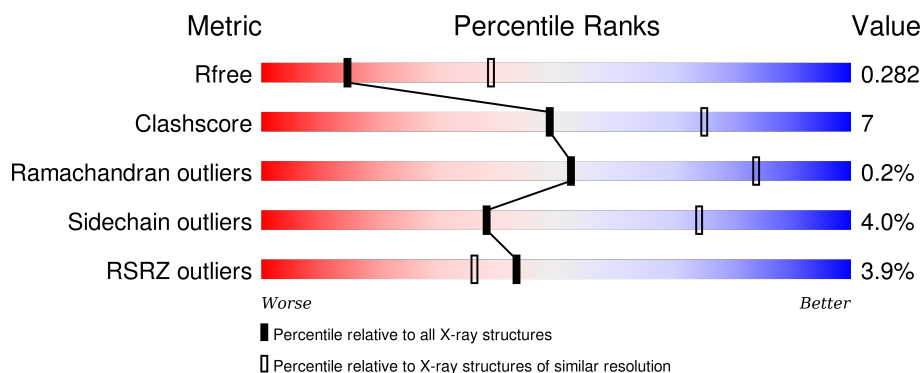
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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 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	748	
1	B	748	
1	C	748	
1	D	748	
1	E	748	

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Mol	Chain	Length	Quality of chain
1	F	748	
1	G	748	

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
10	FUL	C	1771	X	-	-	-
10	NAG	D	1769	X	-	-	-
10	NAG	E	1769	X	-	-	-
3	CA	B	1764	-	-	-	X
4	BMA	D	1767	X	-	-	-
5	NAG	G	1772	X	-	-	-
5	NAG	G	1773	-	-	-	X
9	NAG	B	1769	X	-	-	-

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 39103 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 Membrane primary amine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	705	Total	C	N	O	S	0	3	0
			5494	3539	927	1007	21			
1	B	705	Total	C	N	O	S	0	2	0
			5488	3532	935	1000	21			
1	C	709	Total	C	N	O	S	0	2	0
			5498	3546	927	1004	21			
1	D	711	Total	C	N	O	S	0	1	0
			5510	3546	935	1007	22			
1	E	702	Total	C	N	O	S	0	0	0
			5423	3496	914	992	21			
1	F	701	Total	C	N	O	S	0	3	0
			5390	3460	916	993	21			
1	G	706	Total	C	N	O	S	8	1	0
			5392	3470	907	994	21			

There are 119 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ASP	-	EXPRESSION TAG	UNP Q16853
A	17	ILE	-	EXPRESSION TAG	UNP Q16853
A	18	VAL	-	EXPRESSION TAG	UNP Q16853
A	19	ASP	-	EXPRESSION TAG	UNP Q16853
A	20	TYR	-	EXPRESSION TAG	UNP Q16853
A	21	LYS	-	EXPRESSION TAG	UNP Q16853
A	22	ASP	-	EXPRESSION TAG	UNP Q16853
A	23	ASP	-	EXPRESSION TAG	UNP Q16853
A	24	ASP	-	EXPRESSION TAG	UNP Q16853
A	25	ASP	-	EXPRESSION TAG	UNP Q16853
A	26	LYS	-	EXPRESSION TAG	UNP Q16853
A	27	GLU	-	EXPRESSION TAG	UNP Q16853
A	28	ASN	-	EXPRESSION TAG	UNP Q16853
A	29	LEU	-	EXPRESSION TAG	UNP Q16853
A	30	TYR	-	EXPRESSION TAG	UNP Q16853

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Chain	Residue	Modelled	Actual	Comment	Reference
A	31	PHE	-	EXPRESSION TAG	UNP Q16853
A	32	GLN	-	EXPRESSION TAG	UNP Q16853
B	16	ASP	-	EXPRESSION TAG	UNP Q16853
B	17	ILE	-	EXPRESSION TAG	UNP Q16853
B	18	VAL	-	EXPRESSION TAG	UNP Q16853
B	19	ASP	-	EXPRESSION TAG	UNP Q16853
B	20	TYR	-	EXPRESSION TAG	UNP Q16853
B	21	LYS	-	EXPRESSION TAG	UNP Q16853
B	22	ASP	-	EXPRESSION TAG	UNP Q16853
B	23	ASP	-	EXPRESSION TAG	UNP Q16853
B	24	ASP	-	EXPRESSION TAG	UNP Q16853
B	25	ASP	-	EXPRESSION TAG	UNP Q16853
B	26	LYS	-	EXPRESSION TAG	UNP Q16853
B	27	GLU	-	EXPRESSION TAG	UNP Q16853
B	28	ASN	-	EXPRESSION TAG	UNP Q16853
B	29	LEU	-	EXPRESSION TAG	UNP Q16853
B	30	TYR	-	EXPRESSION TAG	UNP Q16853
B	31	PHE	-	EXPRESSION TAG	UNP Q16853
B	32	GLN	-	EXPRESSION TAG	UNP Q16853
C	16	ASP	-	EXPRESSION TAG	UNP Q16853
C	17	ILE	-	EXPRESSION TAG	UNP Q16853
C	18	VAL	-	EXPRESSION TAG	UNP Q16853
C	19	ASP	-	EXPRESSION TAG	UNP Q16853
C	20	TYR	-	EXPRESSION TAG	UNP Q16853
C	21	LYS	-	EXPRESSION TAG	UNP Q16853
C	22	ASP	-	EXPRESSION TAG	UNP Q16853
C	23	ASP	-	EXPRESSION TAG	UNP Q16853
C	24	ASP	-	EXPRESSION TAG	UNP Q16853
C	25	ASP	-	EXPRESSION TAG	UNP Q16853
C	26	LYS	-	EXPRESSION TAG	UNP Q16853
C	27	GLU	-	EXPRESSION TAG	UNP Q16853
C	28	ASN	-	EXPRESSION TAG	UNP Q16853
C	29	LEU	-	EXPRESSION TAG	UNP Q16853
C	30	TYR	-	EXPRESSION TAG	UNP Q16853
C	31	PHE	-	EXPRESSION TAG	UNP Q16853
C	32	GLN	-	EXPRESSION TAG	UNP Q16853
D	16	ASP	-	EXPRESSION TAG	UNP Q16853
D	17	ILE	-	EXPRESSION TAG	UNP Q16853
D	18	VAL	-	EXPRESSION TAG	UNP Q16853
D	19	ASP	-	EXPRESSION TAG	UNP Q16853
D	20	TYR	-	EXPRESSION TAG	UNP Q16853
D	21	LYS	-	EXPRESSION TAG	UNP Q16853

