



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:45 AM GMT

PDB ID : 2IID
Title : Structure of L-amino acid oxidase from Calloselasma rhodostoma in complex with L-phenylalanine
Authors : Moustafa, I.M.; Foster, S.; Lyubimov, A.Y.; Vrielink, A.
Deposited on : 2006-09-27
Resolution : 1.80 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

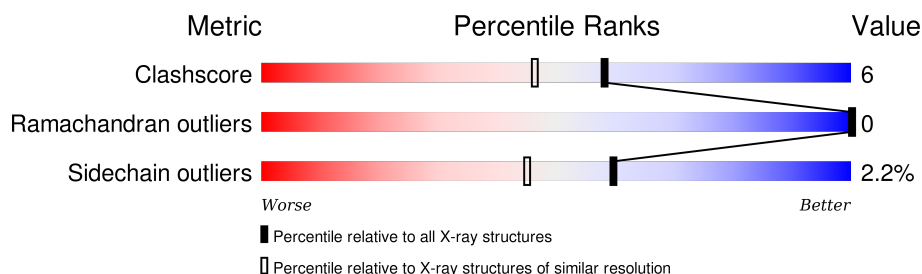
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)

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	498	 87% 10% . .
1	B	498	 86% 10% . .
1	C	498	 87% 9% . .
1	D	498	 87% 9% . .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18055 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 L-amino-acid oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	0	4	0
			3892	2479	666	735	12			
1	B	483	Total	C	N	O	S	0	4	0
			3892	2479	666	735	12			
1	C	483	Total	C	N	O	S	0	4	0
			3892	2479	666	735	12			
1	D	483	Total	C	N	O	S	0	4	0
			3892	2479	666	735	12			

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

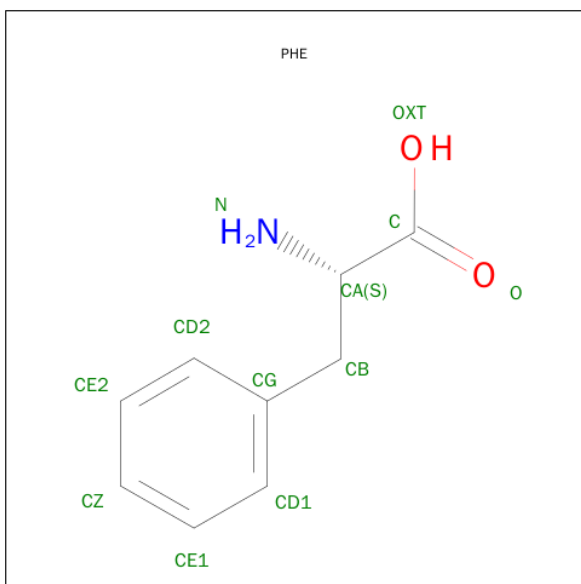
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			24	14	1	9		
2	C	2	Total	C	N	O	0	0
			24	14	1	9		
2	D	2	Total	C	N	O	0	0
			24	14	1	9		

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



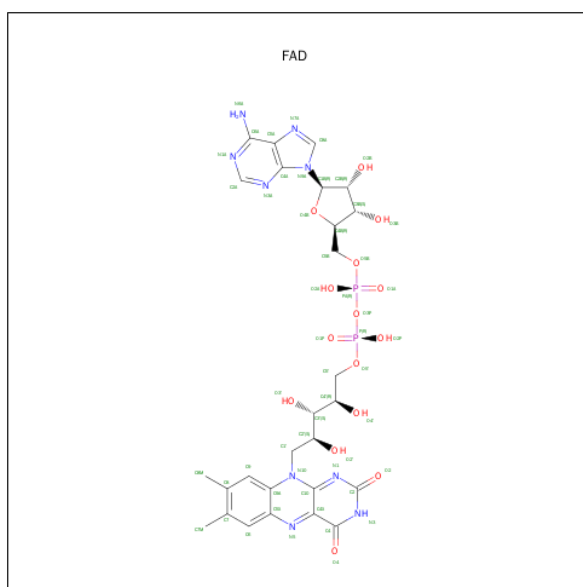
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			12	9	1	2		
4	B	1	Total	C	N	O	0	0
			12	9	1	2		
4	C	1	Total	C	N	O	0	0
			12	9	1	2		
4	D	1	Total	C	N	O	0	0
			12	9	1	2		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	538	Total	O	0	0
			538	538		

