



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 01:00 AM GMT

PDB ID : 1F8S
Title : CRYSTAL STRUCTURE OF L-AMINO ACID OXIDASE FROM CALLOSE-
LASMA RHODOSTOMA, COMPLEXED WITH THREE MOLECULES OF
O-AMINOBENZOATE.
Authors : Pawelek, P.D.; Cheah, J.; Coulombe, R.; Macheroux, P.; Ghisla, S.; Vrielink,
A.
Deposited on : 2000-07-04
Resolution : 2.00 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

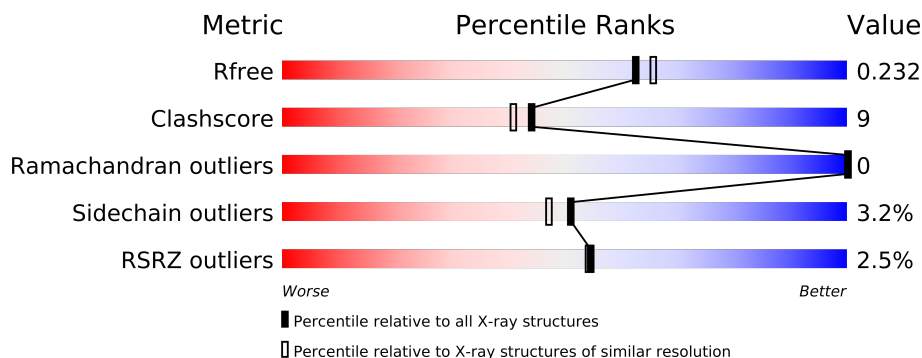
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	498	
1	B	498	
1	C	498	
1	D	498	
1	E	498	
1	F	498	
1	G	498	
1	H	498	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	NAG	A	1543	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
2	NAG	D	1543	-	X
2	NAG	E	1543	-	X
3	BE2	A	1544	-	X
3	BE2	A	1545	-	X
3	BE2	A	1546	-	X
3	BE2	B	1544	-	X
3	BE2	B	1545	-	X
3	BE2	B	1546	-	X
3	BE2	C	1544	-	X
3	BE2	C	1545	-	X
3	BE2	D	1544	-	X
3	BE2	D	1545	-	X
3	BE2	D	1546	-	X
3	BE2	E	1544	-	X
3	BE2	E	1545	-	X
3	BE2	F	1545	-	X
3	BE2	G	1545	-	X
3	BE2	H	1544	-	X
3	BE2	H	1545	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 34018 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

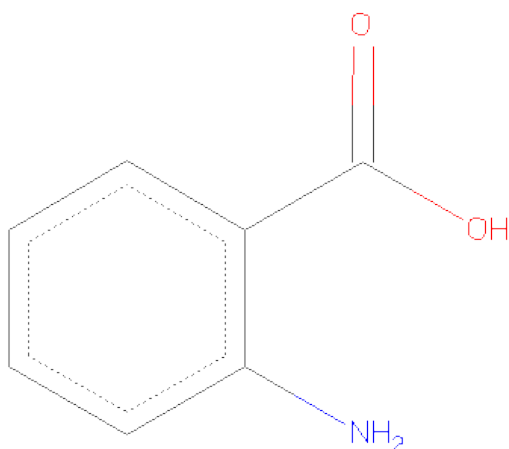
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	1	0
			3858	2461	656	729	12			
1	B	482	Total	C	N	O	S	0	1	0
			3858	2461	656	729	12			
1	C	482	Total	C	N	O	S	0	1	0
			3858	2461	656	729	12			
1	D	482	Total	C	N	O	S	0	1	0
			3858	2461	656	729	12			
1	E	482	Total	C	N	O	S	0	1	0
			3858	2461	656	729	12			
1	F	482	Total	C	N	O	S	0	1	0
			3858	2461	656	729	12			
1	G	482	Total	C	N	O	S	0	1	0
			3858	2461	656	729	12			
1	H	482	Total	C	N	O	S	0	1	0
			3858	2461	656	729	12			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		
2	G	1	Total	C	N	O	0	0
			14	8	1	5		
2	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is 2-AMINOBENZOIC ACID (three-letter code: BE2) (formula: C₇H₇NO₂).