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Chain	Residue	Modelled	Actual	Comment	Reference
D	22	ASP	-	EXPRESSION TAG	UNP Q16853
D	23	ASP	-	EXPRESSION TAG	UNP Q16853
D	24	ASP	-	EXPRESSION TAG	UNP Q16853
D	25	ASP	-	EXPRESSION TAG	UNP Q16853
D	26	LYS	-	EXPRESSION TAG	UNP Q16853
D	27	GLU	-	EXPRESSION TAG	UNP Q16853
D	28	ASN	-	EXPRESSION TAG	UNP Q16853
D	29	LEU	-	EXPRESSION TAG	UNP Q16853
D	30	TYR	-	EXPRESSION TAG	UNP Q16853
D	31	PHE	-	EXPRESSION TAG	UNP Q16853
D	32	GLN	-	EXPRESSION TAG	UNP Q16853
E	16	ASP	-	EXPRESSION TAG	UNP Q16853
E	17	ILE	-	EXPRESSION TAG	UNP Q16853
E	18	VAL	-	EXPRESSION TAG	UNP Q16853
E	19	ASP	-	EXPRESSION TAG	UNP Q16853
E	20	TYR	-	EXPRESSION TAG	UNP Q16853
E	21	LYS	-	EXPRESSION TAG	UNP Q16853
E	22	ASP	-	EXPRESSION TAG	UNP Q16853
E	23	ASP	-	EXPRESSION TAG	UNP Q16853
E	24	ASP	-	EXPRESSION TAG	UNP Q16853
E	25	ASP	-	EXPRESSION TAG	UNP Q16853
E	26	LYS	-	EXPRESSION TAG	UNP Q16853
E	27	GLU	-	EXPRESSION TAG	UNP Q16853
E	28	ASN	-	EXPRESSION TAG	UNP Q16853
E	29	LEU	-	EXPRESSION TAG	UNP Q16853
E	30	TYR	-	EXPRESSION TAG	UNP Q16853
E	31	PHE	-	EXPRESSION TAG	UNP Q16853
E	32	GLN	-	EXPRESSION TAG	UNP Q16853
F	16	ASP	-	EXPRESSION TAG	UNP Q16853
F	17	ILE	-	EXPRESSION TAG	UNP Q16853
F	18	VAL	-	EXPRESSION TAG	UNP Q16853
F	19	ASP	-	EXPRESSION TAG	UNP Q16853
F	20	TYR	-	EXPRESSION TAG	UNP Q16853
F	21	LYS	-	EXPRESSION TAG	UNP Q16853
F	22	ASP	-	EXPRESSION TAG	UNP Q16853
F	23	ASP	-	EXPRESSION TAG	UNP Q16853
F	24	ASP	-	EXPRESSION TAG	UNP Q16853
F	25	ASP	-	EXPRESSION TAG	UNP Q16853
F	26	LYS	-	EXPRESSION TAG	UNP Q16853
F	27	GLU	-	EXPRESSION TAG	UNP Q16853
F	28	ASN	-	EXPRESSION TAG	UNP Q16853
F	29	LEU	-	EXPRESSION TAG	UNP Q16853

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Chain	Residue	Modelled	Actual	Comment	Reference
F	30	TYR	-	EXPRESSION TAG	UNP Q16853
F	31	PHE	-	EXPRESSION TAG	UNP Q16853
F	32	GLN	-	EXPRESSION TAG	UNP Q16853
G	16	ASP	-	EXPRESSION TAG	UNP Q16853
G	17	ILE	-	EXPRESSION TAG	UNP Q16853
G	18	VAL	-	EXPRESSION TAG	UNP Q16853
G	19	ASP	-	EXPRESSION TAG	UNP Q16853
G	20	TYR	-	EXPRESSION TAG	UNP Q16853
G	21	LYS	-	EXPRESSION TAG	UNP Q16853
G	22	ASP	-	EXPRESSION TAG	UNP Q16853
G	23	ASP	-	EXPRESSION TAG	UNP Q16853
G	24	ASP	-	EXPRESSION TAG	UNP Q16853
G	25	ASP	-	EXPRESSION TAG	UNP Q16853
G	26	LYS	-	EXPRESSION TAG	UNP Q16853
G	27	GLU	-	EXPRESSION TAG	UNP Q16853
G	28	ASN	-	EXPRESSION TAG	UNP Q16853
G	29	LEU	-	EXPRESSION TAG	UNP Q16853
G	30	TYR	-	EXPRESSION TAG	UNP Q16853
G	31	PHE	-	EXPRESSION TAG	UNP Q16853
G	32	GLN	-	EXPRESSION TAG	UNP Q16853

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Cu 1 1	0	0
2	D	1	Total Cu 1 1	0	0
2	E	1	Total Cu 1 1	0	0
2	B	1	Total Cu 1 1	0	0
2	C	1	Total Cu 1 1	0	0
2	A	1	Total Cu 1 1	0	0
2	F	1	Total Cu 1 1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	2	Total Ca 2 2	0	0
3	D	2	Total Ca 2 2	0	0
3	E	2	Total Ca 2 2	0	0
3	B	2	Total Ca 2 2	0	0
3	C	2	Total Ca 2 2	0	0
3	A	2	Total Ca 2 2	0	0
3	F	2	Total Ca 2 2	0	0

- 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 39 22 2 15	0	0
4	B	3	Total C N O 39 22 2 15	0	0
4	C	3	Total C N O 39 22 2 15	0	0
4	D	3	Total C N O 39 22 2 15	0	0
4	E	3	Total C N O 39 22 2 15	0	0
4	F	3	Total C N O 39 22 2 15	0	0
4	G	3	Total C N O 39 22 2 15	0	0

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

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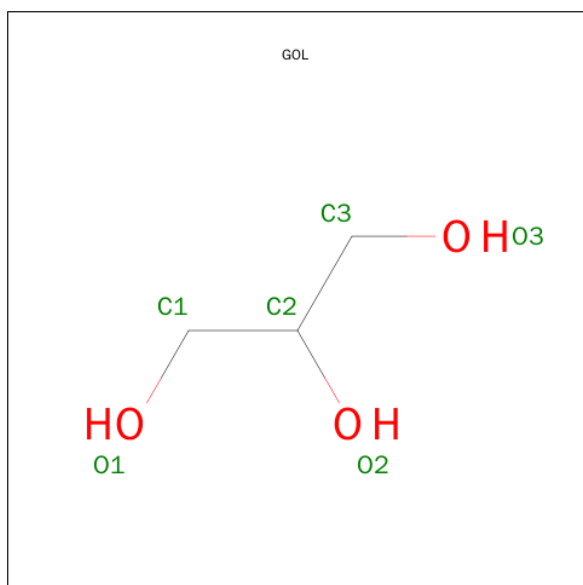
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	F	2	Total	C	N	O	0	0
			28	16	2	10		
5	G	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

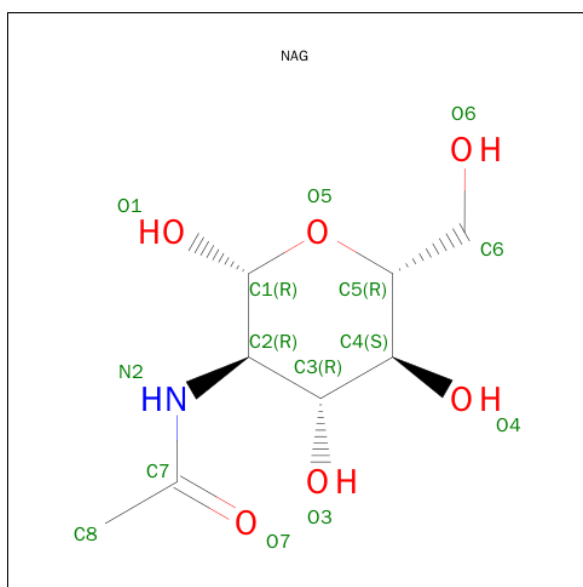
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 9 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 10 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	2	Total	C	N	O	0	0
			24	14	1	9		
10	D	2	Total	C	N	O	0	0
			24	14	1	9		
10	E	2	Total	C	N	O	0	0
			24	14	1	9		
10	F	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 11 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	G	2	Total	C	N	O	0	0
			24	14	1	9		

