



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:47 PM GMT

PDB ID : 1H82
Title : STRUCTURE OF POLYAMINE OXIDASE IN COMPLEX WITH GUAZATINE
Authors : Binda, C.; Coda, A.; Angelini, R.; Federico, R.; Ascenzi, P.; Mattevi, A.
Deposited on : 2001-01-24
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

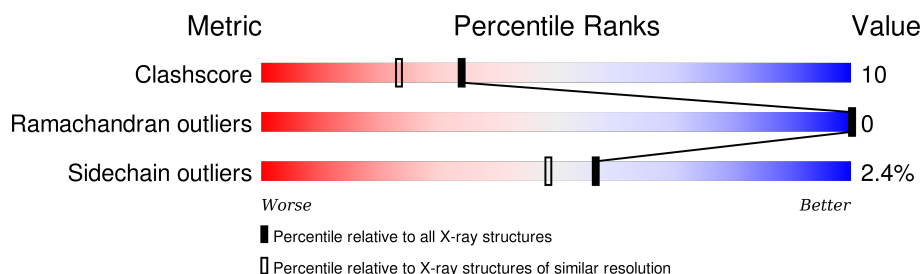
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	472	 77% 19% . .
1	B	472	 76% 20% . .
1	C	472	 81% 15% . .

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
5	NAG	C	601	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MAN	C	604	X	-	-	-

2 Entry composition [i](#)

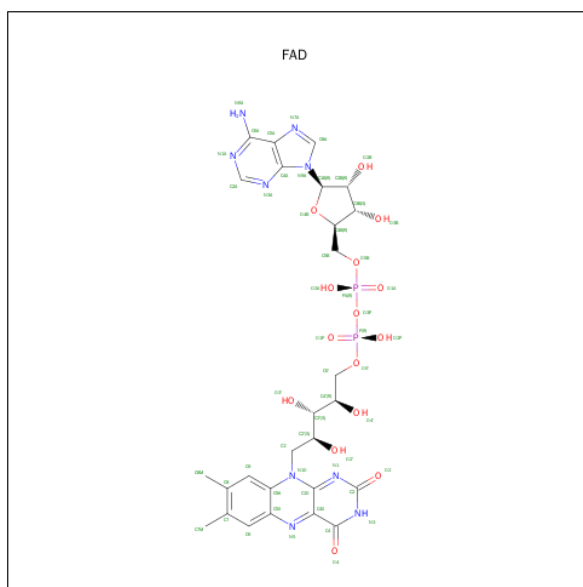
There are 7 unique types of molecules in this entry. The entry contains 12210 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 POLYAMINE OXIDASE.

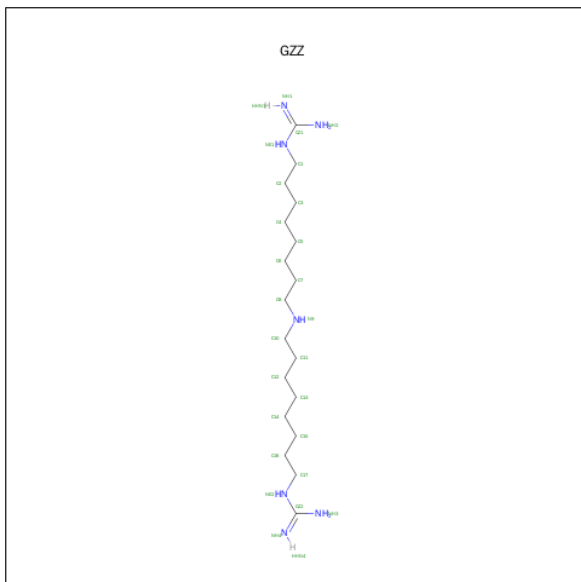
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	54	0	0
			3684	2353	621	696	14			
1	B	462	Total	C	N	O	S	54	0	0
			3715	2374	627	700	14			
1	C	462	Total	C	N	O	S	41	0	0
			3715	2374	627	700	14			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



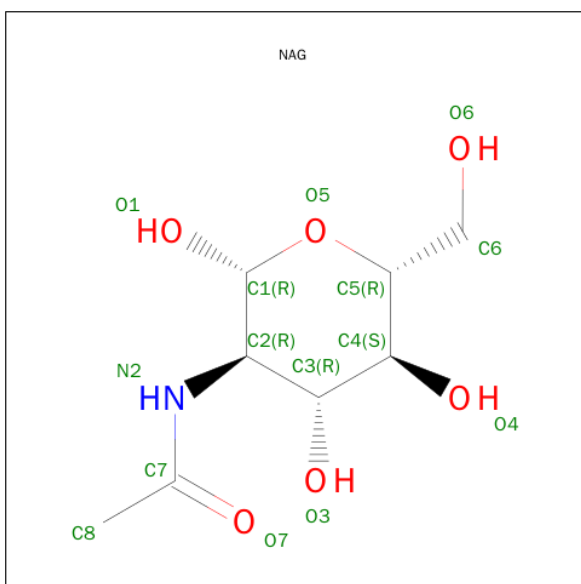
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is N-{8-[(8-{[(E)-AMINO(IMINO)METHYL]AMINO}OCTYL)AMINO]OCTYL}GUANIDINE (three-letter code: GZZ) (formula: $C_{18}H_{41}N_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			25	18	7		
3	B	1	Total	C	N	0	0
			25	18	7		
3	C	1	Total	C	N	0	0
			25	18	7		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

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

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	3	Total	C	N	O	0	0
			36	20	1	15		

- Molecule 7 is water.

