

Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2023 – 10:09 PM JST

PDB ID	:	5YB8
Title	:	L-Amino acid oxidase/monooxygenase from Pseudomonas sp. AIU 813 -
		L-arginine complex
Authors	:	Im, D.; Matsui, D.; Arakawa, T.; Isobe, K.; Asano, Y.; Fushinobu, S.
Deposited on	:	2017-09-03
Resolution	:	2.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.30 Å.

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



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	5042(2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575(2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
1	А	580	81%	13%	• 5%
1	В	580	80%	13%	• 5%
1	С	580	5% 82%	11%	• 5%
1	D	580	8%	13%	• 5%

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 crite-



ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ARG	С	601	-	-	-	Х



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17837 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Λ	540	Total	С	Ν	0	\mathbf{S}	0	0	0
	A	049	4305	2749	742	791	23	0	0	0
1	В	540	Total	С	Ν	0	S	0	0	0
1	D	049	4305	2749	742	791	23	0	0	0
1	C	540	Total	С	Ν	0	S	0	0	0
	C	049	4305	2749	742	791	23	0	0	0
1	П	540	Total	С	Ν	0	S	0	0	0
I D	549	4305	2749	742	791	23	0	0	U	

• Molecule 1 is a protein called L-amino acid oxidase/monooxygenase.

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-19	MET	-	expression tag	UNP W6JQJ6
А	-18	GLY	-	expression tag	UNP W6JQJ6
А	-17	SER	-	expression tag	UNP W6JQJ6
А	-16	SER	-	expression tag	UNP W6JQJ6
А	-15	HIS	-	expression tag	UNP W6JQJ6
А	-14	HIS	-	expression tag	UNP W6JQJ6
А	-13	HIS	-	expression tag	UNP W6JQJ6
А	-12	HIS	-	expression tag	UNP W6JQJ6
А	-11	HIS	-	expression tag	UNP W6JQJ6
А	-10	HIS	-	expression tag	UNP W6JQJ6
А	-9	SER	-	expression tag	UNP W6JQJ6
А	-8	SER	-	expression tag	UNP W6JQJ6
А	-7	GLY	-	expression tag	UNP W6JQJ6
А	-6	LEU	-	expression tag	UNP W6JQJ6
А	-5	VAL	-	expression tag	UNP W6JQJ6
А	-4	PRO	-	expression tag	UNP W6JQJ6
А	-3	ARG	-	expression tag	UNP W6JQJ6
А	-2	GLY	-	expression tag	UNP W6JQJ6
A	-1	SER	-	expression tag	UNP W6JQJ6
A	0	HIS	-	expression tag	UNP W6JQJ6
A	473	PHE	SER	conflict	UNP W6JQJ6



Chain	Residue	Modelled	Actual	Comment	Reference
В	-19	MET	-	expression tag	UNP W6JQJ6
В	-18	GLY	_	expression tag	UNP W6JQJ6
В	-17	SER	-	expression tag	UNP W6JQJ6
В	-16	SER	-	expression tag	UNP W6JQJ6
В	-15	HIS	-	expression tag	UNP W6JQJ6
В	-14	HIS	-	expression tag	UNP W6JQJ6
В	-13	HIS	-	expression tag	UNP W6JQJ6
В	-12	HIS	-	expression tag	UNP W6JQJ6
В	-11	HIS	-	expression tag	UNP W6JQJ6
В	-10	HIS	-	expression tag	UNP W6JQJ6
В	-9	SER	-	expression tag	UNP W6JQJ6
В	-8	SER	-	expression tag	UNP W6JQJ6
В	-7	GLY	-	expression tag	UNP W6JQJ6
В	-6	LEU	-	expression tag	UNP W6JQJ6
В	-5	VAL	-	expression tag	UNP W6JQJ6
В	-4	PRO	-	expression tag	UNP W6JQJ6
В	-3	ARG	-	expression tag	UNP W6JQJ6
В	-2	GLY	-	expression tag	UNP W6JQJ6
В	-1	SER	-	expression tag	UNP W6JQJ6
В	0	HIS	-	expression tag	UNP W6JQJ6
В	473	PHE	SER	conflict	UNP W6JQJ6
С	-19	MET	-	expression tag	UNP W6JQJ6
С	-18	GLY	-	expression tag	UNP W6JQJ6
С	-17	SER	-	expression tag	UNP W6JQJ6
С	-16	SER	-	expression tag	UNP W6JQJ6
С	-15	HIS	-	expression tag	UNP W6JQJ6
С	-14	HIS	-	expression tag	UNP W6JQJ6
С	-13	HIS	-	expression tag	UNP W6JQJ6
С	-12	HIS	-	expression tag	UNP W6JQJ6
С	-11	HIS	-	expression tag	UNP W6JQJ6
C	-10	HIS	-	expression tag	UNP W6JQJ6
C	-9	SER	-	expression tag	UNP W6JQJ6
С	-8	SER	-	expression tag	UNP W6JQJ6
C	-7	GLY	-	expression tag	UNP W6JQJ6
C	-6	LEU	-	expression tag	UNP W6JQJ6
C	-5	VAL	-	expression tag	UNP W6JQJ6
С	-4	PRO	-	expression tag	UNP W6JQJ6
С	-3	ARG	-	expression tag	UNP W6JQJ6
C	-2	GLY		expression tag	UNP W6JQJ6
С	-1	SER	-	expression tag	UNP W6JQJ6
C	0	HIS	-	expression tag	UNP W6JQJ6
С	473	PHE	SER	conflict	UNP W6JQJ6



Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	expression tag	UNP W6JQJ6
D	-18	GLY	-	expression tag	UNP W6JQJ6
D	-17	SER	-	expression tag	UNP W6JQJ6
D	-16	SER	-	expression tag	UNP W6JQJ6
D	-15	HIS	-	expression tag	UNP W6JQJ6
D	-14	HIS	-	expression tag	UNP W6JQJ6
D	-13	HIS	-	expression tag	UNP W6JQJ6
D	-12	HIS	-	expression tag	UNP W6JQJ6
D	-11	HIS	-	expression tag	UNP W6JQJ6
D	-10	HIS	-	expression tag	UNP W6JQJ6
D	-9	SER	-	expression tag	UNP W6JQJ6
D	-8	SER	-	expression tag	UNP W6JQJ6
D	-7	GLY	-	expression tag	UNP W6JQJ6
D	-6	LEU	-	expression tag	UNP W6JQJ6
D	-5	VAL	-	expression tag	UNP W6JQJ6
D	-4	PRO	-	expression tag	UNP W6JQJ6
D	-3	ARG	-	expression tag	UNP W6JQJ6
D	-2	GLY	-	expression tag	UNP W6JQJ6
D	-1	SER	-	expression tag	UNP W6JQJ6
D	0	HIS	-	expression tag	UNP W6JQJ6
D	473	PHE	SER	conflict	UNP W6JQJ6

• Molecule 2 is ARGININE (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	А	1	Total 12	C 6	N 4	O 2	0	0