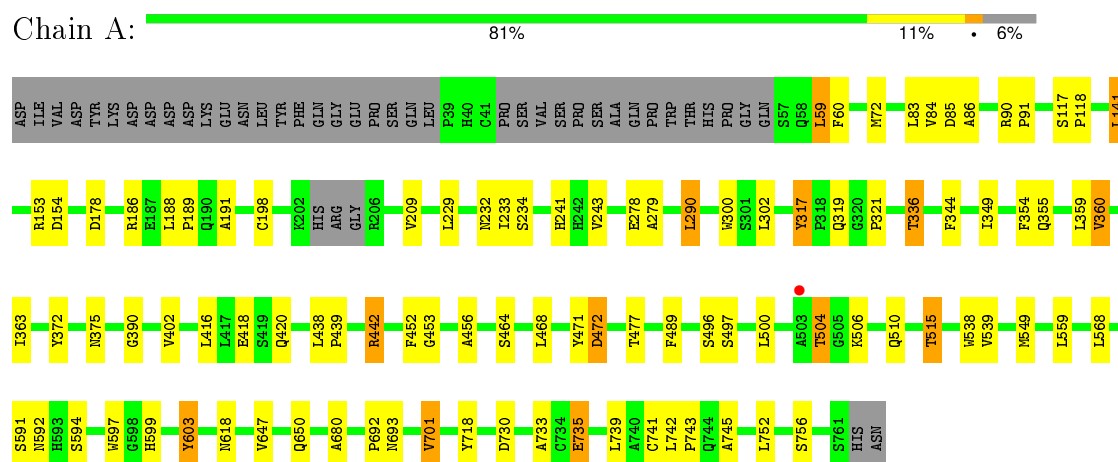
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	49	Total	O	0	0
			49	49		
12	B	47	Total	O	0	0
			47	47		
12	C	33	Total	O	0	0
			33	33		
12	D	40	Total	O	0	0
			40	40		
12	E	23	Total	O	0	0
			23	23		
12	F	23	Total	O	0	0
			23	23		
12	G	15	Total	O	0	0
			15	15		

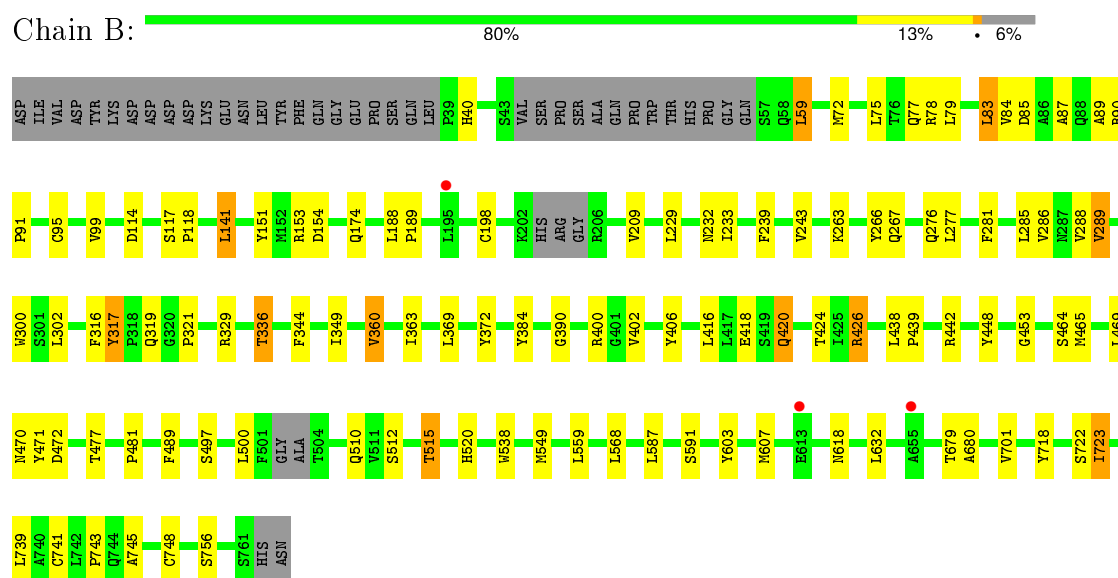
3 Residue-property plots

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

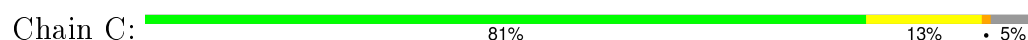
- Molecule 1: Membrane primary amine oxidase

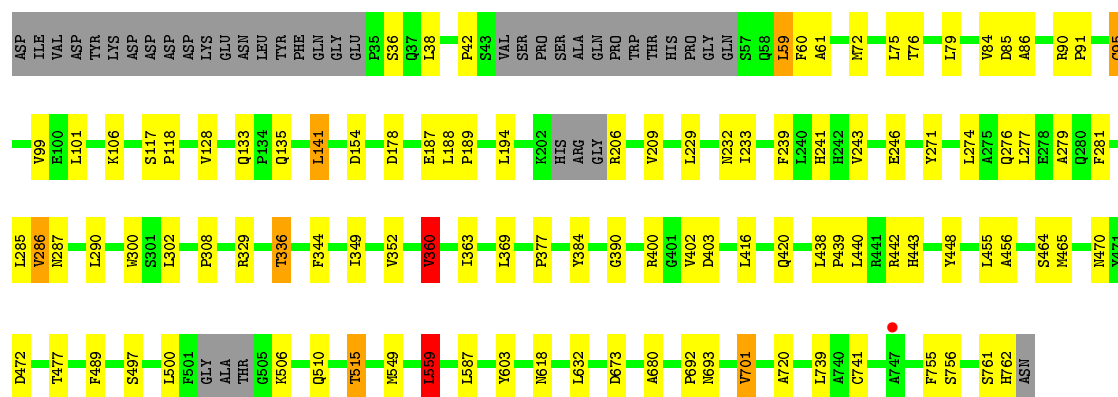


- Molecule 1: Membrane primary amine oxidase

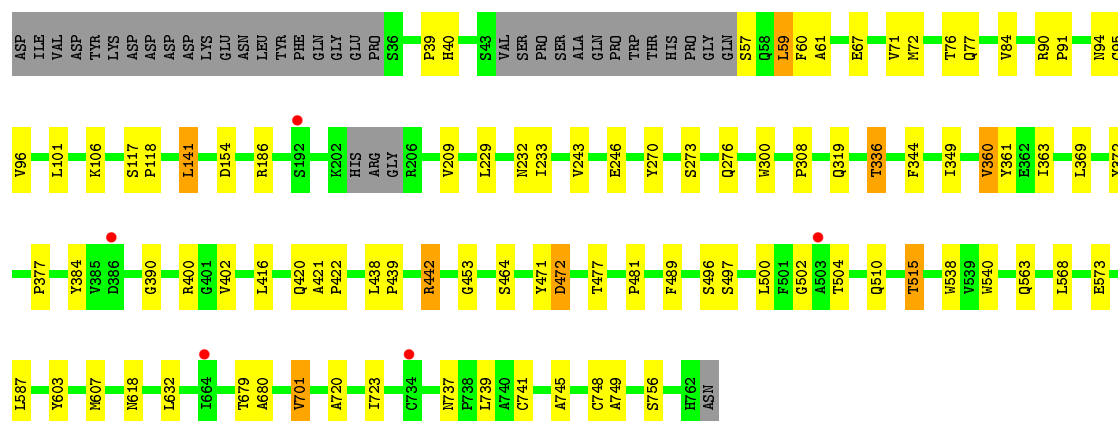
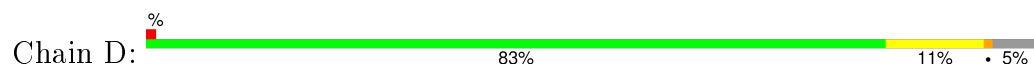