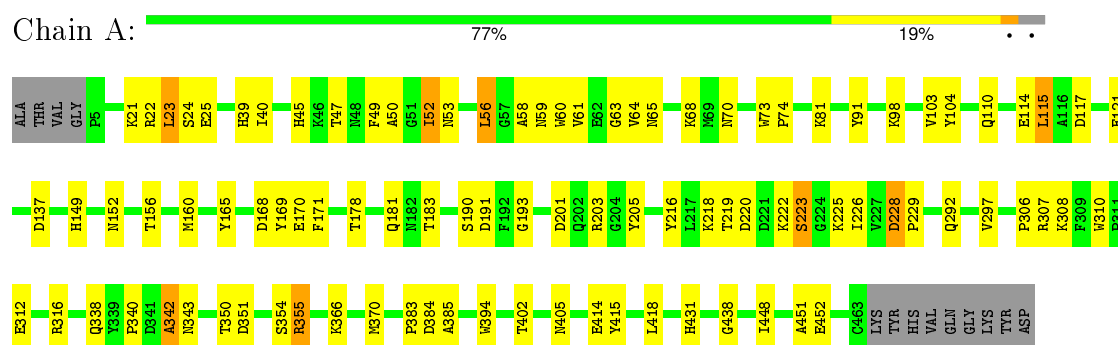
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	234	Total	O	0	0
			234	234		
7	B	243	Total	O	0	0
			243	243		
7	C	269	Total	O	0	0
			269	269		

3 Residue-property plots

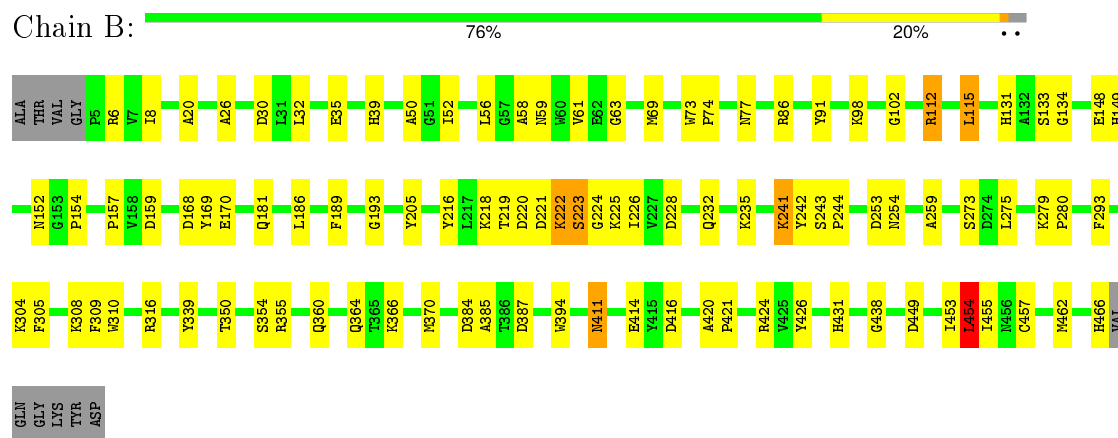
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

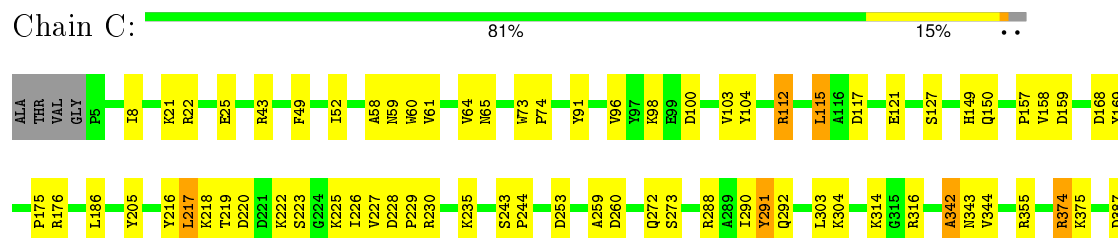
• Molecule 1: POLYAMINE OXIDASE



• Molecule 1: POLYAMINE OXIDASE



• Molecule 1: POLYAMINE OXIDASE



R412	L418	R424	H431	E434	G438	L454	H466	VAL	GLN	GLY	LYS	TYR	ASP
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	184.97Å 184.97Å 282.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.90	Depositor
% Data completeness (in resolution range)	94.3 (50.00-1.90)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5D	Depositor
R, R_{free}	0.199 , 0.231	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12210	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FCA, GZZ, NAG, FAD, 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	0.66	0/3775	1.17	13/5116 (0.3%)
1	B	0.66	0/3808	1.18	17/5160 (0.3%)
1	C	0.68	0/3808	1.17	16/5160 (0.3%)
All	All	0.67	0/11391	1.17	46/15436 (0.3%)

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	1	0
1	C	0	1
6	C	1	0
All	All	2	1