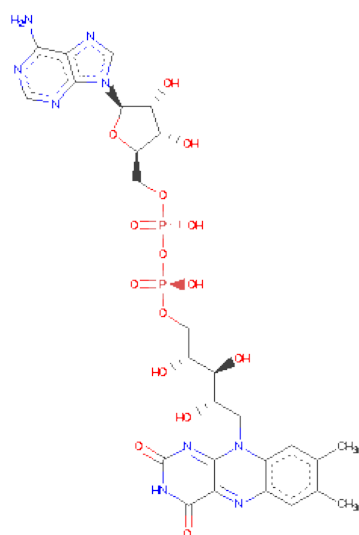
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	7	1	2		
3	A	1	Total	C	N	O	0	0
			10	7	1	2		
3	A	1	Total	C	N	O	0	0
			10	7	1	2		
3	B	1	Total	C	N	O	0	0
			10	7	1	2		
3	B	1	Total	C	N	O	0	0
			10	7	1	2		
3	B	1	Total	C	N	O	0	0
			10	7	1	2		
3	C	1	Total	C	N	O	0	0
			10	7	1	2		
3	C	1	Total	C	N	O	0	0
			10	7	1	2		
3	C	1	Total	C	N	O	0	0
			10	7	1	2		
3	D	1	Total	C	N	O	0	0
			10	7	1	2		
3	D	1	Total	C	N	O	0	0
			10	7	1	2		
3	D	1	Total	C	N	O	0	0
			10	7	1	2		
3	E	1	Total	C	N	O	0	0
			10	7	1	2		
3	E	1	Total	C	N	O	0	0
			10	7	1	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	N	O	0	0
			10	7	1	2		
3	F	1	Total	C	N	O	0	0
			10	7	1	2		
3	F	1	Total	C	N	O	0	0
			10	7	1	2		
3	F	1	Total	C	N	O	0	0
			10	7	1	2		
3	G	1	Total	C	N	O	0	0
			10	7	1	2		
3	G	1	Total	C	N	O	0	0
			10	7	1	2		
3	G	1	Total	C	N	O	0	0
			10	7	1	2		
3	H	1	Total	C	N	O	0	0
			10	7	1	2		
3	H	1	Total	C	N	O	0	0
			10	7	1	2		
3	H	1	Total	C	N	O	0	0
			10	7	1	2		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is water.

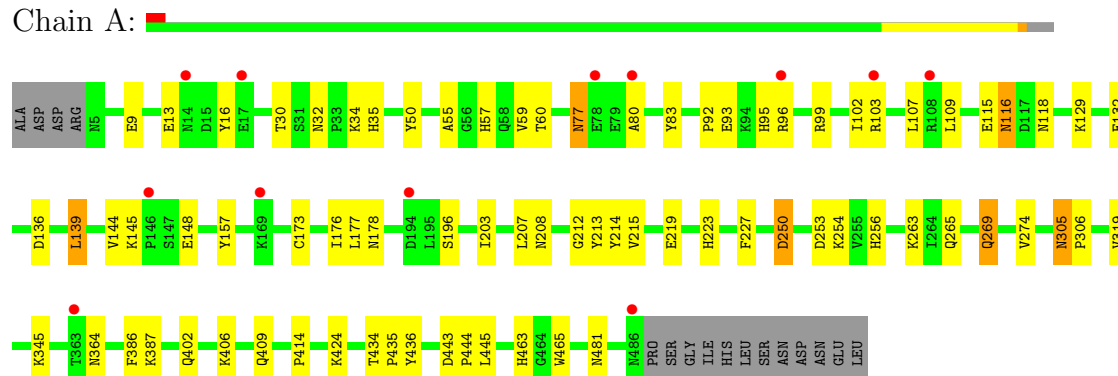
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	292	Total	O	0	0
			292	292		
5	B	305	Total	O	0	0
			305	305		
5	C	350	Total	O	0	0
			350	350		
5	D	341	Total	O	0	0
			341	341		
5	E	281	Total	O	0	0
			281	281		
5	F	292	Total	O	0	0
			292	292		
5	G	285	Total	O	0	0
			285	285		
5	H	232	Total	O	0	0
			232	232		

3 Residue-property plots

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

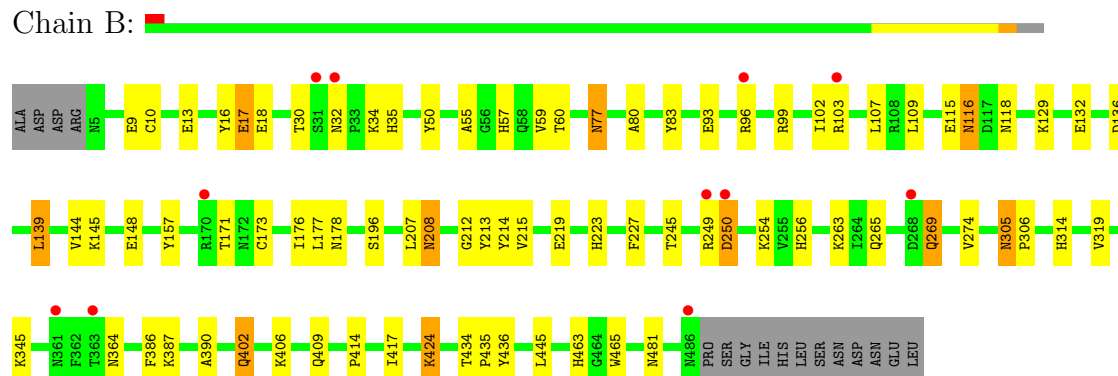
• Molecule 1: L-AMINO ACID OXIDASE

Chain A:



