



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:58 PM UTC

PDB ID : 3CP8 / pdb_00003cp8
Title : Crystal structure of GidA from Chlorobium tepidum
Authors : Meyer, S.; Scrima, A.; Versees, W.; Wittinghofer, A.
Deposited on : 2008-03-31
Resolution : 3.20 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

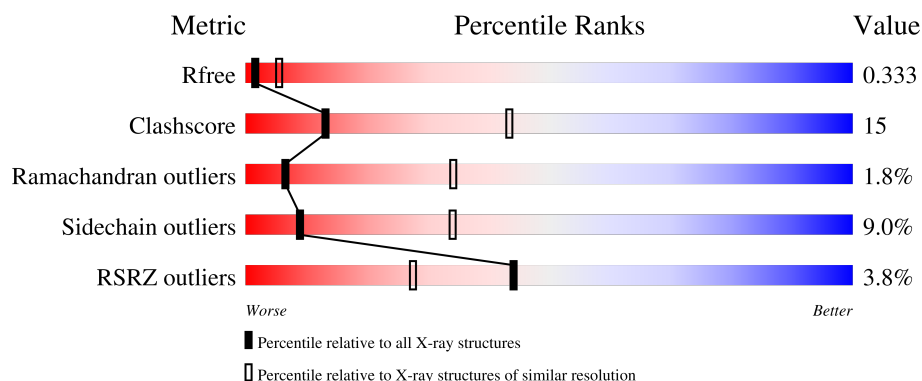
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

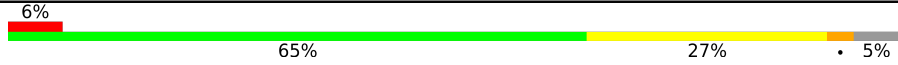
The reported resolution of this entry is 3.20 Å.

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 $\leq 5\%$. 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	641	
1	B	641	
1	C	641	
1	D	641	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18567 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 tRNA uridine 5-carboxymethylaminomethyl modification enzyme gidA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	611	Total	C	N	O	S	0	0	0
			4704	2945	839	896	24			
1	B	611	Total	C	N	O	S	0	0	0
			4704	2945	839	896	24			
1	C	611	Total	C	N	O	S	0	0	0
			4704	2945	839	896	24			
1	D	552	Total	C	N	O	S	0	0	0
			4243	2658	752	810	23			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q8KA85
A	-18	GLY	-	expression tag	UNP Q8KA85
A	-17	SER	-	expression tag	UNP Q8KA85
A	-16	SER	-	expression tag	UNP Q8KA85
A	-15	HIS	-	expression tag	UNP Q8KA85
A	-14	HIS	-	expression tag	UNP Q8KA85
A	-13	HIS	-	expression tag	UNP Q8KA85
A	-12	HIS	-	expression tag	UNP Q8KA85
A	-11	HIS	-	expression tag	UNP Q8KA85
A	-10	HIS	-	expression tag	UNP Q8KA85
A	-9	SER	-	expression tag	UNP Q8KA85
A	-8	SER	-	expression tag	UNP Q8KA85
A	-7	GLY	-	expression tag	UNP Q8KA85
A	-6	LEU	-	expression tag	UNP Q8KA85
A	-5	VAL	-	expression tag	UNP Q8KA85
A	-4	PRO	-	expression tag	UNP Q8KA85
A	-3	ARG	-	expression tag	UNP Q8KA85
A	-2	GLY	-	expression tag	UNP Q8KA85
A	-1	SER	-	expression tag	UNP Q8KA85
A	0	HIS	-	expression tag	UNP Q8KA85

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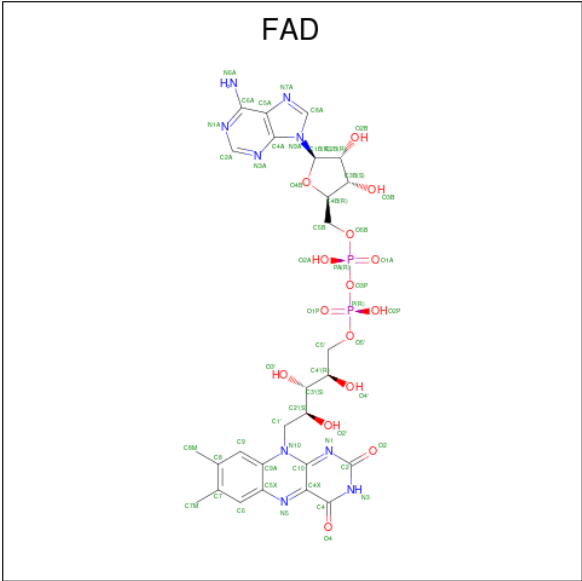
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP Q8KA85
B	-18	GLY	-	expression tag	UNP Q8KA85
B	-17	SER	-	expression tag	UNP Q8KA85
B	-16	SER	-	expression tag	UNP Q8KA85
B	-15	HIS	-	expression tag	UNP Q8KA85
B	-14	HIS	-	expression tag	UNP Q8KA85
B	-13	HIS	-	expression tag	UNP Q8KA85
B	-12	HIS	-	expression tag	UNP Q8KA85
B	-11	HIS	-	expression tag	UNP Q8KA85
B	-10	HIS	-	expression tag	UNP Q8KA85
B	-9	SER	-	expression tag	UNP Q8KA85
B	-8	SER	-	expression tag	UNP Q8KA85
B	-7	GLY	-	expression tag	UNP Q8KA85
B	-6	LEU	-	expression tag	UNP Q8KA85
B	-5	VAL	-	expression tag	UNP Q8KA85
B	-4	PRO	-	expression tag	UNP Q8KA85
B	-3	ARG	-	expression tag	UNP Q8KA85
B	-2	GLY	-	expression tag	UNP Q8KA85
B	-1	SER	-	expression tag	UNP Q8KA85
B	0	HIS	-	expression tag	UNP Q8KA85
C	-19	MET	-	expression tag	UNP Q8KA85
C	-18	GLY	-	expression tag	UNP Q8KA85
C	-17	SER	-	expression tag	UNP Q8KA85
C	-16	SER	-	expression tag	UNP Q8KA85
C	-15	HIS	-	expression tag	UNP Q8KA85
C	-14	HIS	-	expression tag	UNP Q8KA85
C	-13	HIS	-	expression tag	UNP Q8KA85
C	-12	HIS	-	expression tag	UNP Q8KA85
C	-11	HIS	-	expression tag	UNP Q8KA85
C	-10	HIS	-	expression tag	UNP Q8KA85
C	-9	SER	-	expression tag	UNP Q8KA85
C	-8	SER	-	expression tag	UNP Q8KA85
C	-7	GLY	-	expression tag	UNP Q8KA85
C	-6	LEU	-	expression tag	UNP Q8KA85
C	-5	VAL	-	expression tag	UNP Q8KA85
C	-4	PRO	-	expression tag	UNP Q8KA85
C	-3	ARG	-	expression tag	UNP Q8KA85
C	-2	GLY	-	expression tag	UNP Q8KA85
C	-1	SER	-	expression tag	UNP Q8KA85
C	0	HIS	-	expression tag	UNP Q8KA85
D	-19	MET	-	expression tag	UNP Q8KA85
D	-18	GLY	-	expression tag	UNP Q8KA85

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	SER	-	expression tag	UNP Q8KA85
D	-16	SER	-	expression tag	UNP Q8KA85
D	-15	HIS	-	expression tag	UNP Q8KA85
D	-14	HIS	-	expression tag	UNP Q8KA85
D	-13	HIS	-	expression tag	UNP Q8KA85
D	-12	HIS	-	expression tag	UNP Q8KA85
D	-11	HIS	-	expression tag	UNP Q8KA85
D	-10	HIS	-	expression tag	UNP Q8KA85
D	-9	SER	-	expression tag	UNP Q8KA85
D	-8	SER	-	expression tag	UNP Q8KA85
D	-7	GLY	-	expression tag	UNP Q8KA85
D	-6	LEU	-	expression tag	UNP Q8KA85
D	-5	VAL	-	expression tag	UNP Q8KA85
D	-4	PRO	-	expression tag	UNP Q8KA85
D	-3	ARG	-	expression tag	UNP Q8KA85
D	-2	GLY	-	expression tag	UNP Q8KA85
D	-1	SER	-	expression tag	UNP Q8KA85
D	0	HIS	-	expression tag	UNP Q8KA85

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

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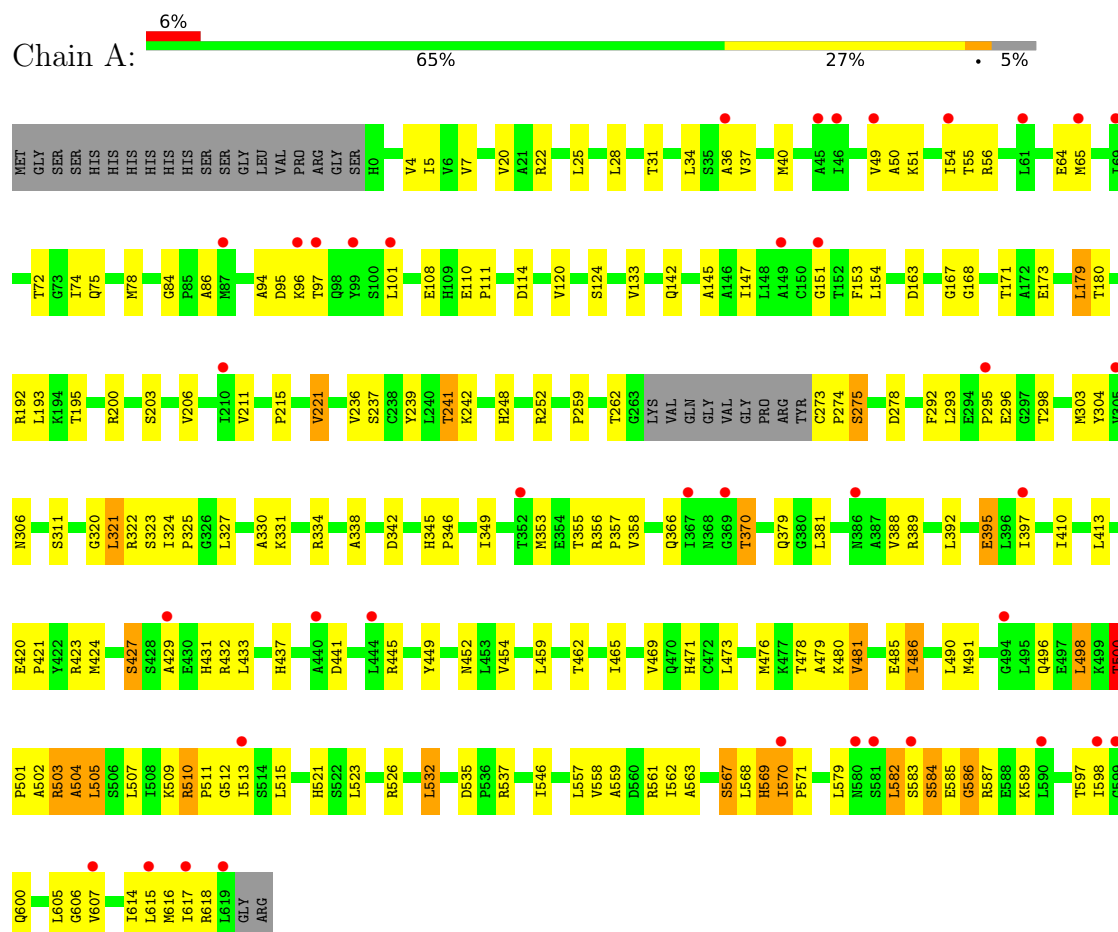
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

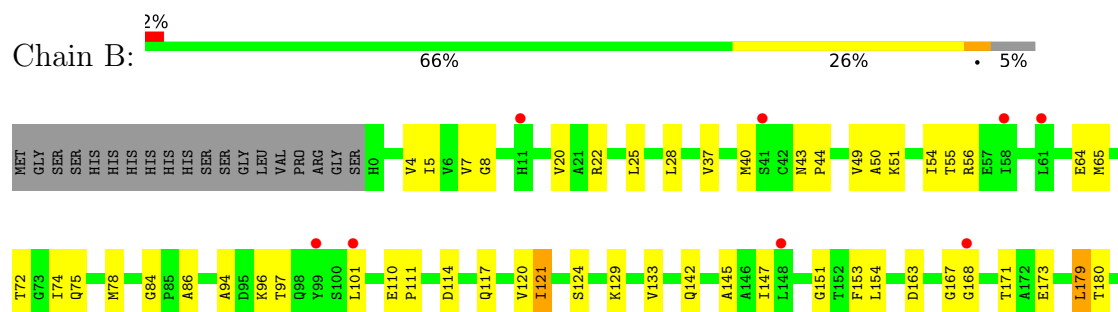
3 Residue-property plots [i](#)

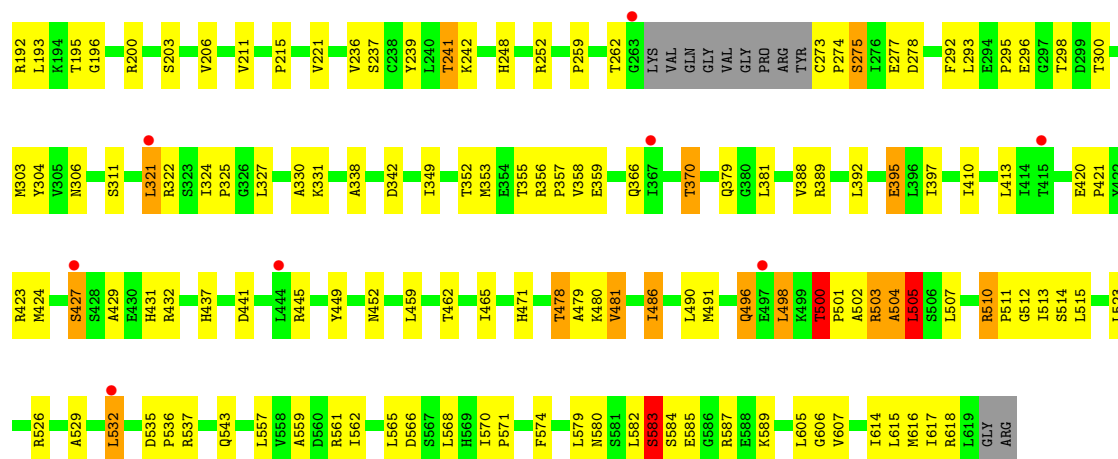
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: tRNA uridine 5-carboxymethylaminomethyl modification enzyme gidA

