



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:31 AM UTC

PDB ID : 3ITJ / pdb_00003itj
Title : Crystal structure of *Saccharomyces cerevisiae* thioredoxin reductase 1 (Trr1)
Authors : Oliveira, M.A.; Discola, K.F.; Alves, S.V.; Medrano, F.J.; Guimaraes, B.G.; Netto, L.E.S.
Deposited on : 2009-08-28
Resolution : 2.40 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

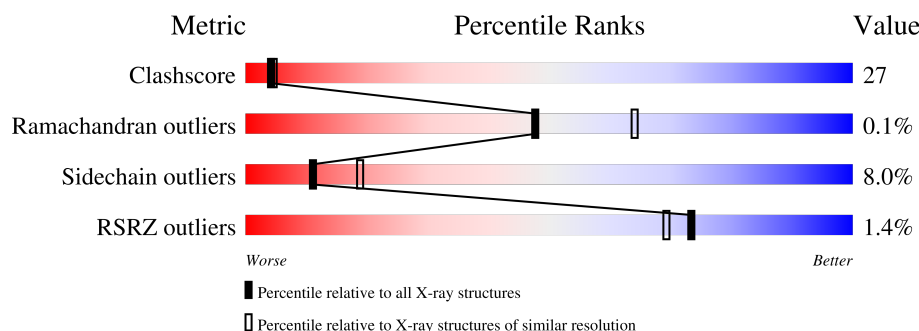
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	338	
1	B	338	
1	C	338	
1	D	338	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CIT	A	501	-	-	X	-
3	CIT	B	506	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9837 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 Thioredoxin reductase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	1	0
			2376	1499	402	463	12			
1	B	319	Total	C	N	O	S	0	0	0
			2373	1496	402	463	12			
1	C	314	Total	C	N	O	S	0	0	0
			2299	1444	388	456	11			
1	D	307	Total	C	N	O	S	0	0	0
			2222	1401	369	442	10			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P29509
A	-18	GLY	-	expression tag	UNP P29509
A	-17	SER	-	expression tag	UNP P29509
A	-16	SER	-	expression tag	UNP P29509
A	-15	HIS	-	expression tag	UNP P29509
A	-14	HIS	-	expression tag	UNP P29509
A	-13	HIS	-	expression tag	UNP P29509
A	-12	HIS	-	expression tag	UNP P29509
A	-11	HIS	-	expression tag	UNP P29509
A	-10	HIS	-	expression tag	UNP P29509
A	-9	SER	-	expression tag	UNP P29509
A	-8	SER	-	expression tag	UNP P29509
A	-7	GLY	-	expression tag	UNP P29509
A	-6	LEU	-	expression tag	UNP P29509
A	-5	VAL	-	expression tag	UNP P29509
A	-4	PRO	-	expression tag	UNP P29509
A	-3	ARG	-	expression tag	UNP P29509
A	-2	GLY	-	expression tag	UNP P29509
A	-1	SER	-	expression tag	UNP P29509
A	0	HIS	-	expression tag	UNP P29509
B	-19	MET	-	expression tag	UNP P29509

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP P29509
B	-17	SER	-	expression tag	UNP P29509
B	-16	SER	-	expression tag	UNP P29509
B	-15	HIS	-	expression tag	UNP P29509
B	-14	HIS	-	expression tag	UNP P29509
B	-13	HIS	-	expression tag	UNP P29509
B	-12	HIS	-	expression tag	UNP P29509
B	-11	HIS	-	expression tag	UNP P29509
B	-10	HIS	-	expression tag	UNP P29509
B	-9	SER	-	expression tag	UNP P29509
B	-8	SER	-	expression tag	UNP P29509
B	-7	GLY	-	expression tag	UNP P29509
B	-6	LEU	-	expression tag	UNP P29509
B	-5	VAL	-	expression tag	UNP P29509
B	-4	PRO	-	expression tag	UNP P29509
B	-3	ARG	-	expression tag	UNP P29509
B	-2	GLY	-	expression tag	UNP P29509
B	-1	SER	-	expression tag	UNP P29509
B	0	HIS	-	expression tag	UNP P29509
C	-19	MET	-	expression tag	UNP P29509
C	-18	GLY	-	expression tag	UNP P29509
C	-17	SER	-	expression tag	UNP P29509
C	-16	SER	-	expression tag	UNP P29509
C	-15	HIS	-	expression tag	UNP P29509
C	-14	HIS	-	expression tag	UNP P29509
C	-13	HIS	-	expression tag	UNP P29509
C	-12	HIS	-	expression tag	UNP P29509
C	-11	HIS	-	expression tag	UNP P29509
C	-10	HIS	-	expression tag	UNP P29509
C	-9	SER	-	expression tag	UNP P29509
C	-8	SER	-	expression tag	UNP P29509
C	-7	GLY	-	expression tag	UNP P29509
C	-6	LEU	-	expression tag	UNP P29509
C	-5	VAL	-	expression tag	UNP P29509
C	-4	PRO	-	expression tag	UNP P29509
C	-3	ARG	-	expression tag	UNP P29509
C	-2	GLY	-	expression tag	UNP P29509
C	-1	SER	-	expression tag	UNP P29509
C	0	HIS	-	expression tag	UNP P29509
D	-19	MET	-	expression tag	UNP P29509
D	-18	GLY	-	expression tag	UNP P29509
D	-17	SER	-	expression tag	UNP P29509