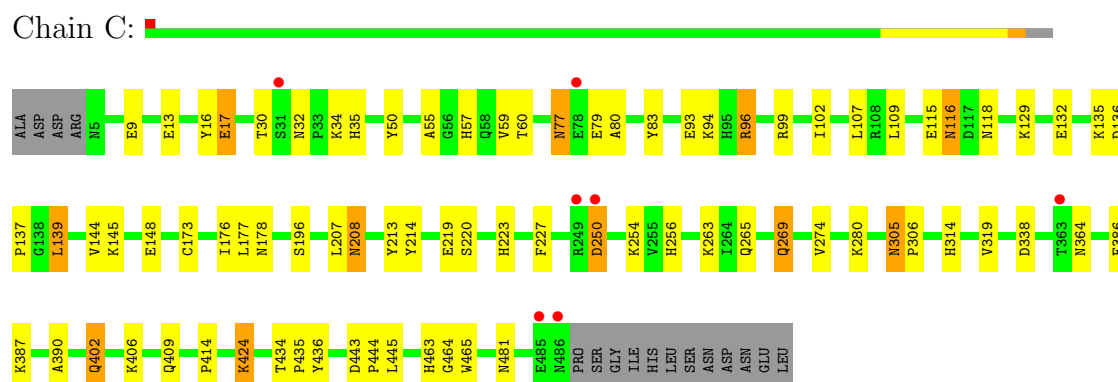
• Molecule 1: L-AMINO ACID OXIDASE

Chain B:



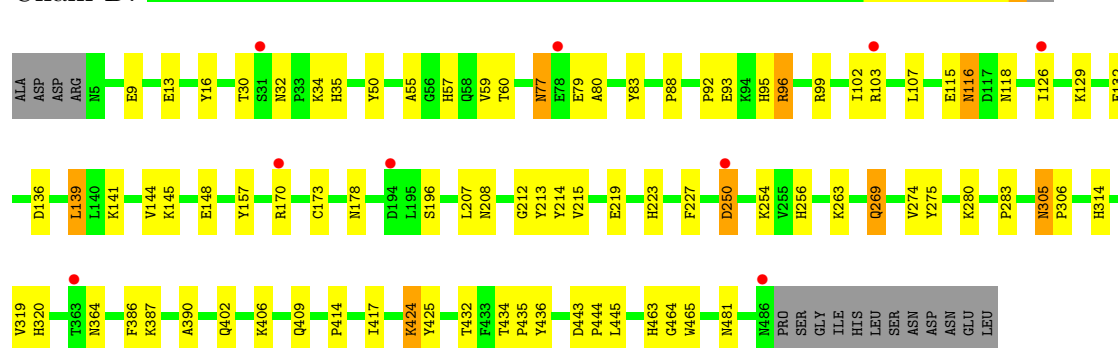
• Molecule 1: L-AMINO ACID OXIDASE

Chain C:



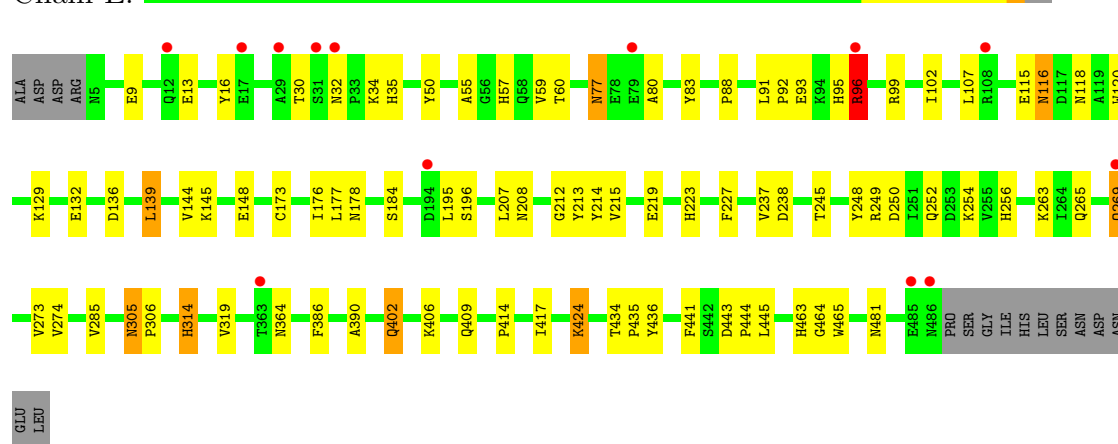
- Molecule 1: L-AMINO ACID OXIDASE

Chain D:



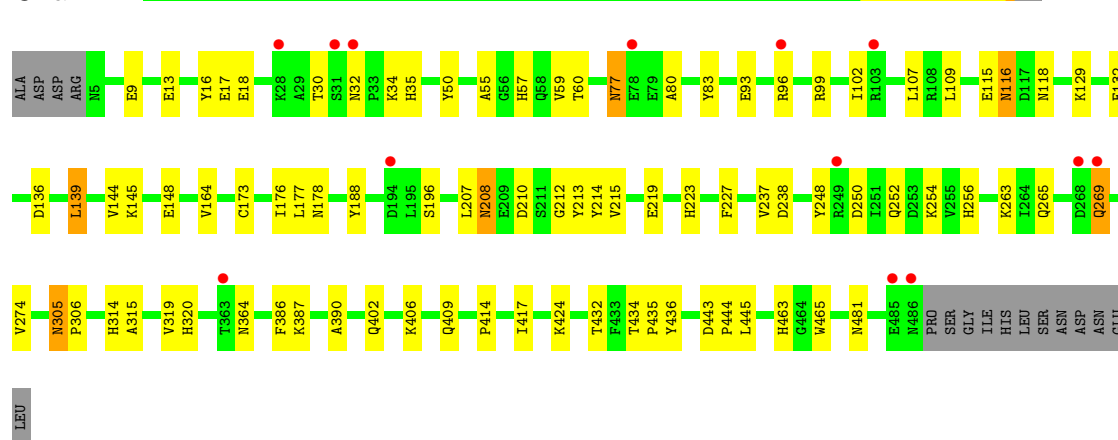
- Molecule 1: L-AMINO ACID OXIDASE

Chain E:



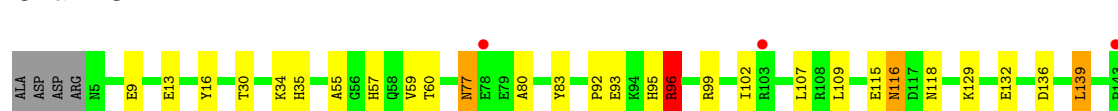
- Molecule 1: L-AMINO ACID OXIDASE

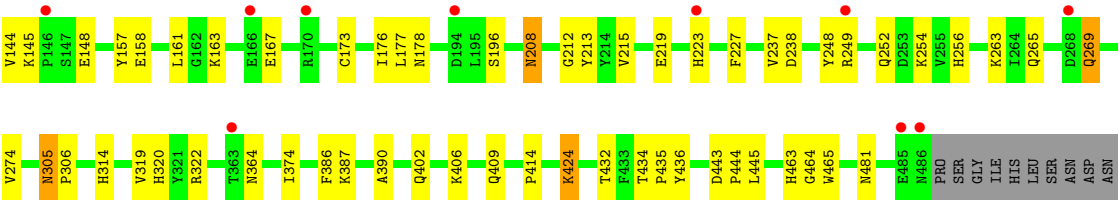
Chain F:



- Molecule 1: L-AMINO ACID OXIDASE

Chain G:

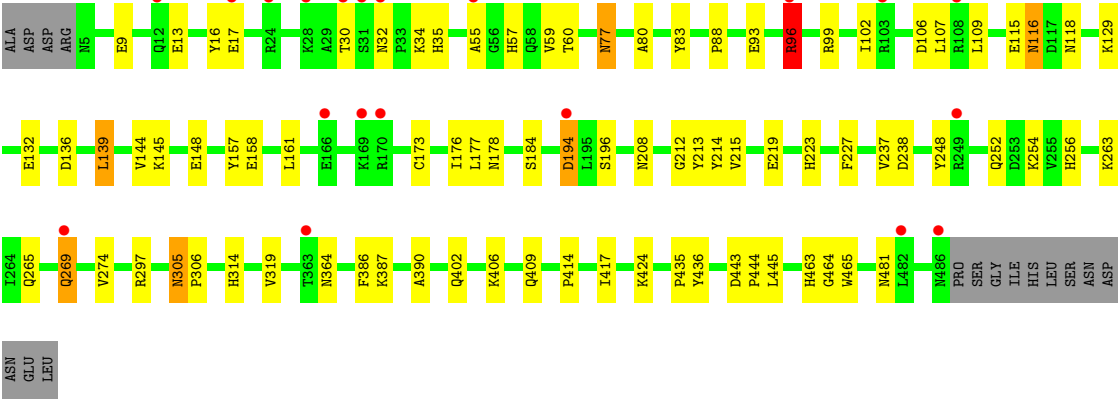




GLU
LEU

• Molecule 1: L-AMINO ACID OXIDASE

Chain H:



ASN
GLU
LEU

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.55Å 137.18Å 212.63Å 90.00° 105.63° 90.00°	Depositor
Resolution (Å)	500.00 – 2.00 48.80 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (500.00-2.00) 85.1 (48.80-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 1.79Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.205 , 0.225 0.213 , 0.232	Depositor DCC
R_{free} test set	33637 reflections (11.13%)	DCC
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 30.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 335933 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	34018	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.15 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.4693e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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: BE2, NAG, FAD

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	0.39	0/3950	0.64	3/5347 (0.1%)
1	B	0.39	2/3950 (0.1%)	0.62	0/5347
1	C	0.39	2/3950 (0.1%)	0.62	1/5347 (0.0%)
1	D	0.41	0/3950	0.63	1/5347 (0.0%)
1	E	0.37	0/3950	0.64	2/5347 (0.0%)
1	F	0.40	2/3950 (0.1%)	0.62	0/5347
1	G	0.40	0/3950	0.63	3/5347 (0.1%)
1	H	0.38	0/3950	0.63	1/5347 (0.0%)
All	All	0.39	6/31600 (0.0%)	0.63	11/42776 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	17	GLU	CD-OE1	-6.33	1.18	1.25
1	B	17	GLU	CB-CG	-6.19	1.40	1.52
1	C	17	GLU	CG-CD	-5.91	1.43	1.51
1	B	17	GLU	CG-CD	-5.90	1.43	1.51
1	F	17	GLU	CD-OE1	-5.66	1.19	1.25

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	E	96	ARG	CG-CD-NE	-6.51	98.13	111.80
1	A	96	ARG	NE-CZ-NH2	6.09	123.34	120.30
1	A	103	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	G	96	ARG	NE-CZ-NH2	5.52	123.06	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	96	ARG	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3858	0	3775	58	1
1	B	3858	0	3775	70	0
1	C	3858	0	3775	67	1
1	D	3858	0	3775	69	2
1	E	3858	0	3775	74	0
1	F	3858	0	3775	68	0
1	G	3858	0	3775	68	0
1	H	3858	0	3775	68	2
2	A	14	0	13	0	0
2	B	14	0	13	1	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
2	E	14	0	13	0	0
2	F	14	0	13	0	0
2	G	14	0	13	0	0
2	H	14	0	13	0	0
3	A	30	0	18	2	0
3	B	30	0	18	4	0
3	C	30	0	18	4	0
3	D	30	0	18	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	30	0	18	2	0
3	F	30	0	18	4	0
3	G	30	0	18	10	0
3	H	30	0	18	2	0
4	A	53	0	31	0	0
4	B	53	0	31	0	0
4	C	53	0	31	0	0
4	D	53	0	31	1	0
4	E	53	0	31	1	0
4	F	53	0	31	0	0
4	G	53	0	31	1	0
4	H	53	0	31	1	0
5	A	292	0	0	4	0
5	B	305	0	0	7	0
5	C	350	0	0	9	0
5	D	341	0	0	4	0
5	E	281	0	0	6	0
5	F	292	0	0	4	0
5	G	285	0	0	8	0
5	H	232	0	0	6	0
All	All	34018	0	30696	536	3

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

The worst 5 of 536 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:96:ARG:CG	1:H:96:ARG:HH11	1.50	1.22
1:E:96:ARG:HG3	1:E:96:ARG:NH1	1.19	1.12
1:E:96:ARG:CG	1:E:96:ARG:HH11	1.58	1.12
1:H:96:ARG:NH1	1:H:96:ARG:HG3	1.31	1.05
1:E:96:ARG:CG	1:E:96:ARG:NH1	2.11	1.02

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:253:ASP:OD1	1:H:106:ASP:OD1[1_655]	2.10	0.10
1:C:338:ASP:OD1	1:D:132:GLU:OE2[2_546]	2.15	0.05
1:D:170:ARG:NH1	1:H:194:ASP:OD1[1_656]	2.15	0.05