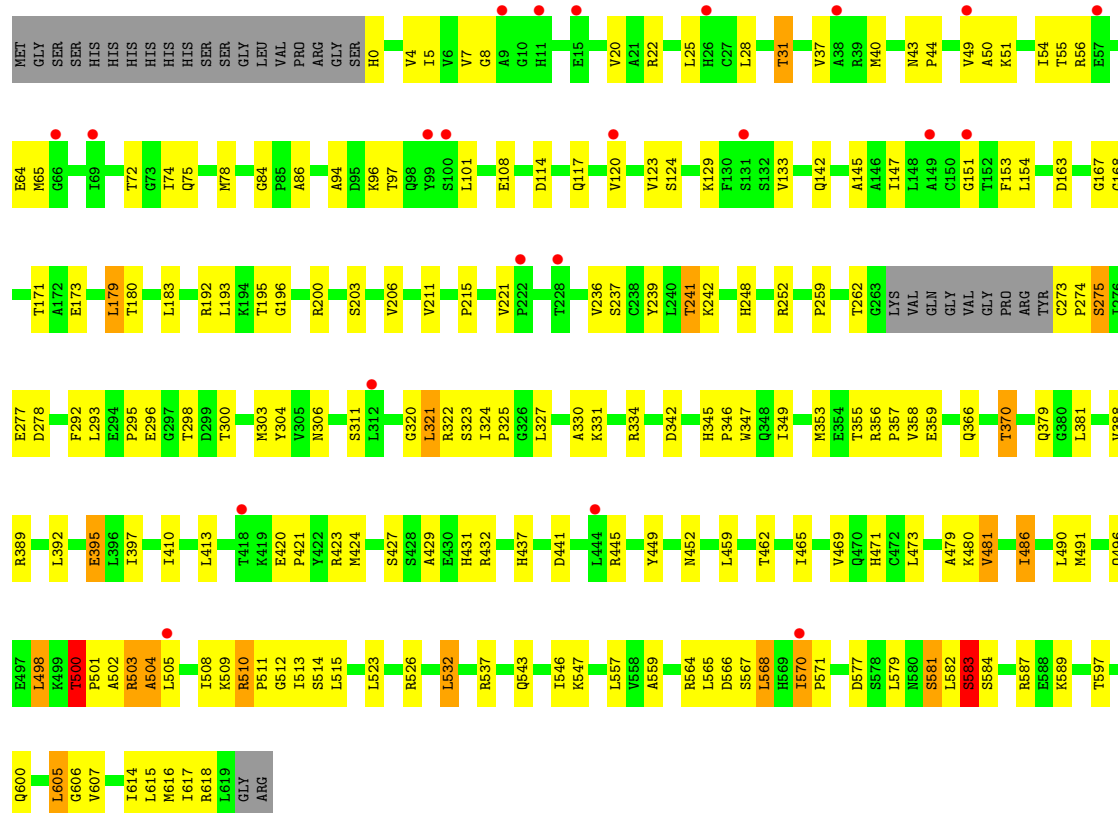


- Molecule 1: tRNA uridine 5-carboxymethylaminomethyl modification enzyme gidA



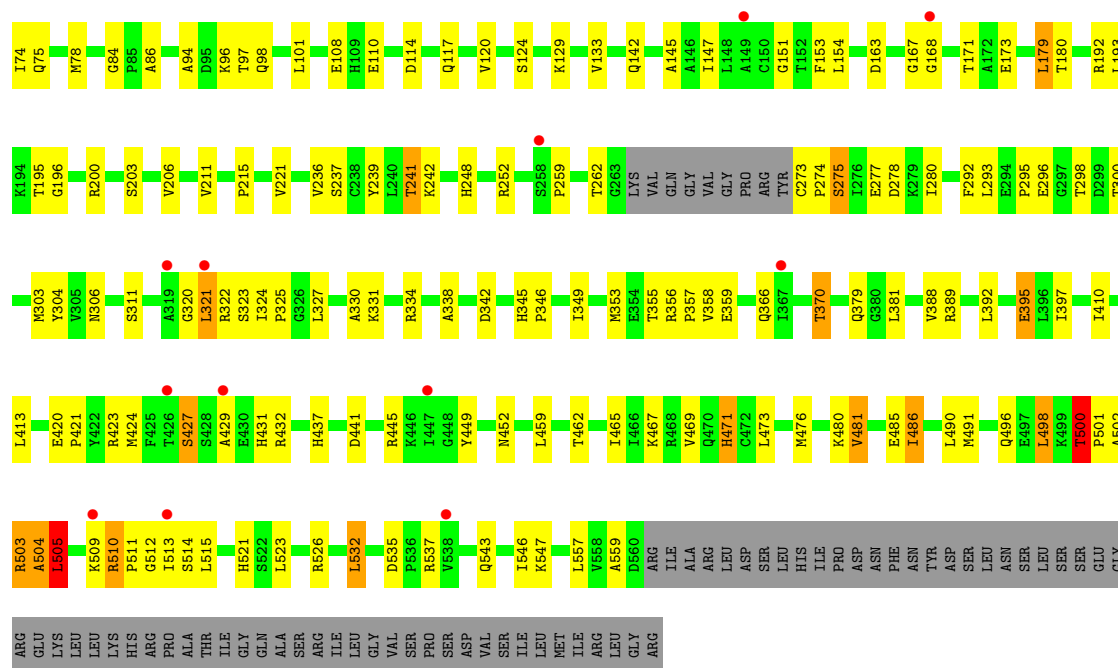


- Molecule 1: tRNA uridine 5-carboxymethylaminomethyl modification enzyme gidA



- Molecule 1: tRNA uridine 5-carboxymethylaminomethyl modification enzyme gidA





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.50Å 71.84Å 171.93Å 90.00° 91.82° 90.00°	Depositor
Resolution (Å)	44.85 – 3.20 44.85 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (44.85-3.20) 99.3 (44.85-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.254 , 0.278 0.325 , 0.333	Depositor DCC
R_{free} test set	2471 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	98.4	Xtriage
Anisotropy	0.860	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	18567	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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

5.1 Standard geometry

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	0.60	0/4785	0.91	5/6468 (0.1%)
1	B	0.58	1/4785 (0.0%)	0.91	7/6468 (0.1%)
1	C	0.55	1/4785 (0.0%)	0.90	6/6468 (0.1%)
1	D	0.52	0/4317	0.89	5/5836 (0.1%)
All	All	0.57	2/18672 (0.0%)	0.90	23/25240 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	2
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	570	ILE	CA-CB	7.79	1.58	1.54
1	B	479	ALA	N-CA	5.91	1.53	1.46

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	570	ILE	N-CA-C	6.49	120.78	112.67
1	B	479	ALA	N-CA-C	6.24	118.35	110.24
1	B	179	LEU	N-CA-C	6.18	118.01	111.28
1	C	583	SER	N-CA-C	5.99	123.56	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	479	ALA	N-CA-C	5.63	118.00	110.35
1	D	179	LEU	N-CA-C	5.58	117.36	111.28
1	B	84	GLY	CA-C-N	5.50	126.71	119.84
1	B	84	GLY	C-N-CA	5.50	126.71	119.84
1	A	179	LEU	N-CA-C	5.44	117.21	111.28
1	B	536	PRO	N-CA-C	-5.42	106.98	113.98
1	A	221	VAL	N-CA-C	5.41	113.89	107.73
1	C	179	LEU	N-CA-C	5.33	117.09	111.28
1	B	478	THR	CA-C-N	5.31	128.62	120.82
1	B	478	THR	C-N-CA	5.31	128.62	120.82
1	C	84	GLY	CA-C-N	5.24	126.39	119.84
1	C	84	GLY	C-N-CA	5.24	126.39	119.84
1	D	84	GLY	CA-C-N	5.08	126.19	119.84
1	D	84	GLY	C-N-CA	5.08	126.19	119.84
1	A	84	GLY	CA-C-N	5.08	126.19	119.84
1	A	84	GLY	C-N-CA	5.08	126.19	119.84
1	D	110	GLU	CA-C-N	5.01	124.80	119.28
1	D	110	GLU	C-N-CA	5.01	124.80	119.28
1	A	570	ILE	N-CA-C	5.00	119.69	108.88

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	582	LEU	Peptide
1	B	582	LEU	Peptide
1	B	583	SER	Peptide
1	C	582	LEU	Peptide
1	C	583	SER	Peptide

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	4704	0	4748	152	0
1	B	4704	0	4748	144	0
1	C	4704	0	4748	138	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4243	0	4269	135	0
2	A	53	0	31	10	0
2	B	53	0	31	13	0
2	C	53	0	31	12	0
2	D	53	0	31	11	0
All	All	18567	0	18637	555	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 15.

