



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:11 PM UTC

PDB ID : 1GAL / pdb_00001gal
Title : CRYSTAL STRUCTURE OF GLUCOSE OXIDASE FROM ASPERGILLUS
NIGER: REFINED AT 2.3 ANGSTROMS RESOLUTION
Authors : Hecht, H.J.; Kalisz, K.; Hendle, J.; Schmid, R.D.; Schomburg, D.
Deposited on : 1992-08-27
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

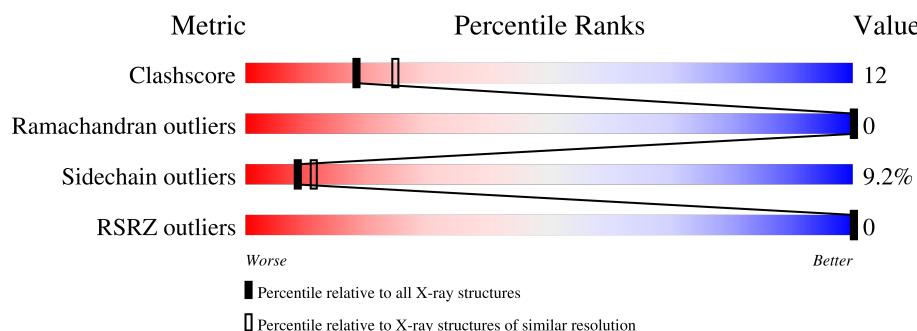
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	583	 52% 37% 9% .
2	B	5	 100%

2 Entry composition [i](#)

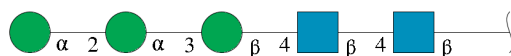
There are 5 unique types of molecules in this entry. The entry contains 4774 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLUCOSE OXIDASE.

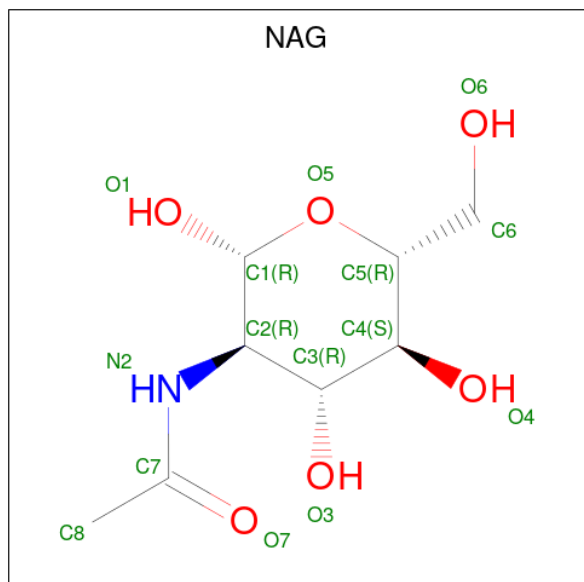
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	0	0
			4452	2801	764	873	14			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



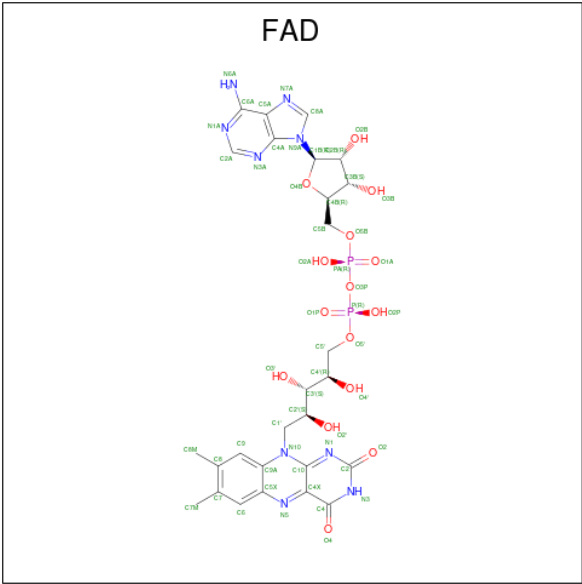
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



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

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 53 27 9 15 2	0	0

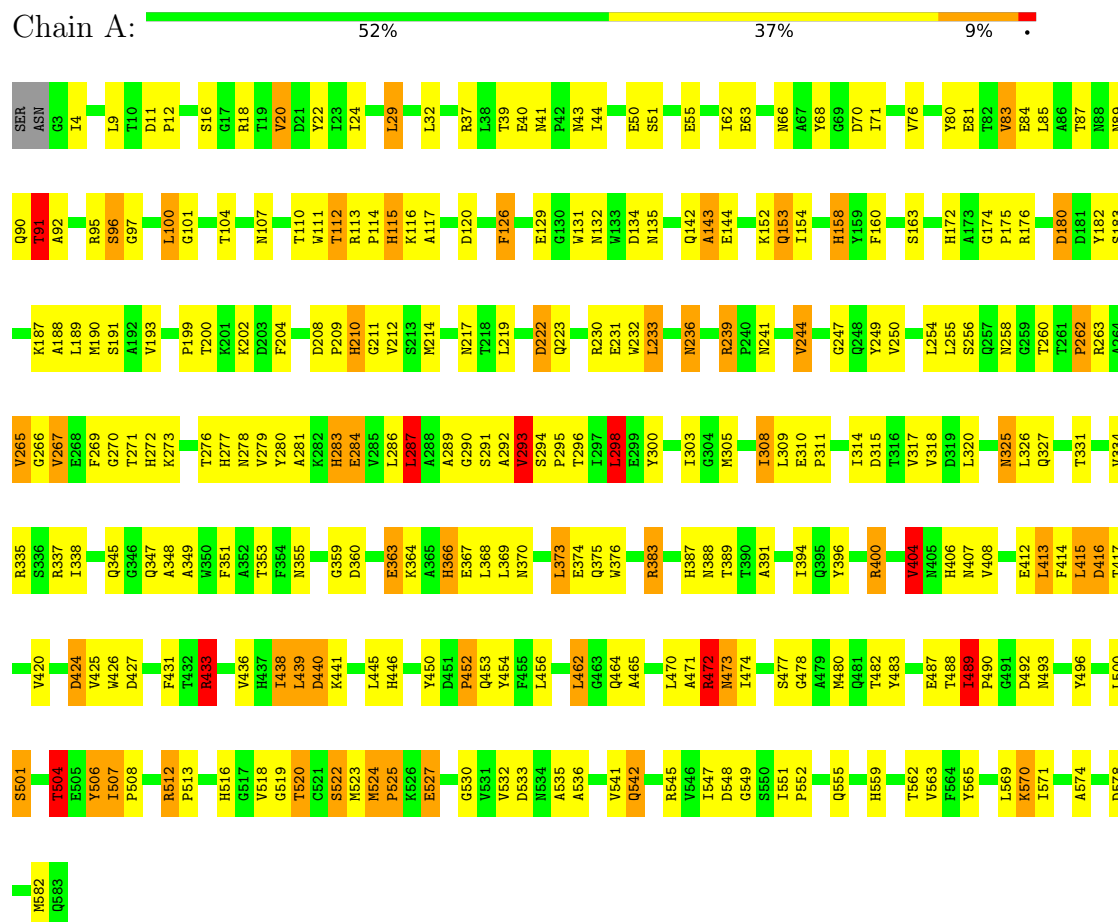
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	152	Total O 152 152	0	0