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	355	ARG	NE-CZ-NH2	-11.84	114.38	120.30
1	A	342	ALA	N-CA-C	8.13	132.95	111.00
1	C	112	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	B	112	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	C	115	LEU	CB-CG-CD1	-6.55	99.86	111.00
1	B	186	LEU	CB-CG-CD2	-6.43	100.07	111.00
1	A	297	VAL	CB-CA-C	-6.39	99.25	111.40
1	B	115	LEU	CB-CG-CD2	-6.38	100.16	111.00
1	C	43	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	B	224	GLY	N-CA-C	-6.20	97.59	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	230	ARG	NE-CZ-NH1	-6.20	117.20	120.30
1	C	374	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	B	273	SER	C-N-CA	-5.99	106.73	121.70
1	B	454	LEU	CA-CB-CG	5.95	128.98	115.30
1	C	273	SER	C-N-CA	-5.91	106.93	121.70
1	B	241	LYS	CD-CE-NZ	5.84	125.13	111.70
1	B	316	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	C	342	ALA	N-CA-C	5.80	126.67	111.00
1	B	56	LEU	CB-CG-CD1	-5.80	101.14	111.00
1	A	61	VAL	N-CA-C	-5.73	95.53	111.00
1	C	22	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	B	86	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	C	176	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	B	222	LYS	N-CA-CB	5.54	120.58	110.60
1	B	273	SER	N-CA-C	-5.45	96.28	111.00
1	C	288	ARG	CG-CD-NE	-5.42	100.41	111.80
1	A	223	SER	CB-CA-C	-5.42	99.80	110.10
1	A	201	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	A	351	ASP	N-CA-CB	-5.41	100.87	110.60
1	A	56	LEU	CB-CG-CD1	-5.37	101.88	111.00
1	C	61	VAL	N-CA-C	-5.34	96.57	111.00
1	A	355	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	C	374	ARG	CG-CD-NE	-5.27	100.73	111.80
1	C	22	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	316	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	B	61	VAL	N-CA-C	-5.22	96.90	111.00
1	B	316	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	C	186	LEU	CB-CG-CD1	-5.20	102.16	111.00
1	C	412	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	A	228	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	B	112	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	C	316	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	60	TRP	CB-CA-C	-5.08	100.24	110.40
1	B	221	ASP	CB-CA-C	5.06	120.51	110.40
1	A	22	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	22	ARG	NE-CZ-NH2	-5.05	117.77	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	341	ASP	CA
6	C	604	MAN	C1

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	291	TYR	Sidechain

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	3684	0	3585	66	0
1	B	3715	0	3614	87	0
1	C	3715	0	3614	55	0
2	A	53	0	31	4	0
2	B	53	0	31	2	0
2	C	53	0	31	2	0
3	A	25	0	39	7	0
3	B	25	0	39	4	0
3	C	25	0	39	2	0
4	A	28	0	26	2	0
4	B	28	0	26	4	0
5	C	24	0	22	8	0
6	C	36	0	31	6	0
7	A	234	0	0	5	0
7	B	243	0	0	5	0
7	C	269	0	0	9	0
All	All	12210	0	11128	221	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 10.