All (555) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:500:THR:HB	1:B:501:PRO:CD	1.73	1.18
1:C:500:THR:HB	1:C:501:PRO:CD	1.73	1.18
1:A:500:THR:HB	1:A:501:PRO:CD	1.73	1.16
1:D:500:THR:HB	1:D:501:PRO:CD	1.70	1.16
1:C:370:THR:HG21	1:C:379:GLN:HE22	1.10	1.15
1:A:498:LEU:HD21	1:A:502:ALA:HB3	1.24	1.12
1:B:498:LEU:HD21	1:B:502:ALA:HB3	1.26	1.12
1:D:498:LEU:HD21	1:D:502:ALA:HB3	1.23	1.12
1:B:370:THR:HG21	1:B:379:GLN:HE22	1.15	1.11
1:D:195:THR:HB	2:D:622:FAD:HM83	1.31	1.10
1:A:500:THR:CB	1:A:501:PRO:HD3	1.83	1.09
1:C:195:THR:HB	2:C:622:FAD:HM83	1.23	1.09
1:C:498:LEU:HD21	1:C:502:ALA:HB3	1.34	1.09
1:B:195:THR:HB	2:B:622:FAD:HM83	1.28	1.09
1:B:500:THR:CB	1:B:501:PRO:HD3	1.83	1.09
1:D:498:LEU:HD21	1:D:502:ALA:CB	1.83	1.09
1:C:500:THR:CB	1:C:501:PRO:HD3	1.82	1.08
1:D:500:THR:CB	1:D:501:PRO:HD3	1.82	1.08
1:D:370:THR:HG21	1:D:379:GLN:HE22	1.12	1.08
1:A:195:THR:HB	2:A:622:FAD:C8M	1.83	1.07
1:B:121:ILE:HD13	1:D:500:THR:CG2	1.85	1.07
1:A:498:LEU:HD21	1:A:502:ALA:CB	1.86	1.06
1:C:583:SER:HB3	1:C:587:ARG:HB2	1.31	1.06
1:B:498:LEU:HD21	1:B:502:ALA:CB	1.86	1.05
1:A:583:SER:HB3	1:A:587:ARG:HB2	1.37	1.05
1:A:370:THR:HG21	1:A:379:GLN:HE22	1.18	1.04
1:A:195:THR:HB	2:A:622:FAD:HM83	1.06	1.03
1:A:583:SER:CB	1:A:587:ARG:HB2	1.88	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ILE:CD1	1:D:500:THR:CG2	2.38	1.02
1:C:501:PRO:O	1:C:503:ARG:HG3	1.61	0.98
1:B:121:ILE:CD1	1:D:500:THR:HG22	1.95	0.97
1:A:532:LEU:HD23	1:A:532:LEU:H	1.30	0.96
1:C:195:THR:HB	2:C:622:FAD:C8M	1.96	0.96
1:C:532:LEU:HD23	1:C:532:LEU:H	1.32	0.95
1:D:532:LEU:HD23	1:D:532:LEU:H	1.30	0.94
1:B:532:LEU:H	1:B:532:LEU:HD23	1.31	0.94
1:A:195:THR:CB	2:A:622:FAD:HM83	1.98	0.92
1:B:195:THR:HB	2:B:622:FAD:C8M	1.99	0.92
1:D:206:VAL:HG21	1:D:303:MET:HE1	1.51	0.91
1:D:153:PHE:HE2	2:D:622:FAD:H3B	1.35	0.91
1:B:153:PHE:HE2	2:B:622:FAD:H3B	1.34	0.91
1:B:121:ILE:HD13	1:D:500:THR:HG21	1.52	0.91
1:A:153:PHE:HE2	2:A:622:FAD:H3B	1.36	0.90
1:A:206:VAL:HG21	1:A:303:MET:HE1	1.53	0.90
1:C:500:THR:HB	1:C:501:PRO:HD3	0.91	0.89
1:C:206:VAL:HG21	1:C:303:MET:HE1	1.53	0.89
1:B:121:ILE:HD13	1:D:500:THR:HG22	1.53	0.89
1:A:500:THR:HB	1:A:501:PRO:HD3	0.91	0.88
1:C:153:PHE:HE2	2:C:622:FAD:H3B	1.38	0.88
1:D:195:THR:HB	2:D:622:FAD:C8M	2.04	0.87
1:B:583:SER:HB2	1:B:584:SER:O	1.74	0.87
1:B:206:VAL:HG21	1:B:303:MET:HE1	1.57	0.87
1:B:500:THR:HB	1:B:501:PRO:HD3	0.91	0.85
1:D:500:THR:HB	1:D:501:PRO:HD3	0.88	0.85
1:A:153:PHE:CE2	2:A:622:FAD:H3B	2.11	0.84
1:C:195:THR:CB	2:C:622:FAD:HM83	2.07	0.82
1:D:153:PHE:CE2	2:D:622:FAD:H3B	2.15	0.81
1:A:583:SER:HB2	1:A:587:ARG:CB	2.11	0.81
1:A:420:GLU:HG3	1:A:421:PRO:HD2	1.64	0.80
1:B:153:PHE:CE2	2:B:622:FAD:H3B	2.16	0.80
1:A:211:VAL:HG11	1:A:239:TYR:HB3	1.64	0.79
1:B:583:SER:HB3	1:B:587:ARG:HB2	1.64	0.79
1:A:515:LEU:HD21	1:A:532:LEU:HD12	1.66	0.78
1:D:211:VAL:HG11	1:D:239:TYR:HB3	1.66	0.77
1:D:498:LEU:CD2	1:D:502:ALA:HB3	2.10	0.77
1:C:583:SER:HB3	1:C:587:ARG:CB	2.13	0.77
1:A:583:SER:CB	1:A:587:ARG:CB	2.62	0.77
1:B:121:ILE:HD12	1:D:500:THR:HG22	1.67	0.76
1:B:514:SER:HA	1:B:543:GLN:NE2	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:VAL:HG11	1:B:239:TYR:HB3	1.67	0.75
1:A:583:SER:HB2	1:A:587:ARG:HB2	1.66	0.75
1:B:583:SER:HB3	1:B:587:ARG:CB	2.17	0.75
1:C:153:PHE:CE2	2:C:622:FAD:H3B	2.22	0.75
1:C:420:GLU:HG3	1:C:421:PRO:HD2	1.69	0.75
1:A:480:LYS:HA	1:A:503:ARG:HB3	1.68	0.74
1:C:515:LEU:HD21	1:C:532:LEU:HD12	1.67	0.74
1:D:480:LYS:HA	1:D:503:ARG:HB3	1.69	0.74
1:B:515:LEU:HD21	1:B:532:LEU:HD12	1.69	0.74
1:A:5:ILE:HG22	1:A:28:LEU:HB3	1.70	0.74
1:C:5:ILE:HG22	1:C:28:LEU:HB3	1.69	0.74
1:B:420:GLU:HG3	1:B:421:PRO:HD2	1.70	0.73
1:A:481:VAL:HB	1:A:486:ILE:HD11	1.70	0.72
1:C:370:THR:HG21	1:C:379:GLN:NE2	1.96	0.72
1:C:211:VAL:HG11	1:C:239:TYR:HB3	1.71	0.72
1:D:515:LEU:HD21	1:D:532:LEU:HD12	1.70	0.72
1:A:498:LEU:CD2	1:A:502:ALA:HB3	2.12	0.72
1:D:420:GLU:HG3	1:D:421:PRO:HD2	1.70	0.72
1:D:481:VAL:HB	1:D:486:ILE:HD11	1.72	0.71
1:B:195:THR:CB	2:B:622:FAD:HM83	2.14	0.71
1:A:56:ARG:HH11	1:A:437:HIS:CD2	2.09	0.71
1:B:5:ILE:HG22	1:B:28:LEU:HB3	1.72	0.70
1:B:481:VAL:HB	1:B:486:ILE:HD11	1.72	0.70
1:A:476:MET:O	1:A:505:LEU:HB2	1.91	0.70
1:C:481:VAL:HB	1:C:486:ILE:HD11	1.73	0.70
1:B:616:MET:C	1:B:618:ARG:H	1.99	0.69
1:B:56:ARG:HH11	1:B:437:HIS:CD2	2.10	0.69
1:A:211:VAL:CG1	1:A:239:TYR:HB3	2.23	0.69
1:B:211:VAL:CG1	1:B:239:TYR:HB3	2.22	0.69
1:B:322:ARG:NH1	1:B:330:ALA:O	2.26	0.69
1:C:153:PHE:HD1	1:C:168:GLY:HA3	1.57	0.69
1:C:616:MET:C	1:C:618:ARG:H	2.00	0.69
1:D:211:VAL:CG1	1:D:239:TYR:HB3	2.23	0.69
1:C:583:SER:HB2	1:C:584:SER:O	1.92	0.69
1:A:153:PHE:CD1	1:A:168:GLY:HA3	2.28	0.68
1:C:56:ARG:HH11	1:C:437:HIS:CD2	2.11	0.68
1:B:535:ASP:OD1	1:B:537:ARG:HB2	1.93	0.68
1:D:5:ILE:HG22	1:D:28:LEU:HB3	1.74	0.68
1:D:322:ARG:NH1	1:D:330:ALA:O	2.27	0.68
1:A:441:ASP:O	1:A:445:ARG:HB2	1.93	0.68
1:D:86:ALA:HB1	1:D:432:ARG:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:616:MET:C	1:A:618:ARG:H	2.01	0.67
1:C:153:PHE:CD1	1:C:168:GLY:HA3	2.29	0.67
1:C:86:ALA:HB1	1:C:432:ARG:HB3	1.75	0.67
1:B:153:PHE:HD1	1:B:168:GLY:HA3	1.60	0.67
1:B:153:PHE:CD1	1:B:168:GLY:HA3	2.29	0.66
1:B:273:CYS:N	1:B:423:ARG:HH12	1.93	0.66
1:A:195:THR:CB	2:A:622:FAD:C8M	2.64	0.66
1:D:56:ARG:HH11	1:D:437:HIS:CD2	2.13	0.66
1:D:153:PHE:CD1	1:D:168:GLY:HA3	2.30	0.66
1:B:498:LEU:CD2	1:B:502:ALA:HB3	2.13	0.66
1:C:273:CYS:N	1:C:423:ARG:HH12	1.94	0.66
1:C:441:ASP:O	1:C:445:ARG:HB2	1.95	0.66
1:C:514:SER:HA	1:C:543:GLN:NE2	2.11	0.66
1:D:195:THR:CB	2:D:622:FAD:HM83	2.18	0.66
1:A:322:ARG:NH1	1:A:330:ALA:O	2.29	0.66
1:B:441:ASP:O	1:B:445:ARG:HB2	1.95	0.66
1:B:86:ALA:HB1	1:B:432:ARG:HB3	1.77	0.65
1:B:480:LYS:HA	1:B:503:ARG:HB3	1.76	0.65
1:A:86:ALA:HB1	1:A:432:ARG:HB3	1.78	0.65
1:C:322:ARG:NH1	1:C:330:ALA:O	2.30	0.65
1:A:72:THR:HG22	1:A:72:THR:O	1.94	0.65
1:A:4:VAL:HA	1:A:145:ALA:O	1.96	0.65
1:B:72:THR:O	1:B:72:THR:HG22	1.96	0.65
1:D:153:PHE:HD1	1:D:168:GLY:HA3	1.63	0.65
1:C:211:VAL:CG1	1:C:239:TYR:HB3	2.26	0.64
1:C:349:ILE:HG22	1:C:355:THR:HG22	1.80	0.64
1:D:40:MET:HE1	1:D:94:ALA:HB3	1.80	0.64
1:C:4:VAL:HA	1:C:145:ALA:O	1.97	0.64
1:C:503:ARG:O	1:C:504:ALA:C	2.38	0.64
1:B:424:MET:O	1:B:427:SER:HB3	1.98	0.64
1:A:153:PHE:HD1	1:A:168:GLY:HA3	1.60	0.64
1:A:480:LYS:CA	1:A:503:ARG:HB3	2.28	0.64
1:B:589:LYS:HG3	1:B:606:GLY:HA3	1.80	0.64
1:C:481:VAL:H	1:C:503:ARG:HB3	1.62	0.64
1:D:273:CYS:N	1:D:423:ARG:HH12	1.96	0.64
1:D:349:ILE:HG22	1:D:355:THR:HG22	1.80	0.64
1:D:370:THR:HG21	1:D:379:GLN:NE2	1.98	0.64
1:D:441:ASP:O	1:D:445:ARG:HB2	1.96	0.64
1:B:56:ARG:HH11	1:B:437:HIS:HD2	1.44	0.63
1:A:349:ILE:HG22	1:A:355:THR:HG22	1.80	0.63
1:A:589:LYS:HG3	1:A:606:GLY:HA3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:VAL:HA	1:D:145:ALA:O	1.98	0.63
1:B:503:ARG:O	1:B:504:ALA:C	2.41	0.63
1:A:503:ARG:O	1:A:504:ALA:C	2.41	0.63
1:B:431:HIS:HE1	1:B:559:ALA:HA	1.64	0.63
1:D:498:LEU:HD21	1:D:502:ALA:HB2	1.77	0.63
1:D:503:ARG:O	1:D:504:ALA:C	2.42	0.63
1:D:480:LYS:CA	1:D:503:ARG:HB3	2.28	0.62
1:A:431:HIS:HE1	1:A:559:ALA:HA	1.63	0.62
1:B:4:VAL:HA	1:B:145:ALA:O	1.98	0.62
1:D:78:MET:HE2	1:D:221:VAL:HG21	1.81	0.62
1:D:431:HIS:HE1	1:D:559:ALA:HA	1.64	0.62
1:A:56:ARG:HH11	1:A:437:HIS:HD2	1.46	0.62
1:A:498:LEU:HD21	1:A:502:ALA:HB2	1.81	0.62
1:C:431:HIS:HE1	1:C:559:ALA:HA	1.65	0.62
1:A:480:LYS:HA	1:A:503:ARG:CB	2.30	0.61
1:B:353:MET:HE3	1:B:410:ILE:HG12	1.82	0.61
1:D:424:MET:O	1:D:427:SER:HB3	2.00	0.61
1:A:532:LEU:H	1:A:532:LEU:CD2	2.09	0.61
1:C:498:LEU:HD21	1:C:502:ALA:CB	2.22	0.61
1:C:589:LYS:HG3	1:C:606:GLY:HA3	1.82	0.61
1:B:50:ALA:HB3	1:B:424:MET:HB3	1.83	0.61
1:A:241:THR:HG21	1:A:325:PRO:O	2.01	0.61
1:C:72:THR:HG22	1:C:72:THR:O	2.00	0.61
1:D:72:THR:O	1:D:72:THR:HG22	2.00	0.61
1:B:22:ARG:HH12	1:B:64:GLU:HG2	1.65	0.61
1:C:195:THR:CB	2:C:622:FAD:C8M	2.74	0.60
1:A:583:SER:HB2	1:A:587:ARG:HB3	1.84	0.60
1:B:370:THR:HG21	1:B:379:GLN:NE2	2.01	0.60
1:D:480:LYS:HA	1:D:503:ARG:CB	2.31	0.60
1:B:349:ILE:HG22	1:B:355:THR:HG22	1.82	0.60
1:B:275:SER:HB3	1:B:278:ASP:H	1.66	0.59
1:C:22:ARG:HH12	1:C:64:GLU:HG2	1.67	0.59
1:A:40:MET:HE1	1:A:94:ALA:HB3	1.83	0.59
1:D:500:THR:CB	1:D:501:PRO:CD	2.55	0.59
1:C:78:MET:HE2	1:C:221:VAL:HG21	1.85	0.59
1:C:96:LYS:HE2	1:C:296:GLU:CD	2.27	0.59
1:D:50:ALA:HB3	1:D:424:MET:HB3	1.85	0.59
1:D:490:LEU:HD21	1:D:513:ILE:HD11	1.85	0.59
1:A:273:CYS:N	1:A:423:ARG:HH12	1.99	0.59
1:C:56:ARG:HH11	1:C:437:HIS:HD2	1.49	0.59
1:C:490:LEU:HD21	1:C:513:ILE:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:LEU:HD22	1:D:421:PRO:HD3	1.84	0.59
1:D:275:SER:HB3	1:D:278:ASP:H	1.67	0.59
1:A:501:PRO:O	1:A:503:ARG:HG3	2.03	0.58
1:D:50:ALA:CB	1:D:424:MET:HB3	2.33	0.58
1:C:50:ALA:CB	1:C:424:MET:HB3	2.33	0.58
1:B:501:PRO:O	1:B:503:ARG:HG3	2.02	0.58
1:C:40:MET:HE1	1:C:94:ALA:HB3	1.85	0.58
1:D:501:PRO:O	1:D:503:ARG:HG3	2.02	0.58
1:C:565:LEU:HD13	1:C:616:MET:HE1	1.85	0.58
1:A:275:SER:HB3	1:A:278:ASP:H	1.68	0.58
1:B:50:ALA:CB	1:B:424:MET:HB3	2.34	0.58
1:B:167:GLY:HA2	1:B:173:GLU:O	2.03	0.58
1:B:241:THR:HG21	1:B:325:PRO:O	2.04	0.58
1:C:50:ALA:HB3	1:C:424:MET:HB3	1.85	0.58
1:D:389:ARG:HD2	1:D:395:GLU:O	2.04	0.58
1:A:50:ALA:CB	1:A:424:MET:HB3	2.34	0.58
1:B:193:LEU:HD22	1:B:421:PRO:HD3	1.86	0.58
1:B:195:THR:CB	2:B:622:FAD:C8M	2.79	0.58
1:D:509:LYS:HG3	1:D:546:ILE:HD11	1.86	0.58
1:A:75:GLN:O	1:A:75:GLN:HG3	2.04	0.57
1:B:78:MET:HE2	1:B:221:VAL:HG21	1.86	0.57
1:C:353:MET:HE3	1:C:410:ILE:HG12	1.86	0.57
1:A:490:LEU:HD21	1:A:513:ILE:HD11	1.87	0.57
1:B:500:THR:CB	1:B:501:PRO:CD	2.56	0.57
1:B:459:LEU:O	1:B:462:THR:HG22	2.03	0.57
1:B:480:LYS:CA	1:B:503:ARG:HB3	2.34	0.57
1:C:167:GLY:HA2	1:C:173:GLU:O	2.03	0.57
1:D:241:THR:HG21	1:D:325:PRO:O	2.05	0.57
1:A:22:ARG:HH12	1:A:64:GLU:HG2	1.68	0.57
1:A:459:LEU:O	1:A:462:THR:HG22	2.04	0.57
1:C:275:SER:HB3	1:C:278:ASP:H	1.68	0.57
1:C:583:SER:CB	1:C:587:ARG:HB2	2.21	0.57
1:A:151:GLY:HA2	1:A:366:GLN:HB3	1.87	0.56
1:D:459:LEU:O	1:D:462:THR:HG22	2.05	0.56
1:A:50:ALA:HB3	1:A:424:MET:HB3	1.86	0.56
1:A:167:GLY:HA2	1:A:173:GLU:O	2.05	0.56
1:B:75:GLN:O	1:B:75:GLN:HG3	2.04	0.56
1:B:498:LEU:HD21	1:B:502:ALA:HB2	1.79	0.56
1:C:193:LEU:HD22	1:C:421:PRO:HD3	1.87	0.56
1:C:459:LEU:O	1:C:462:THR:HG22	2.05	0.56
1:A:78:MET:HE2	1:A:221:VAL:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:GLY:HA2	1:B:366:GLN:HB3	1.86	0.56
1:B:532:LEU:H	1:B:532:LEU:CD2	2.09	0.56
1:C:259:PRO:HD2	1:C:311:SER:HB3	1.88	0.56
1:A:424:MET:O	1:A:427:SER:HB3	2.05	0.56
1:C:241:THR:HG21	1:C:325:PRO:O	2.05	0.56
1:D:22:ARG:HH12	1:D:64:GLU:HG2	1.70	0.56
1:C:424:MET:O	1:C:427:SER:HB3	2.05	0.56
1:D:56:ARG:HH11	1:D:437:HIS:HD2	1.52	0.56
1:C:51:LYS:HA	1:C:54:ILE:HG22	1.88	0.56
1:C:8:GLY:HA2	2:C:622:FAD:H1B	1.88	0.55
1:C:51:LYS:HA	1:C:54:ILE:CG2	2.36	0.55
1:B:490:LEU:HD21	1:B:513:ILE:HD11	1.87	0.55
1:A:96:LYS:HE2	1:A:296:GLU:CD	2.31	0.55
1:C:151:GLY:HA2	1:C:366:GLN:HB3	1.89	0.55
1:C:500:THR:CB	1:C:501:PRO:CD	2.56	0.55
1:A:193:LEU:HD22	1:A:421:PRO:HD3	1.88	0.55
1:B:449:TYR:CG	1:B:459:LEU:HD22	2.42	0.55
1:C:196:GLY:O	2:C:622:FAD:HM72	2.07	0.55
1:D:167:GLY:HA2	1:D:173:GLU:O	2.07	0.55
1:C:75:GLN:O	1:C:75:GLN:HG3	2.06	0.55
1:D:151:GLY:HA2	1:D:366:GLN:HB3	1.87	0.55
1:C:120:VAL:HG13	1:C:133:VAL:HG13	1.89	0.55
1:D:449:TYR:CG	1:D:459:LEU:HD22	2.42	0.54
1:A:353:MET:HE3	1:A:410:ILE:HG12	1.89	0.54
1:A:569:HIS:C	1:A:571:PRO:HD2	2.31	0.54
1:A:583:SER:C	1:A:584:SER:OG	2.50	0.54
1:D:75:GLN:O	1:D:75:GLN:HG3	2.06	0.54
1:A:370:THR:HG21	1:A:379:GLN:NE2	2.03	0.54
1:C:449:TYR:CG	1:C:459:LEU:HD22	2.43	0.54
1:C:389:ARG:HD2	1:C:395:GLU:O	2.07	0.54
1:C:564:ARG:O	1:C:567:SER:HB3	2.07	0.54
1:D:353:MET:HE3	1:D:410:ILE:HG12	1.88	0.54
1:B:121:ILE:CD1	1:D:500:THR:HG21	2.24	0.54
1:C:501:PRO:O	1:C:503:ARG:CG	2.47	0.54
1:A:509:LYS:HZ2	1:A:546:ILE:HD13	1.71	0.54
1:C:236:VAL:HG11	1:C:295:PRO:HG2	1.88	0.54
1:A:389:ARG:HD2	1:A:395:GLU:O	2.08	0.53
1:A:449:TYR:CG	1:A:459:LEU:HD22	2.43	0.53
1:D:532:LEU:H	1:D:532:LEU:CD2	2.09	0.53
1:A:445:ARG:HB3	1:A:462:THR:HG21	1.91	0.53
1:C:445:ARG:HB3	1:C:462:THR:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:LYS:HA	1:B:503:ARG:CB	2.38	0.53
1:A:568:LEU:HD12	1:A:598:ILE:CD1	2.38	0.53
1:B:25:LEU:HD13	1:B:388:VAL:HG13	1.91	0.53
1:B:51:LYS:HA	1:B:54:ILE:HG22	1.91	0.53
1:B:236:VAL:HG11	1:B:295:PRO:HG2	1.90	0.53
