



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2018 – 11:54 AM EDT

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

<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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

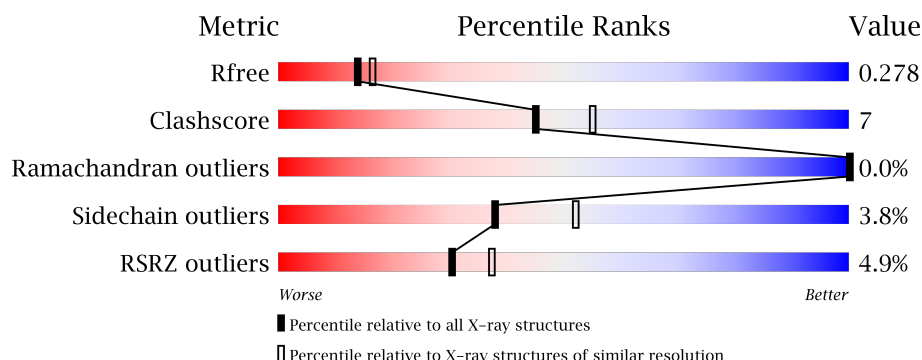
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (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 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.

Mol	Chain	Length	Quality of chain
1	A	580	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>• 5%</div> </div> </div>
1	B	580	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>13%</div> <div>• 5%</div> </div> </div>
1	C	580	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>• 5%</div> </div> </div>
1	D	580	<div> <div>8%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>• 5%</div> </div> </div>

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	A	601	-	-	-	X
2	ARG	A	602	-	-	-	X
2	ARG	B	601	-	-	-	X
2	ARG	B	602	-	-	-	X
2	ARG	C	601	-	-	-	X
2	ARG	C	602	-	-	-	X
2	ARG	D	601	-	-	-	X

2 Entry composition

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.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4305	2749	742	791	23			
1	B	549	Total	C	N	O	S	0	0	0
			4305	2749	742	791	23			
1	C	549	Total	C	N	O	S	0	0	0
			4305	2749	742	791	23			
1	D	549	Total	C	N	O	S	0	0	0
			4305	2749	742	791	23			

There are 84 discrepancies between the modelled and reference sequences:

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

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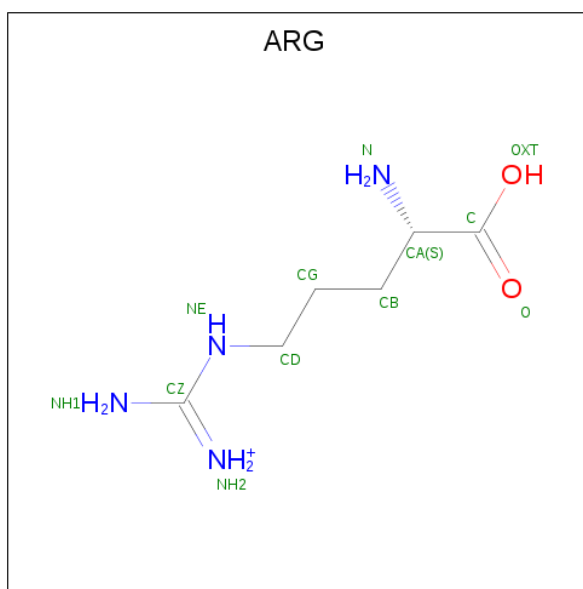
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP W6JQJ6
B	-18	GLY	-	expression tag	UNP W6JQJ6
B	-17	SER	-	expression tag	UNP W6JQJ6
B	-16	SER	-	expression tag	UNP W6JQJ6
B	-15	HIS	-	expression tag	UNP W6JQJ6
B	-14	HIS	-	expression tag	UNP W6JQJ6
B	-13	HIS	-	expression tag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

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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: $C_6H_{15}N_4O_2$).