All (221) 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:272:GLN:HA	7:C:2151:HOH:O	1.25	1.28
1:A:220:ASP:HB3	1:A:223:SER:HB2	1.25	1.12
1:A:308:LYS:HZ3	1:A:312:GLU:HG3	0.94	1.10
1:C:219:THR:HG22	1:C:226:ILE:HA	1.43	1.00
1:B:220:ASP:HB3	1:B:223:SER:HB2	1.44	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:MET:HE2	1:B:74:PRO:HD3	1.44	0.95
5:C:601:NAG:C4	6:C:602:NAG:C1	2.45	0.95
1:A:308:LYS:NZ	1:A:312:GLU:HG3	1.81	0.94
1:B:69:MET:CE	1:B:73:TRP:HB3	1.97	0.93
5:C:601:NAG:H3	5:C:603:FCA:O2	1.72	0.90
1:B:69:MET:HE3	1:B:73:TRP:HB3	1.55	0.89
1:C:291:TYR:CZ	7:C:2151:HOH:O	2.27	0.87
1:A:220:ASP:CB	1:A:223:SER:HB2	2.06	0.84
4:B:601:NAG:C4	4:B:602:NAG:C1	2.58	0.82
1:C:21:LYS:O	1:C:25:GLU:HG3	1.80	0.81
1:A:169:TYR:O	3:A:590:GZZ:H102	1.81	0.80
1:B:220:ASP:CB	1:B:223:SER:HB2	2.12	0.79
1:B:411:ASN:ND2	1:B:414:GLU:H	1.80	0.77
1:C:216:TYR:CD1	1:C:217:LEU:HD13	2.19	0.77
1:C:291:TYR:OH	7:C:2151:HOH:O	2.04	0.76
1:B:220:ASP:HB3	1:B:223:SER:CB	2.15	0.75
1:C:292:GLN:OE1	7:C:2154:HOH:O	2.04	0.74
1:B:131:HIS:CD2	1:B:133:SER:H	2.04	0.74
1:A:171:PHE:HD2	3:A:590:GZZ:HC11	1.53	0.74
1:A:394:TRP:HE1	1:B:152:ASN:ND2	1.85	0.73
1:A:117:ASP:O	1:A:121:GLU:HG3	1.88	0.73
4:A:601:NAG:C4	4:A:602:NAG:C1	2.67	0.72
1:C:412:ARG:NH1	1:C:434:GLU:OE2	2.21	0.71
1:A:308:LYS:HZ3	1:A:312:GLU:CG	1.89	0.69
1:B:223:SER:HB3	1:B:225:LYS:H	1.57	0.69
1:C:219:THR:HG22	1:C:226:ILE:CA	2.21	0.68
1:A:431:HIS:H	1:A:431:HIS:CD2	2.08	0.68
1:C:112:ARG:HD3	1:C:159:ASP:OD1	1.93	0.68
3:B:590:GZZ:HC11	7:B:2084:HOH:O	1.93	0.68
1:A:292:GLN:NE2	1:A:414:GLU:OE2	2.27	0.68
1:A:171:PHE:CD2	3:A:590:GZZ:HC11	2.30	0.67
1:C:220:ASP:OD2	1:C:222:LYS:N	2.26	0.67
1:B:50:ALA:HB1	1:B:304:LYS:HD3	1.77	0.67
1:C:216:TYR:CE1	1:C:217:LEU:HD13	2.29	0.66
1:B:243:SER:HB2	1:B:244:PRO:CD	2.25	0.66
1:B:242:TYR:CZ	1:B:280:PRO:HD2	2.31	0.66
5:C:601:NAG:O4	6:C:602:NAG:C2	2.44	0.65
1:A:220:ASP:OD1	1:A:222:LYS:N	2.30	0.65
3:A:590:GZZ:HC12	7:A:2207:HOH:O	1.97	0.65
1:B:69:MET:CE	1:B:74:PRO:HD3	2.22	0.65
1:A:355:ARG:NH1	7:A:2182:HOH:O	2.04	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:GLN:OE1	7:A:2138:HOH:O	2.15	0.64
1:C:218:LYS:H	1:C:228:ASP:HB2	1.63	0.64
1:A:47:THR:O	1:A:53:ASN:HA	1.98	0.63
1:B:243:SER:HB2	1:B:244:PRO:HD2	1.79	0.63
1:B:424:ARG:HG3	7:B:2225:HOH:O	1.99	0.63
1:B:360:GLN:NE2	7:B:2184:HOH:O	2.31	0.63
1:C:218:LYS:O	1:C:227:VAL:N	2.25	0.63
1:C:21:LYS:HB2	1:C:216:TYR:CE2	2.34	0.63
1:B:218:LYS:H	1:B:228:ASP:HB2	1.62	0.63
1:B:131:HIS:HD2	1:B:133:SER:OG	1.82	0.62
4:A:601:NAG:HO4	4:A:602:NAG:C1	2.11	0.62
1:A:308:LYS:NZ	1:A:310:TRP:O	2.25	0.62
1:C:291:TYR:CE2	7:C:2151:HOH:O	2.48	0.61
1:A:73:TRP:HB3	1:A:74:PRO:HD3	1.82	0.61
1:C:228:ASP:OD1	1:C:229:PRO:HD2	2.01	0.61
1:B:131:HIS:HD2	1:B:133:SER:H	1.46	0.61
1:B:169:TYR:O	3:B:590:GZZ:H102	1.99	0.61
1:B:308:LYS:HE2	1:B:310:TRP:O	1.99	0.61
1:B:431:HIS:H	1:B:431:HIS:CD2	2.18	0.61
1:B:360:GLN:NE2	1:B:364:GLN:NE2	2.48	0.61
1:C:431:HIS:CD2	1:C:431:HIS:H	2.17	0.61
1:A:218:LYS:H	1:A:228:ASP:HB2	1.66	0.61
1:B:457:CYS:HA	1:B:462:MET:O	2.00	0.61
1:B:387:ASP:HB2	7:B:2199:HOH:O	2.00	0.61
1:A:219:THR:HG22	1:A:226:ILE:HA	1.81	0.60
1:A:110:GLN:O	1:A:114:GLU:HG3	2.00	0.60
1:B:370:MET:HG3	1:B:384:ASP:OD2	2.01	0.60
1:B:218:LYS:N	1:B:228:ASP:HB2	2.17	0.60
1:B:20:ALA:HB3	1:B:216:TYR:OH	2.01	0.60
1:C:91:TYR:OH	1:C:314:LYS:HE2	2.01	0.60
1:B:219:THR:HG22	1:B:226:ILE:HA	1.84	0.60
1:A:307:ARG:HA	1:A:343:ASN:ND2	2.18	0.59
1:C:150:GLN:NE2	7:C:2081:HOH:O	2.34	0.59
1:A:152:ASN:ND2	1:B:394:TRP:HE1	2.01	0.59
1:B:98:LYS:HG3	1:B:102:GLY:O	2.03	0.58
1:A:58:ALA:HA	2:A:579:FAD:C4X	2.33	0.58
1:A:223:SER:HB3	1:A:225:LYS:H	1.68	0.58
1:B:411:ASN:HD22	1:B:414:GLU:H	1.48	0.58
1:A:394:TRP:HE1	1:B:152:ASN:HD22	1.51	0.58
1:B:131:HIS:CD2	1:B:133:SER:OG	2.58	0.57
1:A:98:LYS:HE3	1:A:103:VAL:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:THR:CG2	1:C:226:ILE:HA	2.28	0.57
1:B:223:SER:HB3	1:B:225:LYS:HB2	1.87	0.56
1:C:169:TYR:O	3:C:590:GZZ:H102	2.05	0.56
1:A:307:ARG:HA	1:A:343:ASN:HD21	1.70	0.56
1:C:117:ASP:O	1:C:121:GLU:HG3	2.05	0.56
1:C:303:LEU:O	1:C:344:VAL:HA	2.06	0.55
5:C:601:NAG:O6	6:C:602:NAG:C1	2.54	0.55
1:A:21:LYS:HB2	1:A:216:TYR:CE2	2.40	0.55
1:A:342:ALA:O	1:A:343:ASN:HB2	2.05	0.55
1:B:69:MET:HE2	1:B:74:PRO:CD	2.30	0.54
1:A:306:PRO:HG2	1:A:383:PRO:HB2	1.88	0.54
1:B:69:MET:HE2	1:B:73:TRP:HB3	1.86	0.54
1:A:91:TYR:N	1:A:91:TYR:CD1	2.75	0.54
1:B:241:LYS:HA	1:B:279:LYS:O	2.08	0.54
1:B:112:ARG:HD3	1:B:159:ASP:OD1	2.08	0.54
5:C:601:NAG:H3	5:C:603:FCA:HO2	1.71	0.54
1:A:81:LYS:O	1:A:203:ARG:NH2	2.42	0.53
1:C:304:LYS:HE2	1:C:342:ALA:O	2.09	0.53
4:B:601:NAG:O4	4:B:602:NAG:C2	2.54	0.52
1:B:366:LYS:HD2	1:B:385:ALA:HB3	1.91	0.52
1:B:454:LEU:C	1:B:454:LEU:HD12	2.29	0.52
1:A:63:GLY:HA2	1:A:193:GLY:O	2.09	0.52
1:C:73:TRP:HB3	1:C:74:PRO:HD3	1.91	0.52
1:C:374:ARG:HD2	7:C:2215:HOH:O	2.10	0.51
1:B:411:ASN:C	1:B:411:ASN:HD22	2.14	0.51
1:B:69:MET:HE3	1:B:73:TRP:CB	2.35	0.51
1:B:63:GLY:HA2	1:B:193:GLY:O	2.10	0.51
1:B:148:GLU:O	1:B:149:HIS:HB2	2.12	0.50