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Δ	1	Total C N C	O C	0
	Л	1	12 6 4 2	2 0	0
2	Δ	1	Total C N C	O C	0
	11	1	12 6 4 2	2 0	0
2	В	1	Total C N C		0
	D	1	12 6 4 2	2 0	0
2	В	1	Total C N (0
	D	1	12 6 4 2	2 0	0
2	С	1	Total C N (0
	0	1	12 6 4 2	2 0	0
2	С	1	Total C N (0 C	0
	0	1	12 6 4 2	2 0	0
2	Л	1	Total C N C	0 C	0
	D		12 6 4 2	$2 \mid 0$	

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
3	Λ	1	Total	С	Ν	Ο	Р	0	0
J	A	1	53	27	9	15	2	0	0
2	Р	1	Total	С	Ν	Ο	Р	0	0
J	D	1	53	27	9	15	2	0	0
9	C	1	Total	С	Ν	Ο	Р	0	0
3	C	1	53	27	9	15	2	0	0
9	р	1	Total	С	Ν	0	Р	0	0
3	D	1	53	27	9	15	2	0	0



• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	98	Total O 98 98	0	0
4	В	108	Total O 108 108	0	0
4	С	53	$\begin{array}{cc} \text{Total} & \text{O} \\ 53 & 53 \end{array}$	0	0
4	D	50	$\begin{array}{cc} {\rm Total} & {\rm O} \\ 50 & 50 \end{array}$	0	0



3 Residue-property plots (i)

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



• Molecule 1: L-amino acid oxidase/monooxygenase

 \bullet Molecule 1: L-amino acid oxidase/monooxygenase

Chain C:



11% • 5%







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	98.20Å 133.00Å 101.50Å	Deperitor
a, b, c, α , β , γ	90.00° 112.00° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	94.11 - 2.30	Depositor
Resolution (A)	45.52 - 2.30	EDS
% Data completeness	99.8 (94.11-2.30)	Depositor
(in resolution range)	$99.8 \ (45.52 - 2.30)$	EDS
R_{merge}	0.08	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.80 (at 2.29 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
D D.	0.220 , 0.273	Depositor
Π, Π_{free}	0.226 , 0.278	DCC
R_{free} test set	2009 reflections $(1.88%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	31.3	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.38 , 40.3	EDS
L-test for twinning ²	$< L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	0.138 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17837	wwPDB-VP
Average B, all atoms $(Å^2)$	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.

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



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: 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	
INIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.82	0/4428	0.88	5/6019~(0.1%)
1	В	0.82	0/4428	0.91	5/6019~(0.1%)
1	С	0.69	0/4428	0.81	4/6019~(0.1%)
1	D	0.69	0/4428	0.81	4/6019~(0.1%)
All	All	0.76	0/17712	0.85	18/24076~(0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	486	ARG	NE-CZ-NH1	8.41	124.50	120.30
1	В	353	MET	CG-SD-CE	8.09	113.14	100.20
1	D	482	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	А	486	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	С	482	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	А	457	ASP	CB-CG-OD1	6.19	123.87	118.30
1	В	28	ASP	CB-CG-OD1	5.98	123.68	118.30
1	С	482	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	D	482	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	С	389	MET	CG-SD-CE	5.57	109.10	100.20
1	В	43	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	А	303	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	D	389	MET	CG-SD-CE	5.33	108.72	100.20
1	D	222	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	А	102	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	А	496	MET	CG-SD-CE	-5.25	91.79	100.20
1	В	322	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	С	204	PHE	CB-CG-CD2	-5.06	117.26	120.80

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	А	4305	0	4166	74	0
1	В	4305	0	4164	64	0
1	С	4305	0	4166	66	0
1	D	4305	0	4166	69	0
2	А	36	0	36	1	0
2	В	24	0	24	2	0
2	С	24	0	24	1	0
2	D	12	0	12	2	0
3	А	53	0	31	5	0
3	В	53	0	31	6	0
3	С	53	0	31	5	0
3	D	53	0	31	6	0
4	А	98	0	0	4	0
4	В	108	0	0	10	0
4	С	53	0	0	1	0
4	D	50	0	0	1	0
All	All	17837	0	16882	253	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (253) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
1:D:472:ALA:HB1	3:D:602:FAD:HM83	1.45	0.97
1:D:203:THR:OG1	1:D:206:ASP:OD2	1.84	0.95
1:B:472:ALA:HB1	3:B:603:FAD:HM83	1.47	0.95
1:C:472:ALA:HB1	3:C:603:FAD:HM83	1.49	0.94
1:A:303:ARG:HG3	1:A:303:ARG:HH11	1.29	0.94
1:A:241:ASN:OD1	1:A:359:ARG:NH2	2.07	0.88
1:C:203:THR:OG1	1:C:206:ASP:OD2	1.91	0.87
1:A:472:ALA:HB1	3:A:604:FAD:HM83	1.58	0.85



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:389:MET:HE3	1:B:391:LEU:HG	1.61	0.82
1:A:464:GLU:OE1	1:A:464:GLU:N	2.14	0.80
1:B:362:GLN:HE22	1:B:464:GLU:HB3	1.46	0.79
1:B:389:MET:CE	1:B:391:LEU:HG	2.13	0.79
1:A:206:ASP:CG	1:D:206:ASP:CG	2.42	0.78
1:B:472:ALA:CB	3:B:603:FAD:HM83	2.15	0.76
1:D:464:GLU:N	1:D:464:GLU:OE1	2.20	0.74
1:B:464:GLU:N	1:B:464:GLU:OE1	2.20	0.74
1:D:238:ASP:OD1	2:D:601:ARG:NH2	2.21	0.73
1:D:358:THR:O	1:D:359:ARG:HD3	1.89	0.73
1:C:337:THR:HG21	1:C:356:ASP:OD1	1.90	0.72
1:C:389:MET:CE	1:C:391:LEU:HG	2.20	0.72
1:D:334:TRP:O	1:D:338:THR:HG23	1.90	0.72
1:A:353:MET:CE	1:A:357:ARG:CZ	2.68	0.72
1:A:389:MET:CE	1:A:391:LEU:HG	2.20	0.71
1:C:464:GLU:OE1	1:C:464:GLU:N	2.21	0.71
1:A:477:LEU:HD12	1:A:480:HIS:CE1	2.26	0.71
1:B:206:ASP:CG	1:C:206:ASP:CG	2.49	0.71
1:A:362:GLN:HE22	1:A:464:GLU:HB3	1.55	0.70
1:C:135:THR:HG23	1:C:389:MET:HE2	1.73	0.70
1:D:337:THR:HG21	1:D:356:ASP:OD1	1.91	0.70
1:D:472:ALA:CB	3:D:602:FAD:HM83	2.19	0.70
1:A:303:ARG:HG3	1:A:303:ARG:NH1	1.99	0.69
1:A:334:TRP:O	1:A:338:THR:HG23	1.92	0.69
1:D:389:MET:CE	1:D:391:LEU:HG	2.23	0.69
1:B:490:HIS:HD2	4:B:794:HOH:O	1.77	0.68
1:B:189:LYS:HD3	4:B:761:HOH:O	1.94	0.68
1:A:356:ASP:OD2	2:A:603:ARG:N	2.25	0.68
1:C:472:ALA:CB	3:C:603:FAD:HM83	2.23	0.68
1:D:362:GLN:HE22	1:D:464:GLU:HB3	1.59	0.68
1:C:353:MET:CE	1:C:357:ARG:CZ	2.72	0.67
1:B:477:LEU:HD12	1:B:480:HIS:CE1	2.29	0.67
1:A:322:ARG:HG2	4:A:777:HOH:O	1.95	0.67
1:B:142:GLN:HB2	4:B:709:HOH:O	1.94	0.65
1:D:135:THR:HG23	1:D:389:MET:HE2	1.79	0.64
1:C:334:TRP:O	1:C:338:THR:HG23	1.97	0.64
1:C:362:GLN:HE22	1:C:464:GLU:HB3	1.62	0.64
1:B:100:GLY:HA2	3:B:603:FAD:C4X	2.27	0.64
1:D:552:GLU:HG2	1:D:553:ILE:HG23	1.79	0.64
1:B:334:TRP:O	1:B:338:THR:HG23	1.98	0.63
1:A:490:HIS:HD2	4:A:780:HOH:O	1.81	0.62