- Molecule 1: Membrane primary amine oxidase

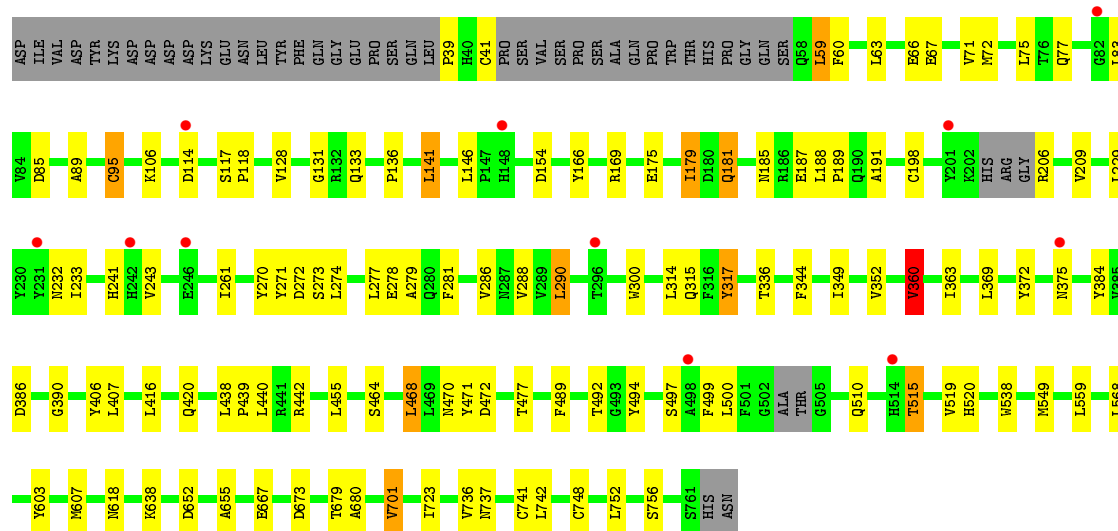
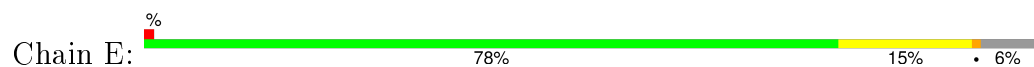




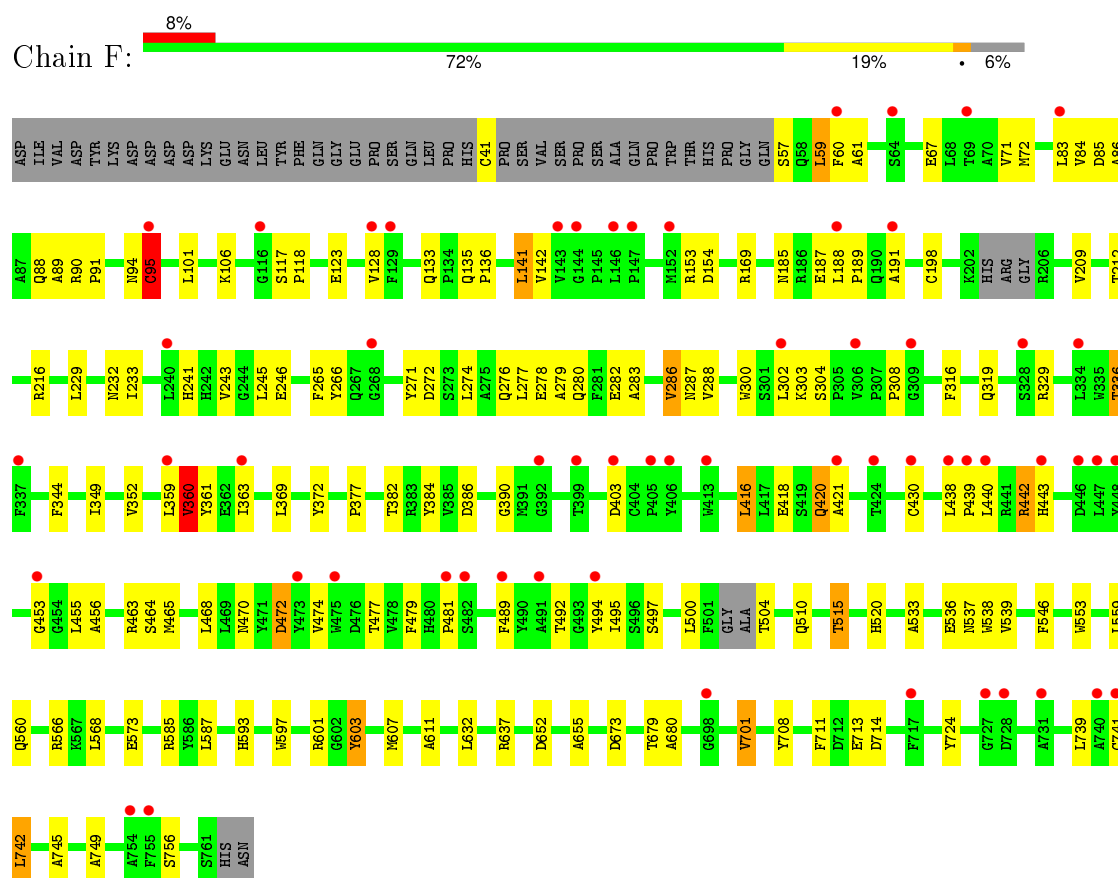
• Molecule 1: Membrane primary amine oxidase