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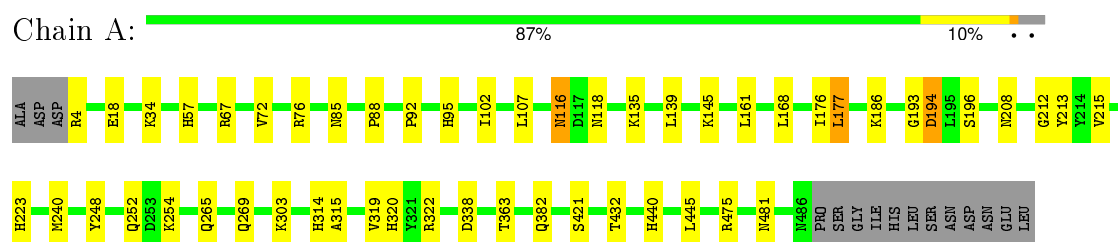
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	541	Total 541	O 541	0	0
6	C	528	Total 528	O 528	0	0
6	D	478	Total 478	O 478	0	0

3 Residue-property plots

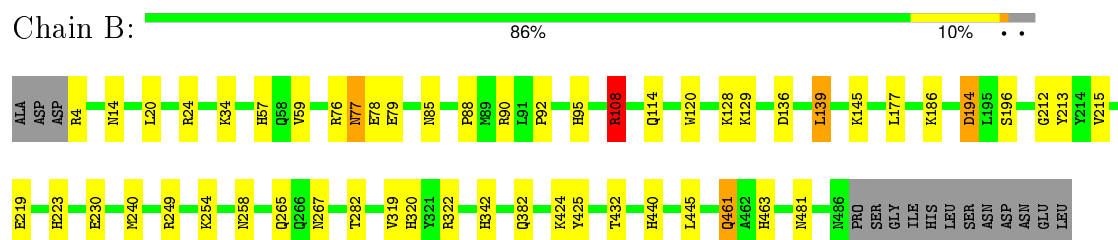
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

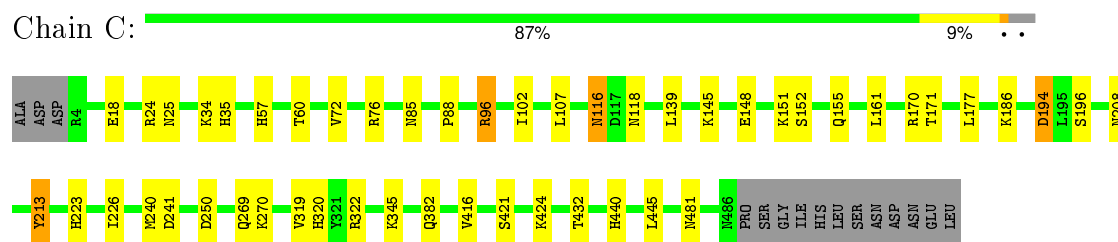
- Molecule 1: L-amino-acid oxidase



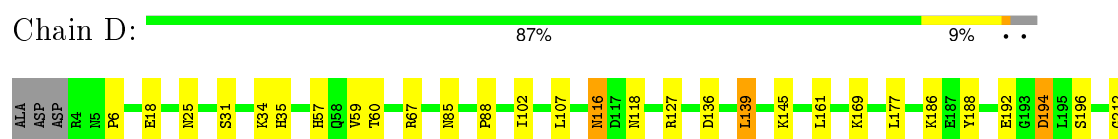
- Molecule 1: L-amino-acid oxidase



- Molecule 1: L-amino-acid oxidase



- Molecule 1: L-amino-acid oxidase



Y213	Y214	Y215	H223	I226	F227	M240	Y248	Q252	D253	K254	Q269	H314	V319	H320	Y321	R322	Q382	K406	T432	H440	L445	I481	H486	PRO	SER	GLY	ILE	HIS	LEU	SER	ASN	ASP	ASN	GLU	LEU
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.76 Å 154.00 Å 103.18 Å 90.00° 109.52° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80	Depositor
% Data completeness (in resolution range)	99.5 (50.00-1.80)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.172 , 0.210	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18055	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

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: NAG, FAD, FUC

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	0.64	0/3984	0.68	1/5391 (0.0%)
1	B	0.66	0/3984	0.69	1/5391 (0.0%)
1	C	0.65	0/3984	0.68	2/5391 (0.0%)
1	D	0.63	0/3984	0.68	2/5391 (0.0%)
All	All	0.64	0/15936	0.68	6/21564 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	127	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	C	96	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	108	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	C	96	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	177	LEU	CB-CG-CD1	5.37	120.12	111.00
1	D	127	ARG	NE-CZ-NH1	5.30	122.95	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3892	0	3808	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3892	0	3808	55	0
1	C	3892	0	3808	45	0
1	D	3892	0	3808	45	0
2	A	24	0	22	0	0
2	C	24	0	22	2	0
2	D	24	0	22	0	0
3	A	14	0	13	0	0
3	B	28	0	26	0	0
3	C	14	0	13	1	0
3	D	14	0	13	0	0
4	A	12	0	8	1	0
4	B	12	0	8	0	0
4	C	12	0	8	1	0
4	D	12	0	8	0	0
5	A	53	0	31	2	0
5	B	53	0	31	1	0
5	C	53	0	31	3	0
5	D	53	0	31	1	0
6	A	538	0	0	18	0
6	B	541	0	0	14	0
6	C	528	0	0	15	0
6	D	478	0	0	14	0
All	All	18055	0	15519	187	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 6.