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP P29509
D	-15	HIS	-	expression tag	UNP P29509
D	-14	HIS	-	expression tag	UNP P29509
D	-13	HIS	-	expression tag	UNP P29509
D	-12	HIS	-	expression tag	UNP P29509
D	-11	HIS	-	expression tag	UNP P29509
D	-10	HIS	-	expression tag	UNP P29509
D	-9	SER	-	expression tag	UNP P29509
D	-8	SER	-	expression tag	UNP P29509
D	-7	GLY	-	expression tag	UNP P29509
D	-6	LEU	-	expression tag	UNP P29509
D	-5	VAL	-	expression tag	UNP P29509
D	-4	PRO	-	expression tag	UNP P29509
D	-3	ARG	-	expression tag	UNP P29509
D	-2	GLY	-	expression tag	UNP P29509
D	-1	SER	-	expression tag	UNP P29509
D	0	HIS	-	expression tag	UNP P29509

- # FAD

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
2	C	1	Total 53	C 27	N 9	O 15	P 2	0	0

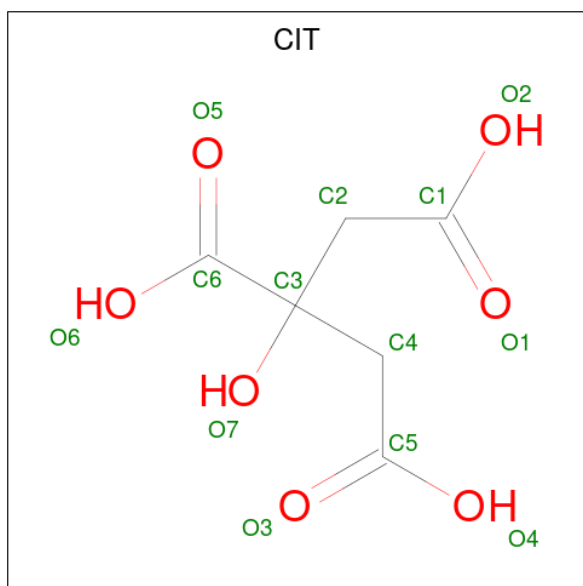


WORLD WIDE
PDB
PROTEIN DATA BANK

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

- Molecule 3 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		
3	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	82	Total	O	0	0
			82	82		
4	B	76	Total	O	0	0
			76	76		

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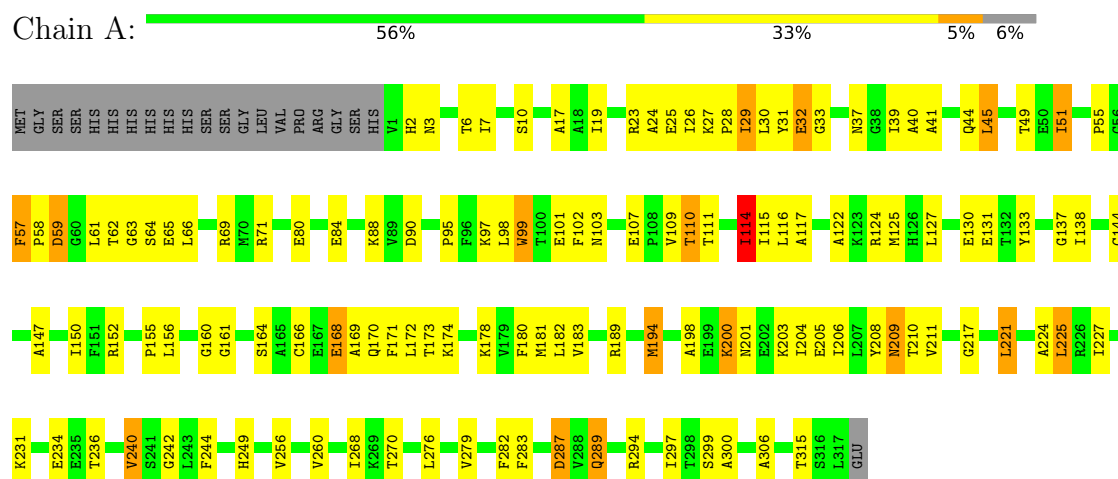
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	65	Total	O	0	0
			65	65		
4	D	54	Total	O	0	0
			54	54		