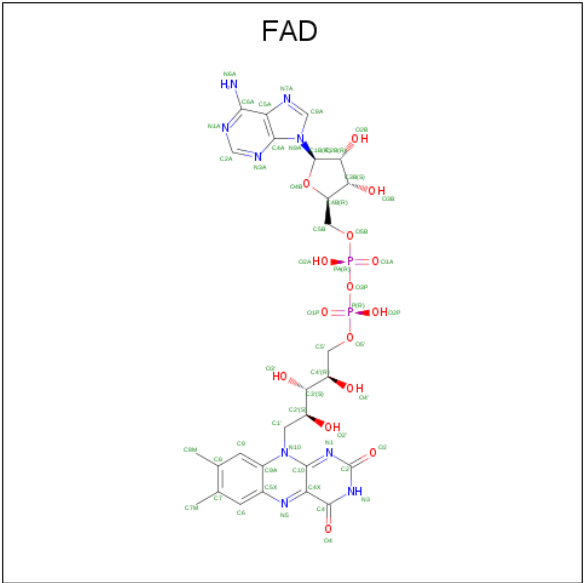
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	6	4	2		

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

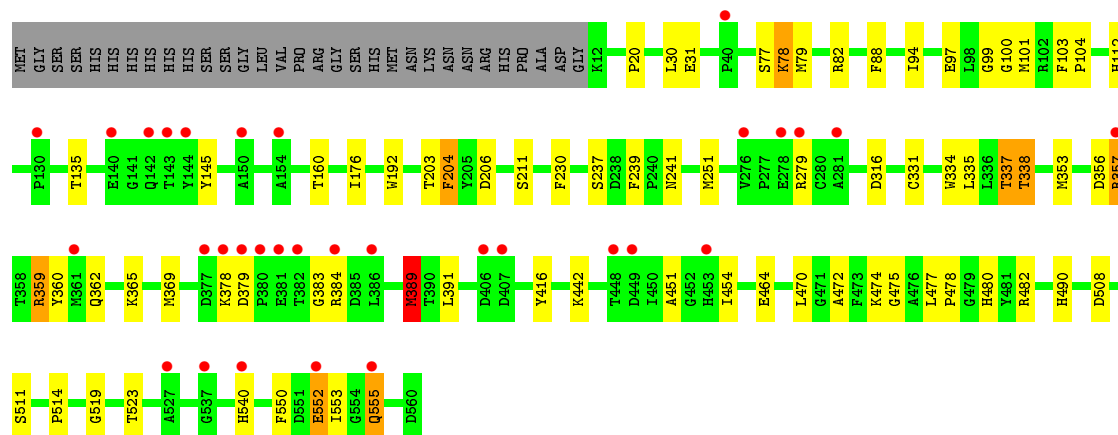
- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



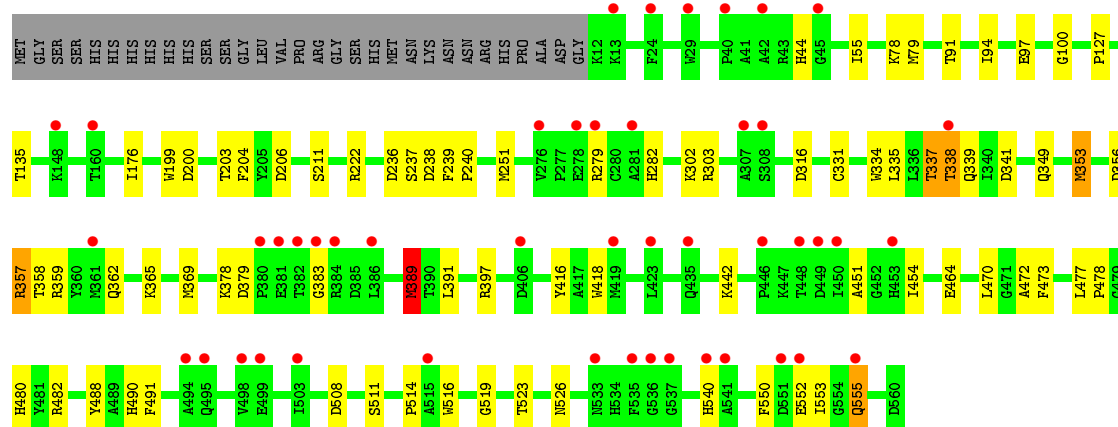
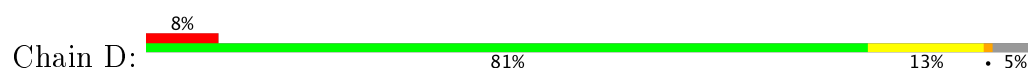
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			53	27	9	15		
3	B	1	Total	C	N	O	0	0
			53	27	9	15		
3	C	1	Total	C	N	O	0	0
			53	27	9	15		
3	D	1	Total	C	N	O	0	0
			53	27	9	15		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	98	Total 98	O 98	0	0
4	B	108	Total 108	O 108	0	0
4	C	53	Total 53	O 53	0	0
4	D	50	Total 50	O 50	0	0