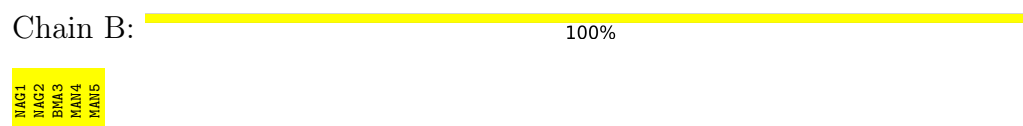
3 Residue-property plots

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: GLUCOSE OXIDASE



• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	66.50Å 66.50Å 214.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.30 10.00 – 2.31	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.30) 83.7 (10.00-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.30Å)	Xtriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.181 , (Not available) 0.163 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.044 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4774	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% 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: FAD, MAN, BMA, 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	1.07	2/4560 (0.0%)	2.27	213/6219 (3.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	507	ILE	CA-CB	8.47	1.58	1.54
1	A	547	ILE	CA-CB	5.17	1.60	1.54

All (213) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	493	ASN	CA-CB-CG	15.26	127.86	112.60
1	A	208	ASP	O-C-N	13.46	130.65	121.23
1	A	545	ARG	NE-CZ-NH2	-13.17	107.35	119.20
1	A	70	ASP	CA-CB-CG	11.61	124.21	112.60
1	A	545	ARG	NE-CZ-NH1	11.09	132.59	121.50
1	A	366	HIS	CA-CB-CG	-10.75	103.05	113.80
1	A	222	ASP	CA-CB-CG	10.64	123.24	112.60
1	A	492	ASP	CA-CB-CG	10.37	122.97	112.60
1	A	208	ASP	CA-CB-CG	9.85	122.45	112.60
1	A	135	ASN	CA-CB-CG	-9.81	102.78	112.60
1	A	388	ASN	OD1-CG-ND2	-9.46	113.14	122.60
1	A	512	ARG	NE-CZ-NH1	9.41	130.91	121.50
1	A	519	GLY	N-CA-C	9.34	127.06	114.92
1	A	95	ARG	NE-CZ-NH1	9.23	130.73	121.50
1	A	446	HIS	CA-CB-CG	-9.19	104.61	113.80
1	A	559	HIS	CA-CB-CG	-9.14	104.66	113.80
1	A	493	ASN	OD1-CG-ND2	-9.13	113.47	122.60
1	A	135	ASN	OD1-CG-ND2	9.08	131.68	122.60
1	A	416	ASP	CA-CB-CG	-8.92	103.68	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	433	ARG	CD-NE-CZ	8.83	136.76	124.40
1	A	334	VAL	CA-C-O	-8.82	111.36	120.27
1	A	551	ILE	N-CA-C	8.58	127.42	108.88
1	A	104	THR	N-CA-C	-8.56	102.28	112.89
1	A	290	GLY	CA-C-O	-8.55	116.33	122.23
1	A	506	TYR	CA-C-N	8.47	128.56	120.43
1	A	506	TYR	C-N-CA	8.47	128.56	120.43
1	A	317	VAL	N-CA-C	-8.37	103.66	111.45
1	A	547	ILE	N-CA-C	8.14	119.91	112.17
1	A	80	TYR	CA-C-O	-8.14	112.04	121.16
1	A	134	ASP	CA-CB-CG	-7.95	104.65	112.60
1	A	236	ASN	OD1-CG-ND2	-7.93	114.67	122.60
1	A	547	ILE	N-CA-CB	-7.89	101.78	112.28
1	A	427	ASP	N-CA-C	-7.85	97.24	109.25
1	A	293	VAL	CB-CA-C	7.82	118.58	110.91
1	A	142	GLN	CG-CD-NE2	7.75	128.02	116.40
1	A	370	ASN	CA-C-O	-7.72	111.09	119.97
1	A	191	SER	N-CA-CB	7.72	121.58	110.16
1	A	208	ASP	N-CA-CB	7.64	122.69	111.77
1	A	18	ARG	CD-NE-CZ	7.57	134.99	124.40
1	A	472	ARG	NE-CZ-NH1	7.54	129.04	121.50
1	A	120	ASP	O-C-N	7.51	130.09	122.12
1	A	190	MET	CA-C-O	-7.51	112.59	120.55
1	A	271	THR	CA-CB-OG1	-7.49	98.37	109.60
1	A	431	PHE	CA-CB-CG	-7.41	106.39	113.80
1	A	160	PHE	CA-CB-CG	7.28	121.08	113.80
1	A	493	ASN	CB-CG-ND2	7.25	127.27	116.40
1	A	542	GLN	CA-CB-CG	7.24	128.57	114.10
1	A	388	ASN	CA-CB-CG	7.18	119.78	112.60
1	A	406	HIS	CA-CB-CG	-7.13	106.67	113.80
1	A	524	MET	N-CA-C	-7.12	101.81	108.22
1	A	217	ASN	CB-CG-ND2	7.08	127.02	116.40
1	A	548	ASP	CA-C-O	-6.95	113.41	120.77
1	A	267	VAL	N-CA-CB	-6.94	99.53	112.36
1	A	258	ASN	CA-CB-CG	6.93	119.53	112.60
1	A	191	SER	CB-CA-C	-6.93	99.07	110.85
1	A	387	HIS	CA-C-O	-6.91	111.10	118.77
1	A	415	LEU	O-C-N	6.88	131.05	123.27
1	A	555	GLN	N-CA-C	-6.83	100.69	110.59
1	A	66	ASN	OD1-CG-ND2	-6.82	115.78	122.60
1	A	512	ARG	CD-NE-CZ	6.78	133.90	124.40
1	A	132	ASN	CA-CB-CG	6.71	119.31	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	ASP	CB-CA-C	6.71	123.19	110.51
1	A	292	ALA	N-CA-C	-6.70	104.92	113.23
1	A	80	TYR	CA-C-N	-6.69	112.68	122.65
1	A	80	TYR	C-N-CA	-6.69	112.68	122.65
1	A	375	GLN	N-CA-C	-6.69	103.91	111.07
1	A	135	ASN	N-CA-C	6.62	118.15	111.07
1	A	334	VAL	N-CA-C	-6.59	98.01	107.77
1	A	95	ARG	NE-CZ-NH2	-6.59	113.27	119.20
1	A	446	HIS	O-C-N	6.56	131.21	122.41
1	A	40	GLU	N-CA-C	-6.52	104.25	111.82
1	A	320	LEU	CA-C-O	-6.40	114.61	120.50
1	A	374	GLU	CG-CD-OE1	-6.40	103.69	118.40
1	A	370	ASN	O-C-N	6.38	130.11	122.27
1	A	388	ASN	CB-CG-ND2	6.37	125.96	116.40
1	A	500	LEU	CA-C-O	-6.37	113.75	120.63
1	A	360	ASP	CA-C-O	-6.34	113.10	120.20
1	A	375	GLN	OE1-CD-NE2	-6.33	116.27	122.60
1	A	414	PHE	CA-C-O	-6.32	113.35	120.43
1	A	488	THR	CA-CB-OG1	-6.32	100.12	109.60
1	A	353	THR	CA-CB-OG1	-6.32	100.12	109.60
1	A	144	GLU	N-CA-C	6.28	120.12	110.20
1	A	293	VAL	N-CA-C	6.26	117.38	112.12
1	A	180	ASP	N-CA-CB	-6.26	100.91	110.42
1	A	404	VAL	N-CA-C	6.24	117.02	110.72
1	A	383	ARG	NE-CZ-NH1	6.23	127.73	121.50
1	A	440	ASP	CA-CB-CG	-6.22	106.38	112.60
1	A	433	ARG	NE-CZ-NH2	-6.14	113.67	119.20
1	A	154	ILE	CA-C-O	6.13	127.35	120.85
1	A	101	GLY	N-CA-C	-6.12	106.59	114.85
1	A	559	HIS	N-CA-C	-6.07	99.39	109.46
1	A	210	HIS	O-C-N	6.05	130.49	123.41
1	A	367	GLU	N-CA-CB	6.01	118.89	109.94
1	A	284	GLU	CA-CB-CG	5.97	126.05	114.10
1	A	231	GLU	N-CA-C	5.97	119.03	111.69
1	A	522	SER	N-CA-C	5.95	118.98	110.24
1	A	265	VAL	N-CA-CB	-5.93	101.72	111.98