All (187) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322[A]:ARG:HD3	6:B:976:HOH:O	1.25	1.32
1:A:34:LYS:H	1:A:57:HIS:HD2	1.12	0.94
1:B:34:LYS:H	1:B:57:HIS:HD2	1.16	0.93
1:A:440:HIS:HD2	1:C:186:LYS:HZ1	1.08	0.93
1:C:34:LYS:H	1:C:57:HIS:HD2	1.17	0.88
1:B:90:ARG:HH11	1:B:114:GLN:HE22	1.24	0.85
1:B:145:LYS:HG3	1:B:196:SER:HB3	1.59	0.84
1:A:254:LYS:HE3	6:A:849:HOH:O	1.78	0.82
1:B:219:GLU:OE2	1:B:463:HIS:HD2	1.62	0.81
1:D:145:LYS:HG3	1:D:196:SER:HB3	1.63	0.81
1:A:116:ASN:HD22	1:A:118:ASN:H	1.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322[A]:ARG:HD3	6:C:778:HOH:O	1.80	0.79
1:D:34:LYS:H	1:D:57:HIS:HD2	1.31	0.79
1:C:145:LYS:HG3	1:C:196:SER:HB3	1.64	0.78
1:B:319:VAL:HG21	1:B:445:LEU:HD11	1.67	0.76
1:B:108:ARG:HH11	1:B:108:ARG:HG3	1.48	0.76
1:C:223[A]:HIS:CE1	6:C:995:HOH:O	2.39	0.75
1:B:59:VAL:HG22	1:B:254:LYS:HD3	1.69	0.75
1:D:116:ASN:HD22	1:D:118:ASN:H	1.33	0.75
1:D:322[A]:ARG:HD3	6:D:994:HOH:O	1.87	0.74
1:C:116:ASN:HD22	1:C:118:ASN:H	1.36	0.74
1:B:282:THR:O	1:B:282:THR:HG23	1.88	0.73
1:A:315:ALA:O	1:A:319:VAL:HG23	1.89	0.73
1:B:186:LYS:NZ	1:D:440:HIS:HD2	1.87	0.73
1:A:145:LYS:HG3	1:A:196:SER:HB3	1.71	0.72
1:D:319:VAL:HG21	1:D:445:LEU:HD11	1.70	0.72
1:B:14:ASN:H	1:B:461:GLN:NE2	1.87	0.71
1:B:108:ARG:HD3	6:B:917:HOH:O	1.89	0.71
1:B:85:ASN:HD21	1:B:240:MET:H	1.39	0.70
1:D:85:ASN:HD21	1:D:240:MET:H	1.38	0.70
1:C:25:ASN:ND2	6:C:702:HOH:O	2.24	0.69
1:A:475:ARG:HG2	6:A:994:HOH:O	1.91	0.69
1:A:440:HIS:HD2	1:C:186:LYS:NZ	1.89	0.69
1:B:57:HIS:HE1	1:B:481:ASN:OD1	1.77	0.67
1:D:57:HIS:HE1	1:D:481:ASN:OD1	1.77	0.67
1:D:322[A]:ARG:HG2	6:D:994:HOH:O	1.94	0.66
1:B:440:HIS:HD2	1:D:186:LYS:HZ3	1.43	0.66
1:A:34:LYS:N	1:A:57:HIS:HD2	1.90	0.65
1:A:319:VAL:HG21	1:A:445:LEU:HD11	1.78	0.65
1:C:85:ASN:HD21	1:C:240:MET:H	1.42	0.65
1:C:319:VAL:HG21	1:C:445:LEU:HD11	1.77	0.65
1:D:59:VAL:HG22	1:D:254:LYS:HD3	1.79	0.64
1:A:440:HIS:CD2	1:C:186:LYS:HZ1	2.01	0.64
1:B:14:ASN:H	1:B:461:GLN:HE21	1.45	0.64
1:A:76:ARG:NH1	6:A:1054:HOH:O	2.30	0.63
1:C:18:GLU:HG3	6:C:975:HOH:O	1.98	0.63
1:B:440:HIS:HD2	1:D:186:LYS:NZ	1.97	0.62
1:A:85:ASN:HD21	1:A:240:MET:H	1.47	0.62
1:B:34:LYS:H	1:B:57:HIS:CD2	2.08	0.61
1:A:248:TYR:CZ	1:A:252:GLN:HG3	2.36	0.61
1:A:116:ASN:ND2	1:A:118:ASN:H	1.96	0.61
4:A:526:PHE:HA	5:A:527:FAD:N5	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:ASN:ND2	1:D:118:ASN:H	1.99	0.60
1:A:322[A]:ARG:HD2	6:A:878:HOH:O	2.02	0.60
4:C:526:PHE:HA	5:C:527:FAD:N5	2.17	0.59
1:A:88:PRO:HA	5:A:527:FAD:C4X	2.32	0.59
1:C:57:HIS:HE1	1:C:481:ASN:OD1	1.85	0.58
1:B:85:ASN:ND2	1:B:240:MET:H	2.01	0.58
1:D:136:ASP:HB3	1:D:139:LEU:HD22	1.86	0.58
1:A:382:GLN:NE2	1:C:382:GLN:NE2	2.52	0.58
1:B:90:ARG:NH1	1:B:114:GLN:HE22	1.98	0.58
1:D:88:PRO:HA	5:D:527:FAD:C4X	2.34	0.57
1:D:85:ASN:ND2	1:D:240:MET:H	2.01	0.57
1:C:76:ARG:NH2	1:C:241:ASP:OD1	2.28	0.57
1:B:219:GLU:OE2	1:B:463:HIS:CD2	2.51	0.56