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	481/498 (97%)	470 (98%)	11 (2%)	0	100	100
1	B	481/498 (97%)	466 (97%)	15 (3%)	0	100	100
1	C	481/498 (97%)	467 (97%)	14 (3%)	0	100	100
1	D	481/498 (97%)	468 (97%)	13 (3%)	0	100	100
1	E	481/498 (97%)	468 (97%)	13 (3%)	0	100	100
1	F	481/498 (97%)	469 (98%)	12 (2%)	0	100	100
1	G	481/498 (97%)	468 (97%)	13 (3%)	0	100	100
1	H	481/498 (97%)	468 (97%)	13 (3%)	0	100	100
All	All	3848/3984 (97%)	3744 (97%)	104 (3%)	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	414/427 (97%)	402 (97%)	12 (3%)	55	52
1	B	414/427 (97%)	400 (97%)	14 (3%)	49	45
1	C	414/427 (97%)	401 (97%)	13 (3%)	52	49
1	D	414/427 (97%)	400 (97%)	14 (3%)	49	45
1	E	414/427 (97%)	401 (97%)	13 (3%)	52	49
1	F	414/427 (97%)	400 (97%)	14 (3%)	49	45
1	G	414/427 (97%)	401 (97%)	13 (3%)	52	49
1	H	414/427 (97%)	400 (97%)	14 (3%)	49	45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3312/3416 (97%)	3205 (97%)	107 (3%)	51 47

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	269	GLN
1	E	208	ASN
1	H	178	ASN
1	D	305	ASN
1	E	96	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	305	ASN
1	E	125	ASN
1	H	208	ASN
1	D	314	HIS
1	E	35	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