1	A	90	GLN	O-C-N	5.92	130.85	123.15
1	A	562	THR	CA-CB-OG1	-5.92	100.72	109.60
1	A	68	TYR	CB-CA-C	5.89	118.67	109.84
1	A	188	ALA	CA-C-O	-5.88	114.32	120.55
1	A	191	SER	CA-C-O	-5.85	114.22	120.42
1	A	293	VAL	CA-C-O	-5.85	115.02	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	562	THR	O-C-N	5.84	128.09	122.07
1	A	115	HIS	N-CA-C	-5.80	101.04	110.20
1	A	214	MET	N-CA-C	-5.77	101.41	110.36
1	A	172	HIS	CA-CB-CG	-5.76	108.04	113.80
1	A	438	ILE	N-CA-C	-5.73	103.73	110.21
1	A	439	LEU	N-CA-CB	-5.73	102.27	110.80
1	A	97	GLY	O-C-N	5.72	128.60	122.93
1	A	291	SER	CA-CB-OG	-5.72	99.65	111.10
1	A	400	ARG	NE-CZ-NH2	-5.72	114.06	119.20
1	A	230	ARG	NE-CZ-NH1	5.71	127.21	121.50
1	A	176	ARG	N-CA-C	-5.71	102.45	110.50
1	A	236	ASN	CA-CB-CG	5.70	118.30	112.60
1	A	367	GLU	CB-CA-C	-5.70	101.69	110.81
1	A	331	THR	CA-CB-OG1	-5.68	101.08	109.60
1	A	287	LEU	CA-C-O	-5.67	114.07	120.43
1	A	337	ARG	NH1-CZ-NH2	5.65	126.65	119.30
1	A	80	TYR	O-C-N	5.64	129.77	122.89
1	A	41	ASN	N-CA-CB	5.63	117.32	110.17
1	A	348	ALA	CA-C-O	-5.62	115.43	121.45
1	A	71	ILE	CB-CG1-CD1	5.62	125.60	113.80
1	A	134	ASP	O-C-N	5.61	128.08	122.08
1	A	489	ILE	CA-CB-CG2	5.60	120.03	110.50
1	A	452	PRO	N-CD-CG	-5.59	94.81	103.20
1	A	83	VAL	N-CA-CB	-5.59	102.00	111.23
1	A	40	GLU	CB-CG-CD	5.59	122.10	112.60
1	A	84	GLU	N-CA-C	-5.58	101.11	109.15
1	A	258	ASN	N-CA-C	-5.58	104.72	112.03
1	A	337	ARG	CD-NE-CZ	-5.58	116.59	124.40
1	A	359	GLY	CA-C-N	5.57	128.51	120.38
1	A	359	GLY	C-N-CA	5.57	128.51	120.38
1	A	507	ILE	CA-C-O	-5.54	114.50	118.71
1	A	126	PHE	N-CA-CB	-5.54	101.97	110.44
1	A	250	VAL	N-CA-C	-5.54	101.58	108.89
1	A	520	THR	N-CA-C	5.52	119.76	113.19
1	A	465	ALA	CA-C-N	5.51	128.11	120.29
1	A	465	ALA	C-N-CA	5.51	128.11	120.29
1	A	279	VAL	CB-CA-C	5.48	119.45	110.69
1	A	389	THR	CA-C-N	5.48	127.89	120.44
1	A	389	THR	C-N-CA	5.48	127.89	120.44
1	A	63	GLU	N-CA-C	5.47	119.22	112.54
1	A	39	THR	CA-CB-OG1	-5.46	101.41	109.60
1	A	464	GLN	CA-C-N	5.45	127.58	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	464	GLN	C-N-CA	5.45	127.58	120.28
1	A	309	LEU	CB-CA-C	5.45	119.43	110.88
1	A	504	THR	CA-CB-OG1	-5.45	101.43	109.60
1	A	391	ALA	N-CA-C	-5.43	105.36	111.28
1	A	578	ASP	CA-C-O	-5.42	114.81	120.55
1	A	433	ARG	NE-CZ-NH1	5.41	126.91	121.50
1	A	424	ASP	N-CA-C	-5.39	99.73	108.52
1	A	183	SER	CA-C-N	5.36	125.02	119.56
1	A	183	SER	C-N-CA	5.36	125.02	119.56
1	A	43	ASN	O-C-N	5.35	129.43	122.42
1	A	314	ILE	O-C-N	-5.35	117.56	123.18
1	A	91	THR	CA-CB-OG1	-5.33	101.60	109.60
1	A	525	PRO	N-CD-CG	-5.33	95.21	103.20
1	A	190	MET	N-CA-C	-5.33	105.48	111.28
1	A	62	ILE	N-CA-C	-5.30	107.00	111.56
1	A	143	ALA	O-C-N	-5.30	115.14	122.46
1	A	153	GLN	CA-CB-CG	-5.30	103.50	114.10
1	A	501	SER	CA-CB-OG	-5.30	100.50	111.10
1	A	163	SER	O-C-N	5.29	128.41	122.22
1	A	244	VAL	O-C-N	5.28	128.47	123.03
1	A	445	LEU	N-CA-C	-5.27	106.35	112.89
1	A	351	PHE	CA-C-O	-5.27	115.15	120.84
1	A	533	ASP	CA-C-O	-5.26	115.45	121.82
1	A	262	PRO	N-CA-C	-5.26	102.84	111.21
1	A	436	VAL	CA-C-O	-5.24	114.23	120.78
1	A	96	SER	CA-CB-OG	-5.24	100.62	111.10
1	A	412	GLU	N-CA-CB	5.24	118.99	110.77
1	A	29	LEU	CA-C-O	-5.24	115.31	121.07
1	A	273	LYS	N-CA-C	-5.24	102.30	110.10
1	A	200	THR	CA-CB-OG1	-5.22	101.77	109.60
1	A	202	LYS	CA-C-O	-5.22	114.81	120.81
1	A	107	ASN	CA-CB-CG	5.20	117.80	112.60
1	A	488	THR	CA-CB-CG2	5.20	119.33	110.50
1	A	570	LYS	CA-C-O	-5.18	115.39	120.82
1	A	284	GLU	CA-C-N	5.16	129.51	122.90
1	A	284	GLU	C-N-CA	5.16	129.51	122.90
1	A	278	ASN	CA-C-N	5.16	130.90	122.69
1	A	278	ASN	C-N-CA	5.16	130.90	122.69
1	A	283	HIS	CA-CB-CG	-5.16	108.64	113.80
1	A	363	GLU	CA-C-N	5.15	127.13	120.44
1	A	363	GLU	C-N-CA	5.15	127.13	120.44
1	A	41	ASN	CA-C-O	5.14	122.63	119.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	THR	CA-CB-CG2	5.14	119.24	110.50
1	A	129	GLU	O-C-N	5.14	129.23	123.06
1	A	292	ALA	CA-C-N	-5.14	117.37	122.77
1	A	292	ALA	C-N-CA	-5.14	117.37	122.77
1	A	462	LEU	O-C-N	5.14	127.57	122.12
1	A	174	GLY	O-C-N	5.13	126.90	121.77
1	A	144	GLU	CA-C-O	5.12	126.89	121.05
1	A	552	PRO	CB-CA-C	5.12	117.17	110.92
1	A	337	ARG	NE-CZ-NH2	-5.11	114.60	119.20
1	A	400	ARG	CA-C-N	5.08	127.36	120.65
1	A	400	ARG	C-N-CA	5.08	127.36	120.65
1	A	112	THR	CA-C-O	-5.08	115.82	121.51
1	A	565	TYR	N-CA-C	-5.08	105.83	111.36
1	A	473	ASN	CA-C-O	-5.06	115.68	121.00
1	A	20	VAL	N-CA-C	-5.06	101.42	108.80
1	A	441	LYS	CA-CB-CG	5.06	124.21	114.10
1	A	407	ASN	CB-CG-ND2	5.05	123.98	116.40
1	A	92	ALA	N-CA-C	-5.05	102.31	110.14
1	A	111	TRP	CA-CB-CG	5.04	123.18	113.60
1	A	272	HIS	ND1-CE1-NE2	-5.04	103.36	108.40
1	A	298	LEU	N-CA-C	-5.03	105.71	111.14
1	A	315	ASP	CA-C-N	5.03	129.01	121.72
1	A	315	ASP	C-N-CA	5.03	129.01	121.72
1	A	376	TRP	CA-C-N	5.01	126.99	120.28
1	A	376	TRP	C-N-CA	5.01	126.99	120.28
1	A	134	ASP	CA-C-O	-5.00	115.56	121.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4452	0	4239	109	0
2	B	61	0	52	0	0
3	A	56	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	53	0	31	1	0
5	A	152	0	0	8	0
All	All	4774	0	4374	109	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 12.