3:C:522:NAG:O7	6:C:676:HOH:O	2.17	0.56
1:A:34:LYS:H	1:A:57:HIS:CD2	2.05	0.56
1:D:223[A]:HIS:CE1	1:D:227:PHE:CD1	2.94	0.56
1:D:34:LYS:H	1:D:57:HIS:CD2	2.19	0.55
1:C:85:ASN:ND2	1:C:240:MET:H	2.04	0.55
1:B:76:ARG:NH1	6:B:1054:HOH:O	2.36	0.55
1:B:186:LYS:HZ1	1:D:440:HIS:HD2	1.52	0.55
1:B:223[B]:HIS:CD2	6:B:1044:HOH:O	2.58	0.54
1:A:85:ASN:ND2	1:A:240:MET:H	2.05	0.54
1:D:406:LYS:HE2	6:D:995:HOH:O	2.07	0.54
1:A:314:HIS:HD2	6:C:688:HOH:O	1.90	0.54
1:D:102:ILE:HG23	1:D:107:LEU:HB2	1.89	0.54
1:D:25:ASN:ND2	6:D:915:HOH:O	2.40	0.54
1:B:463:HIS:HE1	6:B:540:HOH:O	1.89	0.54
1:C:345:LYS:NZ	6:C:961:HOH:O	2.39	0.53
1:B:322[A]:ARG:NE	1:B:432:THR:HG21	2.23	0.53
1:C:35:HIS:HE1	1:C:60:THR:OG1	1.92	0.53
1:D:322[A]:ARG:CG	6:D:994:HOH:O	2.54	0.52
1:A:194:ASP:OD1	1:A:194:ASP:C	2.47	0.52
1:A:363:THR:HG22	6:A:872:HOH:O	2.09	0.52
1:B:319:VAL:CG2	1:B:445:LEU:HD11	2.39	0.52
1:A:475:ARG:NH1	6:A:634:HOH:O	2.42	0.52
1:C:116:ASN:ND2	1:C:118:ASN:H	2.07	0.52
1:B:59:VAL:CG2	1:B:254:LYS:HD3	2.39	0.51
1:A:303:LYS:HE3	6:A:988:HOH:O	2.11	0.51
1:B:77:ASN:C	1:B:77:ASN:HD22	2.14	0.51
1:B:78:GLU:HG2	6:B:1026:HOH:O	2.10	0.51
1:B:258:ASN:OD1	6:B:1041:HOH:O	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:635:HOH:O	1:D:314:HIS:HD2	1.94	0.50
1:A:475:ARG:NH2	6:A:763:HOH:O	2.45	0.50
1:C:226:ILE:HD11	6:C:934:HOH:O	2.10	0.50
1:A:57:HIS:HE1	1:A:481:ASN:OD1	1.94	0.50
1:C:24:ARG:HD2	6:C:702:HOH:O	2.10	0.50
1:D:226:ILE:HD11	6:D:880:HOH:O	2.12	0.50
1:D:186:LYS:NZ	6:D:600:HOH:O	2.42	0.49
1:B:282:THR:O	1:B:282:THR:CG2	2.59	0.49
1:A:76:ARG:HG2	1:A:76:ARG:HH11	1.78	0.48
1:D:31:SER:HA	6:D:977:HOH:O	2.12	0.48
1:B:322[A]:ARG:CD	6:B:976:HOH:O	2.11	0.48
1:A:186:LYS:NZ	1:C:440:HIS:HD2	2.11	0.48
1:B:249:ARG:HD2	6:B:883:HOH:O	2.13	0.48
1:A:186:LYS:HZ3	1:C:440:HIS:HD2	1.61	0.48
1:D:35:HIS:HE1	1:D:60:THR:OG1	1.96	0.48
1:C:116:ASN:HD21	1:C:118:ASN:HD22	1.60	0.48
1:B:76:ARG:HH11	1:B:76:ARG:HG2	1.77	0.47
1:D:18:GLU:HG3	6:D:804:HOH:O	2.14	0.47
1:B:92:PRO:HG2	1:B:95:HIS:CG	2.49	0.47
1:B:382:GLN:NE2	1:D:382:GLN:HE22	2.12	0.47
1:A:102:ILE:HG23	1:A:107:LEU:HB2	1.95	0.47
1:A:72:VAL:HG22	1:A:88:PRO:HG2	1.96	0.47
1:C:226:ILE:HD12	6:C:942:HOH:O	2.14	0.47
1:A:135:LYS:HG3	6:A:778:HOH:O	2.14	0.47
1:C:34:LYS:H	1:C:57:HIS:CD2	2.10	0.47
1:C:72:VAL:HG22	1:C:88:PRO:HG2	1.97	0.47
1:A:475:ARG:CG	6:A:994:HOH:O	2.57	0.46
1:C:88:PRO:HA	5:C:527:FAD:C4X	2.45	0.46
1:B:342:HIS:HD2	6:B:686:HOH:O	1.98	0.46
1:C:424:LYS:HD2	6:C:891:HOH:O	2.14	0.46
1:C:102:ILE:HG23	1:C:107:LEU:HB2	1.97	0.46
1:B:88:PRO:HA	5:B:525:FAD:C4X	2.46	0.46
1:B:186:LYS:NZ	6:B:1024:HOH:O	2.49	0.46
1:D:248:TYR:CZ	1:D:252:GLN:HG3	2.51	0.46
1:A:319:VAL:CG2	1:A:445:LEU:HD11	2.45	0.46
1:B:136:ASP:HB3	1:B:139:LEU:HD22	1.97	0.46
1:A:18:GLU:HG3	6:A:700:HOH:O	2.14	0.46
1:D:322[A]:ARG:CD	6:D:994:HOH:O	2.53	0.45
1:A:76:ARG:HG2	1:A:76:ARG:NH1	2.31	0.45
1:D:320:HIS:HB3	1:D:432:THR:O	2.16	0.45