40 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	NAG	A	1543	1	12,14,15	0.36	0	15,19,21	0.88	1 (6%)
3	BE2	A	1544	-	10,10,10	1.66	3 (30%)	13,13,13	1.44	1 (7%)
3	BE2	A	1545	-	10,10,10	1.64	2 (20%)	13,13,13	1.54	2 (15%)
3	BE2	A	1546	-	10,10,10	1.73	3 (30%)	13,13,13	1.46	1 (7%)
4	FAD	A	520	-	58,58,58	2.04	13 (22%)	85,89,89	1.56	13 (15%)
2	NAG	B	1543	1	12,14,15	0.52	0	15,19,21	0.93	0
3	BE2	B	1544	-	10,10,10	1.62	3 (30%)	13,13,13	1.45	1 (7%)
3	BE2	B	1545	-	10,10,10	1.62	2 (20%)	13,13,13	1.54	1 (7%)
3	BE2	B	1546	-	10,10,10	1.69	3 (30%)	13,13,13	1.44	2 (15%)
4	FAD	B	521	-	58,58,58	2.07	13 (22%)	85,89,89	1.58	13 (15%)
2	NAG	C	1543	1	12,14,15	0.51	0	15,19,21	0.55	0
3	BE2	C	1544	-	10,10,10	1.48	3 (30%)	13,13,13	1.45	1 (7%)
3	BE2	C	1545	-	10,10,10	1.61	2 (20%)	13,13,13	1.52	1 (7%)
3	BE2	C	1546	-	10,10,10	1.71	3 (30%)	13,13,13	1.43	2 (15%)
4	FAD	C	522	-	58,58,58	2.00	12 (20%)	85,89,89	1.55	12 (14%)
2	NAG	D	1543	1	12,14,15	0.46	0	15,19,21	0.78	1 (6%)
3	BE2	D	1544	-	10,10,10	1.54	3 (30%)	13,13,13	1.47	2 (15%)
3	BE2	D	1545	-	10,10,10	1.69	2 (20%)	13,13,13	1.58	2 (15%)
3	BE2	D	1546	-	10,10,10	1.74	4 (40%)	13,13,13	1.40	1 (7%)
4	FAD	D	523	-	58,58,58	2.06	13 (22%)	85,89,89	1.53	13 (15%)
2	NAG	E	1543	1	12,14,15	0.50	0	15,19,21	0.76	0
3	BE2	E	1544	-	10,10,10	1.66	3 (30%)	13,13,13	1.46	1 (7%)
3	BE2	E	1545	-	10,10,10	1.70	2 (20%)	13,13,13	1.50	2 (15%)
3	BE2	E	1546	-	10,10,10	1.76	2 (20%)	13,13,13	1.43	2 (15%)
4	FAD	E	524	-	58,58,58	2.04	14 (24%)	85,89,89	1.58	13 (15%)
2	NAG	F	1543	1	12,14,15	0.52	0	15,19,21	0.77	0
3	BE2	F	1544	-	10,10,10	1.52	2 (20%)	13,13,13	1.56	2 (15%)
3	BE2	F	1545	-	10,10,10	1.83	3 (30%)	13,13,13	1.46	2 (15%)
3	BE2	F	1546	-	10,10,10	1.61	2 (20%)	13,13,13	1.48	2 (15%)
4	FAD	F	525	-	58,58,58	1.98	14 (24%)	85,89,89	1.58	12 (14%)
2	NAG	G	1543	1	12,14,15	0.45	0	15,19,21	0.77	0
3	BE2	G	1544	-	10,10,10	1.57	3 (30%)	13,13,13	1.53	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BE2	G	1545	-	10,10,10	1.63	3 (30%)	13,13,13	1.41	1 (7%)
3	BE2	G	1546	-	10,10,10	1.73	4 (40%)	13,13,13	1.42	2 (15%)
4	FAD	G	526	-	58,58,58	2.00	13 (22%)	85,89,89	1.59	13 (15%)
2	NAG	H	1543	1	12,14,15	0.52	0	15,19,21	0.72	1 (6%)
3	BE2	H	1544	-	10,10,10	1.61	3 (30%)	13,13,13	1.44	1 (7%)
3	BE2	H	1545	-	10,10,10	1.65	2 (20%)	13,13,13	1.46	2 (15%)
3	BE2	H	1546	-	10,10,10	1.69	4 (40%)	13,13,13	1.43	1 (7%)
4	FAD	H	527	-	58,58,58	2.07	13 (22%)	85,89,89	1.53	12 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1543	1	1/1/5/7	0/6/23/26	0/1/1/1
3	BE2	A	1544	-	-	0/4/4/4	0/1/1/1
3	BE2	A	1545	-	-	0/4/4/4	0/1/1/1
3	BE2	A	1546	-	-	0/4/4/4	0/1/1/1
4	FAD	A	520	-	-	0/34/50/50	0/1/6/6
2	NAG	B	1543	1	-	0/6/23/26	0/1/1/1
3	BE2	B	1544	-	-	0/4/4/4	0/1/1/1
3	BE2	B	1545	-	-	0/4/4/4	0/1/1/1
3	BE2	B	1546	-	-	0/4/4/4	0/1/1/1
4	FAD	B	521	-	-	0/34/50/50	0/1/6/6
2	NAG	C	1543	1	-	0/6/23/26	0/1/1/1
3	BE2	C	1544	-	-	0/4/4/4	0/1/1/1
3	BE2	C	1545	-	-	0/4/4/4	0/1/1/1
3	BE2	C	1546	-	-	0/4/4/4	0/1/1/1
4	FAD	C	522	-	-	0/34/50/50	0/1/6/6
2	NAG	D	1543	1	-	0/6/23/26	0/1/1/1
3	BE2	D	1544	-	-	0/4/4/4	0/1/1/1
3	BE2	D	1545	-	-	0/4/4/4	0/1/1/1
3	BE2	D	1546	-	-	0/4/4/4	0/1/1/1
4	FAD	D	523	-	-	0/34/50/50	0/1/6/6
2	NAG	E	1543	1	-	0/6/23/26	0/1/1/1
3	BE2	E	1544	-	-	0/4/4/4	0/1/1/1
3	BE2	E	1545	-	-	0/4/4/4	0/1/1/1
3	BE2	E	1546	-	-	0/4/4/4	0/1/1/1
4	FAD	E	524	-	-	0/34/50/50	0/1/6/6
2	NAG	F	1543	1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BE2	F	1544	-	-	0/4/4/4	0/1/1/1
3	BE2	F	1545	-	-	0/4/4/4	0/1/1/1
3	BE2	F	1546	-	-	0/4/4/4	0/1/1/1
4	FAD	F	525	-	-	0/34/50/50	0/1/6/6
2	NAG	G	1543	1	-	0/6/23/26	0/1/1/1
3	BE2	G	1544	-	-	0/4/4/4	0/1/1/1
3	BE2	G	1545	-	-	0/4/4/4	0/1/1/1
3	BE2	G	1546	-	-	0/4/4/4	0/1/1/1
4	FAD	G	526	-	-	0/34/50/50	0/1/6/6
2	NAG	H	1543	1	-	0/6/23/26	0/1/1/1
3	BE2	H	1544	-	-	0/4/4/4	0/1/1/1
3	BE2	H	1545	-	-	0/4/4/4	0/1/1/1
3	BE2	H	1546	-	-	0/4/4/4	0/1/1/1
4	FAD	H	527	-	-	0/34/50/50	0/1/6/6

The worst 5 of 171 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	526	FAD	P-O3P	-6.51	1.48	1.59
4	D	523	FAD	P-O3P	-6.38	1.48	1.59
4	A	520	FAD	P-O3P	-6.18	1.48	1.59
4	B	521	FAD	C1'-C2'	6.03	1.57	1.51
4	E	524	FAD	P-O3P	-6.01	1.49	1.59

The worst 5 of 141 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	525	FAD	O4B-C1B-N9A	-6.94	101.99	108.44
4	B	521	FAD	O4B-C1B-N9A	-6.86	102.06	108.44
4	E	524	FAD	O4B-C1B-N9A	-6.57	102.33	108.44
4	A	520	FAD	O4B-C1B-N9A	-6.54	102.36	108.44
4	G	526	FAD	O4B-C1B-N9A	-6.41	102.48	108.44