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:472:ALA:CB	3:A:604:FAD:HM83	2.30	0.62
1:C:389:MET:HE1	1:C:391:LEU:HG	1.82	0.62
1:D:389:MET:HE1	1:D:391:LEU:HG	1.80	0.61
1:D:358:THR:C	1:D:359:ARG:HD3	2.21	0.61
1:B:378:LYS:HE3	1:B:383:GLY:O	2.01	0.61
1:C:477:LEU:HD12	1:C:480:HIS:CE1	2.36	0.61
1:A:353:MET:CE	1:A:357:ARG:NH2	2.63	0.60
1:A:206:ASP:OD1	1:D:206:ASP:OD2	2.19	0.60
1:C:353:MET:HE1	1:C:357:ARG:NH1	2.17	0.60
1:D:94:ILE:HG21	1:D:369:MET:CE	2.32	0.59
1:D:378:LYS:HE3	1:D:383:GLY:O	2.02	0.59
1:A:389:MET:HE1	1:A:391:LEU:HG	1.84	0.59
1:A:206:ASP:CG	1:D:206:ASP:OD2	2.41	0.59
1:C:353:MET:HE2	1:C:357:ARG:CZ	2.33	0.58
1:B:100:GLY:HA2	3:B:603:FAD:N5	2.18	0.58
1:B:362:GLN:NE2	1:B:464:GLU:HB3	2.15	0.58
1:A:362:GLN:NE2	1:A:464:GLU:HB3	2.17	0.58
1:B:321:CYS:SG	4:B:781:HOH:O	2.57	0.58
1:C:331:CYS:HB2	1:C:335:LEU:HD12	1.85	0.58
1:C:378:LYS:HE3	1:C:383:GLY:O	2.03	0.58
1:A:206:ASP:OD2	1:D:206:ASP:OD1	2.21	0.58
1:B:206:ASP:OD2	1:C:206:ASP:OD1	2.22	0.57
1:C:362:GLN:NE2	1:C:464:GLU:HB3	2.19	0.57
1:A:353:MET:HE2	1:A:357:ARG:CZ	2.34	0.57
1:A:100:GLY:HA2	3:A:604:FAD:N5	2.20	0.57
1:C:94:ILE:HG21	1:C:369:MET:CE	2.35	0.57
1:C:241:ASN:OD1	1:C:359:ARG:NH1	2.37	0.56
1:C:389:MET:HE3	1:C:391:LEU:HG	1.86	0.56
1:B:256:ASP:HB2	4:B:724:HOH:O	2.05	0.56
1:A:206:ASP:OD2	1:D:206:ASP:CG	2.44	0.56
1:D:362:GLN:NE2	1:D:464:GLU:HB3	2.21	0.56
1:B:135:THR:HG23	1:B:389:MET:HE2	1.87	0.56
1:C:100:GLY:HA2	3:C:603:FAD:N5	2.22	0.55
1:D:334:TRP:HB2	1:D:470:LEU:HD13	1.88	0.55
1:C:362:GLN:OE1	1:C:464:GLU:CD	2.45	0.55
1:A:519:GLY:O	1:A:523:THR:HG23	2.07	0.55
1:B:203:THR:OG1	1:B:206:ASP:OD2	2.12	0.55
1:D:362:GLN:OE1	1:D:464:GLU:CD	2.44	0.55
1:C:94:ILE:HG21	1:C:369:MET:HE2	1.90	0.54
1:C:316:ASP:C	1:C:316:ASP:OD1	2.45	0.54
1:D:204:PHE:HB3	1:D:239:PHE:HA	1.89	0.54