• Molecule 1: L-amino acid oxidase/monooxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.20 Å 133.00 Å 101.50 Å 90.00° 112.00° 90.00°	Depositor
Resolution (Å)	94.11 – 2.30 45.52 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (94.11-2.30) 99.8 (45.52-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.29 Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.220 , 0.273 0.226 , 0.278	Depositor DCC
R_{free} test set	2009 reflections (1.91%)	DCC
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	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD

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	0.82	0/4428	0.88	5/6019 (0.1%)
1	B	0.82	0/4428	0.91	5/6019 (0.1%)
1	C	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(°)	Ideal(°)
1	B	486	ARG	NE-CZ-NH1	8.41	124.50	120.30
1	B	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	A	486	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	C	482	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	A	457	ASP	CB-CG-OD1	6.19	123.87	118.30
1	B	28	ASP	CB-CG-OD1	5.98	123.68	118.30
1	C	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	C	389	MET	CG-SD-CE	5.57	109.10	100.20
1	B	43	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	A	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	A	102	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	496	MET	CG-SD-CE	-5.25	91.79	100.20
1	B	322	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	C	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

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	4305	0	4166	74	0
1	B	4305	0	4164	64	0
1	C	4305	0	4166	66	0
1	D	4305	0	4166	69	0
2	A	36	0	36	1	0
2	B	24	0	24	2	0
2	C	24	0	24	1	0
2	D	12	0	12	2	0
3	A	53	0	31	5	0
3	B	53	0	31	6	0
3	C	53	0	31	5	0
3	D	53	0	31	6	0
4	A	98	0	0	4	0
4	B	108	0	0	10	0
4	C	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 distance (Å)	Clash overlap (Å)
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:HH11	1:A:303:ARG:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:OE1	1:B:464:GLU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:316:ASP:OD1	1:C:316:ASP:C	2.45	0.54
1:C:94:ILE:HG21	1:C:369:MET:HE2	1.90	0.54
1:D:204:PHE:HB3	1:D:239:PHE:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:353:MET:HE1	1:C:357:ARG:CZ	2.39	0.53
1:C:334:TRP:HB2	1:C:470:LEU:HD13	1.89	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:359:ARG:HG2	1:C:360:TYR:N	2.26	0.51
1:C:88:PHE:HB2	1:C:369:MET:HE1	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:331:CYS:HB2	1:D:335:LEU:HD12	1.94	0.48
1:D:303:ARG:HD2	1:D:341:ASP:OD2	2.13	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:91:THR:HG21	1:A:369:MET:CE	2.44	0.47
1:A:88:PHE:HB2	1:A:369:MET:HE1	1.95	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:474:LYS:HG2	1:C:514:PRO:HB3	1.96	0.47
1:C:77:SER:OG	1:C:78:LYS:N	2.48	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: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:A:393:ASP:HB2	1:D:353:MET:HE2	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:379:ASP:OD1	1:B:379:ASP:C	2.55	0.45
1:B:206:ASP:OD2	1:C:206:ASP:OD2	2.34	0.45
1:C:379:ASP:OD1	1:C:379:ASP:C	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:HG3	1:A:555:GLN:H	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:OD1	1:A:316:ASP:C	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:HA	1:D:97:GLU:OE1	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:HG3	1:C:555:GLN:H	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