1:B:438:GLY:O	2:B:579:FAD:H1'2	2.10	0.50
5:C:601:NAG:H4	6:C:602:NAG:C1	2.39	0.50
1:B:131:HIS:HD2	1:B:133:SER:CB	2.25	0.50
1:B:222:LYS:CG	1:B:222:LYS:O	2.59	0.50
1:C:355:ARG:NH1	7:C:2198:HOH:O	2.18	0.50
1:C:220:ASP:HB3	1:C:223:SER:OG	2.12	0.49
1:B:222:LYS:HG3	1:B:222:LYS:O	2.12	0.49
1:B:243:SER:CB	1:B:244:PRO:CD	2.89	0.49
1:A:405:ASN:OD1	3:A:590:GZZ:NH1	2.46	0.49
1:A:338:GLN:C	1:A:340:PRO:HD3	2.34	0.49
1:A:98:LYS:HE2	1:A:104:TYR:HA	1.95	0.48
1:B:58:ALA:HA	2:B:579:FAD:C4X	2.43	0.48
1:B:69:MET:HE3	1:B:73:TRP:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:VAL:HG12	1:A:65:ASN:N	2.28	0.48
1:C:219:THR:HA	1:C:225:LYS:O	2.13	0.48
4:B:601:NAG:H4	4:B:602:NAG:C1	2.41	0.48
1:A:448:ILE:O	1:A:452:GLU:HG3	2.14	0.47
1:B:449:ASP:O	1:B:453:ILE:HG13	2.13	0.47
1:B:223:SER:C	1:B:225:LYS:H	2.11	0.47
1:B:69:MET:CE	1:B:73:TRP:CD1	2.98	0.47
1:A:23:LEU:HD13	1:A:451:ALA:HB1	1.96	0.47
1:B:242:TYR:CE2	1:B:280:PRO:HD2	2.50	0.47
1:C:342:ALA:O	1:C:343:ASN:HB2	2.15	0.47
1:C:235:LYS:NZ	1:C:253:ASP:OD2	2.31	0.47
1:A:415:TYR:O	1:A:418:LEU:HB2	2.15	0.47
1:A:49:PHE:N	1:A:52:ILE:O	2.36	0.47
1:A:220:ASP:OD1	1:A:223:SER:N	2.45	0.46
1:A:170:GLU:OE2	3:A:590:GZZ:H101	2.14	0.46
1:A:152:ASN:HD22	1:B:394:TRP:HE1	1.62	0.46
1:C:218:LYS:N	1:C:228:ASP:HB2	2.31	0.46
1:B:69:MET:CE	1:B:73:TRP:HD1	2.29	0.46
1:C:104:TYR:CZ	1:C:158:VAL:HG23	2.51	0.46
1:B:454:LEU:HD12	1:B:454:LEU:O	2.15	0.46
3:A:590:GZZ:C1	7:A:2207:HOH:O	2.59	0.45
1:B:6:ARG:HA	1:B:30:ASP:O	2.16	0.45
5:C:603:FCA:H5	6:C:602:NAG:H62	1.99	0.45
1:B:52:ILE:CD1	1:B:339:TYR:CD2	2.99	0.45
1:C:219:THR:HA	1:C:227:VAL:HG22	1.98	0.45
1:B:223:SER:C	1:B:225:LYS:N	2.69	0.45
1:C:96:VAL:O	1:C:103:VAL:HA	2.17	0.45
1:B:91:TYR:N	1:B:91:TYR:CD1	2.85	0.44
1:A:178:THR:CG2	1:A:183:THR:HG21	2.48	0.44
1:C:8:ILE:HG13	1:C:259:ALA:HB2	1.98	0.44
1:B:170:GLU:OE2	3:B:590:GZZ:H101	2.17	0.44
1:B:8:ILE:HA	1:B:32:LEU:O	2.18	0.44
1:B:189:PHE:CZ	3:B:590:GZZ:H171	2.53	0.44
1:B:360:GLN:NE2	1:B:364:GLN:HE21	2.14	0.44
1:C:272:GLN:C	7:C:2151:HOH:O	2.50	0.44
1:A:45:HIS:HD2	1:A:56:LEU:HD12	1.83	0.44
1:B:421:PRO:HB3	1:B:426:TYR:CD2	2.53	0.43
1:A:370:MET:HG3	1:A:384:ASP:OD1	2.18	0.43
1:C:219:THR:CA	1:C:227:VAL:HG22	2.47	0.43
1:A:49:PHE:O	1:A:50:ALA:HB3	2.18	0.43
1:B:304:LYS:HG3	1:B:305:PHE:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ILE:HD12	1:B:339:TYR:CD2	2.54	0.43
1:A:68:LYS:HD2	1:A:191:ASP:HB3	1.99	0.43
1:B:73:TRP:CZ2	1:B:77:ASN:HB2	2.53	0.43
1:B:253:ASP:O	1:B:254:ASN:HB2	2.18	0.43
1:B:275:LEU:HA	1:B:275:LEU:HD12	1.78	0.43
1:C:60:TRP:CZ3	3:C:590:GZZ:H112	2.53	0.43
1:B:420:ALA:HA	1:B:421:PRO:HD3	1.81	0.43
1:A:58:ALA:HA	2:A:579:FAD:N5	2.34	0.42
1:A:21:LYS:O	1:A:25:GLU:HG3	2.18	0.42
1:C:104:TYR:CZ	1:C:158:VAL:CG2	3.02	0.42
1:C:98:LYS:HG2	1:C:104:TYR:CE1	2.54	0.42
1:C:100:ASP:OD1	1:C:375:LYS:HE2	2.19	0.42
1:A:366:LYS:HD2	1:A:385:ALA:HB3	2.00	0.42
1:B:134:GLY:HA2	1:B:181:GLN:OE1	2.20	0.42
1:C:219:THR:CA	1:C:225:LYS:O	2.67	0.42
1:A:70:ASN:O	1:A:74:PRO:HD3	2.18	0.42
1:B:308:LYS:HG2	1:B:309:PHE:N	2.33	0.42
1:A:228:ASP:HA	1:A:229:PRO:HD2	1.91	0.42
1:B:154:PRO:HB3	1:B:159:ASP:HB3	2.00	0.42
1:C:58:ALA:HA	2:C:579:FAD:C4X	2.50	0.42
1:B:431:HIS:CD2	7:B:2229:HOH:O	2.72	0.42
1:B:6:ARG:O	1:B:259:ALA:HB1	2.20	0.42
1:C:217:LEU:HA	1:C:217:LEU:HD12	1.90	0.42
1:B:244:PRO:O	1:B:424:ARG:NH1	2.52	0.42
1:C:91:TYR:N	1:C:91:TYR:CD1	2.87	0.42
1:C:64:VAL:HG12	1:C:65:ASN:N	2.35	0.42
1:A:438:GLY:O	2:A:579:FAD:H1'2	2.20	0.42
1:C:454:LEU:HD12	1:C:454:LEU:O	2.20	0.42
5:C:601:NAG:HO4	6:C:602:NAG:C1	2.16	0.41
1:A:218:LYS:N	1:A:228:ASP:HB2	2.31	0.41
1:C:260:ASP:O	1:C:424:ARG:HD3	2.20	0.41
1:C:243:SER:HB2	1:C:244:PRO:CD	2.50	0.41
1:C:290:ILE:HA	1:C:418:LEU:HD21	2.03	0.41
1:B:35:GLU:HG2	1:B:39:HIS:O	2.21	0.41
1:A:219:THR:HA	1:A:225:LYS:O	2.21	0.41
1:A:431:HIS:CD2	7:A:2218:HOH:O	2.74	0.41
1:A:115:LEU:C	1:A:115:LEU:HD12	2.42	0.41
1:A:156:THR:O	1:A:160:MET:HG3	2.20	0.41
1:C:49:PHE:O	1:C:52:ILE:HG12	2.21	0.41
4:B:601:NAG:O6	4:B:602:NAG:C1	2.69	0.41
1:C:438:GLY:O	2:C:579:FAD:H1'2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:GLN:HB3	1:B:235:LYS:HG3	2.02	0.40
1:B:131:HIS:CD2	1:B:133:SER:CB	3.03	0.40
1:B:26:ALA:HB2	1:B:455:ILE:HD13	2.03	0.40
1:C:223:SER:C	1:C:225:LYS:H	2.24	0.40
1:A:73:TRP:N	1:A:74:PRO:CD	2.85	0.40
1:B:350:THR:HA	1:B:354:SER:OG	2.21	0.40
1:A:39:HIS:HD2	1:A:40:ILE:O	2.05	0.40
1:B:416:ASP:OD2	1:B:466:HIS:HD2	2.04	0.40
1:A:350:THR:HA	1:A:354:SER:OG	2.21	0.40
1:A:402:THR:HB	2:A:579:FAD:HM83	2.03	0.40
1:A:137:ASP:OD1	1:A:181:GLN:HB2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	457/472 (97%)	437 (96%)	20 (4%)	0	100	100
1	B	460/472 (98%)	441 (96%)	19 (4%)	0	100	100
1	C	460/472 (98%)	443 (96%)	17 (4%)	0	100	100
All	All	1377/1416 (97%)	1321 (96%)	56 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	394/404 (98%)	384 (98%)	10 (2%)	55	47
1	B	397/404 (98%)	388 (98%)	9 (2%)	58	51
1	C	397/404 (98%)	387 (98%)	10 (2%)	55	47
All	All	1188/1212 (98%)	1159 (98%)	29 (2%)	57	49