All (109) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ARG:NH1	5:A:838:HOH:O	1.84	1.09
1:A:325:ASN:ND2	1:A:433:ARG:HD2	1.91	0.85
1:A:115:HIS:HD2	1:A:117:ALA:H	1.24	0.84
1:A:4:ILE:HD11	1:A:233:LEU:HD13	1.65	0.79
1:A:22:TYR:CE2	1:A:284:GLU:HG2	2.18	0.78
1:A:22:TYR:HE2	1:A:284:GLU:HG2	1.49	0.77
1:A:283:HIS:HD2	1:A:582:MET:SD	2.09	0.76
1:A:400:ARG:O	1:A:404:VAL:HB	1.94	0.67
1:A:50:GLU:HG2	1:A:100:LEU:CD1	2.28	0.64
1:A:417:THR:HA	1:A:420:VAL:O	1.99	0.63
1:A:187:LYS:HD3	5:A:761:HOH:O	1.99	0.63
1:A:490:PRO:HB3	1:A:506:TYR:OH	1.98	0.63
1:A:296:THR:HB	1:A:438:ILE:HG22	1.81	0.61
1:A:81:GLU:HB2	1:A:91:THR:HG23	1.82	0.61
1:A:472:ARG:HD3	1:A:487:GLU:OE1	2.01	0.60
1:A:126:PHE:O	1:A:525:PRO:HD3	2.01	0.60
1:A:4:ILE:CD1	1:A:233:LEU:HD13	2.31	0.60
1:A:325:ASN:HD22	1:A:433:ARG:HD2	1.66	0.60
1:A:305:MET:HE3	1:A:308:ILE:HD13	1.83	0.59
1:A:338:ILE:HA	1:A:483:TYR:O	2.03	0.59
1:A:152:LYS:HE2	1:A:182:TYR:CE1	2.39	0.58
1:A:472:ARG:NH1	1:A:487:GLU:OE2	2.37	0.57
1:A:477:SER:O	1:A:480:MET:HB2	2.05	0.57
1:A:523:MET:HA	1:A:532:VAL:HG23	1.87	0.56
1:A:383:ARG:NH2	5:A:839:HOH:O	2.37	0.56
1:A:355:ASN:OD1	1:A:366:HIS:HE1	1.89	0.56
1:A:189:LEU:HD11	1:A:474:ILE:HD12	1.88	0.56
1:A:143:ALA:HB2	1:A:569:LEU:HD11	1.89	0.55
1:A:383:ARG:HD3	1:A:456:LEU:HD13	1.89	0.55
1:A:16:SER:HB3	1:A:277:HIS:HB3	1.87	0.55
1:A:44:ILE:O	1:A:241:ASN:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:GLU:HG2	1:A:100:LEU:HD12	1.89	0.54
1:A:51:SER:O	1:A:247:GLY:HA2	2.07	0.54
1:A:153:GLN:O	1:A:158:HIS:HB2	2.08	0.54
1:A:152:LYS:HE2	1:A:182:TYR:CD1	2.44	0.54
1:A:289:ALA:HB1	1:A:293:VAL:HG22	1.89	0.54
1:A:364:LYS:HE3	1:A:462:LEU:HD13	1.90	0.53
1:A:269:PHE:O	1:A:276:THR:HA	2.08	0.53
1:A:193:VAL:HG21	1:A:212:VAL:HG23	1.91	0.53
1:A:115:HIS:CD2	1:A:117:ALA:H	2.16	0.53
1:A:284:GLU:HG3	1:A:286:LEU:HD21	1.90	0.53
1:A:158:HIS:CE1	1:A:175:PRO:HB3	2.45	0.52
1:A:236:ASN:O	1:A:239:ARG:HB2	2.10	0.52
1:A:50:GLU:OE1	4:A:600:FAD:H1B	2.10	0.52
1:A:325:ASN:ND2	1:A:433:ARG:CD	2.68	0.52
1:A:472:ARG:HH11	1:A:487:GLU:CD	2.18	0.52
1:A:522:SER:CB	1:A:524:MET:HE2	2.40	0.52
1:A:295:PRO:HG3	1:A:520:THR:HB	1.92	0.52
1:A:522:SER:HB3	1:A:524:MET:HE2	1.92	0.52
1:A:263:ARG:HG3	1:A:542:GLN:OE1	2.10	0.51
1:A:222:ASP:O	1:A:223:GLN:HB2	2.10	0.51
1:A:408:VAL:O	5:A:834:HOH:O	2.19	0.51
1:A:489:ILE:HA	1:A:490:PRO:C	2.36	0.51
1:A:4:ILE:HD11	1:A:233:LEU:CD1	2.38	0.50
1:A:76:VAL:HG12	1:A:76:VAL:O	2.12	0.50
1:A:373:LEU:HG	1:A:396:TYR:HB3	1.94	0.50
1:A:212:VAL:HA	1:A:349:ALA:O	2.12	0.49
1:A:294:SER:N	1:A:295:PRO:HD2	2.28	0.49
1:A:501:SER:O	1:A:504:THR:HB	2.13	0.49
1:A:287:LEU:CD2	1:A:298:LEU:HD13	2.43	0.49
1:A:325:ASN:HD21	1:A:433:ARG:HD2	1.74	0.48
1:A:255:LEU:HD11	1:A:303:ILE:HD11	1.94	0.48
1:A:413:LEU:HD13	1:A:471:ALA:HB2	1.95	0.48
1:A:232:TRP:O	1:A:236:ASN:ND2	2.44	0.48
1:A:300:TYR:HE1	1:A:440:ASP:O	1.95	0.48
1:A:383:ARG:HD2	1:A:453:GLN:OE1	2.14	0.48
1:A:87:THR:OG1	1:A:508:PRO:HB3	2.14	0.47
1:A:490:PRO:HB3	1:A:506:TYR:CZ	2.49	0.47
1:A:571:ILE:O	1:A:574:ALA:HB3	2.14	0.47
1:A:527:GLU:H	1:A:527:GLU:CD	2.23	0.47
1:A:453:GLN:HB3	1:A:456:LEU:HD12	1.96	0.46
1:A:474:ILE:O	1:A:480:MET:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:GLN:HA	1:A:415:LEU:O	2.15	0.46
1:A:310:GLU:HB3	1:A:311:PRO:HD3	1.98	0.46
1:A:249:TYR:HB2	1:A:270:GLY:O	2.15	0.46
1:A:85:LEU:O	1:A:89:ASN:N	2.48	0.46
1:A:204:PHE:CD1	1:A:209:PRO:HA	2.51	0.46
1:A:55:GLU:OE2	5:A:854:HOH:O	2.21	0.45
1:A:112:THR:HB	1:A:204:PHE:HB3	1.98	0.45
1:A:489:ILE:HD11	5:A:766:HOH:O	2.15	0.45
1:A:373:LEU:HB2	5:A:846:HOH:O	2.17	0.45
1:A:472:ARG:HD2	1:A:496:TYR:CE1	2.52	0.45
1:A:450:TYR:CE2	1:A:452:PRO:HG3	2.52	0.45
1:A:335:ARG:HB3	1:A:489:ILE:HG23	1.99	0.44
1:A:266:GLY:HA3	1:A:280:TYR:HA	1.98	0.44
1:A:269:PHE:CZ	1:A:277:HIS:HB2	2.53	0.44
1:A:11:ASP:HA	1:A:12:PRO:HD2	1.81	0.44
1:A:424:ASP:HB3	1:A:426:TRP:HZ3	1.82	0.44
1:A:518:VAL:HA	1:A:549:GLY:O	2.18	0.43
1:A:20:VAL:O	1:A:281:ALA:HA	2.18	0.43
1:A:24:ILE:HG12	1:A:286:LEU:HD12	1.99	0.43
1:A:29:LEU:C	1:A:29:LEU:HD23	2.44	0.43
1:A:369:LEU:O	1:A:373:LEU:HD13	2.19	0.43
1:A:81:GLU:HB2	1:A:91:THR:CG2	2.49	0.43
1:A:318:VAL:HG21	1:A:541:VAL:HG22	2.01	0.43
1:A:477:SER:O	1:A:478:GLY:C	2.63	0.42
1:A:182:TYR:HA	1:A:345:GLN:O	2.19	0.42
1:A:113:ARG:HB3	1:A:114:PRO:HD2	2.02	0.42
1:A:116:LYS:NZ	5:A:827:HOH:O	2.53	0.42
1:A:325:ASN:HD22	1:A:433:ARG:CD	2.29	0.41
1:A:326:LEU:C	1:A:327:GLN:HG3	2.45	0.41
1:A:256:SER:O	1:A:262:PRO:HA	2.21	0.41
1:A:535:ALA:O	1:A:536:ALA:HB3	2.21	0.41
1:A:131:TRP:CZ2	1:A:570:LYS:HD3	2.56	0.41
1:A:210:HIS:CD2	1:A:211:GLY:N	2.89	0.41
1:A:524:MET:O	1:A:530:GLY:HA3	2.21	0.41
1:A:454:TYR:OH	1:A:513:PRO:HB3	2.21	0.41
1:A:199:PRO:O	1:A:211:GLY:HA3	2.20	0.40
1:A:24:ILE:HA	1:A:286:LEU:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	579/583 (99%)	554 (96%)	25 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	466/468 (100%)	423 (91%)	43 (9%)	8	11