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	547/580 (94%)	531 (97%)	16 (3%)	0	100	100
1	B	547/580 (94%)	530 (97%)	17 (3%)	0	100	100
1	C	547/580 (94%)	537 (98%)	10 (2%)	0	100	100
1	D	547/580 (94%)	533 (97%)	13 (2%)	1 (0%)	51	63
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

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	448/474 (94%)	431 (96%)	17 (4%)	38	52
1	B	448/474 (94%)	432 (96%)	16 (4%)	40	55
1	C	448/474 (94%)	432 (96%)	16 (4%)	40	55
1	D	448/474 (94%)	433 (97%)	15 (3%)	43	59
All	All	1792/1896 (94%)	1728 (96%)	64 (4%)	38	55

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

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

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Mol	Chain	Res	Type
1	C	389	MET
1	C	442	LYS
1	C	511	SER
1	C	540	HIS
1	C	552	GLU
1	C	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

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

Mol	Chain	Res	Type
1	A	267	GLN
1	A	275	HIS
1	A	362	GLN
1	A	480	HIS
1	A	490	HIS
1	B	267	GLN
1	B	435	GLN
1	B	480	HIS
1	B	485	GLN
1	B	490	HIS
1	C	267	GLN
1	C	362	GLN
1	C	428	HIS
1	C	468	HIS
1	C	480	HIS
1	C	490	HIS
1	D	267	GLN

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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 ⓘ

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ARG	A	601	-	6,11,11	0.41	0	5,13,13	0.41	0
2	ARG	A	602	-	6,11,11	0.59	0	5,13,13	0.81	0
2	ARG	A	603	-	6,11,11	0.35	0	5,13,13	0.63	0
3	FAD	A	604	-	51,58,58	1.30	5 (9%)	54,89,89	3.23	17 (31%)
2	ARG	B	601	-	6,11,11	0.46	0	5,13,13	0.64	0
2	ARG	B	602	-	6,11,11	0.45	0	5,13,13	0.80	0
3	FAD	B	603	-	51,58,58	1.55	8 (15%)	54,89,89	3.59	17 (31%)
2	ARG	C	601	-	6,11,11	0.71	0	5,13,13	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ARG	C	602	-	6,11,11	0.41	0	5,13,13	0.20	0
3	FAD	C	603	-	51,58,58	1.49	6 (11%)	54,89,89	2.77	19 (35%)
2	ARG	D	601	-	6,11,11	0.45	0	5,13,13	0.65	0
3	FAD	D	602	-	51,58,58	1.50	7 (13%)	54,89,89	2.62	15 (27%)

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	A	601	-	-	0/7/11/11	0/0/0/0
2	ARG	A	602	-	-	0/7/11/11	0/0/0/0
2	ARG	A	603	-	-	0/7/11/11	0/0/0/0
3	FAD	A	604	-	-	0/28/50/50	0/6/6/6
2	ARG	B	601	-	-	0/7/11/11	0/0/0/0
2	ARG	B	602	-	-	0/7/11/11	0/0/0/0
3	FAD	B	603	-	-	0/28/50/50	0/6/6/6
2	ARG	C	601	-	-	0/7/11/11	0/0/0/0
2	ARG	C	602	-	-	0/7/11/11	0/0/0/0
3	FAD	C	603	-	-	0/28/50/50	0/6/6/6
2	ARG	D	601	-	-	0/7/11/11	0/0/0/0
3	FAD	D	602	-	-	0/28/50/50	0/6/6/6