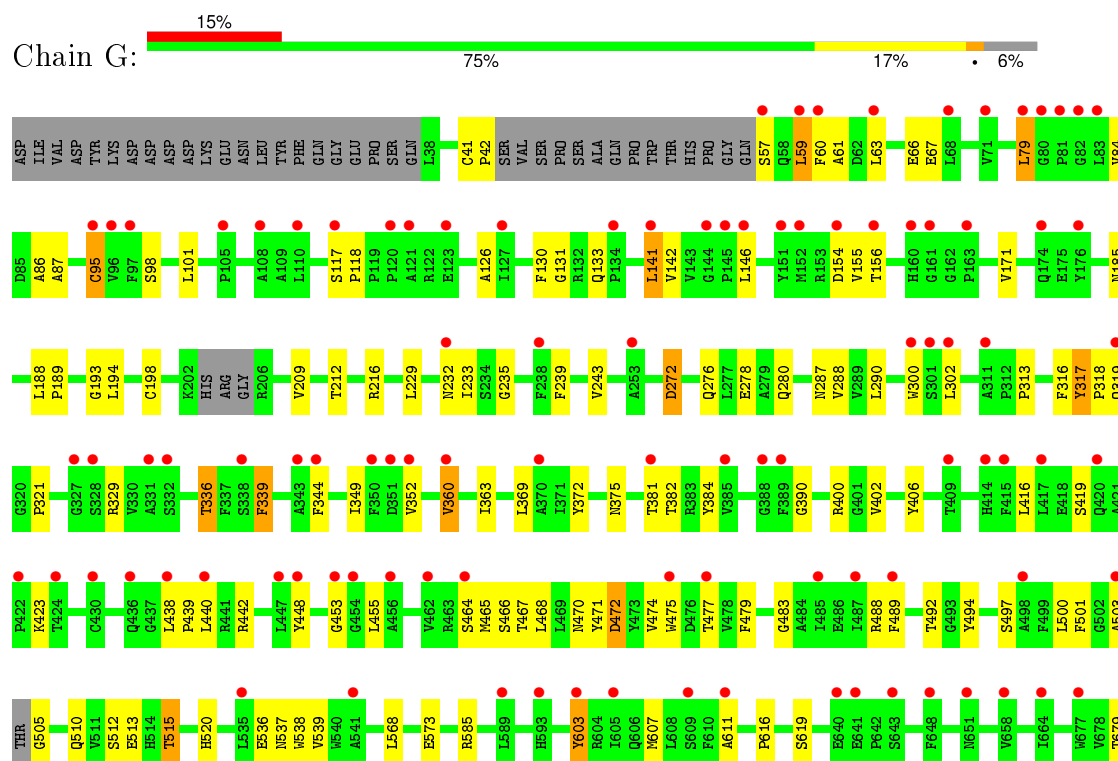
• Molecule 1: Membrane primary amine oxidase

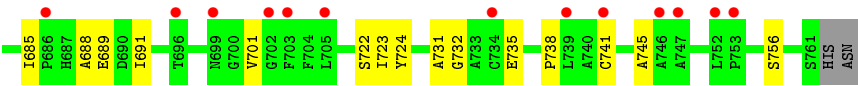


• Molecule 1: Membrane primary amine oxidase



- Molecule 1: Membrane primary amine oxidase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	394.47Å 115.83Å 179.29Å 90.00° 112.34° 90.00°	Depositor
Resolution (Å)	110.40 – 2.90 110.40 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.3 (110.40-2.90) 98.3 (110.40-2.90)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	0.19	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.5.0063	Depositor
R, R_{free}	0.250 , 0.286 0.249 , 0.282	Depositor DCC
R_{free} test set	8187 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 162838 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	39103	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BMA, NAG, CA, NDG, FUC, TPQ, FUL, CU

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	0.76	1/5660 (0.0%)	0.72	2/7728 (0.0%)
1	B	0.76	2/5653 (0.0%)	0.73	2/7716 (0.0%)
1	C	0.70	2/5665 (0.0%)	0.71	1/7737 (0.0%)
1	D	0.69	0/5672	0.72	2/7746 (0.0%)
1	E	0.70	1/5582 (0.0%)	0.72	2/7622 (0.0%)
1	F	0.83	1/5551 (0.0%)	0.76	1/7583 (0.0%)
1	G	0.85	0/5553	0.77	1/7590 (0.0%)
All	All	0.76	7/39336 (0.0%)	0.73	11/53722 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
4	D	1	0
5	G	1	0
9	B	1	0
10	C	1	0
10	D	1	0
10	E	1	0
All	All	6	1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	430	CYS	CB-SG	-8.73	1.67	1.82
1	B	95	CYS	CB-SG	-7.45	1.69	1.82
1	C	95	CYS	CB-SG	-7.08	1.70	1.82
1	A	360	VAL	CB-CG1	-6.40	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	95	CYS	CB-SG	-5.80	1.72	1.81

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	701	VAL	CG1-CB-CG2	9.11	125.48	110.90
1	A	360	VAL	CG1-CB-CG2	6.69	121.61	110.90
1	D	360	VAL	CG1-CB-CG2	6.38	121.11	110.90
1	C	559	LEU	CB-CG-CD1	6.27	121.66	111.00
1	B	426	ARG	NE-CZ-NH1	6.23	123.41	120.30

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	B	1769	NAG	C1
10	C	1771	FUL	C1
4	D	1767	BMA	C1
10	D	1769	NAG	C1
10	E	1769	NAG	C1

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	95	CYS	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	5494	0	5167	65	0
1	B	5488	0	5174	79	0
1	C	5498	0	5157	77	0
1	D	5510	0	5162	61	0
1	E	5423	0	5067	82	0
1	F	5390	0	4995	125	0
1	G	5392	0	4980	110	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
4	A	39	0	34	0	0
4	B	39	0	34	0	0
4	C	39	0	34	3	0
4	D	39	0	34	5	0
4	E	39	0	34	2	0
4	F	39	0	34	0	0
4	G	39	0	34	4	0
5	A	28	0	25	1	0
5	C	28	0	25	6	0
5	D	28	0	25	3	0
5	E	28	0	25	6	0
5	F	28	0	25	1	0
5	G	28	0	25	0	0
6	A	24	0	22	0	0
7	A	6	0	8	0	0
8	B	14	0	13	4	0
8	D	14	0	13	0	0
9	B	38	0	34	0	0
10	C	24	0	22	0	0
10	D	24	0	22	0	0
10	E	24	0	22	0	0
10	F	24	0	22	1	0
11	G	24	0	22	0	0
12	A	49	0	0	0	0
12	B	47	0	0	1	0
12	C	33	0	0	0	0
12	D	40	0	0	0	0
12	E	23	0	0	0	0
12	F	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	G	15	0	0	3	0
All	All	39103	0	36290	544	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.

The worst 5 of 544 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:C:232:ASN:ND2	5:C:1772:NAG:H83	1.56	1.20
1:C:232:ASN:HD22	5:C:1772:NAG:H83	0.90	1.06
1:E:206:ARG:O	5:E:1772:NAG:H81	1.58	1.03
1:D:72:MET:HE1	1:D:416:LEU:HD11	1.41	1.01
1:D:232:ASN:HD22	5:D:1772:NAG:H83	1.19	1.01

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	701/748 (94%)	660 (94%)	40 (6%)	1 (0%)	56	87
1	B	698/748 (93%)	653 (94%)	44 (6%)	1 (0%)	56	87
1	C	702/748 (94%)	659 (94%)	40 (6%)	3 (0%)	39	74
1	D	705/748 (94%)	666 (94%)	38 (5%)	1 (0%)	56	87
1	E	693/748 (93%)	655 (94%)	35 (5%)	3 (0%)	39	74
1	F	696/748 (93%)	658 (94%)	37 (5%)	1 (0%)	56	87
1	G	698/748 (93%)	650 (93%)	47 (7%)	1 (0%)	56	87
All	All	4893/5236 (93%)	4601 (94%)	281 (6%)	11 (0%)	52	84