1:C:170:ARG:NH1	2:C:525:FUC:H62	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:VAL:CG2	1:D:445:LEU:HD11	2.43	0.45
1:D:192:GLU:OE2	6:D:824:HOH:O	2.21	0.45
1:D:212:GLY:O	1:D:215:VAL:HG22	2.16	0.45
1:B:120:TRP:CH2	1:B:129:LYS:HE2	2.52	0.44
1:D:169:LYS:HG3	6:D:649:HOH:O	2.17	0.44
1:C:322[A]:ARG:NE	1:C:432:THR:HG21	2.32	0.44
1:C:194:ASP:C	1:C:194:ASP:OD1	2.55	0.44
1:B:424:LYS:HE3	1:B:425:TYR:CE2	2.52	0.44
1:B:194:ASP:HA	6:B:932:HOH:O	2.17	0.44
1:B:265:GLN:HE21	1:B:267:ASN:HD21	1.66	0.43
1:C:96:ARG:HD2	6:C:924:HOH:O	2.18	0.43
1:A:92:PRO:HG2	1:A:95:HIS:CG	2.53	0.43
1:B:128:LYS:HE3	1:B:139:LEU:HG	2.00	0.43
1:D:223[A]:HIS:NE2	1:D:227:PHE:CE1	2.87	0.43
1:A:67:ARG:NH2	6:A:598:HOH:O	2.51	0.43
1:B:212:GLY:O	1:B:215:VAL:HG22	2.18	0.43
1:B:20:LEU:O	1:B:24:ARG:HG2	2.19	0.43
1:A:223[B]:HIS:CD2	6:A:907:HOH:O	2.72	0.42
1:B:461:GLN:HG2	6:B:734:HOH:O	2.19	0.42
1:A:382:GLN:CD	1:C:382:GLN:NE2	2.73	0.42
1:A:382:GLN:NE2	1:C:382:GLN:CD	2.72	0.42
1:A:193:GLY:O	1:A:194:ASP:HB3	2.18	0.42
1:C:171:THR:HG22	2:C:525:FUC:H5	2.02	0.42
1:D:188:TYR:C	1:D:188:TYR:CD2	2.92	0.42
1:B:320:HIS:HB3	1:B:432:THR:O	2.20	0.42
1:C:320:HIS:HB3	1:C:432:THR:O	2.20	0.41
1:B:79:GLU:HG2	6:C:718:HOH:O	2.19	0.41
1:A:4:ARG:N	6:A:953:HOH:O	2.53	0.41
1:D:194:ASP:OD1	1:D:194:ASP:C	2.58	0.41
1:C:213:TYR:HA	1:C:213:TYR:HD1	1.73	0.41
1:D:67:ARG:NH2	6:D:604:HOH:O	2.49	0.41
1:C:269:GLN:O	1:C:270:LYS:HD3	2.20	0.41
1:C:34:LYS:N	1:C:57:HIS:HD2	1.99	0.41
1:A:116:ASN:C	1:A:116:ASN:HD22	2.23	0.41
1:B:76:ARG:NH1	1:B:76:ARG:HG2	2.34	0.41
1:B:92:PRO:HB3	1:B:230:GLU:HG2	2.03	0.41
1:D:116:ASN:HD22	1:D:118:ASN:N	2.10	0.41
1:A:322[A]:ARG:CD	6:A:878:HOH:O	2.66	0.41
5:C:527:FAD:H8A	6:C:534:HOH:O	2.19	0.41
1:B:382:GLN:CD	1:D:382:GLN:NE2	2.75	0.41
1:A:168:LEU:HB2	1:A:176:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223[A]:HIS:HE1	6:C:995:HOH:O	1.93	0.41
1:A:338:ASP:HB2	6:A:1012:HOH:O	2.21	0.41
1:A:265:GLN:HG2	6:A:1064:HOH:O	2.20	0.41
1:C:152:SER:OG	1:C:155:GLN:HG3	2.20	0.40
1:B:440:HIS:CD2	1:D:186:LYS:HZ3	2.29	0.40
1:A:382:GLN:NE2	1:A:421[B]:SER:OG	2.55	0.40
1:A:303:LYS:NZ	6:A:932:HOH:O	2.54	0.40
1:A:212:GLY:O	1:A:215:VAL:HG22	2.22	0.40
1:C:382:GLN:NE2	1:C:421[B]:SER:OG	2.54	0.40
1:A:320:HIS:HB3	1:A:432:THR:O	2.21	0.40
1:D:6:PRO:HG2	6:D:951:HOH:O	2.21	0.40
1:C:148:GLU:HA	1:C:151:LYS:HD2	2.04	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	485/498 (97%)	474 (98%)	11 (2%)	0	100	100
1	B	485/498 (97%)	474 (98%)	11 (2%)	0	100	100
1	C	485/498 (97%)	471 (97%)	14 (3%)	0	100	100
1	D	485/498 (97%)	474 (98%)	11 (2%)	0	100	100
All	All	1940/1992 (97%)	1893 (98%)	47 (2%)	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	418/427 (98%)	410 (98%)	8 (2%)	65	52
1	B	418/427 (98%)	410 (98%)	8 (2%)	65	52
1	C	418/427 (98%)	409 (98%)	9 (2%)	60	45
1	D	418/427 (98%)	411 (98%)	7 (2%)	68	57
All	All	1672/1708 (98%)	1640 (98%)	32 (2%)	60	52