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	603	FAD	C6-C5X	-3.98	1.35	1.41
3	D	602	FAD	C6-C5X	-3.12	1.37	1.41
3	B	603	FAD	C2-N1	-3.00	1.32	1.38
3	B	603	FAD	C5A-N7A	-2.60	1.30	1.39
3	A	604	FAD	C2-N1	-2.02	1.34	1.38
3	D	602	FAD	C4-C4X	2.01	1.45	1.41
3	B	603	FAD	C9A-N10	2.11	1.41	1.38
3	A	604	FAD	C4-C4X	2.15	1.45	1.41
3	B	603	FAD	O4'-C4'	2.36	1.48	1.43
3	C	603	FAD	C8-C7	2.42	1.47	1.41
3	A	604	FAD	O4B-C1B	2.49	1.44	1.41
3	A	604	FAD	C8-C7	2.78	1.48	1.41
3	D	602	FAD	C5A-C4A	2.80	1.46	1.40
3	C	603	FAD	C5A-C4A	2.96	1.47	1.40
3	D	602	FAD	C8-C7	3.09	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	FAD	C8-C7	3.17	1.49	1.41
3	B	603	FAD	C9A-C5X	3.34	1.49	1.42
3	C	603	FAD	C9A-C5X	3.37	1.49	1.42
3	C	603	FAD	C4X-C10	3.75	1.47	1.41
3	A	604	FAD	C4X-C10	3.88	1.47	1.41
3	D	602	FAD	C9A-N10	3.90	1.43	1.38
3	D	602	FAD	C9A-C5X	4.17	1.51	1.42
3	B	603	FAD	O4B-C1B	4.19	1.47	1.41
3	C	603	FAD	C9A-N10	4.38	1.44	1.38
3	D	602	FAD	C4X-C10	4.46	1.48	1.41
3	B	603	FAD	C4X-C10	4.70	1.49	1.41