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	618	ASN
1	G	87	ALA
1	C	618	ASN
1	C	279	ALA
1	E	272	ASP

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	568/625 (91%)	545 (96%)	23 (4%)	38	74
1	B	569/625 (91%)	549 (96%)	20 (4%)	43	78
1	C	565/625 (90%)	546 (97%)	19 (3%)	44	79
1	D	567/625 (91%)	546 (96%)	21 (4%)	41	77
1	E	555/625 (89%)	533 (96%)	22 (4%)	38	74
1	F	549/625 (88%)	524 (95%)	25 (5%)	33	69
1	G	545/625 (87%)	519 (95%)	26 (5%)	31	67
All	All	3918/4375 (90%)	3762 (96%)	156 (4%)	38	74

5 of 156 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	442	ARG
1	E	141	LEU
1	G	416	LEU
1	D	472	ASP
1	D	701	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	319	GLN

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Mol	Chain	Res	Type
1	D	563	GLN
1	F	319	GLN
1	C	693	ASN
1	G	319	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 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	TPQ	A	471	1	13,14,15	1.48	2 (15%)	15,19,21	2.61	4 (26%)
1	TPQ	B	471	1	13,14,15	1.49	2 (15%)	15,19,21	3.18	3 (20%)
1	TPQ	C	471	1	13,14,15	1.45	2 (15%)	15,19,21	2.90	4 (26%)
1	TPQ	D	471	1	13,14,15	1.43	1 (7%)	15,19,21	2.58	3 (20%)
1	TPQ	E	471	1	13,14,15	1.66	2 (15%)	15,19,21	2.82	4 (26%)
1	TPQ	F	471	1	13,14,15	1.68	4 (30%)	15,19,21	2.06	5 (33%)
1	TPQ	G	471	1	13,14,15	1.47	2 (15%)	15,19,21	2.75	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPQ	A	471	1	-	0/4/22/24	0/1/1/1
1	TPQ	B	471	1	-	0/4/22/24	0/1/1/1
1	TPQ	C	471	1	-	0/4/22/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPQ	D	471	1	-	0/4/22/24	0/1/1/1
1	TPQ	E	471	1	-	0/4/22/24	0/1/1/1
1	TPQ	F	471	1	-	0/4/22/24	0/1/1/1
1	TPQ	G	471	1	-	0/4/22/24	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	471	TPQ	O4-C4	-3.98	1.23	1.34
1	C	471	TPQ	O4-C4	-3.85	1.24	1.34
1	A	471	TPQ	O4-C4	-3.81	1.24	1.34
1	E	471	TPQ	O4-C4	-3.68	1.24	1.34
1	B	471	TPQ	O4-C4	-3.50	1.25	1.34

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	471	TPQ	C1-C6-C5	-8.84	117.58	122.97
1	B	471	TPQ	C1-C6-C5	-8.17	118.00	122.97
1	E	471	TPQ	C1-C6-C5	-7.28	118.53	122.97
1	G	471	TPQ	C1-C6-C5	-7.15	118.61	122.97
1	A	471	TPQ	C1-C6-C5	-6.90	118.77	122.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	471	TPQ	1	0
1	B	471	TPQ	1	0
1	D	471	TPQ	1	0
1	E	471	TPQ	2	0
1	G	471	TPQ	2	0