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	24	SER
1	A	52	ILE
1	A	59	ASN
1	A	115	LEU
1	A	149	HIS
1	A	165	TYR
1	A	168	ASP
1	A	190	SER
1	A	205	TYR
1	B	59	ASN
1	B	115	LEU
1	B	157	PRO
1	B	168	ASP
1	B	205	TYR
1	B	223	SER
1	B	293	PHE
1	B	411	ASN
1	B	454	LEU
1	C	59	ASN
1	C	115	LEU
1	C	127	SER
1	C	149	HIS
1	C	157	PRO
1	C	168	ASP
1	C	175	PRO
1	C	205	TYR
1	C	217	LEU
1	C	387	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	HIS
1	A	152	ASN
1	A	292	GLN
1	A	343	ASN
1	A	360	GLN
1	A	431	HIS
1	B	131	HIS
1	B	152	ASN
1	B	292	GLN
1	B	360	GLN
1	B	364	GLN
1	B	411	ASN
1	B	431	HIS
1	B	466	HIS
1	C	360	GLN
1	C	371	GLN
1	C	431	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

5 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	$\# Z > 2$
5	NAG	C	601	1,5,6	14,14,15	1.28	2 (14%)	15,19,21	1.61	5 (33%)
6	NAG	C	602	5,6	14,14,15	0.97	1 (7%)	15,19,21	1.58	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FCA	C	603	5	10,10,11	1.23	1 (10%)	14,14,16	1.81	5 (35%)
6	MAN	C	604	6	11,11,12	0.64	0	14,15,17	2.66	3 (21%)
6	MAN	C	605	6	11,11,12	0.57	0	14,15,17	1.59	3 (21%)