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	603	FAD	C4B-O4B-C1B	-17.09	91.58	109.77
3	A	604	FAD	C4B-O4B-C1B	-11.03	98.03	109.77
3	A	604	FAD	N3A-C2A-N1A	-7.64	122.20	128.86
3	D	602	FAD	N3A-C2A-N1A	-7.55	122.28	128.86
3	B	603	FAD	N3A-C2A-N1A	-7.00	122.76	128.86
3	C	603	FAD	N3A-C2A-N1A	-6.91	122.84	128.86
3	C	603	FAD	C4B-O4B-C1B	-6.55	102.80	109.77
3	D	602	FAD	C4B-O4B-C1B	-6.38	102.98	109.77
3	A	604	FAD	C4X-C4-N3	-6.20	114.65	123.48
3	B	603	FAD	C4X-C4-N3	-6.15	114.73	123.48
3	A	604	FAD	C4X-C10-N10	-5.13	116.95	120.52
3	D	602	FAD	C4X-C4-N3	-4.67	116.84	123.48
3	C	603	FAD	C4X-C4-N3	-4.28	117.39	123.48
3	C	603	FAD	O2'-C2'-C1'	-3.84	100.92	109.79
3	B	603	FAD	O3B-C3B-C4B	-3.16	101.85	111.09
3	A	604	FAD	C4A-C5A-N7A	-3.12	106.39	109.41
3	D	602	FAD	C1B-N9A-C4A	-3.00	121.45	126.64
3	C	603	FAD	C6-C5X-N5	-2.99	115.46	118.97
3	B	603	FAD	C4A-C5A-N7A	-2.96	106.55	109.41
3	C	603	FAD	C4A-C5A-N7A	-2.80	106.71	109.41
3	D	602	FAD	O2'-C2'-C1'	-2.73	103.47	109.79
3	C	603	FAD	C4-C4X-C10	-2.73	117.75	119.96
3	D	602	FAD	C6-C5X-N5	-2.41	116.14	118.97
3	B	603	FAD	O3'-C3'-C2'	-2.15	103.49	108.82
3	C	603	FAD	C1B-N9A-C4A	-2.13	122.95	126.64
3	C	603	FAD	C7-C6-C5X	-2.08	117.86	121.08
3	C	603	FAD	C4X-N5-C5X	2.02	118.89	116.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	FAD	C4X-N5-C5X	2.04	118.92	116.76
3	C	603	FAD	O2'-C2'-C3'	2.05	114.17	109.09
3	C	603	FAD	O2A-PA-O1A	2.13	123.31	112.28
3	C	603	FAD	O2P-P-O1P	2.15	123.38	112.28
3	D	602	FAD	O4B-C4B-C3B	2.27	109.67	105.17
3	B	603	FAD	O2A-PA-O1A	2.36	124.50	112.28
3	A	604	FAD	C6-C5X-C9A	2.38	122.08	119.00
3	A	604	FAD	O2A-PA-O1A	2.38	124.60	112.28
3	A	604	FAD	O4'-C4'-C5'	2.40	115.35	110.00
3	B	603	FAD	O4'-C4'-C5'	2.53	115.63	110.00
3	D	602	FAD	C2A-N1A-C6A	2.54	123.21	118.77
3	C	603	FAD	C2A-N1A-C6A	2.56	123.24	118.77
3	A	604	FAD	O2'-C2'-C3'	2.56	115.45	109.09
3	B	603	FAD	C6-C5X-C9A	2.59	122.36	119.00
3	B	603	FAD	N6A-C6A-N1A	2.59	123.91	118.77
3	A	604	FAD	C10-C4X-N5	2.61	123.60	120.59
3	B	603	FAD	O4'-C4'-C3'	2.72	115.84	109.09
3	D	602	FAD	C10-C4X-N5	2.96	124.00	120.59
3	D	602	FAD	C6-C5X-C9A	3.26	123.23	119.00
3	B	603	FAD	C10-C4X-N5	3.29	124.38	120.59
3	D	602	FAD	O2A-PA-O1A	3.32	129.45	112.28
3	B	603	FAD	O5B-PA-O1A	3.35	122.78	109.25
3	A	604	FAD	C4X-N5-C5X	3.47	120.43	116.76
3	A	604	FAD	O5B-PA-O1A	3.52	123.46	109.25
3	A	604	FAD	O5B-C5B-C4B	3.54	121.57	109.00
3	C	603	FAD	C10-C4X-N5	3.59	124.72	120.59
3	D	602	FAD	C5X-C9A-N10	4.05	120.66	117.66
3	C	603	FAD	C5X-C9A-N10	4.06	120.67	117.66
3	C	603	FAD	C6-C5X-C9A	4.07	124.28	119.00
3	A	604	FAD	O4B-C4B-C5B	4.30	123.92	109.40
3	B	603	FAD	O4B-C4B-C5B	4.37	124.16	109.40
3	A	604	FAD	C5X-C9A-N10	4.48	120.98	117.66
3	B	603	FAD	C5X-C9A-N10	5.05	121.41	117.66
3	A	604	FAD	C1'-N10-C9A	5.13	123.05	118.35
3	D	602	FAD	C4-N3-C2	7.72	121.91	115.16
3	C	603	FAD	C4-N3-C2	7.75	121.94	115.16
3	D	602	FAD	C1'-N10-C9A	8.02	125.69	118.35
3	B	603	FAD	C1'-N10-C9A	8.40	126.04	118.35
3	C	603	FAD	C1'-N10-C9A	9.04	126.63	118.35
3	B	603	FAD	C4-N3-C2	9.05	123.07	115.16
3	A	604	FAD	C4-N3-C2	11.29	125.03	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	603	ARG	1	0
3	A	604	FAD	5	0
2	B	601	ARG	1	0
2	B	602	ARG	1	0
3	B	603	FAD	6	0
2	C	602	ARG	1	0
3	C	603	FAD	5	0
2	D	601	ARG	2	0
3	D	602	FAD	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	549/580 (94%)	0.19	12 (2%) 62 69	14, 29, 53, 85	0
1	B	549/580 (94%)	0.18	17 (3%) 49 56	15, 29, 51, 83	0
1	C	549/580 (94%)	0.55	32 (5%) 24 30	20, 39, 62, 112	0
1	D	549/580 (94%)	0.59	46 (8%) 12 16	22, 38, 60, 91	0
All	All	2196/2320 (94%)	0.38	107 (4%) 30 37	14, 35, 58, 112	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	380	PRO	4.9
1	C	279	ARG	4.7
1	B	279	ARG	4.6
1	C	381	GLU	4.3
1	A	279	ARG	4.1
1	D	537	GLY	4.1
1	C	278	GLU	4.0
1	D	279	ARG	3.9
1	D	381	GLU	3.7
1	A	380	PRO	3.7
1	D	278	GLU	3.6
1	D	383	GLY	3.5
1	D	380	PRO	3.4
1	A	381	GLU	3.4
1	B	380	PRO	3.4
1	D	382	THR	3.4
1	C	382	THR	3.4
1	D	536	GLY	3.3
1	C	154	ALA	3.2
1	C	143	THR	3.1
1	C	276	VAL	3.1