5.5 Carbohydrates

48 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$
4	NAG	A	1765	1,4	14,14,15	0.67	0	15,19,21	2.32	2 (13%)
4	NAG	A	1766	4	14,14,15	0.76	1 (7%)	15,19,21	1.33	2 (13%)
4	BMA	A	1767	4	11,11,12	0.96	0	14,15,17	2.49	5 (35%)
6	NDG	A	1769	1,6	14,14,15	2.27	3 (21%)	15,19,21	2.94	8 (53%)
6	FUL	A	1771	6	10,10,11	1.27	1 (10%)	14,14,16	2.45	4 (28%)
5	NAG	A	1772	1,5	14,14,15	0.96	1 (7%)	15,19,21	2.03	5 (33%)
5	NAG	A	1773	5	14,14,15	0.82	1 (7%)	15,19,21	1.10	0
4	NAG	B	1765	1,4	14,14,15	0.71	0	15,19,21	2.15	3 (20%)
4	NAG	B	1766	4	14,14,15	0.73	0	15,19,21	2.67	4 (26%)
4	BMA	B	1767	4	11,11,12	1.12	1 (9%)	14,15,17	2.01	4 (28%)
9	NAG	B	1769	9,1	14,14,15	0.76	0	15,19,21	1.78	3 (20%)
9	NAG	B	1770	9	14,14,15	0.64	0	15,19,21	1.49	4 (26%)
9	FUL	B	1771	9	10,10,11	1.77	2 (20%)	14,14,16	2.58	5 (35%)
4	NAG	C	1765	1,4	14,14,15	0.99	1 (7%)	15,19,21	1.99	6 (40%)
4	NAG	C	1766	4	14,14,15	0.89	1 (7%)	15,19,21	2.38	4 (26%)
4	BMA	C	1767	4	11,11,12	1.23	1 (9%)	14,15,17	1.90	5 (35%)
10	NAG	C	1769	1,10	14,14,15	1.51	4 (28%)	15,19,21	1.52	3 (20%)
10	FUL	C	1771	10	10,10,11	0.87	0	14,14,16	1.95	4 (28%)
5	NAG	C	1772	1,5	14,14,15	0.69	0	15,19,21	1.35	2 (13%)
5	NAG	C	1773	5	14,14,15	0.89	1 (7%)	15,19,21	2.91	5 (33%)
4	NAG	D	1765	1,4	14,14,15	1.00	1 (7%)	15,19,21	2.52	4 (26%)
4	NAG	D	1766	4	14,14,15	0.50	0	15,19,21	1.92	5 (33%)
4	BMA	D	1767	4	11,11,12	0.83	0	14,15,17	3.10	3 (21%)
10	NAG	D	1769	1,10	14,14,15	1.38	3 (21%)	15,19,21	1.55	4 (26%)
10	FUL	D	1771	10	10,10,11	2.34	5 (50%)	14,14,16	2.42	6 (42%)
5	NAG	D	1772	1,5	14,14,15	0.81	0	15,19,21	2.14	4 (26%)
5	NAG	D	1773	5	14,14,15	0.92	1 (7%)	15,19,21	1.51	3 (20%)
4	NAG	E	1765	1,4	14,14,15	0.51	0	15,19,21	2.25	6 (40%)
4	NAG	E	1766	4	14,14,15	0.57	0	15,19,21	1.01	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BMA	E	1767	4	11,11,12	0.73	0	14,15,17	1.08	1 (7%)
10	NAG	E	1769	1,10	14,14,15	1.37	3 (21%)	15,19,21	2.61	3 (20%)
10	FUL	E	1771	10	10,10,11	1.68	1 (10%)	14,14,16	2.37	4 (28%)
5	NAG	E	1772	1,5	14,14,15	0.53	0	15,19,21	1.21	1 (6%)
5	NAG	E	1773	5	14,14,15	0.74	0	15,19,21	1.56	3 (20%)
4	NAG	F	1765	1,4	14,14,15	0.79	0	15,19,21	1.48	2 (13%)
4	NAG	F	1766	4	14,14,15	0.73	0	15,19,21	2.21	1 (6%)
4	BMA	F	1767	4	11,11,12	1.06	1 (9%)	14,15,17	1.29	1 (7%)
10	NAG	F	1769	1,10	14,14,15	1.12	2 (14%)	15,19,21	3.09	6 (40%)
10	FUL	F	1771	10	10,10,11	1.18	0	14,14,16	3.07	5 (35%)
5	NAG	F	1772	1,5	14,14,15	0.56	0	15,19,21	2.06	5 (33%)
5	NAG	F	1773	5	14,14,15	0.82	1 (7%)	15,19,21	2.28	3 (20%)
4	NAG	G	1765	1,4	14,14,15	0.67	0	15,19,21	1.63	2 (13%)
4	NAG	G	1766	4	14,14,15	0.69	0	15,19,21	1.65	3 (20%)
4	BMA	G	1767	4	11,11,12	0.73	0	14,15,17	1.89	2 (14%)
11	NAG	G	1769	11,1	14,14,15	1.07	2 (14%)	15,19,21	1.94	3 (20%)
11	FUC	G	1771	11	10,10,11	1.88	1 (10%)	14,14,16	1.95	4 (28%)
5	NAG	G	1772	1,5	14,14,15	0.57	0	15,19,21	2.54	8 (53%)
5	NAG	G	1773	5	14,14,15	0.56	0	15,19,21	0.89	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1765	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1766	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1767	4	-	0/2/19/22	0/1/1/1
6	NDG	A	1769	1,6	-	0/6/23/26	0/1/1/1
6	FUL	A	1771	6	-	0/0/17/20	0/1/1/1
5	NAG	A	1772	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1773	5	-	0/6/23/26	0/1/1/1
4	NAG	B	1765	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1766	4	-	0/6/23/26	0/1/1/1
4	BMA	B	1767	4	-	0/2/19/22	0/1/1/1
9	NAG	B	1769	9,1	1/1/5/7	0/6/23/26	0/1/1/1
9	NAG	B	1770	9	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	FUL	B	1771	9	-	0/0/17/20	0/1/1/1
4	NAG	C	1765	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	1766	4	-	0/6/23/26	0/1/1/1
4	BMA	C	1767	4	-	0/2/19/22	0/1/1/1
10	NAG	C	1769	1,10	-	0/6/23/26	0/1/1/1
10	FUL	C	1771	10	1/1/4/5	0/0/17/20	0/1/1/1
5	NAG	C	1772	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1773	5	-	0/6/23/26	0/1/1/1
4	NAG	D	1765	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	1766	4	-	0/6/23/26	0/1/1/1
4	BMA	D	1767	4	1/1/4/5	0/2/19/22	0/1/1/1
10	NAG	D	1769	1,10	1/1/5/7	0/6/23/26	0/1/1/1
10	FUL	D	1771	10	-	0/0/17/20	0/1/1/1
5	NAG	D	1772	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	1773	5	-	0/6/23/26	0/1/1/1
4	NAG	E	1765	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	1766	4	-	0/6/23/26	0/1/1/1
4	BMA	E	1767	4	-	0/2/19/22	0/1/1/1
10	NAG	E	1769	1,10	1/1/5/7	0/6/23/26	0/1/1/1
10	FUL	E	1771	10	-	0/0/17/20	0/1/1/1
5	NAG	E	1772	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	1773	5	-	0/6/23/26	0/1/1/1
4	NAG	F	1765	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	1766	4	-	0/6/23/26	0/1/1/1
4	BMA	F	1767	4	-	0/2/19/22	0/1/1/1
10	NAG	F	1769	1,10	-	0/6/23/26	0/1/1/1
10	FUL	F	1771	10	-	0/0/17/20	0/1/1/1
5	NAG	F	1772	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	1773	5	-	0/6/23/26	0/1/1/1
4	NAG	G	1765	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	1766	4	-	0/6/23/26	0/1/1/1
4	BMA	G	1767	4	-	0/2/19/22	0/1/1/1
11	NAG	G	1769	11,1	-	0/6/23/26	0/1/1/1
11	FUC	G	1771	11	-	0/0/17/20	0/1/1/1
5	NAG	G	1772	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	G	1773	5	-	0/6/23/26	0/1/1/1

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1765	NAG	O5-C1	-2.79	1.39	1.43
4	C	1765	NAG	O5-C1	-2.64	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1772	NAG	O5-C1	-2.25	1.40	1.43
4	A	1766	NAG	O5-C1	-2.23	1.40	1.43
4	C	1766	NAG	O5-C1	-2.14	1.40	1.43

The worst 5 of 172 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	F	1769	NAG	O5-C5-C6	-9.39	87.03	107.35
4	D	1767	BMA	C1-C2-C3	-9.04	98.85	109.54
10	F	1771	FUL	C1-O5-C5	-6.20	102.80	112.38
5	G	1772	NAG	C4-C3-C2	-5.50	102.69	111.23
10	F	1771	FUL	O5-C5-C4	-5.27	100.39	109.53

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	G	1772	NAG	C1
4	D	1767	BMA	C1
10	C	1771	FUL	C1
10	D	1769	NAG	C1
9	B	1769	NAG	C1

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1772	NAG	1	0
4	C	1765	NAG	3	0
5	C	1772	NAG	6	0
4	D	1766	NAG	5	0
4	D	1767	BMA	1	0
5	D	1772	NAG	3	0
4	E	1765	NAG	2	0
5	E	1772	NAG	6	0
10	F	1769	NAG	1	0
5	F	1772	NAG	1	0
4	G	1765	NAG	1	0
4	G	1766	NAG	3	0

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 21 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	GOL	A	764	-	5,5,5	0.47	0	5,5,5	0.45	0
8	NAG	B	1772	1	14,14,15	0.72	0	15,19,21	3.16	7 (46%)
8	NAG	D	1775	1	14,14,15	0.66	0	15,19,21	2.24	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	A	764	-	-	0/4/4/4	0/0/0/0
8	NAG	B	1772	1	-	0/6/23/26	0/1/1/1
8	NAG	D	1775	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1772	NAG	C4-C3-C2	-7.31	99.87	111.23
8	B	1772	NAG	C3-C4-C5	-2.46	105.92	110.20
8	B	1772	NAG	O7-C7-C8	-2.22	118.00	122.06
8	B	1772	NAG	O3-C3-C4	2.14	115.16	110.34
8	B	1772	NAG	O3-C3-C2	2.45	113.97	109.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1772	NAG	4	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 [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	704/748 (94%)	0.49	1 (0%) 95 96	13, 39, 43, 63	0
1	B	704/748 (94%)	0.36	3 (0%) 93 92	12, 39, 43, 65	0
1	C	708/748 (94%)	0.34	1 (0%) 95 96	16, 39, 45, 73	0
1	D	710/748 (94%)	0.41	5 (0%) 89 88	16, 39, 46, 68	0
1	E	701/748 (93%)	0.30	11 (1%) 74 72	22, 39, 49, 76	0
1	F	700/748 (93%)	0.79	58 (8%) 14 9	26, 39, 47, 69	0
1	G	704/748 (94%)	1.05	114 (16%) 3 1	32, 39, 49, 82	0
All	All	4931/5236 (94%)	0.54	193 (3%) 43 36	12, 39, 46, 82	0