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
1	A	139	LEU
1	A	161	LEU
1	A	177	LEU
1	A	194	ASP
1	A	208	ASN
1	A	213	TYR
1	A	269	GLN
1	B	4	ARG
1	B	77	ASN
1	B	108	ARG
1	B	139	LEU
1	B	177	LEU
1	B	194	ASP
1	B	213	TYR
1	B	461	GLN
1	C	116	ASN
1	C	139	LEU
1	C	161	LEU
1	C	177	LEU
1	C	194	ASP
1	C	208	ASN
1	C	213	TYR
1	C	250	ASP
1	C	416	VAL
1	D	116	ASN
1	D	139	LEU
1	D	161	LEU

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Mol	Chain	Res	Type
1	D	177	LEU
1	D	194	ASP
1	D	213	TYR
1	D	269	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	57	HIS
1	A	85	ASN
1	A	116	ASN
1	A	208	ASN
1	A	252	GLN
1	A	269	GLN
1	A	314	HIS
1	A	382	GLN
1	A	440	HIS
1	B	57	HIS
1	B	77	ASN
1	B	85	ASN
1	B	114	GLN
1	B	118	ASN
1	B	208	ASN
1	B	258	ASN
1	B	267	ASN
1	B	342	HIS
1	B	402	GLN
1	B	440	HIS
1	B	461	GLN
1	B	463	HIS
1	C	35	HIS
1	C	57	HIS
1	C	85	ASN
1	C	116	ASN
1	C	208	ASN
1	C	252	GLN
1	C	269	GLN
1	C	314	HIS
1	C	382	GLN
1	C	440	HIS
1	D	35	HIS