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
5	NAG	C	601	1,5,6	-	0/6/23/26	0/1/1/1
6	NAG	C	602	5,6	-	0/6/23/26	0/1/1/1
5	FCA	C	603	5	-	0/0/17/20	0/1/1/1
6	MAN	C	604	6	1/1/4/5	0/2/19/22	0/1/1/1
6	MAN	C	605	6	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	601	NAG	O5-C1	-2.77	1.39	1.43
5	C	603	FCA	C2-C3	-2.77	1.48	1.52
6	C	602	NAG	O5-C1	-2.75	1.39	1.43
5	C	601	NAG	C1-C2	-2.62	1.48	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	602	NAG	C2-N2-C7	-5.32	116.21	123.04
6	C	605	MAN	C1-C2-C3	-3.53	105.36	109.54
6	C	605	MAN	C2-C3-C4	-2.83	106.24	111.04
5	C	601	NAG	O4-C4-C3	-2.50	104.71	110.34
5	C	603	FCA	O5-C1-C2	-2.31	107.10	110.86
5	C	601	NAG	C8-C7-N2	-2.26	111.79	116.11
5	C	601	NAG	O5-C5-C6	-2.15	102.69	107.35
5	C	603	FCA	O3-C3-C2	2.17	113.91	110.00
5	C	603	FCA	O5-C5-C4	2.30	113.52	109.53
6	C	604	MAN	O2-C2-C1	2.46	114.14	109.21
6	C	604	MAN	C1-O5-C5	2.49	115.41	112.25
5	C	601	NAG	C3-C4-C5	2.54	114.63	110.20
5	C	603	FCA	C1-C2-C3	2.63	112.65	109.54
6	C	605	MAN	O2-C2-C3	2.72	115.58	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	601	NAG	O3-C3-C4	3.24	117.64	110.34
5	C	603	FCA	C1-O5-C5	3.31	117.49	112.38
6	C	604	MAN	O2-C2-C3	8.82	127.86	110.12

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	604	MAN	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	601	NAG	7	0
6	C	602	NAG	6	0
5	C	603	FCA	3	0

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	A	579	-	48,58,58	0.99	1 (2%)	54,89,89	2.15	10 (18%)
3	GZZ	A	590	-	18,24,24	1.03	2 (11%)	17,25,25	1.44	3 (17%)
4	NAG	A	601	1,4	14,14,15	0.94	1 (7%)	15,19,21	1.68	4 (26%)
4	NAG	A	602	4	14,14,15	0.90	0	15,19,21	1.85	3 (20%)
2	FAD	B	579	-	48,58,58	0.95	1 (2%)	54,89,89	1.88	5 (9%)
3	GZZ	B	590	-	18,24,24	1.25	2 (11%)	17,25,25	1.37	2 (11%)
4	NAG	B	601	1,4	14,14,15	1.26	3 (21%)	15,19,21	2.49	3 (20%)
4	NAG	B	602	4	14,14,15	0.96	1 (7%)	15,19,21	1.37	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	C	579	-	48,58,58	1.01	2 (4%)	54,89,89	2.24	10 (18%)
3	GZZ	C	590	-	18,24,24	1.21	2 (11%)	17,25,25	0.98	1 (5%)