2:C:622:FAD:H9	2:C:622:FAD:O2'	2.09	0.52
1:D:40:MET:HB2	1:D:96:LYS:HD2	1.91	0.52
1:D:25:LEU:HD13	1:D:388:VAL:HG13	1.91	0.52
1:D:51:LYS:HA	1:D:54:ILE:HG22	1.92	0.52
1:D:96:LYS:HE2	1:D:296:GLU:CD	2.34	0.52
1:D:196:GLY:O	2:D:622:FAD:HM72	2.10	0.52
1:D:51:LYS:HA	1:D:54:ILE:CG2	2.40	0.52
1:D:514:SER:HA	1:D:543:GLN:NE2	2.24	0.52
1:A:120:VAL:HG13	1:A:133:VAL:HG13	1.92	0.52
1:B:445:ARG:HB3	1:B:462:THR:HG21	1.90	0.52
1:B:259:PRO:HD2	1:B:311:SER:HB3	1.91	0.52
1:B:616:MET:C	1:B:618:ARG:N	2.68	0.52
1:C:8:GLY:HA2	2:C:622:FAD:C1B	2.40	0.52
1:D:120:VAL:HG13	1:D:133:VAL:HG13	1.92	0.51
1:A:215:PRO:HA	1:A:237:SER:HB3	1.92	0.51
1:A:322:ARG:HA	1:A:327:LEU:O	2.10	0.51
1:C:577:ASP:HA	1:C:587:ARG:HD3	1.91	0.51
1:D:445:ARG:HB3	1:D:462:THR:HG21	1.91	0.51
1:A:500:THR:CB	1:A:501:PRO:CD	2.57	0.51
1:C:514:SER:HA	1:C:543:GLN:HE21	1.74	0.51
1:D:389:ARG:CZ	1:D:397:ILE:HD11	2.40	0.51
1:C:616:MET:C	1:C:618:ARG:N	2.69	0.51
1:A:583:SER:O	1:A:584:SER:OG	2.27	0.51
1:B:96:LYS:HE2	1:B:296:GLU:CD	2.35	0.51
1:C:192:ARG:NH1	1:C:342:ASP:OD1	2.43	0.51
1:D:259:PRO:HD2	1:D:311:SER:HB3	1.93	0.51
1:D:476:MET:O	1:D:505:LEU:HB2	2.10	0.51
1:A:51:LYS:HA	1:A:54:ILE:HG22	1.93	0.51
1:B:389:ARG:CZ	1:B:397:ILE:HD11	2.41	0.51
1:B:431:HIS:NE2	1:B:562:ILE:HD12	2.26	0.51
1:C:509:LYS:HZ2	1:C:546:ILE:HD13	1.76	0.51
1:D:200:ARG:NH1	1:D:304:TYR:CD2	2.79	0.51
1:A:236:VAL:HG11	1:A:295:PRO:HG2	1.92	0.51
1:A:509:LYS:HG3	1:A:546:ILE:HD11	1.92	0.51
1:C:331:LYS:HD3	1:D:114:ASP:OD2	2.11	0.51
1:A:389:ARG:CZ	1:A:397:ILE:HD11	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:ILE:N	1:A:571:PRO:CD	2.74	0.51
1:C:420:GLU:CG	1:C:421:PRO:HD2	2.41	0.50
1:B:74:ILE:HG23	1:B:236:VAL:HG23	1.93	0.50
1:C:347:TRP:HB3	1:C:605:LEU:HD13	1.93	0.50
1:B:120:VAL:HG12	1:B:179:LEU:HD13	1.93	0.50
1:A:206:VAL:HG21	1:A:303:MET:CE	2.36	0.50
1:B:215:PRO:HA	1:B:237:SER:HB3	1.94	0.50
1:C:503:ARG:O	1:C:505:LEU:N	2.45	0.50
1:D:510:ARG:H	1:D:511:PRO:CD	2.25	0.50
1:A:420:GLU:CG	1:A:421:PRO:HD2	2.38	0.50
1:D:195:THR:CB	2:D:622:FAD:C8M	2.84	0.50
1:B:51:LYS:HA	1:B:54:ILE:CG2	2.42	0.50
1:C:215:PRO:HA	1:C:237:SER:HB3	1.94	0.50
1:C:481:VAL:HG23	1:C:503:ARG:HA	1.93	0.50
1:C:389:ARG:CZ	1:C:397:ILE:HD11	2.42	0.50
1:A:25:LEU:HD13	1:A:388:VAL:HG13	1.93	0.50
1:A:51:LYS:HA	1:A:54:ILE:CG2	2.41	0.50
1:C:25:LEU:HD13	1:C:388:VAL:HG13	1.93	0.49
1:C:40:MET:HB2	1:C:96:LYS:HD2	1.93	0.49
1:C:334:ARG:HG2	1:D:117:GLN:HB3	1.93	0.49
1:D:532:LEU:O	1:D:535:ASP:O	2.30	0.49
1:D:236:VAL:HG11	1:D:295:PRO:HG2	1.93	0.49
1:D:420:GLU:CG	1:D:421:PRO:HD2	2.42	0.49
1:A:616:MET:C	1:A:618:ARG:N	2.70	0.49
1:A:200:ARG:NH1	1:A:304:TYR:CD2	2.81	0.49
1:A:321:LEU:HA	1:A:324:ILE:HD12	1.94	0.49
1:A:568:LEU:HD12	1:A:598:ILE:HD11	1.95	0.49
1:B:120:VAL:HG13	1:B:133:VAL:HG13	1.94	0.49
1:B:389:ARG:HD2	1:B:395:GLU:O	2.13	0.49
1:C:322:ARG:HA	1:C:327:LEU:O	2.11	0.49
1:C:583:SER:CB	1:C:587:ARG:CB	2.88	0.49
1:A:478:THR:O	1:A:479:ALA:C	2.54	0.49
1:B:40:MET:HE1	1:B:94:ALA:HB3	1.94	0.49
2:D:622:FAD:H9	2:D:622:FAD:O2'	2.12	0.48
1:A:120:VAL:HG12	1:A:179:LEU:HD13	1.94	0.48
1:C:465:ILE:HD11	1:C:537:ARG:HB3	1.96	0.48
1:D:120:VAL:HG12	1:D:179:LEU:HD13	1.95	0.48
1:A:108:GLU:OE1	1:B:300:THR:HA	2.12	0.48
1:A:153:PHE:CE2	2:A:622:FAD:H51A	2.47	0.48
2:A:622:FAD:H9	2:A:622:FAD:O2'	2.13	0.48
1:A:465:ILE:HD11	1:A:537:ARG:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:LYS:NZ	1:A:546:ILE:HD13	2.28	0.48
1:C:509:LYS:NZ	1:C:546:ILE:HD13	2.28	0.48
1:B:153:PHE:CE2	2:B:622:FAD:C3B	2.94	0.48
1:C:300:THR:HA	1:D:108:GLU:OE1	2.14	0.48
1:D:322:ARG:HA	1:D:327:LEU:O	2.14	0.48
1:A:509:LYS:HG3	1:A:546:ILE:CD1	2.44	0.48
1:D:321:LEU:HA	1:D:324:ILE:HD12	1.96	0.48
1:A:510:ARG:H	1:A:511:PRO:CD	2.26	0.48
1:C:321:LEU:HA	1:C:324:ILE:HD12	1.96	0.48
1:B:4:VAL:HB	1:B:20:VAL:HG11	1.96	0.48
1:B:55:THR:HG23	1:B:65:MET:HG2	1.95	0.48
1:D:215:PRO:HA	1:D:237:SER:HB3	1.95	0.47
1:D:293:LEU:HB3	1:D:303:MET:HE3	1.95	0.47
1:D:345:HIS:HA	1:D:346:PRO:HD3	1.77	0.47
1:A:153:PHE:HE2	2:A:622:FAD:H51A	1.79	0.47
1:C:200:ARG:NH1	1:C:304:TYR:CD2	2.83	0.47
1:A:192:ARG:NH1	1:A:342:ASP:OD1	2.47	0.47
1:B:420:GLU:CG	1:B:421:PRO:HD2	2.43	0.47
1:C:120:VAL:HG12	1:C:179:LEU:HD13	1.97	0.47
1:D:509:LYS:NZ	1:D:546:ILE:HD13	2.29	0.47
2:B:622:FAD:H9	2:B:622:FAD:O2'	2.14	0.47
1:C:445:ARG:CB	1:C:462:THR:HG21	2.44	0.47
1:B:200:ARG:NH1	1:B:304:TYR:CD2	2.82	0.47
1:B:311:SER:OG	1:B:338:ALA:HB2	2.15	0.47
1:C:108:GLU:OE1	1:D:300:THR:HA	2.14	0.47
1:D:509:LYS:HG3	1:D:546:ILE:CD1	2.44	0.47
1:B:504:ALA:O	1:B:505:LEU:C	2.58	0.47
1:C:74:ILE:HG23	1:C:236:VAL:HG23	1.95	0.47
1:C:532:LEU:H	1:C:532:LEU:CD2	2.10	0.47
1:D:465:ILE:HD11	1:D:537:ARG:HB3	1.97	0.47
1:B:321:LEU:HA	1:B:324:ILE:HD12	1.96	0.46
1:B:40:MET:HB2	1:B:96:LYS:HD2	1.97	0.46
1:B:535:ASP:C	1:B:537:ARG:N	2.69	0.46
1:D:4:VAL:HB	1:D:20:VAL:HG11	1.96	0.46
1:A:570:ILE:N	1:A:571:PRO:HD2	2.30	0.46
1:C:480:LYS:HA	1:C:503:ARG:HB2	1.95	0.46
1:A:72:THR:O	1:A:72:THR:CG2	2.63	0.46
1:B:241:THR:HG22	1:B:242:LYS:H	1.80	0.46
1:A:259:PRO:HD2	1:A:311:SER:HB3	1.98	0.46
1:B:153:PHE:HD2	2:B:622:FAD:H8A	1.79	0.46
1:B:514:SER:HA	1:B:543:GLN:HE21	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:HIS:HA	1:C:346:PRO:HD3	1.77	0.46
1:D:292:PHE:HB2	1:D:306:ASN:HB3	1.98	0.46
1:C:4:VAL:HB	1:C:20:VAL:HG11	1.97	0.46
1:A:331:LYS:HD3	1:B:114:ASP:OD2	2.15	0.46
1:B:570:ILE:N	1:B:571:PRO:CD	2.79	0.46
1:C:462:THR:HA	1:C:465:ILE:HG22	1.98	0.46
1:C:510:ARG:H	1:C:511:PRO:CD	2.29	0.45
1:A:4:VAL:HB	1:A:20:VAL:HG11	1.97	0.45
1:C:566:ASP:O	1:C:597:THR:OG1	2.34	0.45
1:A:462:THR:O	1:A:465:ILE:HG22	2.16	0.45
1:C:292:PHE:HB2	1:C:306:ASN:HB3	1.98	0.45
1:A:292:PHE:HB2	1:A:306:ASN:HB3	1.98	0.45
1:B:56:ARG:NH1	1:B:437:HIS:HD2	2.11	0.45
1:B:584:SER:HB3	1:B:585:GLU:H	1.55	0.45
1:B:292:PHE:HB2	1:B:306:ASN:HB3	1.98	0.45
1:D:462:THR:HA	1:D:465:ILE:HG22	1.99	0.45
1:A:56:ARG:NH1	1:A:437:HIS:HD2	2.14	0.45
1:B:72:THR:O	1:B:72:THR:CG2	2.64	0.45
1:B:561:ARG:HG3	1:B:561:ARG:HH11	1.81	0.45
1:C:481:VAL:H	1:C:503:ARG:CB	2.29	0.45
1:D:50:ALA:O	1:D:54:ILE:HG22	2.17	0.45
1:B:192:ARG:NH1	1:B:342:ASP:OD1	2.50	0.45
1:B:535:ASP:C	1:B:537:ARG:H	2.24	0.45
1:D:445:ARG:CB	1:D:462:THR:HG21	2.47	0.45
1:D:476:MET:SD	1:D:505:LEU:HD12	2.57	0.45
1:D:504:ALA:O	1:D:505:LEU:C	2.59	0.45
1:A:50:ALA:O	1:A:54:ILE:HG22	2.17	0.45
1:A:74:ILE:CG2	1:A:236:VAL:HB	2.47	0.45
1:D:320:GLY:O	1:D:323:SER:OG	2.31	0.45
1:A:153:PHE:CE2	2:A:622:FAD:C3B	2.93	0.44
1:A:479:ALA:HB3	1:A:505:LEU:HG	1.98	0.44
1:C:56:ARG:NH1	1:C:437:HIS:HD2	2.15	0.44
1:A:586:GLY:O	1:A:589:LYS:N	2.50	0.44
1:A:114:ASP:OD2	1:B:331:LYS:HD3	2.17	0.44
1:D:74:ILE:HG23	1:D:236:VAL:HG23	1.99	0.44
1:A:504:ALA:O	1:A:505:LEU:C	2.61	0.44
1:D:192:ARG:NH1	1:D:342:ASP:OD1	2.50	0.44
1:A:248:HIS:O	1:A:252:ARG:HG3	2.18	0.44
1:A:320:GLY:O	1:A:323:SER:OG	2.32	0.44
1:A:532:LEU:O	1:A:535:ASP:O	2.36	0.44
1:B:196:GLY:O	2:B:622:FAD:HM72	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:GLN:HB3	1:D:334:ARG:HG2	1.99	0.44
1:C:129:LYS:HG3	1:C:359:GLU:HB3	1.99	0.44
1:C:320:GLY:O	1:C:323:SER:OG	2.36	0.44
1:D:241:THR:HG22	1:D:242:LYS:H	1.83	0.44
1:B:510:ARG:H	1:B:511:PRO:CD	2.30	0.44
1:B:570:ILE:N	1:B:571:PRO:HD2	2.33	0.44
1:A:498:LEU:HD23	1:A:498:LEU:HA	1.82	0.44
1:D:129:LYS:HG3	1:D:359:GLU:HB3	1.99	0.44
1:B:248:HIS:O	1:B:252:ARG:HG3	2.18	0.44
1:B:322:ARG:HA	1:B:327:LEU:O	2.18	0.44
1:C:248:HIS:O	1:C:252:ARG:HG3	2.18	0.44
1:B:462:THR:HA	1:B:465:ILE:HG22	2.00	0.43
1:D:55:THR:HG23	1:D:65:MET:HG2	1.99	0.43
1:A:241:THR:HG22	1:A:242:LYS:H	1.83	0.43
1:B:565:LEU:HA	1:B:568:LEU:HD12	2.00	0.43
1:B:129:LYS:HG3	1:B:359:GLU:HB3	2.00	0.43
1:C:55:THR:HG23	1:C:65:MET:HG2	1.99	0.43
1:C:241:THR:HG22	1:C:242:LYS:H	1.83	0.43
1:A:445:ARG:CB	1:A:462:THR:HG21	2.49	0.43
1:B:75:GLN:HB3	1:B:236:VAL:O	2.18	0.43
1:B:153:PHE:CE2	2:B:622:FAD:H51A	2.53	0.43
1:C:74:ILE:CG2	1:C:236:VAL:HB	2.48	0.43
1:C:513:ILE:O	1:C:547:LYS:HE3	2.19	0.43
1:A:597:THR:HG23	1:A:600:GLN:H	1.83	0.43
1:C:581:SER:O	1:C:581:SER:OG	2.36	0.43
1:D:485:GLU:HG2	1:D:521:HIS:O	2.18	0.43
1:B:462:THR:O	1:B:465:ILE:HG22	2.19	0.43
1:B:503:ARG:O	1:B:505:LEU:N	2.51	0.43
1:C:40:MET:HE3	1:C:44:PRO:HA	2.00	0.43
1:B:121:ILE:HD12	1:D:500:THR:CG2	2.27	0.43
1:A:356:ARG:HB2	1:A:357:PRO:HD3	2.00	0.43
1:A:462:THR:HA	1:A:465:ILE:HG22	2.00	0.43
1:A:476:MET:SD	1:A:505:LEU:HD12	2.59	0.43
1:D:3:ASP:OD2	1:D:26:HIS:N	2.52	0.43
1:A:40:MET:HB2	1:A:96:LYS:HD2	2.00	0.42
1:A:481:VAL:H	1:A:503:ARG:HB3	1.84	0.42
1:C:50:ALA:O	1:C:54:ILE:HG22	2.19	0.42
1:A:95:ASP:O	1:A:96:LYS:C	2.60	0.42
1:B:273:CYS:N	1:B:423:ARG:NH1	2.65	0.42
1:B:445:ARG:CB	1:B:462:THR:HG21	2.48	0.42
1:B:465:ILE:HD11	1:B:537:ARG:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:GLN:HB3	1:C:236:VAL:O	2.19	0.42
1:C:273:CYS:N	1:C:423:ARG:NH1	2.65	0.42
1:D:469:VAL:O	1:D:473:LEU:HG	2.19	0.42
1:C:40:MET:CE	1:C:44:PRO:HA	2.48	0.42
1:C:462:THR:O	1:C:465:ILE:HG22	2.19	0.42
1:D:56:ARG:NH1	1:D:437:HIS:HD2	2.15	0.42
1:D:153:PHE:CE2	2:D:622:FAD:C3B	2.95	0.42
1:A:485:GLU:HG2	1:A:521:HIS:O	2.19	0.42
1:A:568:LEU:HB2	1:A:598:ILE:HG12	2.02	0.42
1:C:153:PHE:HE2	2:C:622:FAD:C3B	2.21	0.42
1:A:75:GLN:HB3	1:A:236:VAL:O	2.20	0.42
1:A:579:LEU:HD13	1:A:582:LEU:HD11	2.02	0.42
1:B:352:THR:O	1:B:353:MET:HB2	2.19	0.42
1:A:110:GLU:HA	1:A:111:PRO:HD3	1.89	0.42
1:B:293:LEU:HB3	1:B:303:MET:HE3	2.02	0.42
1:C:236:VAL:CG1	1:C:295:PRO:HG2	2.50	0.42
1:C:509:LYS:HG3	1:C:546:ILE:HD11	2.02	0.42
1:C:597:THR:HG23	1:C:600:GLN:H	1.85	0.42
1:D:75:GLN:HB3	1:D:236:VAL:O	2.19	0.42
1:A:34:LEU:C	1:A:36:ALA:H	2.27	0.42
1:D:509:LYS:HZ2	1:D:546:ILE:HD13	1.85	0.41
1:A:293:LEU:HB3	1:A:303:MET:HE3	2.02	0.41
1:B:110:GLU:HA	1:B:111:PRO:HD3	1.91	0.41
1:C:72:THR:O	1:C:72:THR:CG2	2.67	0.41
1:C:293:LEU:HB3	1:C:303:MET:HE3	2.02	0.41
1:D:206:VAL:HG21	1:D:303:MET:CE	2.36	0.41
1:D:248:HIS:O	1:D:252:ARG:HG3	2.20	0.41
1:D:480:LYS:CB	1:D:503:ARG:HB3	2.50	0.41
1:A:311:SER:OG	1:A:338:ALA:HB2	2.19	0.41
1:A:503:ARG:O	1:A:505:LEU:N	2.53	0.41
1:D:72:THR:HG23	1:D:98:GLN:HB3	2.02	0.41
1:D:498:LEU:HD11	1:D:502:ALA:HB3	2.02	0.41
1:A:56:ARG:NH1	1:A:437:HIS:CD2	2.85	0.41
1:B:356:ARG:HB2	1:B:357:PRO:HD3	2.00	0.41
1:A:55:THR:HG23	1:A:65:MET:HG2	2.03	0.41
1:D:248:HIS:CD2	1:D:280:ILE:HG12	2.55	0.41
1:D:510:ARG:HA	1:D:547:LYS:HG2	2.03	0.41
1:A:345:HIS:HA	1:A:346:PRO:HD3	1.79	0.41
1:A:469:VAL:O	1:A:473:LEU:HG	2.21	0.41
1:A:563:ALA:O	1:A:567:SER:HB2	2.21	0.41
1:D:510:ARG:H	1:D:511:PRO:HD3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:LYS:HE2	1:A:296:GLU:OE1	2.20	0.41
1:B:584:SER:O	1:B:585:GLU:C	2.63	0.41
1:A:480:LYS:CB	1:A:503:ARG:HB3	2.51	0.41
1:B:480:LYS:CB	1:B:503:ARG:HB3	2.51	0.41
1:B:583:SER:HB3	1:B:587:ARG:HB3	1.99	0.41
1:C:96:LYS:HE2	1:C:296:GLU:OE1	2.19	0.41
1:C:469:VAL:O	1:C:473:LEU:HG	2.20	0.41
1:A:78:MET:HE1	1:A:437:HIS:CE1	2.56	0.41
1:A:437:HIS:CD2	1:A:437:HIS:C	2.98	0.41
1:B:236:VAL:CG1	1:B:295:PRO:HG2	2.51	0.41
1:B:496:GLN:HE21	1:B:496:GLN:HB2	1.63	0.41
1:B:504:ALA:O	1:B:507:LEU:N	2.49	0.41
1:B:529:ALA:HB1	1:B:532:LEU:CD2	2.51	0.41
1:C:114:ASP:OD2	1:D:331:LYS:HD3	2.21	0.41
1:C:570:ILE:N	1:C:571:PRO:HD2	2.36	0.41
1:D:467:LYS:O	1:D:471:HIS:HB2	2.20	0.41
1:B:8:GLY:HA2	2:B:622:FAD:H1B	2.03	0.41
1:B:498:LEU:HA	1:B:498:LEU:HD23	1.83	0.41
1:C:356:ARG:HB2	1:C:357:PRO:HD3	2.03	0.41
1:D:311:SER:OG	1:D:338:ALA:HB2	2.21	0.41
1:D:481:VAL:H	1:D:503:ARG:HB3	1.85	0.41
1:A:445:ARG:HG3	1:A:454:VAL:HG11	2.04	0.40
1:B:40:MET:CE	1:B:44:PRO:HA	2.51	0.40
1:B:498:LEU:HD11	1:B:502:ALA:HB3	2.02	0.40
1:C:31:THR:HA	2:C:622:FAD:N3A	2.36	0.40
1:D:8:GLY:HA2	2:D:622:FAD:H1B	2.03	0.40
1:B:153:PHE:HE2	2:B:622:FAD:H51A	1.85	0.40
1:D:356:ARG:HB2	1:D:357:PRO:HD3	2.03	0.40
1:A:504:ALA:O	1:A:507:LEU:N	2.50	0.40
1:A:510:ARG:H	1:A:511:PRO:HD3	1.85	0.40
1:A:558:VAL:HG12	1:A:562:ILE:HD13	2.03	0.40
1:D:153:PHE:CE2	2:D:622:FAD:H51A	2.56	0.40
1:D:498:LEU:HA	1:D:498:LEU:HD23	1.84	0.40
1:A:334:ARG:HG2	1:B:117:GLN:HB3	2.03	0.40
1:C:123:VAL:HG12	1:C:183:LEU:CD1	2.52	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	607/641 (95%)	545 (90%)	50 (8%)	12 (2%)	6	31
1	B	607/641 (95%)	552 (91%)	43 (7%)	12 (2%)	6	31
1	C	607/641 (95%)	553 (91%)	44 (7%)	10 (2%)	7	36
1	D	548/641 (86%)	505 (92%)	34 (6%)	9 (2%)	7	36
All	All	2369/2564 (92%)	2155 (91%)	171 (7%)	43 (2%)	6	34