The worst 5 of 193 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	741	CYS	5.2
1	G	352	VAL	4.2
1	G	79	LEU	4.2
1	F	489	PHE	4.1
1	F	147	PRO	3.9

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	TPQ	C	471	14/15	0.92	0.28	-	22,47,61,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	TPQ	E	471	14/15	0.94	0.26	-	36,45,58,65	0
1	TPQ	B	471	14/15	0.95	0.24	-	24,31,57,62	0
1	TPQ	G	471	14/15	0.86	0.44	-	44,60,67,84	0
1	TPQ	D	471	14/15	0.95	0.23	-	21,31,48,64	0
1	TPQ	F	471	14/15	0.90	0.29	-	36,40,50,58	0
1	TPQ	A	471	14/15	0.97	0.20	-	17,28,56,58	0

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
5	NAG	C	1773	14/15	0.76	0.31	1.18	56,75,81,82	0
10	NAG	E	1769	14/15	0.81	0.24	1.14	39,72,84,89	0
5	NAG	G	1773	14/15	0.71	0.41	0.87	83,100,107,111	0
4	NAG	B	1765	14/15	0.97	0.17	-0.22	15,23,40,42	0
4	NAG	G	1765	14/15	0.89	0.26	-0.41	65,73,76,78	0
5	NAG	C	1772	14/15	0.96	0.20	-0.65	34,48,72,77	0
6	NDG	A	1769	14/15	0.86	0.17	-0.71	21,56,68,72	0
5	NAG	E	1772	14/15	0.85	0.20	-0.73	68,77,87,88	0
5	NAG	G	1772	14/15	0.85	0.22	-0.85	70,79,85,92	0
5	NAG	F	1772	14/15	0.81	0.20	-0.94	48,66,75,79	0
4	NAG	D	1765	14/15	0.95	0.15	-1.05	18,40,55,56	0
4	NAG	C	1765	14/15	0.97	0.15	-1.30	15,23,37,49	0
4	NAG	E	1765	14/15	0.94	0.14	-1.34	34,50,64,74	0
9	NAG	B	1769	14/15	0.95	0.15	-1.36	27,39,51,51	0
5	NAG	D	1772	14/15	0.94	0.18	-1.56	7,32,40,50	0
5	NAG	A	1773	14/15	0.92	0.17	-1.62	39,54,56,60	0
4	NAG	F	1765	14/15	0.90	0.16	-1.67	32,56,60,67	0
5	NAG	A	1772	14/15	0.95	0.15	-2.20	14,37,43,46	0
4	NAG	A	1765	14/15	0.96	0.14	-3.53	20,26,34,41	0
4	NAG	F	1766	14/15	0.90	0.18	-	49,66,83,86	0
9	FUL	B	1771	10/11	0.94	0.17	-	21,29,43,47	0
4	BMA	C	1767	11/12	0.73	0.23	-	58,73,74,75	0
4	NAG	E	1766	14/15	0.84	0.22	-	74,85,87,88	0
4	BMA	D	1767	11/12	0.77	0.18	-	42,68,74,76	0
4	BMA	A	1767	11/12	0.73	0.22	-	57,73,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	A	1766	14/15	0.93	0.14	-	31,46,56,62	0
4	NAG	C	1766	14/15	0.86	0.21	-	43,53,66,67	0
4	BMA	G	1767	11/12	0.59	0.25	-	76,88,92,93	0
11	FUC	G	1771	10/11	0.86	0.24	-	39,68,73,76	0
5	NAG	F	1773	14/15	0.70	0.31	-	73,85,91,91	0
10	FUL	C	1771	10/11	0.98	0.12	-	16,28,30,30	0
4	BMA	F	1767	11/12	0.49	0.26	-	97,102,107,110	0
10	NAG	D	1769	14/15	0.86	0.18	-	34,68,74,90	0
4	NAG	G	1766	14/15	0.89	0.24	-	63,80,85,89	0
11	NAG	G	1769	14/15	0.81	0.18	-	55,76,89,89	0
5	NAG	E	1773	14/15	0.78	0.22	-	60,80,85,86	0
10	FUL	F	1771	10/11	0.90	0.13	-	33,47,56,57	0
4	NAG	D	1766	14/15	0.87	0.24	-	45,68,74,77	0
10	NAG	F	1769	14/15	0.92	0.14	-	33,45,55,59	0
6	FUL	A	1771	10/11	0.95	0.16	-	14,34,41,44	0
9	NAG	B	1770	14/15	0.88	0.22	-	51,59,71,74	0
4	NAG	B	1766	14/15	0.88	0.19	-	34,55,65,66	0
5	NAG	D	1773	14/15	0.83	0.25	-	46,72,77,78	0
10	FUL	E	1771	10/11	0.92	0.16	-	46,55,58,61	0
4	BMA	B	1767	11/12	0.74	0.18	-	53,61,69,71	0
10	NAG	C	1769	14/15	0.87	0.19	-	29,40,47,51	0
4	BMA	E	1767	11/12	0.78	0.17	-	58,76,83,87	0
10	FUL	D	1771	10/11	0.90	0.16	-	15,51,58,58	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	CA	B	1764	1/1	0.93	0.32	2.92	88,88,88,88	0
3	CA	G	1764	1/1	0.93	0.16	-1.07	94,94,94,94	0
3	CA	D	1763	1/1	0.97	0.13	-1.16	39,39,39,39	0
3	CA	E	1763	1/1	0.96	0.12	-2.09	43,43,43,43	0
7	GOL	A	764	6/6	0.91	0.16	-2.14	43,43,43,43	0
3	CA	B	1763	1/1	0.96	0.14	-2.20	35,35,35,35	0
3	CA	D	1764	1/1	0.96	0.08	-2.25	65,65,65,65	0
3	CA	C	1763	1/1	0.95	0.11	-2.34	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	CA	G	1763	1/1	0.89	0.09	-2.40	51,51,51,51	0
3	CA	F	1763	1/1	0.94	0.10	-2.48	42,42,42,42	0
3	CA	F	1764	1/1	0.94	0.09	-2.77	91,91,91,91	0
3	CA	A	1764	1/1	0.98	0.12	-3.10	50,50,50,50	0
3	CA	E	1764	1/1	0.98	0.06	-3.17	46,46,46,46	0
3	CA	A	1763	1/1	0.98	0.08	-5.10	32,32,32,32	0
3	CA	C	1764	1/1	0.97	0.10	-5.74	53,53,53,53	0
8	NAG	B	1772	14/15	0.81	0.36	-	50,66,69,72	0
2	CU	F	1762	1/1	0.97	0.08	-	60,60,60,60	0
2	CU	C	1762	1/1	0.96	0.06	-	58,58,58,58	0
2	CU	E	1762	1/1	0.97	0.05	-	49,49,49,49	0
2	CU	G	1762	1/1	0.92	0.05	-	69,69,69,69	0
8	NAG	D	1775	14/15	0.82	0.19	-	74,84,90,90	0
2	CU	B	1762	1/1	0.98	0.07	-	49,49,49,49	0
2	CU	D	1762	1/1	1.00	0.10	-	44,44,44,44	0
2	CU	A	1762	1/1	0.97	0.08	-	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.