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Mol	Chain	Res	Type
1	D	57	HIS
1	D	85	ASN
1	D	116	ASN
1	D	208	ASN
1	D	265	GLN
1	D	269	GLN
1	D	314	HIS
1	D	382	GLN
1	D	440	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 ⓘ

6 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	A	523	1,2	14,14,15	0.54	0	15,19,21	1.04	0
2	FUC	A	525	2	10,10,11	0.77	0	14,14,16	2.11	5 (35%)
2	NAG	C	523	1,2	14,14,15	0.48	0	15,19,21	0.69	0
2	FUC	C	525	2	10,10,11	0.66	0	14,14,16	0.78	0
2	NAG	D	523	1,2	14,14,15	0.54	0	15,19,21	1.12	1 (6%)
2	FUC	D	525	2	10,10,11	0.72	0	14,14,16	2.17	4 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	523	1,2	-	0/6/23/26	0/1/1/1
2	FUC	A	525	2	-	0/0/17/20	0/1/1/1
2	NAG	C	523	1,2	-	0/6/23/26	0/1/1/1
2	FUC	C	525	2	-	0/0/17/20	0/1/1/1
2	NAG	D	523	1,2	-	0/6/23/26	0/1/1/1
2	FUC	D	525	2	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	525	FUC	C1-C2-C3	-2.60	106.47	109.54
2	D	525	FUC	O2-C2-C3	-2.40	105.30	110.12
2	D	523	NAG	C2-N2-C7	2.55	126.32	123.04
2	A	525	FUC	O5-C5-C6	2.62	110.47	106.13
2	A	525	FUC	C3-C4-C5	2.72	114.30	109.72
2	D	525	FUC	C3-C4-C5	3.05	114.86	109.72
2	A	525	FUC	O5-C5-C4	3.58	115.74	109.53
2	D	525	FUC	O5-C5-C4	3.89	116.28	109.53
2	A	525	FUC	C1-O5-C5	4.78	119.76	112.38
2	D	525	FUC	C1-O5-C5	4.93	119.99	112.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	525	FUC	2	0

5.6 Ligand geometry [i](#)

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	522	1	14,14,15	0.45	0	15,19,21	1.11	2 (13%)
4	PHE	A	526	-	9,12,12	0.50	0	9,15,15	0.80	1 (11%)
5	FAD	A	527	-	48,58,58	1.32	7 (14%)	54,89,89	2.25	9 (16%)
3	NAG	B	522	1	14,14,15	0.52	0	15,19,21	1.01	0
3	NAG	B	523	1	14,14,15	0.49	0	15,19,21	1.16	1 (6%)
4	PHE	B	524	-	9,12,12	0.77	0	9,15,15	0.86	1 (11%)
5	FAD	B	525	-	48,58,58	1.34	6 (12%)	54,89,89	2.49	6 (11%)
3	NAG	C	522	1	14,14,15	0.59	0	15,19,21	1.76	4 (26%)
4	PHE	C	526	-	9,12,12	0.48	0	9,15,15	0.40	0
5	FAD	C	527	-	48,58,58	1.35	6 (12%)	54,89,89	2.15	10 (18%)
3	NAG	D	522	1	14,14,15	0.46	0	15,19,21	1.38	3 (20%)
4	PHE	D	526	-	9,12,12	0.63	0	9,15,15	0.90	1 (11%)
5	FAD	D	527	-	48,58,58	1.37	6 (12%)	54,89,89	2.38	9 (16%)

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	522	1	-	0/6/23/26	0/1/1/1
4	PHE	A	526	-	-	0/4/8/8	0/1/1/1
5	FAD	A	527	-	-	0/30/50/50	0/6/6/6
3	NAG	B	522	1	-	0/6/23/26	0/1/1/1
3	NAG	B	523	1	-	0/6/23/26	0/1/1/1
4	PHE	B	524	-	-	0/4/8/8	0/1/1/1
5	FAD	B	525	-	-	0/30/50/50	0/6/6/6
3	NAG	C	522	1	-	0/6/23/26	0/1/1/1
4	PHE	C	526	-	-	0/4/8/8	0/1/1/1
5	FAD	C	527	-	-	0/30/50/50	0/6/6/6
3	NAG	D	522	1	-	0/6/23/26	0/1/1/1
4	PHE	D	526	-	-	0/4/8/8	0/1/1/1
5	FAD	D	527	-	-	0/30/50/50	0/6/6/6

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	527	FAD	C1'-N10	2.06	1.50	1.48
5	D	527	FAD	C1'-N10	2.07	1.50	1.48
5	B	525	FAD	C10-N1	2.09	1.39	1.35
5	A	527	FAD	C2A-N1A	2.22	1.38	1.33
5	A	527	FAD	C10-N1	2.23	1.39	1.35
5	A	527	FAD	O4B-C1B	2.29	1.44	1.41
5	A	527	FAD	C1'-N10	2.30	1.50	1.48
5	C	527	FAD	C10-N1	2.60	1.39	1.35
5	B	525	FAD	C5X-N5	2.64	1.39	1.35
5	B	525	FAD	C2A-N1A	2.71	1.39	1.33
5	D	527	FAD	C5X-N5	2.78	1.39	1.35
5	B	525	FAD	C2A-N3A	2.94	1.37	1.32
5	B	525	FAD	C4-N3	3.09	1.38	1.33
5	D	527	FAD	C10-N1	3.09	1.40	1.35
5	C	527	FAD	C2A-N3A	3.14	1.37	1.32
5	C	527	FAD	C4-N3	3.26	1.39	1.33
5	A	527	FAD	C5X-N5	3.29	1.40	1.35
5	D	527	FAD	C4-N3	3.32	1.39	1.33
5	C	527	FAD	C5X-N5	3.45	1.40	1.35
5	D	527	FAD	C2A-N3A	3.55	1.38	1.32
5	A	527	FAD	C2A-N3A	4.01	1.39	1.32
5	A	527	FAD	C4X-N5	4.07	1.39	1.33
5	C	527	FAD	C4X-N5	4.22	1.40	1.33
5	D	527	FAD	C4X-N5	4.50	1.40	1.33
5	B	525	FAD	C4X-N5	5.01	1.41	1.33