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1543	NAG	C1

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	482/498 (96%)	-0.18	12 (2%) 54 54	8, 17, 32, 52	0
1	B	482/498 (96%)	-0.34	11 (2%) 57 57	9, 17, 31, 52	0
1	C	482/498 (96%)	-0.33	7 (1%) 70 70	8, 16, 31, 52	0
1	D	482/498 (96%)	-0.16	9 (1%) 64 64	8, 17, 31, 52	0
1	E	482/498 (96%)	-0.25	13 (2%) 52 52	10, 18, 32, 52	0
1	F	482/498 (96%)	-0.32	13 (2%) 52 52	10, 18, 31, 52	0
1	G	482/498 (96%)	-0.25	13 (2%) 52 52	10, 18, 31, 52	0
1	H	482/498 (96%)	-0.10	20 (4%) 35 35	10, 19, 32, 52	0
All	All	3856/3984 (96%)	-0.24	98 (2%) 54 54	8, 17, 31, 52	0

The worst 5 of 98 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	486	ASN	8.9
1	E	486	ASN	8.6
1	A	363	THR	7.9
1	D	363	THR	7.3
1	B	486	ASN	6.9

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	D	1543	14/15	0.19	11.29	35,38,40,40	0
3	BE2	E	1545	10/10	0.40	5.97	57,57,57,57	0
2	NAG	A	1543	14/15	0.41	5.26	42,45,48,48	0
3	BE2	G	1545	10/10	0.51	5.06	53,54,54,55	0
3	BE2	B	1545	10/10	0.29	4.71	42,43,43,44	0
3	BE2	F	1545	10/10	0.41	4.60	51,51,52,53	0
3	BE2	H	1545	10/10	0.34	3.94	57,57,57,57	0
3	BE2	C	1545	10/10	0.27	3.87	42,43,43,44	0
3	BE2	H	1544	10/10	0.28	3.73	43,43,44,44	0
3	BE2	E	1544	10/10	0.29	3.66	46,46,46,47	0
3	BE2	A	1545	10/10	0.30	3.17	48,49,49,49	0
2	NAG	E	1543	14/15	0.25	3.14	37,40,43,43	0
3	BE2	B	1544	10/10	0.23	3.09	34,35,35,35	0
3	BE2	D	1545	10/10	0.28	2.98	40,40,41,42	0
3	BE2	A	1544	10/10	0.24	2.69	33,33,34,34	0
3	BE2	A	1546	10/10	0.24	2.58	47,47,48,48	0
3	BE2	C	1544	10/10	0.20	2.52	34,35,35,36	0
3	BE2	D	1544	10/10	0.23	2.38	30,31,32,32	0
3	BE2	D	1546	10/10	0.23	2.29	38,40,40,41	0
3	BE2	B	1546	10/10	0.19	2.06	47,48,48,48	0
2	NAG	H	1543	14/15	0.23	1.95	37,39,40,41	0
3	BE2	H	1546	10/10	0.20	1.86	49,49,50,50	0
3	BE2	F	1544	10/10	0.23	1.64	33,34,35,35	0
3	BE2	G	1544	10/10	0.25	1.47	38,39,39,39	0
3	BE2	E	1546	10/10	0.18	1.39	47,48,48,48	0
3	BE2	C	1546	10/10	0.17	1.35	42,42,43,43	0
2	NAG	C	1543	14/15	0.17	1.22	31,33,37,38	0
3	BE2	F	1546	10/10	0.20	0.89	42,42,42,43	0
2	NAG	B	1543	14/15	0.16	0.86	33,35,37,38	0
2	NAG	F	1543	14/15	0.19	0.67	34,36,37,39	0
3	BE2	G	1546	10/10	0.18	0.52	39,39,40,40	0
4	FAD	H	527	53/53	0.09	0.46	11,14,16,17	0
4	FAD	A	520	53/53	0.11	0.12	7,9,10,10	0
2	NAG	G	1543	14/15	0.16	-0.00	29,31,32,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	FAD	G	526	53/53	0.07	-0.10	9,10,11,12	0
4	FAD	D	523	53/53	0.10	-0.21	6,8,10,11	0
4	FAD	E	524	53/53	0.07	-0.29	10,12,14,15	0
4	FAD	F	525	53/53	0.07	-0.44	8,10,12,13	0
4	FAD	C	522	53/53	0.07	-1.01	4,8,9,10	0
4	FAD	B	521	53/53	0.06	-1.21	6,8,10,11	0

6.5 Other polymers ⓘ

There are no such residues in this entry.