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:145:TYR:CD1	1:B:384:ARG:HD3	2.43	0.54
1:C:176:ILE:HG21	1:C:251:MET:SD	2.48	0.54
1:C:362:GLN:OE1	1:C:464:GLU:OE1	2.25	0.54
1:B:338:THR:OG1	1:B:339:GLN:N	2.41	0.54
1:C:100:GLY:HA2	3:C:603:FAD:C4X	2.38	0.54
1:D:477:LEU:HD12	1:D:480:HIS:CE1	2.42	0.53
1:C:552:GLU:HG2	1:C:553:ILE:HG23	1.89	0.53
1:A:337:THR:HG21	1:A:356:ASP:OD1	2.09	0.53
1:C:334:TRP:HB2	1:C:470:LEU:HD13	1.89	0.53
1:C:353:MET:HE1	1:C:357:ARG:CZ	2.39	0.53
1:A:206:ASP:CG	1:D:206:ASP:OD1	2.47	0.53
1:D:94:ILE:HG21	1:D:369:MET:HE2	1.90	0.52
1:A:389:MET:HE3	1:A:391:LEU:HG	1.91	0.52
1:B:206:ASP:OD2	1:C:206:ASP:CG	2.47	0.52
1:A:206:ASP:OD2	1:D:206:ASP:OD2	2.28	0.52
1:B:331:CYS:HB2	1:B:335:LEU:HD12	1.90	0.52
1:D:362:GLN:OE1	1:D:464:GLU:OE1	2.28	0.52
1:C:508:ASP:OD1	1:C:514:PRO:O	2.28	0.52
1:D:100:GLY:HA2	3:D:602:FAD:C4X	2.40	0.52
1:A:362:GLN:OE1	1:A:464:GLU:CD	2.48	0.51
1:B:486:ARG:HD3	4:B:806:HOH:O	2.09	0.51
1:A:135:THR:HG23	1:A:389:MET:HE2	1.90	0.51
1:B:372:ARG:HB2	1:B:373:PRO:HD2	1.92	0.51
1:D:508:ASP:OD1	1:D:514:PRO:O	2.28	0.51
1:A:338:THR:OG1	1:A:339:GLN:N	2.43	0.51
1:B:472:ALA:CA	3:B:603:FAD:HM83	2.41	0.51
1:C:88:PHE:HB2	1:C:369:MET:HE1	1.93	0.51
1:C:359:ARG:HG2	1:C:360:TYR:N	2.26	0.51
1:B:206:ASP:OD1	1:C:206:ASP:OD2	2.28	0.51
1:B:206:ASP:CG	1:C:206:ASP:OD2	2.48	0.50
1:B:241:ASN:OD1	1:B:359:ARG:NH1	2.43	0.50
1:B:337:THR:HG21	1:B:356:ASP:OD1	2.10	0.50
1:B:362:GLN:OE1	1:B:464:GLU:CD	2.50	0.50
1:D:100:GLY:HA2	3:D:602:FAD:N5	2.25	0.50
1:A:100:GLY:HA2	3:A:604:FAD:C4X	2.41	0.50
1:B:303:ARG:HD2	1:B:341:ASP:OD2	2.12	0.50
1:D:199:TRP:O	1:D:200:ASP:C	2.51	0.50
1:A:206:ASP:OD1	1:D:206:ASP:CG	2.50	0.49
1:A:490:HIS:HE1	4:A:743:HOH:O	1.93	0.49
1:C:334:TRP:HB2	1:C:470:LEU:CD1	2.43	0.49
1:A:378:LYS:HE3	1:A:383:GLY:O	2.12	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:334:TRP:HB2	1:D:470:LEU:CD1	2.41	0.49
1:B:221:HIS:CE1	4:B:793:HOH:O	2.65	0.49
1:A:334:TRP:HB2	1:A:470:LEU:HD13	1.95	0.49
1:D:379:ASP:OD1	1:D:379:ASP:C	2.51	0.49
1:B:461:ILE:HG13	1:B:462:SER:N	2.28	0.49
1:A:268:VAL:HB	1:A:269:PRO:CD	2.42	0.48
1:C:359:ARG:HD3	1:C:475:GLY:O	2.13	0.48
1:D:516:TRP:CZ2	2:D:601:ARG:HB3	2.48	0.48
1:A:39:ILE:HG23	1:A:40:PRO:HD2	1.95	0.48
1:B:474:LYS:HG2	1:B:514:PRO:HB3	1.95	0.48
1:A:100:GLY:HA2	3:A:604:FAD:C5X	2.43	0.48
1:C:353:MET:CE	1:C:357:ARG:NH1	2.77	0.48
1:C:490:HIS:HE1	4:C:705:HOH:O	1.95	0.48
1:D:303:ARG:HD2	1:D:341:ASP:OD2	2.13	0.48
1:D:331:CYS:HB2	1:D:335:LEU:HD12	1.94	0.48
1:A:203:THR:OG1	1:A:206:ASP:OD2	2.14	0.48
1:B:91:THR:HG21	1:B:369:MET:CE	2.44	0.48
1:B:142:GLN:NE2	4:B:709:HOH:O	2.46	0.48
1:B:334:TRP:CZ2	1:B:358:THR:O	2.67	0.48
1:D:94:ILE:CG2	1:D:369:MET:CE	2.92	0.48
1:A:88:PHE:HB2	1:A:369:MET:HE1	1.95	0.47
1:A:91:THR:HG21	1:A:369:MET:CE	2.44	0.47
1:A:94:ILE:HG21	1:A:369:MET:HE2	1.95	0.47
1:D:316:ASP:C	1:D:316:ASP:OD1	2.52	0.47
1:B:519:GLY:O	1:B:523:THR:HG23	2.15	0.47
1:C:100:GLY:HA2	3:C:603:FAD:C5X	2.44	0.47
1:D:389:MET:HE3	1:D:391:LEU:HG	1.95	0.47
1:A:393:ASP:HB2	1:D:353:MET:CE	2.44	0.47
1:C:77:SER:OG	1:C:78:LYS:N	2.48	0.47
1:C:474:LYS:HG2	1:C:514:PRO:HB3	1.96	0.47
1:D:490:HIS:HD2	4:D:744:HOH:O	1.98	0.46
1:B:397:ARG:NH1	1:B:421:ASP:OD2	2.46	0.46
1:A:176:ILE:HG21	1:A:251:MET:SD	2.55	0.46
1:B:365:LYS:HG2	1:B:416:TYR:CD1	2.50	0.46
1:A:393:ASP:HB2	1:D:353:MET:HE2	1.97	0.46
1:C:204:PHE:HB3	1:C:239:PHE:HA	1.97	0.46
1:D:176:ILE:HG21	1:D:251:MET:SD	2.55	0.46
1:B:238:ASP:OD2	2:B:601:ARG:NH2	2.48	0.46
2:B:602:ARG:N	1:C:337:THR:HB	2.31	0.46
1:B:190:GLU:O	1:B:194:THR:HG23	2.15	0.46
1:C:94:ILE:CG2	1:C:369:MET:CE	2.93	0.46



	i ageni	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:365:LYS:HG2	1:C:416:TYR:CD1	2.51	0.46
1:D:236:ASP:HA	1:D:239:PHE:CD2	2.50	0.46
1:D:365:LYS:HG2	1:D:416:TYR:CD1	2.51	0.46
1:A:145:TYR:CD1	1:A:384:ARG:HD3	2.51	0.45
1:B:206:ASP:OD2	1:C:206:ASP:OD2	2.34	0.45
1:B:379:ASP:OD1	1:B:379:ASP:C	2.55	0.45
1:C:379:ASP:C	1:C:379:ASP:OD1	2.55	0.45
1:A:94:ILE:HG21	1:A:369:MET:CE	2.47	0.45
1:B:102:ARG:HD2	1:B:258:GLN:OE1	2.17	0.45
1:B:334:TRP:HB2	1:B:470:LEU:HD13	1.99	0.45
1:B:206:ASP:CG	1:C:206:ASP:OD1	2.54	0.45
1:C:145:TYR:CD1	1:C:384:ARG:HD3	2.51	0.45
1:D:338:THR:OG1	1:D:339:GLN:N	2.49	0.45
1:B:337:THR:HB	2:C:602:ARG:HB3	1.98	0.44
1:B:353:MET:HE3	1:B:357:ARG:HE	1.82	0.44
1:C:97:GLU:HB3	1:C:101:MET:HB3	1.99	0.44
1:C:353:MET:CE	1:C:357:ARG:NH2	2.81	0.44
1:A:353:MET:HE1	1:A:357:ARG:CZ	2.46	0.44
1:B:160:THR:HB	1:B:230:PHE:CG	2.52	0.44
1:D:55:ILE:HG22	3:D:602:FAD:O5'	2.18	0.44
1:B:540:HIS:NE2	4:B:702:HOH:O	2.36	0.44
1:D:203:THR:HG22	1:D:478:PRO:HG3	2.00	0.44
1:A:420:SER:HB3	1:D:334:TRP:CZ2	2.52	0.44
1:A:461:ILE:HG13	1:A:462:SER:N	2.33	0.43
1:D:357:ARG:HE	1:D:357:ARG:HA	1.82	0.43
1:A:160:THR:HB	1:A:230:PHE:CG	2.54	0.43
1:A:353:MET:HE1	1:A:357:ARG:NH1	2.33	0.43
1:D:488:TYR:HB3	1:D:555:GLN:OE1	2.18	0.43
1:A:334:TRP:CZ2	1:A:358:THR:O	2.71	0.43
1:A:474:LYS:HG2	1:A:514:PRO:HB3	2.00	0.43
1:B:540:HIS:CD2	4:B:702:HOH:O	2.72	0.43
1:D:416:TYR:HH	1:D:418:TRP:HH2	1.64	0.43
1:A:298:ARG:NH1	4:A:703:HOH:O	2.43	0.43
1:A:353:MET:CE	1:A:357:ARG:NH1	2.82	0.43
1:C:451:ALA:HA	1:C:454:ILE:HD12	2.01	0.43
1:C:519:GLY:O	1:C:523:THR:HG23	2.18	0.43
1:D:302:LYS:HB3	1:D:302:LYS:HE3	1.81	0.43
1:C:30:LEU:HD13	1:C:112:HIS:CD2	2.54	0.43
1:B:268:VAL:HB	1:B:269:PRO:CD	2.49	0.42
1:A:190:GLU:O	1:A:194:THR:HG23	2.20	0.42
1:B:424:LYS:HG2	1:C:334:TRP:CE3	2.54	0.42