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	525	FAD	N3A-C2A-N1A	-14.10	118.10	128.89
5	D	527	FAD	N3A-C2A-N1A	-12.21	119.55	128.89
5	A	527	FAD	N3A-C2A-N1A	-11.16	120.35	128.89
5	C	527	FAD	N3A-C2A-N1A	-9.18	121.86	128.89
5	C	527	FAD	C4X-C4-N3	-4.21	117.83	123.59
5	B	525	FAD	C4X-C4-N3	-3.35	119.00	123.59
5	A	527	FAD	C4X-C4-N3	-3.23	119.17	123.59
5	D	527	FAD	C4X-C4-N3	-3.19	119.22	123.59
5	A	527	FAD	C4B-O4B-C1B	-3.06	106.35	109.72
5	A	527	FAD	C1B-N9A-C4A	-2.85	122.65	126.94
5	A	527	FAD	C4A-C5A-N7A	-2.40	107.27	109.48
3	C	522	NAG	C4-C3-C2	-2.32	107.63	111.23
5	C	527	FAD	C1B-N9A-C4A	-2.25	123.55	126.94
5	C	527	FAD	C9A-C5X-N5	-2.14	119.19	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	527	FAD	C4B-O4B-C1B	-2.11	107.40	109.72
3	D	522	NAG	C2-N2-C7	-2.11	120.33	123.04
5	C	527	FAD	C2B-C3B-C4B	2.01	106.74	102.61
5	D	527	FAD	C2A-N1A-C6A	2.09	122.50	118.77
5	A	527	FAD	C2B-C1B-N9A	2.10	117.50	114.29
5	C	527	FAD	O3'-C3'-C2'	2.13	114.11	108.75
5	C	527	FAD	O3P-P-O5'	2.19	108.74	102.94
3	D	522	NAG	C3-C4-C5	2.20	114.04	110.20
3	A	522	NAG	C2-N2-C7	2.29	125.98	123.04
5	D	527	FAD	O2A-PA-O3P	2.31	115.56	105.09
4	A	526	PHE	CG-CB-CA	2.32	119.71	114.34
5	B	525	FAD	C5X-C9A-N10	2.33	119.39	117.62
5	C	527	FAD	C4-C4X-N5	2.35	121.57	118.72
4	B	524	PHE	CG-CB-CA	2.45	120.01	114.34
3	C	522	NAG	O3-C3-C2	2.50	114.07	109.11
4	D	526	PHE	CG-CB-CA	2.55	120.24	114.34
3	B	523	NAG	C1-O5-C5	2.62	115.58	112.25
5	B	525	FAD	C4-C4X-N5	2.63	121.91	118.72
5	B	525	FAD	C1'-N10-C9A	2.74	121.93	118.86
5	D	527	FAD	C1'-N10-C9A	2.75	121.95	118.86
3	A	522	NAG	O5-C5-C6	2.82	113.45	107.35
5	D	527	FAD	O3P-P-O5'	3.00	110.89	102.94
5	C	527	FAD	C1'-N10-C9A	3.01	122.24	118.86
3	D	522	NAG	C1-O5-C5	3.03	116.10	112.25
5	A	527	FAD	C5X-C9A-N10	3.13	119.99	117.62
3	C	522	NAG	C2-N2-C7	3.16	127.09	123.04
5	D	527	FAD	C5X-C9A-N10	3.32	120.14	117.62
3	C	522	NAG	C3-C2-N2	4.05	120.26	110.56
5	A	527	FAD	C1'-N10-C9A	4.27	123.66	118.86
5	A	527	FAD	C4-N3-C2	7.27	121.53	115.25
5	B	525	FAD	C4-N3-C2	7.92	122.10	115.25
5	D	527	FAD	C4-N3-C2	8.28	122.40	115.25
5	C	527	FAD	C4-N3-C2	8.70	122.77	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	526	PHE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	527	FAD	2	0
5	B	525	FAD	1	0
3	C	522	NAG	1	0
4	C	526	PHE	1	0
5	C	527	FAD	3	0
5	D	527	FAD	1	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](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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