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	32	LEU
1	A	37	ARG
1	A	83	VAL
1	A	91	THR
1	A	96	SER
1	A	100	LEU
1	A	158	HIS
1	A	180	ASP
1	A	219	LEU
1	A	233	LEU
1	A	239	ARG
1	A	244	VAL

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Mol	Chain	Res	Type
1	A	254	LEU
1	A	260	THR
1	A	265	VAL
1	A	267	VAL
1	A	287	LEU
1	A	293	VAL
1	A	298	LEU
1	A	308	ILE
1	A	325	ASN
1	A	363	GLU
1	A	368	LEU
1	A	373	LEU
1	A	394	ILE
1	A	404	VAL
1	A	413	LEU
1	A	416	ASP
1	A	425	VAL
1	A	433	ARG
1	A	439	LEU
1	A	470	LEU
1	A	472	ARG
1	A	473	ASN
1	A	482	THR
1	A	489	ILE
1	A	504	THR
1	A	507	ILE
1	A	512	ARG
1	A	516	HIS
1	A	527	GLU
1	A	563	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	HIS
1	A	158	HIS
1	A	248	GLN
1	A	275	ASN
1	A	278	ASN
1	A	283	HIS
1	A	325	ASN
1	A	327	GLN

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Mol	Chain	Res	Type
1	A	406	HIS
1	A	446	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

5 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	B	1	2,1	14,14,15	1.18	1 (7%)	17,19,21	0.86	0
2	NAG	B	2	2	14,14,15	1.06	1 (7%)	17,19,21	1.86	5 (29%)
2	BMA	B	3	2	11,11,12	0.75	0	15,15,17	2.15	5 (33%)
2	MAN	B	4	2	11,11,12	0.91	0	15,15,17	1.69	3 (20%)
2	MAN	B	5	2	11,11,12	0.95	0	15,15,17	2.06	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
2	NAG	B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	3/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1
2	MAN	B	5	2	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	O7-C7	-3.13	1.16	1.23
2	B	2	NAG	O7-C7	-2.96	1.16	1.23

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5	MAN	C1-O5-C5	4.71	118.49	112.19
2	B	3	BMA	C1-C2-C3	-4.48	103.13	109.64
2	B	4	MAN	O2-C2-C3	4.08	118.61	110.15
2	B	2	NAG	C1-C2-N2	3.98	116.71	110.43
2	B	3	BMA	C2-C3-C4	3.83	117.59	110.86
2	B	4	MAN	C1-C2-C3	-3.69	104.27	109.64
2	B	3	BMA	O3-C3-C2	-3.63	102.64	110.05
2	B	2	NAG	O7-C7-C8	-3.12	116.49	122.05
2	B	2	NAG	O5-C1-C2	-3.00	106.66	111.29
2	B	5	MAN	O2-C2-C3	2.95	116.25	110.15
2	B	2	NAG	O7-C7-N2	2.78	126.90	121.98
2	B	5	MAN	C1-C2-C3	-2.69	105.73	109.64
2	B	5	MAN	C2-C3-C4	2.43	115.14	110.86
2	B	2	NAG	C1-O5-C5	2.43	115.44	112.19
2	B	3	BMA	O5-C1-C2	-2.42	105.01	110.79
2	B	5	MAN	O3-C3-C4	2.42	116.08	110.38
2	B	4	MAN	C6-C5-C4	2.15	118.31	113.02
2	B	3	BMA	O5-C5-C4	-2.13	105.66	110.83