	,	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:303:ARG:NE	1:A:305:ALA:HB2	2.33	0.42
1:A:552:GLU:HG2	1:A:553:ILE:HG23	2.01	0.42
1:B:353:MET:CE	1:B:357:ARG:NE	2.75	0.42
1:B:472:ALA:O	3:B:603:FAD:HM81	2.20	0.42
1:D:127:PRO:HB3	1:D:389:MET:CE	2.49	0.42
1:D:519:GLY:O	1:D:523:THR:HG23	2.20	0.42
1:D:550:PHE:CZ	1:D:555:GLN:NE2	2.87	0.42
1:A:474:LYS:HE2	1:A:514:PRO:HB3	2.02	0.42
1:A:555:GLN:H	1:A:555:GLN:HG3	1.41	0.42
1:A:353:MET:HE1	1:A:357:ARG:NH2	2.35	0.42
1:D:91:THR:HG21	1:D:369:MET:CE	2.50	0.42
1:A:372:ARG:HB2	1:A:373:PRO:HD2	2.02	0.42
1:C:160:THR:HB	1:C:230:PHE:CG	2.55	0.42
1:A:334:TRP:HB2	1:A:470:LEU:CD1	2.50	0.42
1:A:205:TYR:CD2	1:D:478:PRO:HG2	2.55	0.41
1:D:100:GLY:HA2	3:D:602:FAD:C5X	2.50	0.41
1:A:316:ASP:C	1:A:316:ASP:OD1	2.58	0.41
1:C:82:ARG:O	1:C:99:GLY:HA3	2.19	0.41
1:A:203:THR:OG1	1:A:205:TYR:HB2	2.20	0.41
1:B:27:ASP:OD1	1:B:28:ASP:N	2.51	0.41
1:C:103:PHE:HA	1:C:104:PRO:HD2	1.99	0.41
1:D:97:GLU:OE1	1:D:97:GLU:HA	2.20	0.41
1:D:44:HIS:ND1	1:D:282:HIS:HB2	2.35	0.41
1:A:362:GLN:OE1	1:A:464:GLU:OE1	2.38	0.41
1:B:176:ILE:HG21	1:B:251:MET:SD	2.61	0.41
1:C:203:THR:HG22	1:C:478:PRO:HG3	2.02	0.41
1:D:349:GLN:HA	1:D:349:GLN:OE1	2.20	0.41
1:A:397:ARG:NH1	1:A:421:ASP:OD2	2.47	0.41
1:A:60:ALA:HB2	1:A:524:SER:OG	2.21	0.41
1:D:239:PHE:N	1:D:240:PRO:CD	2.84	0.41
1:A:331:CYS:HB2	1:A:335:LEU:HD12	2.02	0.41
1:C:555:GLN:H	1:C:555:GLN:HG3	1.45	0.41
1:B:326:ALA:HA	1:B:502:GLY:O	2.21	0.40
1:B:492:MET:HG3	1:B:550:PHE:CD2	2.55	0.40
1:C:550:PHE:CZ	1:C:555:GLN:NE2	2.90	0.40
1:A:464:GLU:N	1:A:464:GLU:CD	2.75	0.40
1:B:47:GLU:HA	1:B:70:LYS:O	2.20	0.40
1:C:20:PRO:HB2	1:C:192:TRP:CG	2.56	0.40
1:D:451:ALA:HA	1:D:454:ILE:HD12	2.04	0.40
1:D:491:PHE:CE2	1:D:526:ASN:HB3	2.57	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	Perce	ntiles
1	А	547/580~(94%)	531~(97%)	16 (3%)	0	100	100
1	В	547/580~(94%)	530~(97%)	17 (3%)	0	100	100
1	С	547/580~(94%)	537~(98%)	10 (2%)	0	100	100
1	D	547/580~(94%)	533~(97%)	13~(2%)	1 (0%)	47	58
All	All	2188/2320~(94%)	2131 (97%)	56~(3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	397	ARG

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	А	448/474~(94%)	431 (96%)	17 (4%)	33 47
1	В	448/474~(94%)	432 (96%)	16 (4%)	35 49
1	С	448/474~(94%)	432 (96%)	16 (4%)	35 49
1	D	448/474~(94%)	433~(97%)	15 (3%)	38 53
All	All	1792/1896~(94%)	1728 (96%)	64 (4%)	33 49

All (64) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	31	GLU
1	А	78	LYS
1	А	79	MET
1	А	279	ARG
1	А	280	CYS
1	А	298	ARG
1	А	302	LYS
1	А	303	ARG
1	А	338	THR
1	А	357	ARG
1	А	359	ARG
1	А	442	LYS
1	А	486	ARG
1	А	498	VAL
1	А	511	SER
1	А	540	HIS
1	А	555	GLN
1	В	79	MET
1	В	279	ARG
1	В	280	CYS
1	В	298	ARG
1	В	303	ARG
1	В	322	ARG
1	В	337	THR
1	В	338	THR
1	В	357	ARG
1	В	359	ARG
1	В	435	GLN
1	В	442	LYS
1	В	486	ARG
1	В	511	SER
1	В	540	HIS
1	В	555	GLN
1	С	31	GLU
1	С	78	LYS
1	С	79	MET
1	С	211	SER
1	С	237	SER
1	С	279	ARG
1	С	337	THR
1	С	338	THR
1	С	357	ARG
1	С	359	ARG



Mol	Chain	Res	Type
1	С	389	MET
1	С	442	LYS
1	С	511	SER
1	С	540	HIS
1	С	552	GLU
1	С	555	GLN
1	D	78	LYS
1	D	79	MET
1	D	211	SER
1	D	237	SER
1	D	279	ARG
1	D	337	THR
1	D	338	THR
1	D	353	MET
1	D	357	ARG
1	D	389	MET
1	D	442	LYS
1	D	473	PHE
1	D	511	SER
1	D	540	HIS
1	D	555	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	267	GLN
1	А	275	HIS
1	А	362	GLN
1	А	480	HIS
1	А	490	HIS
1	В	267	GLN
1	В	435	GLN
1	В	480	HIS
1	В	485	GLN
1	В	490	HIS
1	С	267	GLN
1	С	362	GLN
1	С	428	HIS
1	С	468	HIS
1	С	480	HIS
1	С	490	HIS
1	D	267	GLN



Continued from previous page...