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	500	THR
1	B	500	THR
1	C	500	THR
1	C	504	ALA
1	D	500	THR
1	A	585	GLU
1	A	586	GLY
1	A	617	ILE
1	B	617	ILE
1	C	617	ILE
1	A	49	VAL
1	A	274	PRO
1	A	429	ALA
1	A	505	LEU
1	A	510	ARG
1	B	274	PRO
1	B	429	ALA
1	B	505	LEU
1	B	510	ARG
1	C	429	ALA
1	C	510	ARG
1	C	568	LEU

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Mol	Chain	Res	Type
1	D	274	PRO
1	D	429	ALA
1	D	505	LEU
1	D	510	ARG
1	A	427	SER
1	A	504	ALA
1	B	49	VAL
1	B	504	ALA
1	C	274	PRO
1	D	427	SER
1	B	580	ASN
1	D	49	VAL
1	D	504	ALA
1	A	512	GLY
1	B	427	SER
1	B	512	GLY
1	B	583	SER
1	C	49	VAL
1	C	512	GLY
1	D	512	GLY
1	C	508	ILE

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	515/539 (96%)	469 (91%)	46 (9%)	9	34
1	B	515/539 (96%)	467 (91%)	48 (9%)	8	33
1	C	515/539 (96%)	468 (91%)	47 (9%)	9	34
1	D	462/539 (86%)	422 (91%)	40 (9%)	9	36
All	All	2007/2156 (93%)	1826 (91%)	181 (9%)	9	34

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	31	THR
1	A	37	VAL
1	A	97	THR
1	A	101	LEU
1	A	124	SER
1	A	142	GLN
1	A	147	ILE
1	A	154	LEU
1	A	163	ASP
1	A	171	THR
1	A	180	THR
1	A	203	SER
1	A	241	THR
1	A	262	THR
1	A	275	SER
1	A	298	THR
1	A	321	LEU
1	A	358	VAL
1	A	370	THR
1	A	381	LEU
1	A	392	LEU
1	A	395	GLU
1	A	413	LEU
1	A	433	LEU
1	A	452	ASN
1	A	471	HIS
1	A	481	VAL
1	A	486	ILE
1	A	491	MET
1	A	496	GLN
1	A	498	LEU
1	A	500	THR
1	A	503	ARG
1	A	523	LEU
1	A	526	ARG
1	A	532	LEU
1	A	557	LEU
1	A	561	ARG
1	A	567	SER
1	A	569	HIS
1	A	584	SER
1	A	605	LEU

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Mol	Chain	Res	Type
1	A	607	VAL
1	A	614	ILE
1	A	615	LEU
1	B	7	VAL
1	B	37	VAL
1	B	43	ASN
1	B	97	THR
1	B	101	LEU
1	B	121	ILE
1	B	124	SER
1	B	142	GLN
1	B	147	ILE
1	B	154	LEU
1	B	163	ASP
1	B	171	THR
1	B	180	THR
1	B	203	SER
1	B	241	THR
1	B	262	THR
1	B	275	SER
1	B	277	GLU
1	B	298	THR
1	B	321	LEU
1	B	358	VAL
1	B	370	THR
1	B	381	LEU
1	B	392	LEU
1	B	395	GLU
1	B	413	LEU
1	B	452	ASN
1	B	471	HIS
1	B	478	THR
1	B	481	VAL
1	B	486	ILE
1	B	491	MET
1	B	496	GLN
1	B	498	LEU
1	B	500	THR
1	B	503	ARG
1	B	505	LEU
1	B	523	LEU
1	B	526	ARG

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Mol	Chain	Res	Type
1	B	532	LEU
1	B	557	LEU
1	B	566	ASP
1	B	574	PHE
1	B	579	LEU
1	B	605	LEU
1	B	607	VAL
1	B	614	ILE
1	B	615	LEU
1	C	0	HIS
1	C	7	VAL
1	C	31	THR
1	C	37	VAL
1	C	43	ASN
1	C	97	THR
1	C	101	LEU
1	C	124	SER
1	C	142	GLN
1	C	147	ILE
1	C	154	LEU
1	C	163	ASP
1	C	171	THR
1	C	180	THR
1	C	203	SER
1	C	241	THR
1	C	262	THR
1	C	275	SER
1	C	277	GLU
1	C	298	THR
1	C	321	LEU
1	C	358	VAL
1	C	370	THR
1	C	381	LEU
1	C	392	LEU
1	C	395	GLU
1	C	413	LEU
1	C	452	ASN
1	C	471	HIS
1	C	481	VAL
1	C	486	ILE
1	C	491	MET
1	C	496	GLN