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	FAD	A	579	-	-	0/30/50/50	0/6/6/6
3	GZZ	A	590	-	-	0/18/22/22	0/0/0/0
4	NAG	A	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	602	4	-	0/6/23/26	0/1/1/1
2	FAD	B	579	-	-	0/30/50/50	0/6/6/6
3	GZZ	B	590	-	-	0/18/22/22	0/0/0/0
4	NAG	B	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	602	4	-	0/6/23/26	0/1/1/1
2	FAD	C	579	-	-	0/30/50/50	0/6/6/6
3	GZZ	C	590	-	-	0/18/22/22	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	NAG	O5-C1	-2.74	1.39	1.43
4	B	601	NAG	C1-C2	-2.29	1.49	1.52
4	B	602	NAG	O5-C1	-2.18	1.40	1.43
4	A	601	NAG	O3-C3	2.05	1.47	1.43
3	A	590	GZZ	C8-N9	2.27	1.54	1.46
4	B	601	NAG	O3-C3	2.28	1.48	1.43
3	A	590	GZZ	C10-N9	2.49	1.55	1.46
2	C	579	FAD	C4-N3	2.73	1.38	1.33
2	C	579	FAD	C4X-N5	2.85	1.37	1.33
3	C	590	GZZ	C10-N9	2.93	1.56	1.46
3	C	590	GZZ	C8-N9	2.95	1.56	1.46
3	B	590	GZZ	C10-N9	3.02	1.56	1.46
3	B	590	GZZ	C8-N9	3.21	1.57	1.46
2	B	579	FAD	C4-N3	3.82	1.40	1.33
2	A	579	FAD	C4-N3	4.09	1.40	1.33

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	579	FAD	C4X-C10-N10	-8.29	115.64	120.52
4	B	601	NAG	C2-N2-C7	-7.29	113.67	123.04
2	A	579	FAD	C4X-C4-N3	-6.38	114.86	123.59
2	A	579	FAD	C4X-C10-N10	-6.26	116.83	120.52
2	B	579	FAD	C4X-C4-N3	-5.79	115.67	123.59
4	A	602	NAG	C2-N2-C7	-5.50	115.97	123.04
2	C	579	FAD	C4-C4X-C10	-4.81	116.86	119.94
2	C	579	FAD	C4X-C4-N3	-4.35	117.64	123.59
2	A	579	FAD	C9A-C5X-N5	-3.52	117.16	122.36
2	B	579	FAD	C4X-C10-N10	-3.33	118.56	120.52
3	A	590	GZZ	C10-N9-C8	-3.17	102.13	113.35
2	C	579	FAD	C9A-C5X-N5	-2.77	118.26	122.36
3	C	590	GZZ	C10-N9-C8	-2.43	104.75	113.35
4	A	601	NAG	C8-C7-N2	-2.39	111.53	116.11
4	A	602	NAG	C8-C7-N2	-2.39	111.54	116.11
4	B	601	NAG	O5-C5-C6	-2.27	102.42	107.35
3	B	590	GZZ	C10-N9-C8	-2.20	105.56	113.35
3	A	590	GZZ	C6-C7-C8	-2.15	103.39	113.69
4	A	602	NAG	C4-C3-C2	-2.10	107.97	111.23
3	A	590	GZZ	C4-C3-C2	-2.01	104.14	114.53
2	C	579	FAD	O2A-PA-O1A	2.06	123.71	112.53
2	A	579	FAD	C4X-N5-C5X	2.12	119.21	116.76
4	A	601	NAG	O3-C3-C4	2.21	115.30	110.34
4	B	602	NAG	O7-C7-N2	2.32	126.59	121.86
2	A	579	FAD	O2A-PA-O1A	2.33	125.17	112.53
4	A	601	NAG	O3-C3-C2	2.42	113.91	109.11
2	C	579	FAD	O2P-P-O1P	2.43	125.69	112.53
2	B	579	FAD	O2A-PA-O3P	2.46	116.25	105.09
2	A	579	FAD	C4A-C5A-N7A	2.58	111.85	109.48
2	B	579	FAD	N3A-C2A-N1A	2.66	130.93	128.89
2	A	579	FAD	C2B-C1B-N9A	2.80	118.57	114.29
2	A	579	FAD	C6-C5X-C9A	2.84	122.72	118.98
2	C	579	FAD	N3A-C2A-N1A	3.10	131.26	128.89
4	B	602	NAG	C1-O5-C5	3.26	116.39	112.25
4	A	601	NAG	C1-O5-C5	3.59	116.80	112.25
2	A	579	FAD	C1'-N10-C9A	3.59	122.89	118.86
3	B	590	GZZ	C7-C8-N9	3.65	121.08	111.96
2	C	579	FAD	C4X-N5-C5X	3.90	121.25	116.76
2	C	579	FAD	C4-C4X-N5	4.14	123.74	118.72
4	B	601	NAG	O3-C3-C2	4.18	117.39	109.11
2	C	579	FAD	C4-N3-C2	8.16	122.30	115.25
2	A	579	FAD	C4-N3-C2	9.16	123.17	115.25
2	B	579	FAD	C4-N3-C2	9.45	123.41	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	579	FAD	4	0
3	A	590	GZZ	7	0
4	A	601	NAG	2	0
4	A	602	NAG	2	0
2	B	579	FAD	2	0
3	B	590	GZZ	4	0
4	B	601	NAG	4	0
4	B	602	NAG	4	0
2	C	579	FAD	2	0
3	C	590	GZZ	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.