Mol	Chain	Res	Type
1	D	362	GLN
1	D	428	HIS
1	D	468	HIS
1	D	480	HIS
1	D	490	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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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).

Mal	Mol Type Chai		hain Ros		Bo	ond leng	ths	E	Bond ang	gles
INIOI	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	ARG	С	602	-	10,11,11	0.69	0	11,13,13	1.87	2 (18%)
3	FAD	А	604	-	53,58,58	1.48	8 (15%)	68,89,89	1.94	19 (27%)
2	ARG	В	601	-	10,11,11	0.92	1 (10%)	11,13,13	0.99	1 (9%)
2	ARG	D	601	-	10,11,11	0.67	0	11,13,13	1.36	2 (18%)
3	FAD	С	603	-	$53,\!58,\!58$	1.44	<mark>9 (16%)</mark>	68,89,89	1.87	21 (30%)
2	ARG	С	601	-	10,11,11	0.91	0	11,13,13	1.43	2 (18%)
2	ARG	В	602	-	10,11,11	0.82	1 (10%)	11,13,13	1.18	1 (9%)



Mol Turo		Chain	Dec	Tink	Bo	ond leng	$_{\rm ths}$	B	ond ang	gles
WIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	ARG	А	601	-	$10,\!11,\!11$	0.76	0	11,13,13	1.16	2 (18%)
3	FAD	В	603	-	$53,\!58,\!58$	1.56	8 (15%)	68,89,89	2.02	21 (30%)
3	FAD	D	602	-	53,58,58	1.50	7 (13%)	68,89,89	1.75	19 (27%)
2	ARG	А	602	-	10,11,11	0.90	0	11,13,13	1.22	1 (9%)
2	ARG	А	603	-	10,11,11	0.90	1 (10%)	11,13,13	1.24	1 (9%)

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	ARG	С	602	-	-	3/11/11/11	-
3	FAD	А	604	-	-	6/30/50/50	0/6/6/6
2	ARG	В	601	-	-	6/11/11/11	-
2	ARG	D	601	-	-	4/11/11/11	-
3	FAD	С	603	-	-	6/30/50/50	0/6/6/6
2	ARG	С	601	-	-	5/11/11/11	-
2	ARG	В	602	-	-	0/11/11/11	-
2	ARG	А	601	-	-	0/11/11/11	-
3	FAD	В	603	-	-	4/30/50/50	0/6/6/6
3	FAD	D	602	-	-	1/30/50/50	0/6/6/6
2	ARG	А	602	-	-	2/11/11/11	-
2	ARG	А	603	-	-	8/11/11/11	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
3	D	602	FAD	C9A-C5X	5.95	1.51	1.41
3	С	603	FAD	C9A-C5X	4.96	1.49	1.41
3	В	603	FAD	C9A-C5X	4.94	1.49	1.41
3	В	603	FAD	O4B-C1B	4.29	1.47	1.41
3	А	604	FAD	C1'-C2'	-4.01	1.47	1.52
3	С	603	FAD	C5X-N5	-3.64	1.32	1.39
3	В	603	FAD	C1'-C2'	-3.48	1.47	1.52
3	В	603	FAD	C8-C7	3.24	1.49	1.40
3	D	602	FAD	C8-C7	3.16	1.48	1.40
3	D	602	FAD	C1'-C2'	-3.09	1.48	1.52
3	А	604	FAD	C4-N3	-3.09	1.33	1.38



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	А	604	FAD	C5X-N5	-3.06	1.33	1.39
3	А	604	FAD	C9A-C5X	2.95	1.46	1.41
3	А	604	FAD	C8-C7	2.85	1.48	1.40
3	D	602	FAD	C5X-N5	-2.65	1.34	1.39
3	D	602	FAD	C4-N3	-2.64	1.33	1.38
3	С	603	FAD	C6-C5X	-2.62	1.35	1.40
3	А	604	FAD	O4B-C1B	2.60	1.44	1.41
3	В	603	FAD	C5A-N7A	-2.52	1.30	1.39
3	С	603	FAD	C8-C7	2.48	1.47	1.40
3	В	603	FAD	O4'-C4'	2.45	1.48	1.43
3	С	603	FAD	C5A-C4A	2.36	1.47	1.40
3	D	602	FAD	C6-C7	-2.27	1.36	1.39
3	С	603	FAD	C6-C7	-2.24	1.36	1.39
3	D	602	FAD	C5A-C4A	2.23	1.46	1.40
2	А	603	ARG	OXT-C	-2.23	1.23	1.30
3	С	603	FAD	C1'-C2'	-2.22	1.49	1.52
3	В	603	FAD	C4-N3	-2.21	1.34	1.38
2	В	601	ARG	OXT-C	-2.20	1.23	1.30
3	В	603	FAD	C5X-N5	-2.17	1.35	1.39
2	В	602	ARG	OXT-C	-2.17	1.23	1.30
3	А	604	FAD	O2-C2	2.13	1.28	1.24
3	С	603	FAD	C4-N3	-2.13	1.34	1.38
3	А	604	FAD	O4'-C4'	2.08	1.47	1.43
3	С	603	FAD	C4A-N3A	-2.06	1.32	1.35

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
3	А	604	FAD	O4B-C1B-C2B	-5.31	99.17	106.93
3	В	603	FAD	C5'-C4'-C3'	-4.90	102.73	112.20
3	А	604	FAD	C5'-C4'-C3'	-4.50	103.51	112.20
3	В	603	FAD	O4B-C4B-C5B	4.49	124.16	109.37
3	А	604	FAD	O4B-C4B-C5B	4.42	123.92	109.37
3	С	603	FAD	O4-C4-C4X	-4.23	115.38	126.60
3	С	603	FAD	O2-C2-N1	-4.19	114.89	121.83
3	А	604	FAD	N3A-C2A-N1A	-4.14	122.20	128.68
3	В	603	FAD	O4B-C1B-C2B	-4.12	100.91	106.93
2	С	602	ARG	OXT-C-O	-4.09	114.79	124.09
3	D	602	FAD	N3A-C2A-N1A	-4.09	122.28	128.68
2	С	602	ARG	OXT-C-CA	4.07	127.25	113.38
3	D	602	FAD	O2-C2-N1	-4.00	115.19	121.83
3	В	603	FAD	O2-C2-N1	-3.86	115.43	121.83