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	5	MAN	O5-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
2	B	5	MAN	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C3-C2-N2-C7

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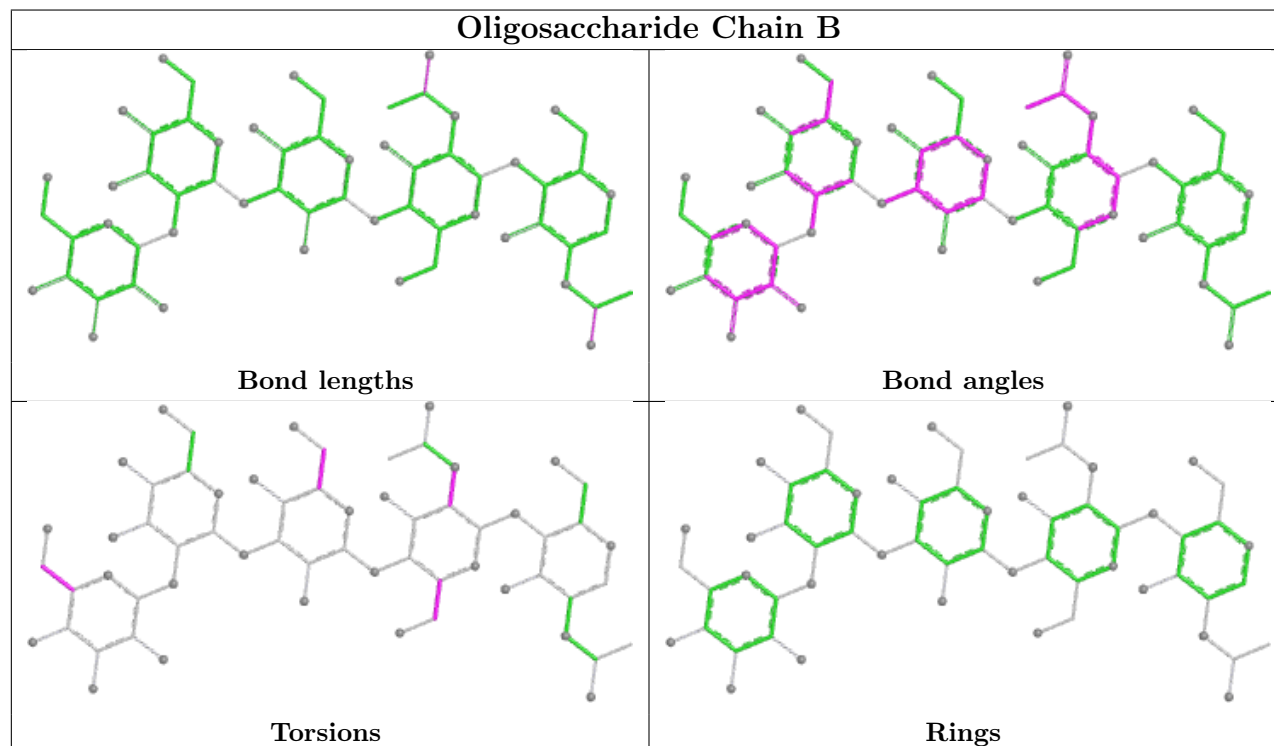
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Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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



5.6 Ligand geometry [i](#)

5 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	605	1	14,14,15	1.39	3 (21%)	17,19,21	2.00	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	608	1	14,14,15	1.10	1 (7%)	17,19,21	3.06	5 (29%)
4	FAD	A	600	-	58,58,58	1.87	13 (22%)	85,89,89	2.36	29 (34%)
3	NAG	A	609	1	14,14,15	1.17	1 (7%)	17,19,21	1.52	2 (11%)
3	NAG	A	604	1	14,14,15	1.23	2 (14%)	17,19,21	2.57	11 (64%)

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	605	1	-	0/6/23/26	0/1/1/1
3	NAG	A	608	1	-	2/6/23/26	0/1/1/1
4	FAD	A	600	-	-	6/34/50/50	0/6/6/6
3	NAG	A	609	1	-	4/6/23/26	0/1/1/1
3	NAG	A	604	1	-	2/6/23/26	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	FAD	P-O3P	-5.39	1.53	1.59
4	A	600	FAD	C6-C7	-4.71	1.33	1.39
4	A	600	FAD	C8-C7	4.38	1.51	1.40
4	A	600	FAD	O5'-C5'	3.85	1.59	1.44
4	A	600	FAD	PA-O2A	-3.83	1.37	1.55
4	A	600	FAD	C1'-C2'	3.82	1.58	1.52
3	A	605	NAG	O7-C7	-3.66	1.15	1.23
3	A	604	NAG	O7-C7	-3.25	1.16	1.23
4	A	600	FAD	P-O2P	-2.81	1.42	1.55
3	A	609	NAG	O7-C7	-2.77	1.17	1.23
4	A	600	FAD	PA-O5B	-2.75	1.48	1.59
3	A	608	NAG	O7-C7	-2.73	1.17	1.23
4	A	600	FAD	C6A-N6A	-2.43	1.28	1.34
4	A	600	FAD	C6-C5X	2.42	1.43	1.40
4	A	600	FAD	O3B-C3B	-2.33	1.37	1.43
4	A	600	FAD	C9-C9A	-2.24	1.36	1.39
3	A	605	NAG	C2-N2	2.22	1.49	1.46
3	A	605	NAG	O5-C5	-2.20	1.39	1.43
3	A	604	NAG	O5-C1	2.19	1.47	1.43
4	A	600	FAD	C4X-N5	2.11	1.35	1.30