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Mol	Chain	Res	Type
1	C	498	LEU
1	C	500	THR
1	C	503	ARG
1	C	523	LEU
1	C	526	ARG
1	C	532	LEU
1	C	557	LEU
1	C	568	LEU
1	C	579	LEU
1	C	581	SER
1	C	605	LEU
1	C	607	VAL
1	C	614	ILE
1	C	615	LEU
1	D	7	VAL
1	D	31	THR
1	D	37	VAL
1	D	43	ASN
1	D	97	THR
1	D	101	LEU
1	D	124	SER
1	D	142	GLN
1	D	147	ILE
1	D	154	LEU
1	D	163	ASP
1	D	171	THR
1	D	180	THR
1	D	203	SER
1	D	241	THR
1	D	262	THR
1	D	275	SER
1	D	277	GLU
1	D	298	THR
1	D	321	LEU
1	D	358	VAL
1	D	370	THR
1	D	381	LEU
1	D	392	LEU
1	D	395	GLU
1	D	413	LEU
1	D	452	ASN
1	D	471	HIS

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Mol	Chain	Res	Type
1	D	481	VAL
1	D	486	ILE
1	D	491	MET
1	D	496	GLN
1	D	498	LEU
1	D	500	THR
1	D	503	ARG
1	D	505	LEU
1	D	523	LEU
1	D	526	ARG
1	D	532	LEU
1	D	557	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	93	GLN
1	A	142	GLN
1	A	431	HIS
1	A	437	HIS
1	A	471	HIS
1	A	569	HIS
1	B	26	HIS
1	B	93	GLN
1	B	142	GLN
1	B	214	GLN
1	B	437	HIS
1	B	543	GLN
1	B	569	HIS
1	B	600	GLN
1	C	11	HIS
1	C	26	HIS
1	C	93	GLN
1	C	126	ASN
1	C	142	GLN
1	C	431	HIS
1	C	437	HIS
1	C	543	GLN
1	C	569	HIS
1	D	11	HIS
1	D	26	HIS

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Mol	Chain	Res	Type
1	D	93	GLN
1	D	142	GLN
1	D	431	HIS
1	D	437	HIS
1	D	471	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FAD	B	622	-	58,58,58	1.24	6 (10%)	85,89,89	1.81	23 (27%)
2	FAD	A	622	-	58,58,58	1.21	6 (10%)	85,89,89	1.83	22 (25%)
2	FAD	D	622	-	58,58,58	1.32	8 (13%)	85,89,89	1.78	22 (25%)
2	FAD	C	622	-	58,58,58	1.29	7 (12%)	85,89,89	1.80	21 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	622	-	-	14/34/50/50	0/5/6/6
2	FAD	A	622	-	-	14/34/50/50	0/5/6/6
2	FAD	D	622	-	-	14/34/50/50	0/5/6/6
2	FAD	C	622	-	-	15/34/50/50	0/5/6/6

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	622	FAD	C2A-N3A	3.40	1.40	1.33
2	B	622	FAD	C4X-N5	3.37	1.38	1.30
2	D	622	FAD	C4X-N5	3.34	1.38	1.30
2	C	622	FAD	C4X-N5	3.33	1.38	1.30
2	A	622	FAD	C4X-N5	3.28	1.37	1.30
2	D	622	FAD	C2A-N1A	3.21	1.39	1.33
2	C	622	FAD	C2A-N3A	3.17	1.39	1.33
2	B	622	FAD	C2A-N3A	3.05	1.39	1.33
2	A	622	FAD	C2A-N1A	3.01	1.39	1.33
2	C	622	FAD	C2A-N1A	2.99	1.39	1.33
2	D	622	FAD	C10-N1	2.98	1.39	1.33
2	A	622	FAD	C2A-N3A	2.97	1.39	1.33
2	B	622	FAD	C2A-N1A	2.96	1.39	1.33
2	B	622	FAD	C10-N1	2.96	1.39	1.33
2	C	622	FAD	C10-N1	2.94	1.39	1.33
2	A	622	FAD	C10-N1	2.89	1.39	1.33
2	C	622	FAD	C5'-C4'	2.72	1.55	1.51
2	B	622	FAD	C5'-C4'	2.66	1.55	1.51
2	D	622	FAD	C8A-N7A	2.52	1.36	1.31
2	D	622	FAD	C5'-C4'	2.50	1.55	1.51
2	C	622	FAD	C8A-N7A	2.47	1.36	1.31
2	D	622	FAD	P-O3P	2.43	1.62	1.59
2	D	622	FAD	PA-O3P	2.38	1.62	1.59
2	A	622	FAD	C5'-C4'	2.21	1.54	1.51
2	C	622	FAD	C5A-N7A	-2.15	1.35	1.39
2	A	622	FAD	C8A-N7A	2.09	1.35	1.31
2	B	622	FAD	C5A-N7A	-2.05	1.35	1.39

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	622	FAD	N3A-C2A-N1A	-5.39	120.43	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	622	FAD	N3A-C2A-N1A	-5.15	120.78	128.58
2	D	622	FAD	N3A-C2A-N1A	-5.05	120.94	128.58
2	A	622	FAD	C5X-C9A-N10	5.05	122.53	117.97
2	B	622	FAD	C5X-C9A-N10	5.01	122.49	117.97
2	C	622	FAD	C5X-C9A-N10	4.95	122.44	117.97
2	C	622	FAD	C5A-C4A-N3A	-4.88	119.99	126.72
2	C	622	FAD	N3A-C2A-N1A	-4.87	121.20	128.58
2	A	622	FAD	C5A-C4A-N3A	-4.79	120.12	126.72
2	D	622	FAD	C5X-C9A-N10	4.78	122.29	117.97
2	D	622	FAD	C5A-C4A-N3A	-4.78	120.13	126.72
2	B	622	FAD	C5A-C4A-N3A	-4.50	120.53	126.72
2	B	622	FAD	C2A-N3A-C4A	3.41	120.16	111.83
2	A	622	FAD	N9A-C8A-N7A	-3.38	109.14	113.94
2	D	622	FAD	C2A-N3A-C4A	3.38	120.08	111.83
2	D	622	FAD	C4-N3-C2	-3.37	119.66	125.64
2	A	622	FAD	C4-N3-C2	-3.34	119.70	125.64
2	C	622	FAD	C4-N3-C2	-3.31	119.76	125.64
2	B	622	FAD	C4-N3-C2	-3.31	119.77	125.64
2	A	622	FAD	C2A-N3A-C4A	3.28	119.83	111.83
2	C	622	FAD	C4X-C10-N10	3.27	121.17	116.48
2	A	622	FAD	C5A-N7A-C8A	3.26	108.57	103.45
2	B	622	FAD	N9A-C8A-N7A	-3.24	109.34	113.94
2	D	622	FAD	C4X-C10-N10	3.22	121.10	116.48
2	A	622	FAD	C4X-C10-N10	3.20	121.06	116.48
2	B	622	FAD	C4X-C10-N10	3.19	121.05	116.48
2	C	622	FAD	C2A-N3A-C4A	3.18	119.60	111.83
2	A	622	FAD	N3A-C4A-N9A	3.13	132.49	127.17
2	B	622	FAD	C5A-N7A-C8A	3.12	108.36	103.45
2	D	622	FAD	N3A-C4A-N9A	3.12	132.47	127.17
2	D	622	FAD	N9A-C8A-N7A	-3.09	109.55	113.94
2	A	622	FAD	C1'-N10-C9A	-3.07	114.66	120.63
2	C	622	FAD	C9A-N10-C10	-3.04	116.11	120.75
2	D	622	FAD	C1'-N10-C9A	-3.02	114.76	120.63
2	C	622	FAD	C1'-N10-C9A	-3.01	114.78	120.63
2	A	622	FAD	C9A-N10-C10	-3.00	116.17	120.75
2	C	622	FAD	N3A-C4A-N9A	2.98	132.23	127.17
2	B	622	FAD	C9A-N10-C10	-2.97	116.22	120.75
2	B	622	FAD	C1'-N10-C9A	-2.96	114.88	120.63
2	D	622	FAD	C9A-N10-C10	-2.87	116.37	120.75
2	B	622	FAD	N3A-C4A-N9A	2.86	132.03	127.17
2	C	622	FAD	C8M-C8-C9	-2.85	114.56	119.57
2	C	622	FAD	N9A-C8A-N7A	-2.77	110.00	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	622	FAD	C5A-N7A-C8A	2.77	107.81	103.45
2	C	622	FAD	C5A-N7A-C8A	2.75	107.77	103.45
2	D	622	FAD	C4X-C10-N1	-2.70	117.97	124.59
2	D	622	FAD	O5B-C5B-C4B	-2.70	99.81	108.99
2	C	622	FAD	C4X-C10-N1	-2.69	117.98	124.59
2	B	622	FAD	C8M-C8-C9	-2.69	114.83	119.57
2	C	622	FAD	C4'-C3'-C2'	2.67	118.02	113.57
2	A	622	FAD	C4X-C10-N1	-2.66	118.07	124.59
2	D	622	FAD	C4X-C4-N3	2.65	119.99	113.25
2	B	622	FAD	C4'-C3'-C2'	2.64	117.96	113.57
2	B	622	FAD	C4X-C10-N1	-2.64	118.13	124.59
2	C	622	FAD	C6A-C5A-C4A	2.62	120.76	117.18
2	A	622	FAD	C8M-C8-C9	-2.61	114.97	119.57
2	A	622	FAD	C4A-C5A-N7A	-2.61	107.60	110.58
2	C	622	FAD	C4X-C4-N3	2.60	119.86	113.25
2	A	622	FAD	C4X-C4-N3	2.59	119.84	113.25
2	B	622	FAD	C4X-C4-N3	2.56	119.77	113.25
2	A	622	FAD	C4'-C3'-C2'	2.53	117.78	113.57
2	C	622	FAD	O5B-C5B-C4B	-2.49	100.53	108.99
2	D	622	FAD	C8M-C8-C9	-2.48	115.20	119.57
2	A	622	FAD	C4-C4X-C10	2.39	121.03	116.93
2	C	622	FAD	O4-C4-C4X	-2.38	120.26	126.53
2	C	622	FAD	C4-C4X-C10	2.36	120.98	116.93
2	A	622	FAD	O4-C4-C4X	-2.35	120.32	126.53
2	B	622	FAD	C9A-C5X-N5	-2.35	119.97	122.45
2	B	622	FAD	C4-C4X-C10	2.34	120.94	116.93
2	D	622	FAD	C4-C4X-C10	2.32	120.92	116.93
2	D	622	FAD	C9A-C5X-N5	-2.32	119.99	122.45
2	A	622	FAD	O2A-PA-O3P	2.31	113.50	107.27
2	B	622	FAD	O4-C4-C4X	-2.30	120.47	126.53
2	A	622	FAD	C9A-C5X-N5	-2.30	120.02	122.45
2	D	622	FAD	O4-C4-C4X	-2.30	120.47	126.53
2	D	622	FAD	C6A-C5A-C4A	2.24	120.23	117.18
2	B	622	FAD	C4A-C5A-N7A	-2.22	108.04	110.58
2	C	622	FAD	C9A-C5X-N5	-2.20	120.12	122.45
2	A	622	FAD	C6A-C5A-C4A	2.19	120.17	117.18
2	C	622	FAD	C4A-C5A-N7A	-2.18	108.09	110.58
2	A	622	FAD	O5B-C5B-C4B	-2.12	101.78	108.99
2	D	622	FAD	C4'-C3'-C2'	2.09	117.05	113.57
2	B	622	FAD	C6A-C5A-C4A	2.09	120.03	117.18
2	B	622	FAD	O2A-PA-O3P	2.05	112.80	107.27
2	B	622	FAD	O5B-C5B-C4B	-2.04	102.03	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	622	FAD	C6-C5X-C9A	2.04	121.85	119.05
2	D	622	FAD	O4B-C4B-C3B	2.02	109.15	105.15
2	D	622	FAD	C4A-C5A-N7A	-2.01	108.29	110.58

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	622	FAD	C5B-O5B-PA-O1A
2	A	622	FAD	O4B-C4B-C5B-O5B
2	A	622	FAD	C1'-C2'-C3'-O3'
2	A	622	FAD	C1'-C2'-C3'-C4'
2	A	622	FAD	O2'-C2'-C3'-O3'
2	A	622	FAD	O2'-C2'-C3'-C4'
2	A	622	FAD	C3'-C4'-C5'-O5'
2	A	622	FAD	O4'-C4'-C5'-O5'
2	B	622	FAD	C5B-O5B-PA-O1A
2	B	622	FAD	C5B-O5B-PA-O3P
2	B	622	FAD	O4B-C4B-C5B-O5B
2	B	622	FAD	C1'-C2'-C3'-O3'
2	B	622	FAD	C1'-C2'-C3'-C4'
2	B	622	FAD	O2'-C2'-C3'-O3'
2	B	622	FAD	O2'-C2'-C3'-C4'
2	B	622	FAD	C3'-C4'-C5'-O5'
2	B	622	FAD	O4'-C4'-C5'-O5'
2	B	622	FAD	PA-O3P-P-O5'
2	C	622	FAD	C5B-O5B-PA-O1A
2	C	622	FAD	C5B-O5B-PA-O3P
2	C	622	FAD	O4B-C4B-C5B-O5B
2	C	622	FAD	C3B-C4B-C5B-O5B
2	C	622	FAD	C1'-C2'-C3'-O3'
2	C	622	FAD	C1'-C2'-C3'-C4'
2	C	622	FAD	O2'-C2'-C3'-O3'
2	C	622	FAD	O2'-C2'-C3'-C4'
2	C	622	FAD	C3'-C4'-C5'-O5'
2	C	622	FAD	O4'-C4'-C5'-O5'
2	C	622	FAD	PA-O3P-P-O5'
2	D	622	FAD	C5B-O5B-PA-O1A
2	D	622	FAD	O4B-C4B-C5B-O5B
2	D	622	FAD	C1'-C2'-C3'-O3'
2	D	622	FAD	C1'-C2'-C3'-C4'
2	D	622	FAD	O2'-C2'-C3'-O3'