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	В	603	FAD	N3A-C2A-N1A	-3.79	122.76	128.68
3	С	603	FAD	C6-C5X-C9A	3.78	124.28	118.94
3	В	603	FAD	O4-C4-N3	3.74	127.29	120.12
3	С	603	FAD	N3A-C2A-N1A	-3.74	122.84	128.68
3	С	603	FAD	O4-C4-N3	3.71	127.23	120.12
3	А	604	FAD	O5B-PA-O1A	3.68	123.46	109.07
3	С	603	FAD	O2'-C2'-C1'	-3.67	100.92	109.80
3	С	603	FAD	C1'-N10-C9A	3.67	126.63	120.51
3	А	604	FAD	O5B-C5B-C4B	3.65	121.57	108.99
3	D	602	FAD	O4-C4-C4X	-3.65	116.91	126.60
2	С	601	ARG	OXT-C-O	-3.65	115.80	124.09
3	В	603	FAD	O5B-PA-O1A	3.51	122.78	109.07
3	D	602	FAD	O2A-PA-O1A	3.48	129.45	112.24
3	В	603	FAD	C5X-C9A-N10	3.35	121.41	117.95
3	В	603	FAD	C1'-N10-C9A	3.32	126.04	120.51
3	В	603	FAD	O4-C4-C4X	-3.28	117.90	126.60
3	В	603	FAD	O3B-C3B-C4B	-3.18	101.85	111.05
3	D	602	FAD	O4-C4-N3	3.17	126.19	120.12
2	А	603	ARG	OXT-C-O	-3.13	116.98	124.09
3	D	602	FAD	C1'-N10-C9A	3.11	125.69	120.51
3	В	603	FAD	C9A-N10-C10	-3.08	115.96	120.77
3	D	602	FAD	C6-C5X-C9A	3.03	123.23	118.94
3	D	602	FAD	C1B-N9A-C4A	-2.95	121.45	126.64
3	D	602	FAD	C9A-N10-C10	-2.94	116.18	120.77
3	А	604	FAD	C5X-C9A-N10	2.93	120.98	117.95
2	D	601	ARG	OXT-C-CA	2.92	123.32	113.38
3	С	603	FAD	C9A-N10-C10	-2.91	116.23	120.77
3	А	604	FAD	C4A-C5A-N7A	-2.89	106.39	109.40
3	В	603	FAD	N3-C2-N1	2.86	124.99	119.38
3	В	603	FAD	O4'-C4'-C3'	2.77	115.84	109.10
2	А	602	ARG	OXT-C-O	-2.76	117.81	124.09
3	В	603	FAD	C4A-C5A-N7A	-2.74	106.55	109.40
2	В	602	ARG	OXT-C-O	-2.71	117.94	124.09
3	C	603	FAD	C9-C8-C7	2.67	123.50	119.67
2	А	601	ARG	OXT-C-O	-2.67	118.02	124.09
3	C	603	FAD	C5X-C9A-N10	2.63	120.67	117.95
3	С	603	FAD	C2A-N1A-C6A	2.62	123.24	118.75
3	D	602	FAD	C5X-C9A-N10	2.62	120.66	117.95
3	D	602	FAD	O2'-C2'-C1'	-2.62	103.47	109.80
3	А	604	FAD	O2'-C2'-C3'	2.61	115.45	109.10
3	D	602	FAD	C2A-N1A-C6A	2.61	123.21	118.75
3	D	602	FAD	N3-C2-N1	2.60	124.48	119.38



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	С	603	FAD	C4A-C5A-N7A	-2.58	106.71	109.40
3	А	604	FAD	C3B-C2B-C1B	2.58	104.86	100.98
3	В	603	FAD	N6A-C6A-N1A	2.57	123.91	118.57
3	А	604	FAD	O4-C4-N3	2.56	125.02	120.12
3	В	603	FAD	O4'-C4'-C5'	2.54	115.63	109.92
2	С	601	ARG	OXT-C-CA	2.52	121.96	113.38
3	А	604	FAD	O2A-PA-O1A	2.50	124.60	112.24
3	В	603	FAD	O2A-PA-O1A	2.48	124.50	112.24
2	D	601	ARG	OXT-C-O	-2.48	118.46	124.09
3	В	603	FAD	C6-C5X-C9A	2.42	122.36	118.94
3	А	604	FAD	O4'-C4'-C5'	2.42	115.35	109.92
3	D	602	FAD	C4X-C10-N1	-2.40	119.16	124.73
2	А	601	ARG	OXT-C-CA	2.39	121.53	113.38
3	А	604	FAD	O4-C4-C4X	-2.37	120.31	126.60
3	D	602	FAD	O4B-C4B-C3B	2.30	109.67	105.11
3	А	604	FAD	P-O3P-PA	-2.29	124.97	132.83
3	С	603	FAD	O2P-P-O1P	2.25	123.38	112.24
3	С	603	FAD	P-O3P-PA	-2.25	125.12	132.83
3	С	603	FAD	O2A-PA-O1A	2.24	123.31	112.24
3	А	604	FAD	C6-C5X-C9A	2.22	122.08	118.94
3	В	603	FAD	O3'-C3'-C2'	-2.20	103.49	108.81
3	D	602	FAD	C9-C8-C7	2.20	122.82	119.67
3	А	604	FAD	C9A-C5X-N5	-2.16	120.09	122.43
3	А	604	FAD	C6-C7-C8	-2.15	116.59	119.67
3	D	602	FAD	C4X-C10-N10	2.14	119.61	116.48
3	С	603	FAD	C3B-C2B-C1B	-2.13	97.77	100.98
3	А	604	FAD	C9-C8-C7	2.12	122.71	119.67
3	С	603	FAD	C1B-N9A-C4A	-2.10	122.95	126.64
3	С	603	FAD	O2'-C2'-C3'	2.08	114.17	109.10
3	В	603	FAD	C9-C8-C7	2.06	122.63	119.67
2	В	601	ARG	OXT-C-O	-2.05	119.43	124.09
3	С	603	FAD	N3-C2-N1	2.05	123.41	119.38
3	D	602	FAD	O2P-P-O1P	2.05	122.36	112.24
3	D	602	FAD	C4-N3-C2	-2.02	121.91	125.64
3	С	603	FAD	C4-N3-C2	-2.00	121.94	125.64
3	С	603	FAD	C9A-C5X-N5	-2.00	120.25	122.43

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms				
2	А	603	ARG	O-C-CA-N				



Mol	Chain	Res	Type	Atoms
2	А	603	ARG	N-CA-CB-CG
2	А	603	ARG	C-CA-CB-CG
2	В	601	ARG	C-CA-CB-CG
2	С	602	ARG	C-CA-CB-CG
3	А	604	FAD	C5B-O5B-PA-O2A
3	А	604	FAD	C5B-O5B-PA-O3P
3	В	603	FAD	C5B-O5B-PA-O2A
3	В	603	FAD	C5B-O5B-PA-O3P
2	С	602	ARG	NE-CD-CG-CB
2	А	603	ARG	NE-CD-CG-CB
2	D	601	ARG	NE-CD-CG-CB
2	А	603	ARG	CG-CD-NE-CZ
2	С	602	ARG	CG-CD-NE-CZ
2	А	603	ARG	OXT-C-CA-N
2	В	601	ARG	CA-CB-CG-CD
2	В	601	ARG	NE-CD-CG-CB
2	А	602	ARG	NE-CD-CG-CB
3	С	603	FAD	O3'-C3'-C4'-C5'
3	С	603	FAD	C2'-C3'-C4'-C5'
3	А	604	FAD	O3'-C3'-C4'-O4'
3	А	604	FAD	C4B-C5B-O5B-PA
3	С	603	FAD	C2'-C3'-C4'-O4'
2	В	601	ARG	N-CA-CB-CG
2	С	601	ARG	N-CA-CB-CG
3	А	604	FAD	N10-C1'-C2'-O2'
3	В	603	FAD	N10-C1'-C2'-O2'
2	D	601	ARG	CA-CB-CG-CD
2	D	601	ARG	O-C-CA-CB
2	А	603	ARG	OXT-C-CA-CB
2	D	601	ARG	OXT-C-CA-CB
3	В	603	FAD	C4B-C5B-O5B-PA
3	D	602	FAD	O4B-C4B-C5B-O5B
2	C	601	ARG	O-C-CA-N
2	A	602	ARG	CG-CD-NE-CZ
2	A	603	ARG	O-C-CA-CB
2	С	601	ARG	O-C-CA-CB
2	В	601	ARG	OXT-C-CA-N
2	С	601	ARG	OXT-C-CA-N
3	С	603	FAD	O4B-C4B-C5B-O5B
2	С	601	ARG	OXT-C-CA-CB
2	В	601	ARG	CG-CD-NE-CZ
3	С	603	FAD	C5'-O5'-P-O1P