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	FAD	C2A-N1A-C6A	8.70	133.02	118.73
3	A	608	NAG	C1-C2-N2	7.08	121.59	110.43
4	A	600	FAD	O4B-C1B-N9A	-6.58	95.46	108.09
3	A	608	NAG	C4-C3-C2	-6.25	101.86	111.02
3	A	608	NAG	C1-O5-C5	5.74	119.89	112.19
4	A	600	FAD	O4B-C1B-C2B	-5.63	94.56	106.62
4	A	600	FAD	C9-C9A-N10	5.52	129.27	121.85
3	A	604	NAG	C2-N2-C7	5.16	129.82	122.90
4	A	600	FAD	C5A-C6A-N1A	-4.97	104.89	117.51
3	A	608	NAG	O5-C1-C2	-4.77	103.91	111.29
3	A	605	NAG	O5-C1-C2	-4.63	104.12	111.29
3	A	609	NAG	O6-C6-C5	4.37	126.22	111.33
3	A	604	NAG	O5-C1-C2	-4.03	105.06	111.29
4	A	600	FAD	N6A-C6A-N1A	3.85	126.96	118.38
3	A	605	NAG	C1-O5-C5	3.78	117.25	112.19
4	A	600	FAD	C6-C5X-C9A	3.70	124.14	119.05
4	A	600	FAD	O3B-C3B-C4B	3.66	121.59	111.08
4	A	600	FAD	C9-C9A-C5X	-3.50	113.84	120.03
4	A	600	FAD	C1B-N9A-C8A	3.48	134.83	127.09
4	A	600	FAD	C4A-N9A-C1B	-3.31	118.90	126.63
4	A	600	FAD	C5'-C4'-C3'	-3.30	106.00	112.22
4	A	600	FAD	C9A-C9-C8	3.30	125.85	119.22
4	A	600	FAD	O5B-C5B-C4B	-3.16	98.23	108.99
4	A	600	FAD	C5A-C4A-N3A	3.13	131.03	126.72
4	A	600	FAD	C4-C4X-C10	2.97	122.02	116.93
3	A	604	NAG	C6-C5-C4	-2.93	105.83	113.02
3	A	604	NAG	C4-C3-C2	-2.90	106.78	111.02
3	A	605	NAG	C1-C2-N2	-2.87	105.91	110.43
3	A	604	NAG	C8-C7-N2	-2.85	111.39	116.12
4	A	600	FAD	C10-C4X-N5	-2.80	119.09	124.81
3	A	605	NAG	O5-C5-C4	-2.78	104.07	110.83
3	A	604	NAG	O3-C3-C2	2.76	115.14	109.40
3	A	609	NAG	C1-C2-N2	2.71	114.71	110.43
3	A	604	NAG	O3-C3-C4	-2.69	104.04	110.38
3	A	608	NAG	O3-C3-C2	2.68	114.97	109.40
4	A	600	FAD	O2B-C2B-C3B	2.68	120.40	111.82
4	A	600	FAD	C1'-C2'-C3'	-2.64	102.51	109.66
4	A	600	FAD	O2P-P-O1P	2.62	124.63	112.44
4	A	600	FAD	C2B-C3B-C4B	-2.54	97.70	102.61
4	A	600	FAD	O2A-PA-O3P	2.46	113.93	107.27
3	A	604	NAG	O4-C4-C5	-2.45	103.30	109.32
3	A	604	NAG	C1-O5-C5	-2.44	108.91	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	604	NAG	O7-C7-C8	2.35	126.23	122.05
4	A	600	FAD	O2B-C2B-C1B	-2.32	102.11	110.10
4	A	600	FAD	C2A-N3A-C4A	-2.29	106.24	111.83
4	A	600	FAD	O3'-C3'-C4'	2.28	114.12	108.93
4	A	600	FAD	N3A-C2A-N1A	-2.23	125.20	128.58
4	A	600	FAD	C7M-C7-C6	2.20	123.44	119.57
3	A	604	NAG	C1-C2-N2	2.08	113.71	110.43
4	A	600	FAD	C4X-C10-N1	-2.06	119.55	124.59
3	A	605	NAG	O7-C7-C8	2.04	125.69	122.05
4	A	600	FAD	O3'-C3'-C2'	-2.04	104.31	108.93
3	A	605	NAG	O7-C7-N2	-2.02	118.41	121.98

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	609	NAG	O5-C5-C6-O6
3	A	608	NAG	O5-C5-C6-O6
3	A	609	NAG	C4-C5-C6-O6
3	A	608	NAG	C4-C5-C6-O6
3	A	609	NAG	C8-C7-N2-C2
3	A	609	NAG	O7-C7-N2-C2
3	A	604	NAG	O5-C5-C6-O6
4	A	600	FAD	PA-O3P-P-O5'
4	A	600	FAD	C2B-C1B-N9A-C8A
4	A	600	FAD	P-O3P-PA-O2A
3	A	604	NAG	C3-C2-N2-C7
4	A	600	FAD	P-O3P-PA-O1A
4	A	600	FAD	C2B-C1B-N9A-C4A
4	A	600	FAD	O4B-C4B-C5B-O5B

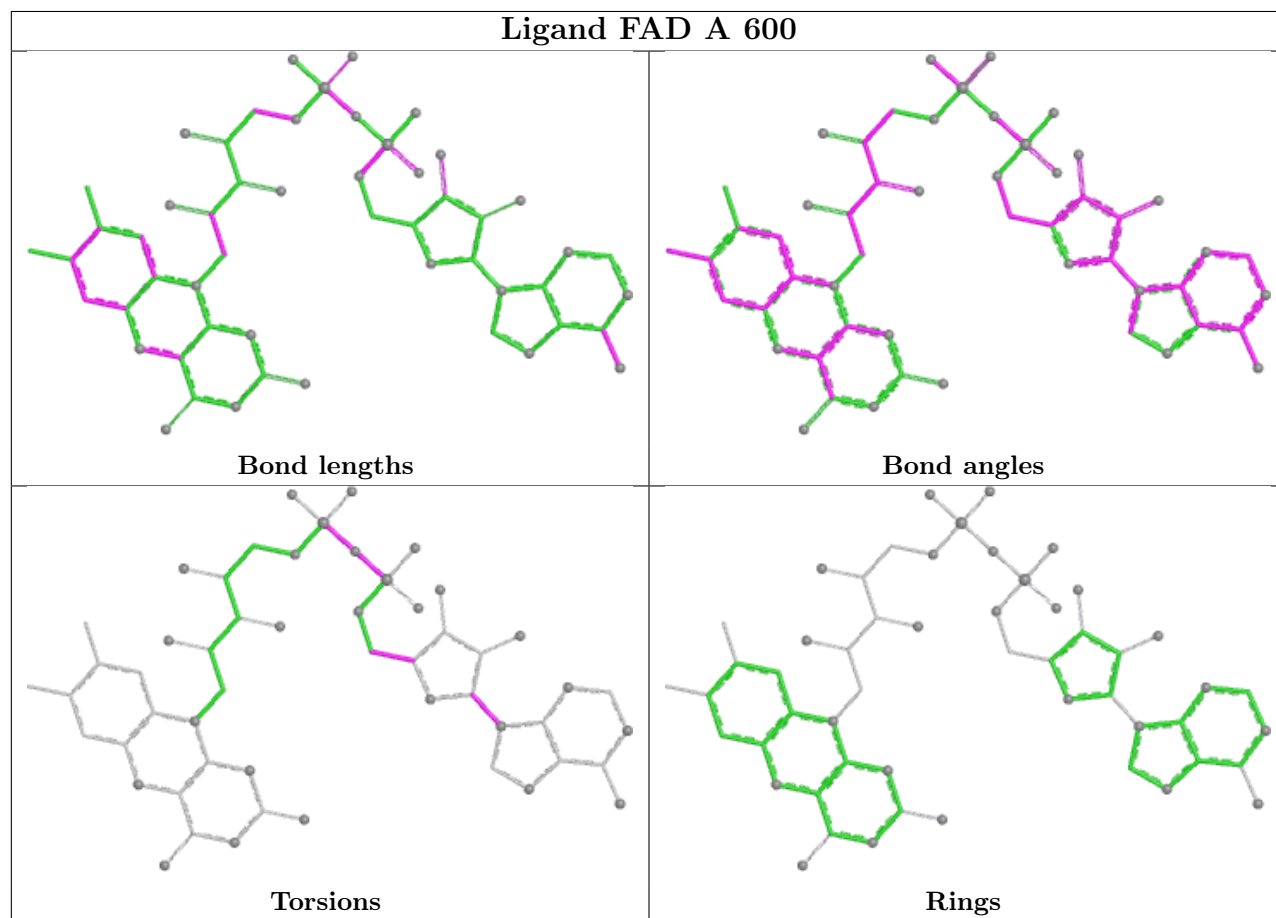
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	FAD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	581/583 (99%)	-0.66	0 100 100	2, 11, 29, 67	0

There are no RSRZ outliers to report.