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Mol	Chain	Res	Type	Atoms
2	D	622	FAD	O2'-C2'-C3'-C4'
2	D	622	FAD	C3'-C4'-C5'-O5'
2	D	622	FAD	O4'-C4'-C5'-O5'
2	D	622	FAD	PA-O3P-P-O5'
2	A	622	FAD	C3B-C4B-C5B-O5B
2	B	622	FAD	C3B-C4B-C5B-O5B
2	D	622	FAD	C3B-C4B-C5B-O5B
2	A	622	FAD	PA-O3P-P-O5'
2	A	622	FAD	C5B-O5B-PA-O2A
2	A	622	FAD	C5B-O5B-PA-O3P
2	B	622	FAD	C5B-O5B-PA-O2A
2	C	622	FAD	C5B-O5B-PA-O2A
2	C	622	FAD	C2'-C1'-N10-C10
2	D	622	FAD	C5B-O5B-PA-O2A
2	D	622	FAD	C5B-O5B-PA-O3P
2	C	622	FAD	P-O3P-PA-O2A
2	D	622	FAD	P-O3P-PA-O2A
2	C	622	FAD	P-O3P-PA-O1A
2	A	622	FAD	P-O3P-PA-O1A
2	A	622	FAD	P-O3P-PA-O2A
2	B	622	FAD	P-O3P-PA-O1A
2	B	622	FAD	P-O3P-PA-O2A
2	D	622	FAD	P-O3P-PA-O1A

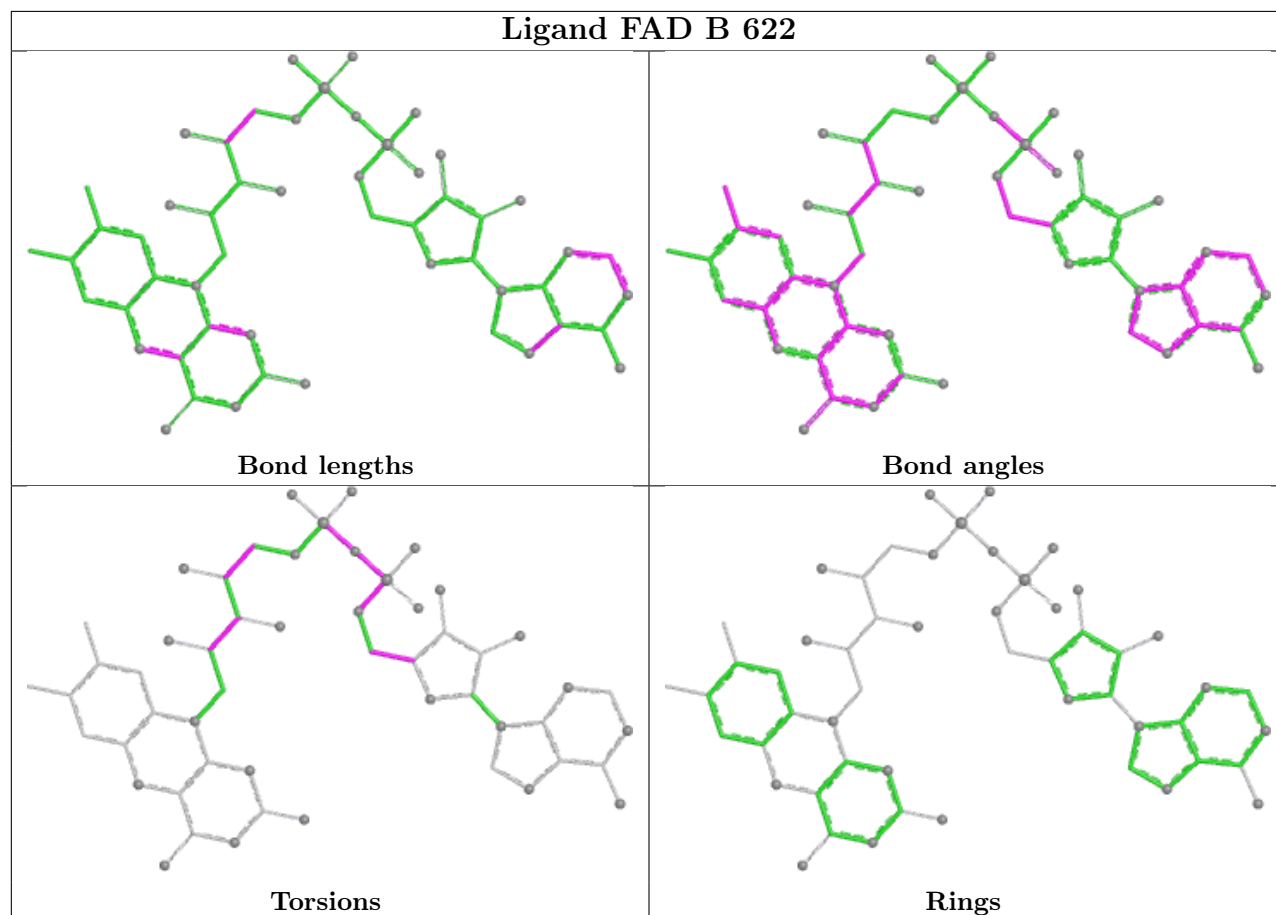
There are no ring outliers.

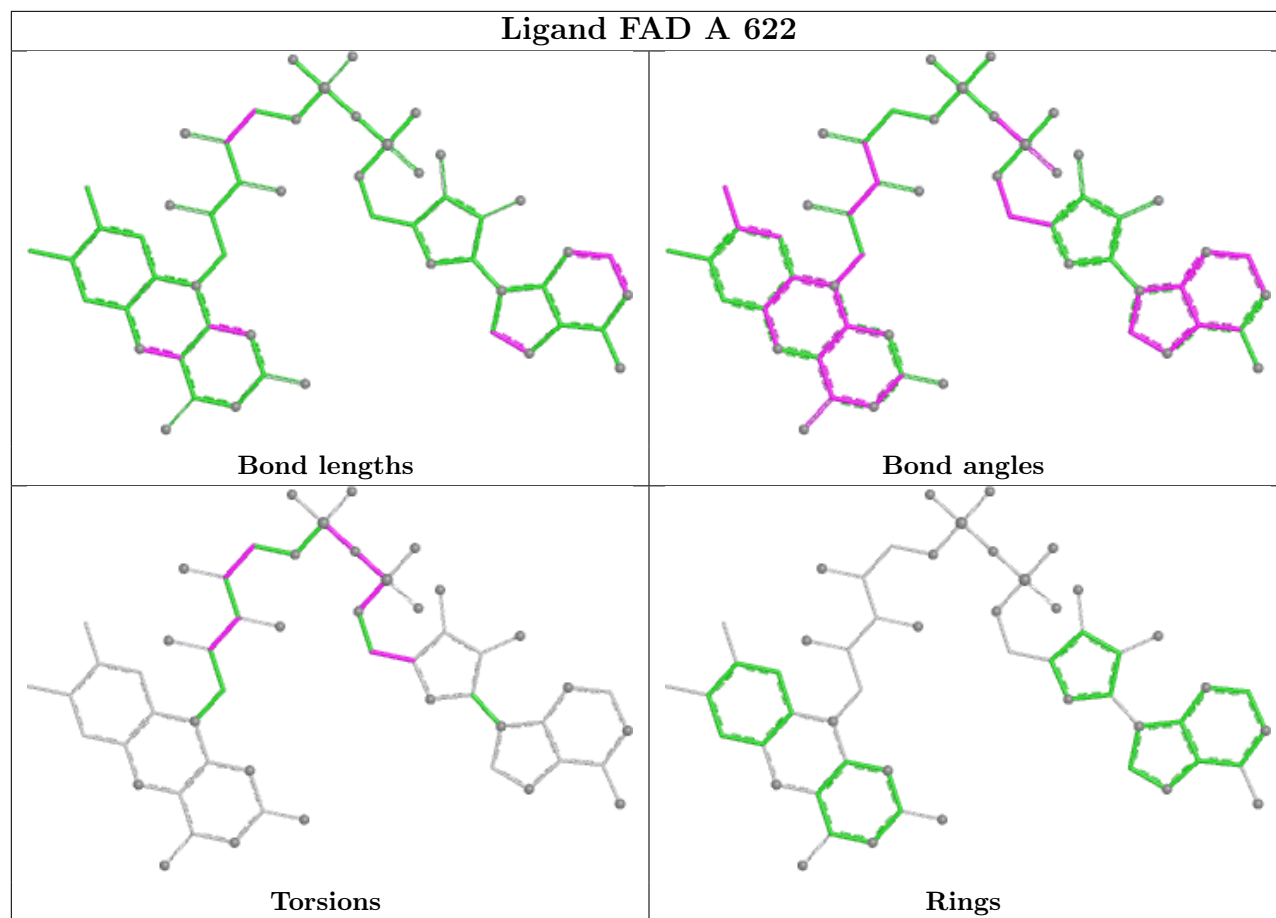
4 monomers are involved in 46 short contacts:

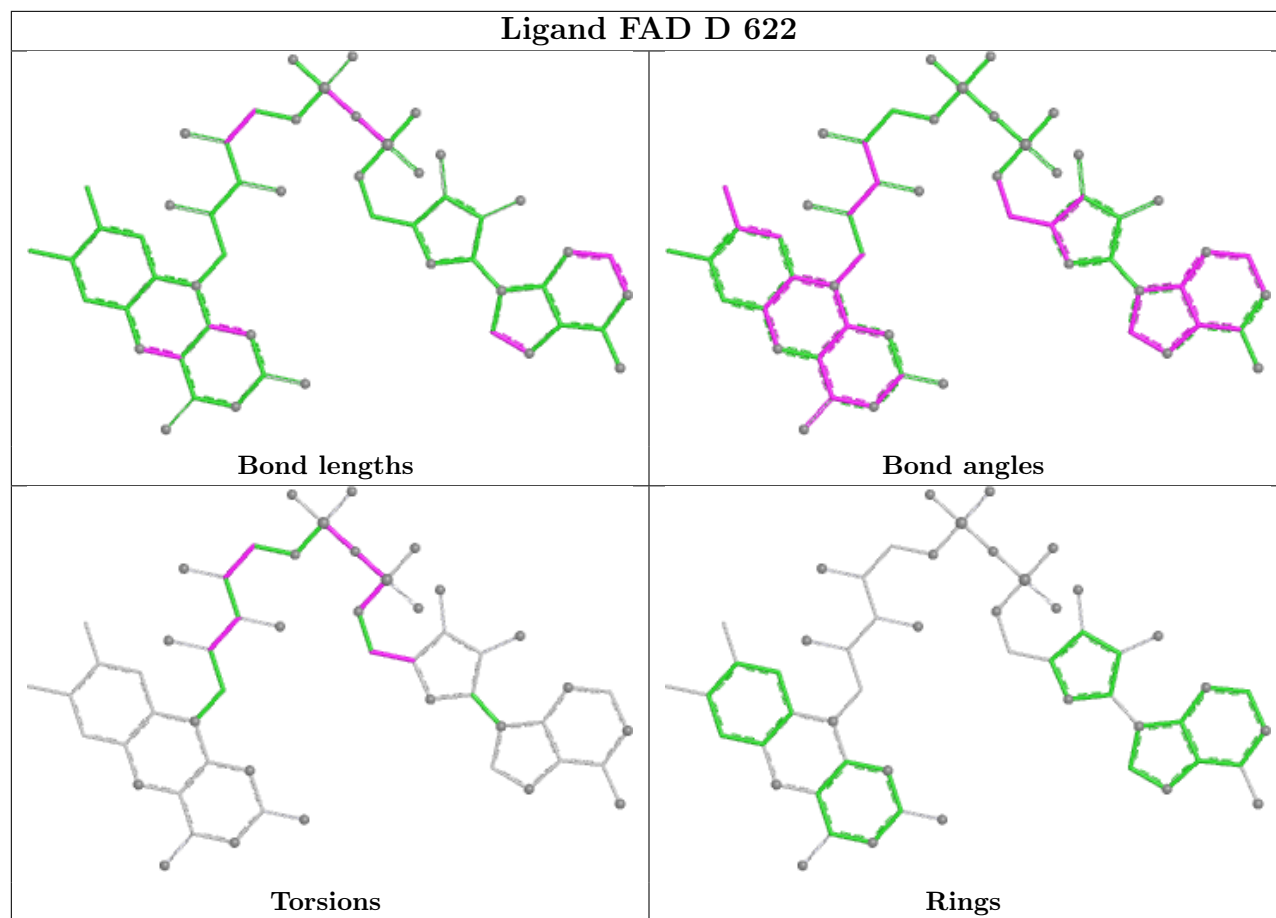
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	622	FAD	13	0
2	A	622	FAD	10	0
2	D	622	FAD	11	0
2	C	622	FAD	12	0

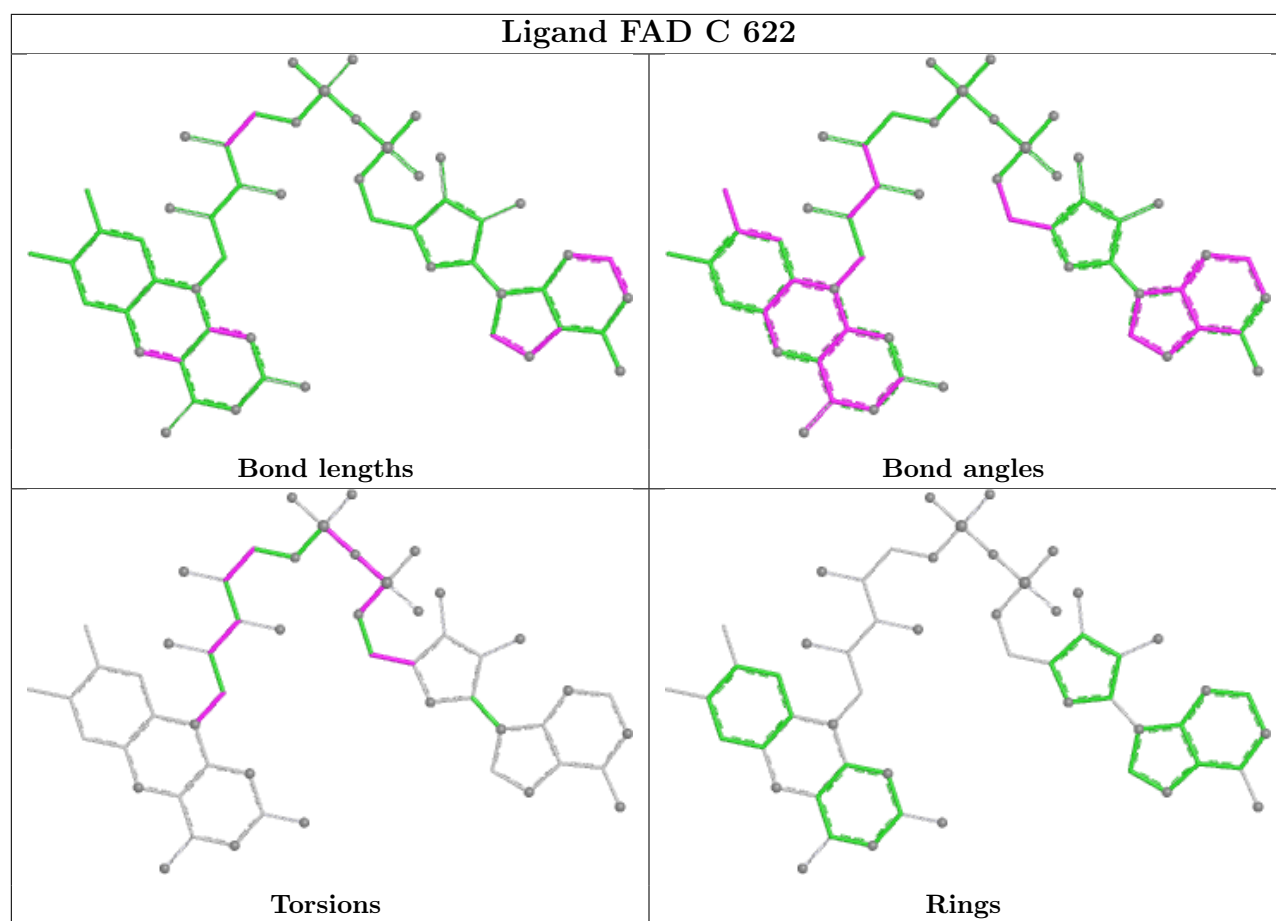
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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