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Mol	Chain	Res	Type	Atoms
3	С	603	FAD	O3'-C3'-C4'-O4'
3	А	604	FAD	O3'-C3'-C4'-C5'

There are no ring outliers.

9 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	С	602	ARG	1	0
3	А	604	FAD	5	0
2	В	601	ARG	1	0
2	D	601	ARG	2	0
3	С	603	FAD	5	0
2	В	602	ARG	1	0
3	В	603	FAD	6	0
3	D	602	FAD	6	0
2	А	603	ARG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





















5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	А	549/580~(94%)	0.19	12 (2%) 62 69	14, 29, 53, 85	0
1	В	549/580~(94%)	0.18	17 (3%) 49 56	15, 29, 51, 83	0
1	С	549/580~(94%)	0.55	31 (5%) 24 30	20, 39, 62, 112	0
1	D	549/580~(94%)	0.58	46 (8%) 11 15	22, 38, 60, 91	0
All	All	2196/2320~(94%)	0.38	106 (4%) 30 37	14, 35, 58, 112	0

All (106) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	С	380	PRO	4.9
1	С	279	ARG	4.6
1	В	279	ARG	4.6
1	С	381	GLU	4.3
1	А	279	ARG	4.1
1	С	278	GLU	4.0
1	D	537	GLY	4.0
1	D	279	ARG	3.9
1	D	381	GLU	3.8
1	А	380	PRO	3.7
1	D	278	GLU	3.6
1	D	383	GLY	3.5
1	D	380	PRO	3.5
1	А	381	GLU	3.4
1	В	380	PRO	3.4
1	С	382	THR	3.4
1	D	382	THR	3.4
1	D	536	GLY	3.2
1	С	154	ALA	3.2
1	С	143	THR	3.1
1	В	382	THR	3.1



Mol	Chain	Res	Type	RSRZ
1	D	446	PRO	3.1
1	С	276	VAL	3.1
1	D	42	ALA	3.0
1	В	381	GLU	3.0
1	А	205	TYR	2.9
1	С	540	HIS	2.8
1	D	338	THR	2.8
1	D	540	HIS	2.8
1	С	537	GLY	2.7
1	С	449	ASP	2.7
1	D	535	PHE	2.7
1	А	353	MET	2.7
1	D	450	ILE	2.7
1	D	552	GLU	2.7
1	В	353	MET	2.7
1	А	338	THR	2.7
1	D	448	THR	2.6
1	С	357	ARG	2.6
1	А	382	THR	2.6
1	А	407	ASP	2.6
1	В	540	HIS	2.6
1	С	386	LEU	2.6
1	D	24	PHE	2.6
1	D	498	VAL	2.6
1	С	555	GLN	2.6
1	С	361	MET	2.5
1	С	150	ALA	2.5
1	С	406	ASP	2.5
1	С	384	ARG	2.4
1	А	278	GLU	2.4
1	В	278	GLU	2.4
1	D	494	ALA	2.4
1	D	40	PRO	2.4
1	С	281	ALA	2.4
1	В	160	THR	2.4
1	D	515	ALA	2.4
1	D	160	THR	2.4
1	В	205	TYR	2.4
1	A	160	THR	2.4
1	D	435	GLN	2.4
1	D	13	LYS	2.3
1	С	453	HIS	2.3



Mol	Chain	Res	Type	RSRZ
1	D	276	VAL	2.3
1	D	386	LEU	2.3
1	С	377	ASP	2.3
1	D	499	GLU	2.3
1	В	150	ALA	2.3
1	С	527	ALA	2.3
1	С	40	PRO	2.3
1	С	552	GLU	2.3
1	В	338	THR	2.2
1	С	142	GLN	2.2
1	С	140	GLU	2.2
1	С	378	LYS	2.2
1	С	379	ASP	2.2
1	D	533	ASN	2.2
1	D	361	MET	2.2
1	В	334	TRP	2.2
1	В	407	ASP	2.2
1	D	453	HIS	2.2
1	D	384	ARG	2.2
1	D	419	MET	2.2
1	А	334	TRP	2.2
1	А	285	GLU	2.2
1	В	144	TYR	2.2
1	D	495	GLN	2.2
1	С	448	THR	2.2
1	D	307	ALA	2.2
1	D	541	ALA	2.2
1	D	308	SER	2.1
1	В	285	GLU	2.1
1	В	379	ASP	2.1
1	D	423	LEU	2.1
1	D	45	GLY	2.1
1	D	29	TRP	2.1
1	D	503	ILE	2.1
1	D	406	ASP	2.1
1	D	555	GLN	2.1
1	D	551	ASP	2.1
1	D	148	LYS	2.1
1	D	281	ALA	2.1
1	С	130	PRO	2.1
1	D	449	ASP	2.0
1	В	419	MET	2.0



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Mol	Chain	\mathbf{Res}	Type	RSRZ
1	\mathbf{C}	144	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
2	ARG	C	601	12/12	0.54	0.42	$58,\!68,\!78,\!80$	0
2	ARG	С	602	12/12	0.65	0.32	68,77,78,80	0
2	ARG	А	601	12/12	0.69	0.34	59,70,85,86	0
2	ARG	D	601	12/12	0.72	0.37	$55,\!64,\!78,\!80$	0
2	ARG	A	603	12/12	0.74	0.26	$69,\!78,\!82,\!83$	0
2	ARG	А	602	12/12	0.76	0.25	40,51,53,55	0
2	ARG	В	601	12/12	0.76	0.29	57,61,74,75	0
2	ARG	В	602	12/12	0.76	0.29	45,55,63,63	0
3	FAD	С	603	53/53	0.94	0.15	23,29,32,34	0
3	FAD	D	602	53/53	0.94	0.15	$21,\!30,\!37,\!38$	0
3	FAD	A	604	53/53	0.96	0.14	17,21,27,31	0
3	FAD	В	603	53/53	0.96	0.13	15,21,29,29	0

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











6.5 Other polymers (i)

There are no such residues in this entry.