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

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Mol	Chain	Res	Type	RSRZ
1	D	386	LEU	2.3
1	C	377	ASP	2.3
1	D	13	LYS	2.3
1	B	150	ALA	2.3
1	D	499	GLU	2.3
1	C	40	PRO	2.3
1	C	527	ALA	2.3
1	C	552	GLU	2.3
1	C	140	GLU	2.2
1	B	407	ASP	2.2
1	D	533	ASN	2.2
1	B	338	THR	2.2
1	C	379	ASP	2.2
1	C	142	GLN	2.2
1	C	378	LYS	2.2
1	B	334	TRP	2.2
1	D	541	ALA	2.2
1	D	361	MET	2.2
1	D	384	ARG	2.2
1	C	448	THR	2.2
1	D	307	ALA	2.2
1	D	453	HIS	2.2
1	D	495	GLN	2.2
1	A	334	TRP	2.2
1	A	285	GLU	2.2
1	B	144	TYR	2.2
1	B	285	GLU	2.2
1	D	419	MET	2.2
1	B	379	ASP	2.1
1	D	308	SER	2.1
1	D	45	GLY	2.1
1	D	423	LEU	2.1
1	D	29	TRP	2.1
1	D	503	ILE	2.1
1	D	281	ALA	2.1
1	D	148	LYS	2.1
1	D	551	ASP	2.1
1	D	555	GLN	2.1
1	C	130	PRO	2.1
1	D	406	ASP	2.0
1	D	449	ASP	2.0
1	B	419	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	144	TYR	2.0
1	C	407	ASP	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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ARG	A	601	12/12	0.68	0.34	10.86	59,70,85,86	0
2	ARG	C	601	12/12	0.54	0.42	6.05	58,68,78,80	0
2	ARG	D	601	12/12	0.72	0.37	4.65	55,64,78,80	0
2	ARG	C	602	12/12	0.65	0.32	4.64	68,77,78,80	0
2	ARG	B	601	12/12	0.76	0.29	3.54	57,61,74,75	0
2	ARG	B	602	12/12	0.76	0.29	3.19	45,55,63,63	0
2	ARG	A	602	12/12	0.76	0.25	2.64	40,51,53,55	0
2	ARG	A	603	12/12	0.74	0.26	1.41	69,78,82,83	0
3	FAD	C	603	53/53	0.94	0.15	-0.37	23,29,32,34	0
3	FAD	A	604	53/53	0.96	0.14	-0.38	17,21,27,31	0
3	FAD	D	602	53/53	0.94	0.15	-0.65	21,30,37,38	0
3	FAD	B	603	53/53	0.96	0.13	-0.69	15,21,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.