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	611/641 (95%)	0.67	39 (6%) 25 16	123, 126, 129, 133	0
1	B	611/641 (95%)	0.55	16 (2%) 57 37	123, 126, 129, 134	0
1	C	611/641 (95%)	0.57	22 (3%) 46 28	117, 126, 129, 133	0
1	D	552/641 (86%)	0.51	13 (2%) 59 40	123, 126, 129, 134	0
All	All	2385/2564 (93%)	0.58	90 (3%) 44 27	117, 126, 129, 134	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	581	SER	4.1
1	A	619	LEU	4.0
1	A	570	ILE	3.5
1	C	57	GLU	3.1
1	D	447	ILE	3.1
1	A	54	ILE	3.1
1	C	418	THR	2.9
1	A	513	ILE	2.9
1	D	61	LEU	2.8
1	A	369	GLY	2.8
1	B	263	GLY	2.8
1	C	99	TYR	2.7
1	D	538	VAL	2.7
1	C	444	LEU	2.7
1	D	321	LEU	2.7
1	D	426	THR	2.7
1	A	101	LEU	2.7
1	A	590	LEU	2.6
1	A	87	MET	2.6
1	A	444	LEU	2.6
1	C	570	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	99	TYR	2.6
1	A	599	GLY	2.6
1	A	97	THR	2.6
1	C	120	VAL	2.5
1	B	101	LEU	2.5
1	B	148	LEU	2.5
1	B	427	SER	2.4
1	A	386	ASN	2.4
1	A	580	ASN	2.4
1	A	583	SER	2.4
1	A	96	LYS	2.3
1	A	617	ILE	2.3
1	B	367	ILE	2.3
1	A	149	ALA	2.3
1	A	397	ILE	2.3
1	C	11	HIS	2.3
1	A	61	LEU	2.3
1	A	367	ILE	2.3
1	A	429	ALA	2.3
1	B	415	THR	2.3
1	A	615	LEU	2.3
1	D	258	SER	2.3
1	A	607	VAL	2.3
1	C	9	ALA	2.2
1	C	228	THR	2.2
1	C	100	SER	2.2
1	A	46	ILE	2.2
1	A	210	ILE	2.2
1	A	151	GLY	2.2
1	A	295	PRO	2.2
1	C	312	LEU	2.2
1	D	168	GLY	2.2
1	C	131	SER	2.2
1	A	69	ILE	2.2
1	A	36	ALA	2.2
1	A	45	ALA	2.2
1	B	444	LEU	2.2
1	C	151	GLY	2.2
1	C	505	LEU	2.2
1	C	49	VAL	2.2
1	B	58	ILE	2.2
1	D	367	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	598	ILE	2.2
1	B	61	LEU	2.2
1	C	15	GLU	2.2
1	D	319	ALA	2.2
1	A	494	GLY	2.2
1	C	222	PRO	2.2
1	B	11	HIS	2.1
1	C	69	ILE	2.1
1	A	65	MET	2.1
1	A	49	VAL	2.1
1	C	26	HIS	2.1
1	B	532	LEU	2.1
1	D	513	ILE	2.1
1	C	38	ALA	2.1
1	B	497	GLU	2.1
1	A	305	VAL	2.1
1	C	149	ALA	2.1
1	D	149	ALA	2.1
1	B	168	GLY	2.1
1	B	41	SER	2.0
1	A	99	TYR	2.0
1	A	352	THR	2.0
1	D	429	ALA	2.0
1	B	321	LEU	2.0
1	A	440	ALA	2.0
1	C	66	GLY	2.0
1	D	509	LYS	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 oligosaccharides in this entry.

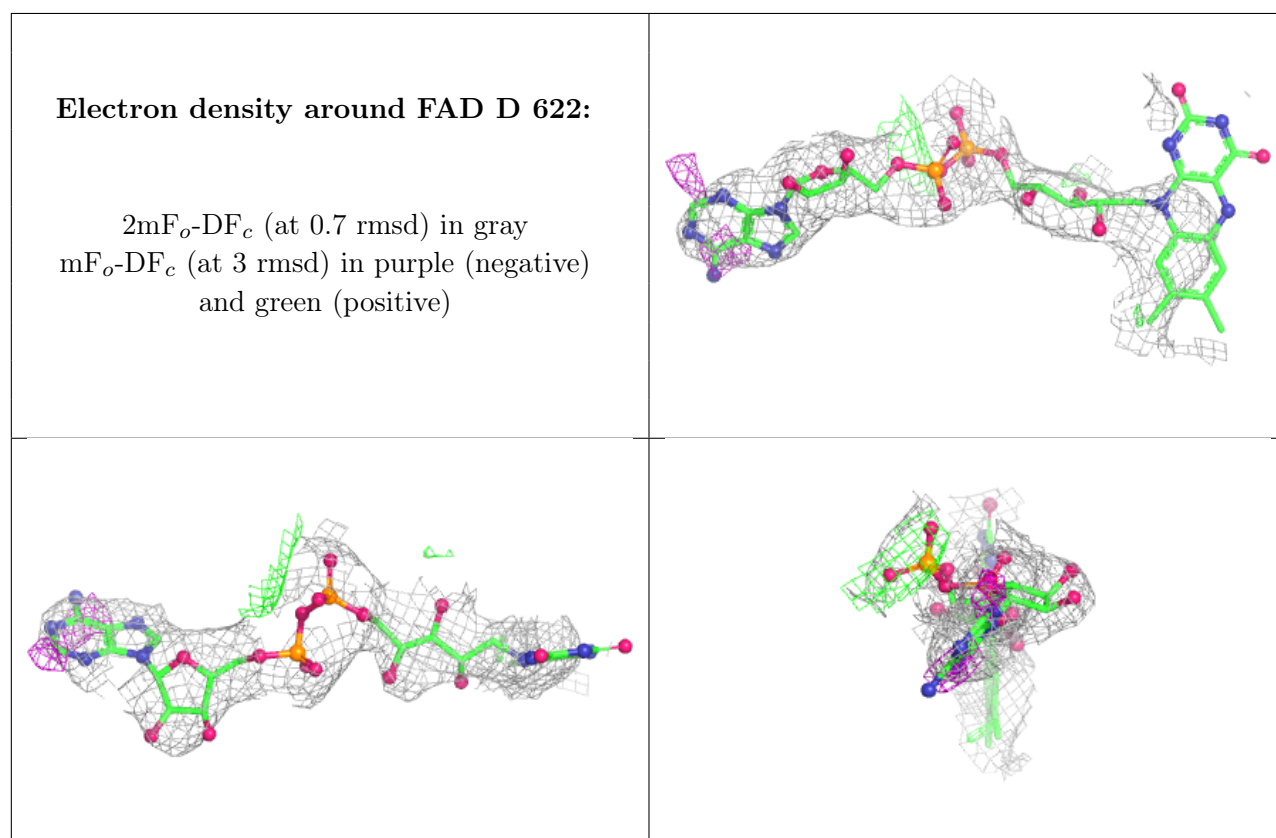
6.4 Ligands [i](#)

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, 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.

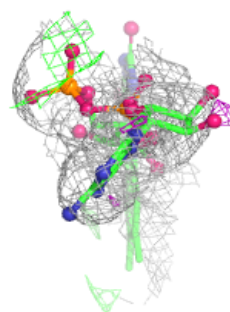
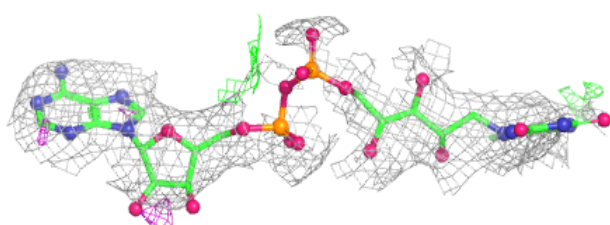
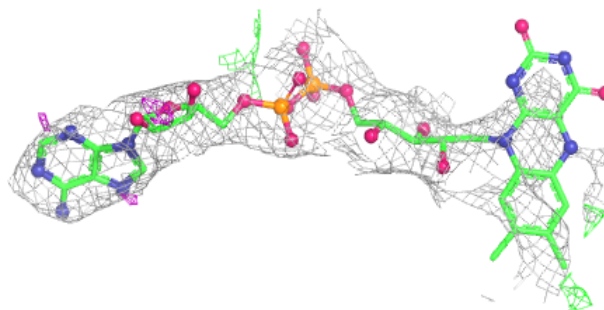
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	D	622	53/53	0.85	0.13	81,87,251,251	0
2	FAD	C	622	53/53	0.87	0.13	81,86,251,251	0
2	FAD	B	622	53/53	0.88	0.13	81,86,251,251	0
2	FAD	A	622	53/53	0.90	0.12	82,86,251,251	0

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.

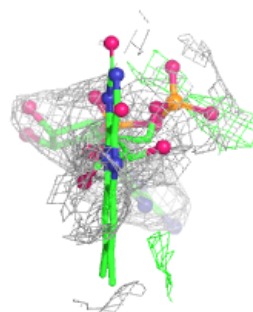
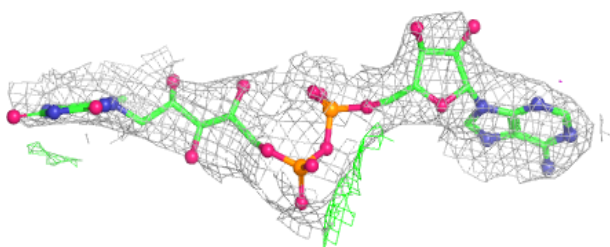
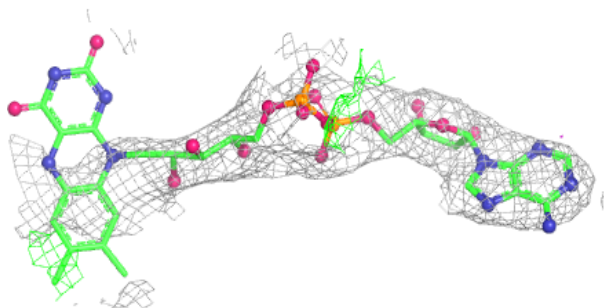


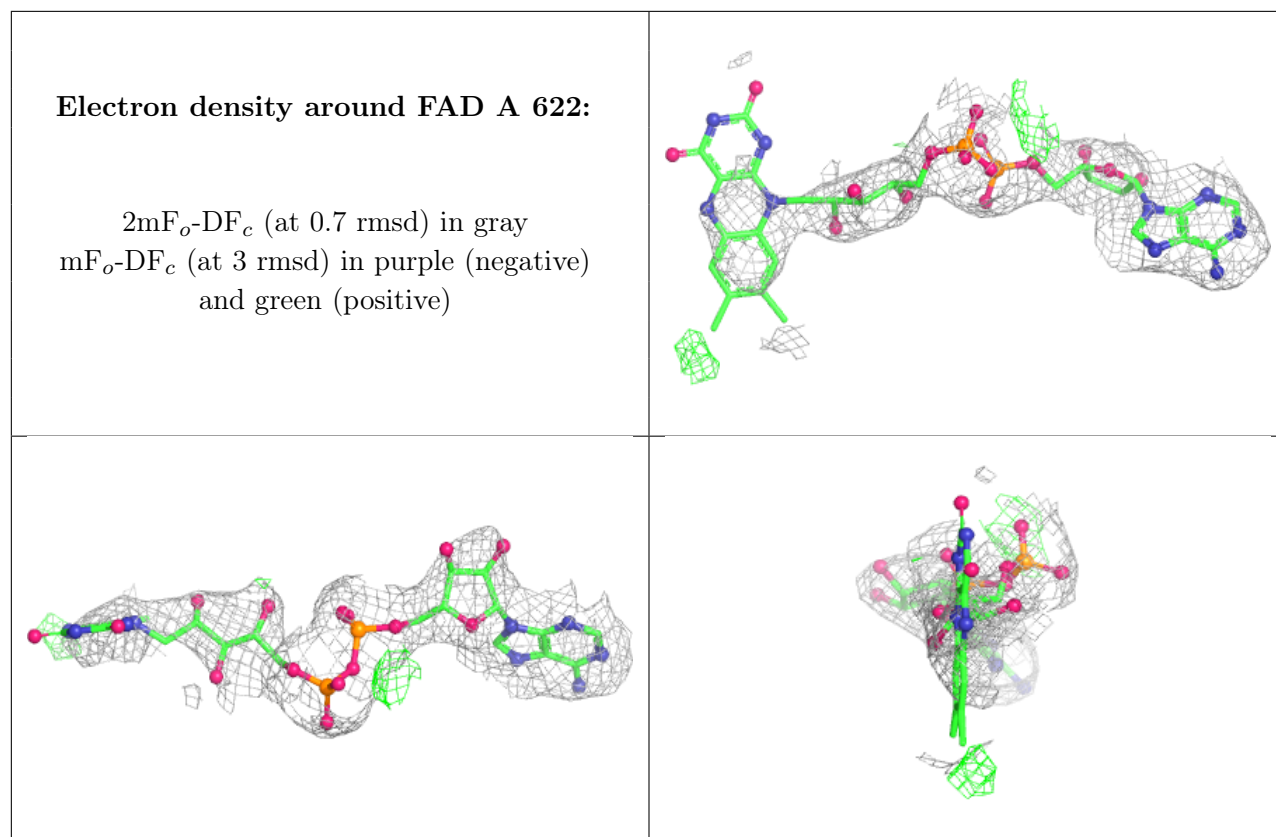
Electron density around FAD C 622:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around FAD B 622:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.