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

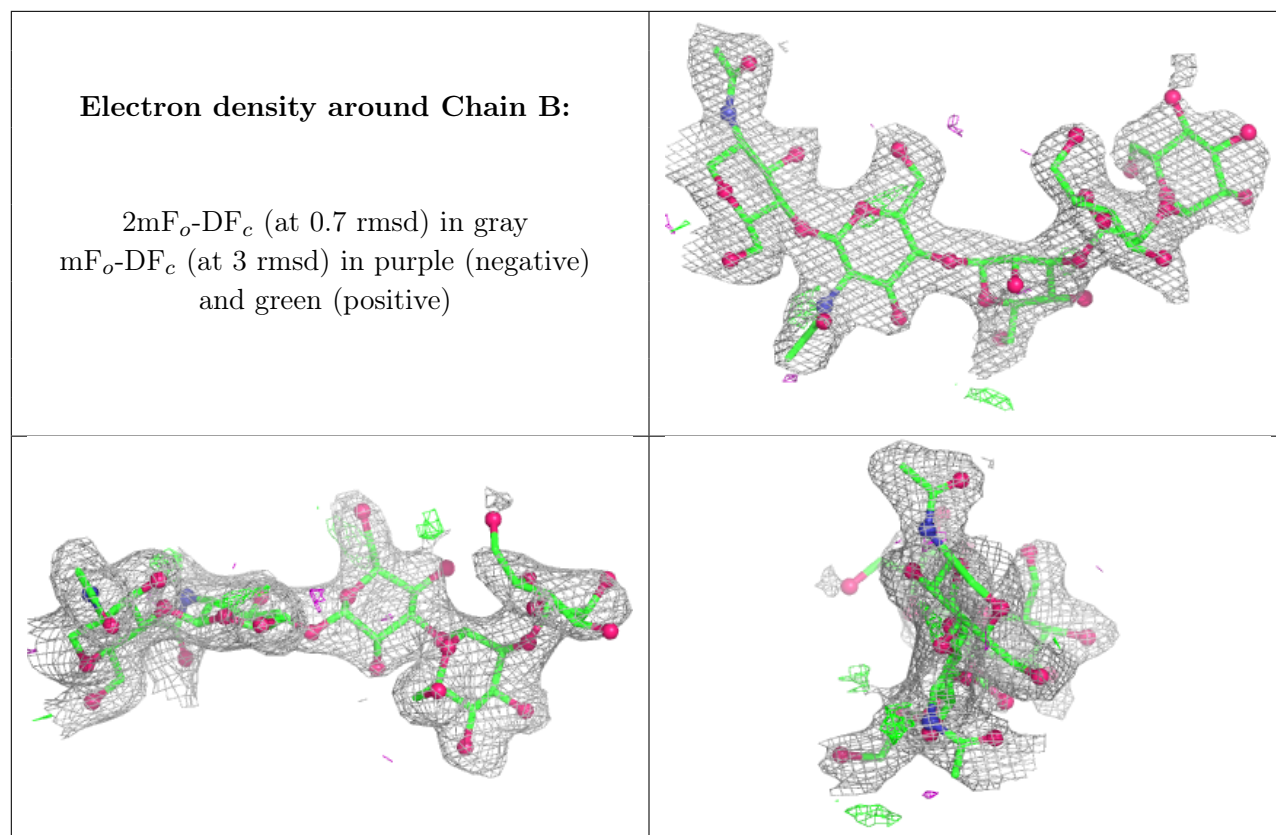
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	B	5	11/12	0.76	0.09	68,68,68,68	0
2	BMA	B	3	11/12	0.82	0.10	54,54,54,54	0
2	NAG	B	2	14/15	0.83	0.10	30,30,30,30	0
2	MAN	B	4	11/12	0.85	0.10	57,57,57,57	0
2	NAG	B	1	14/15	0.89	0.07	22,22,22,22	0

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

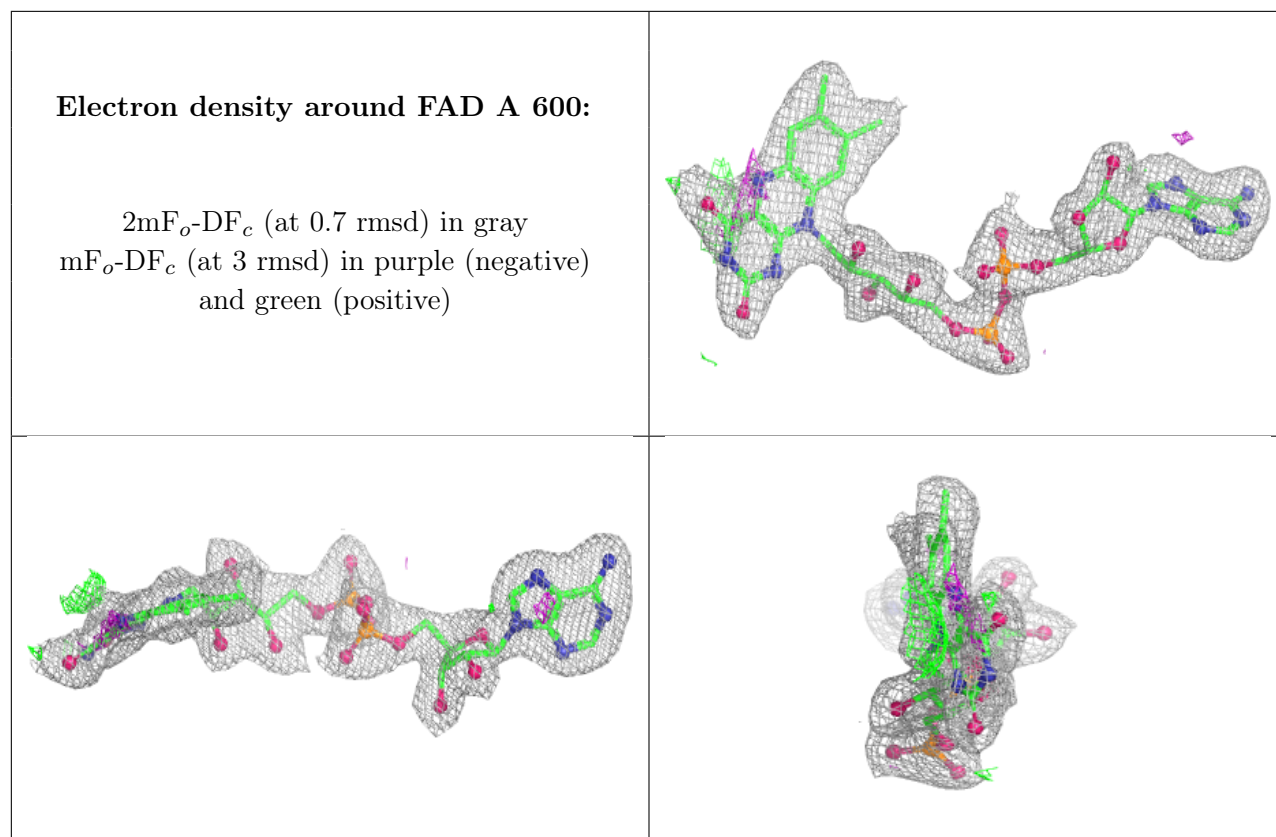


6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	A	609	14/15	0.56	0.14	76,76,76,76	0
3	NAG	A	608	14/15	0.66	0.12	65,65,65,65	0
3	NAG	A	604	14/15	0.86	0.08	23,23,23,23	0
3	NAG	A	605	14/15	0.94	0.06	17,17,17,17	0
4	FAD	A	600	53/53	0.96	0.06	5,5,5,5	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.