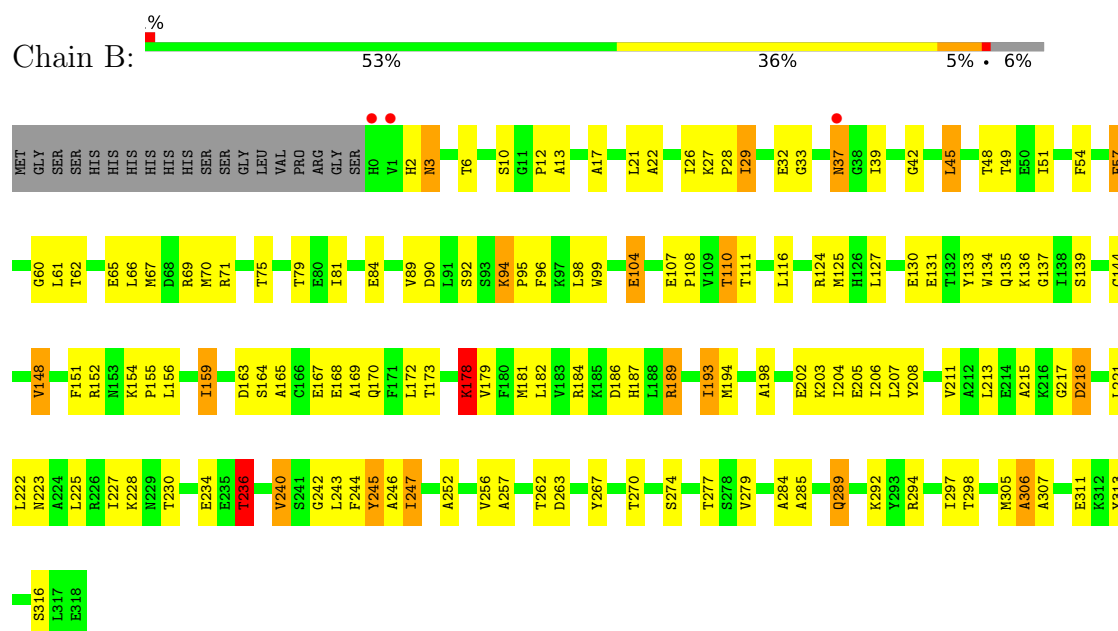
3 Residue-property plots

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.

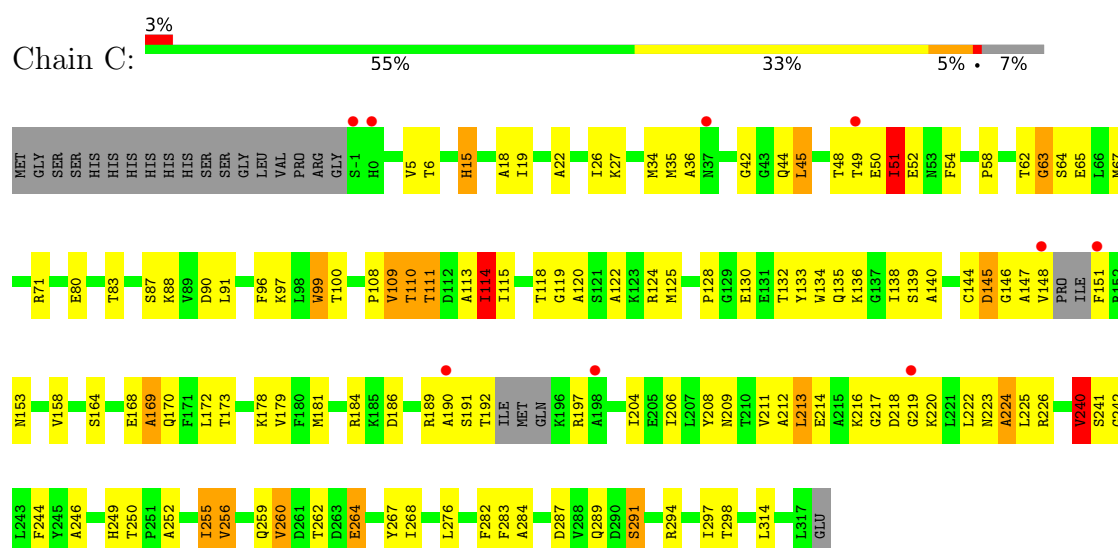
- Molecule 1: Thioredoxin reductase 1



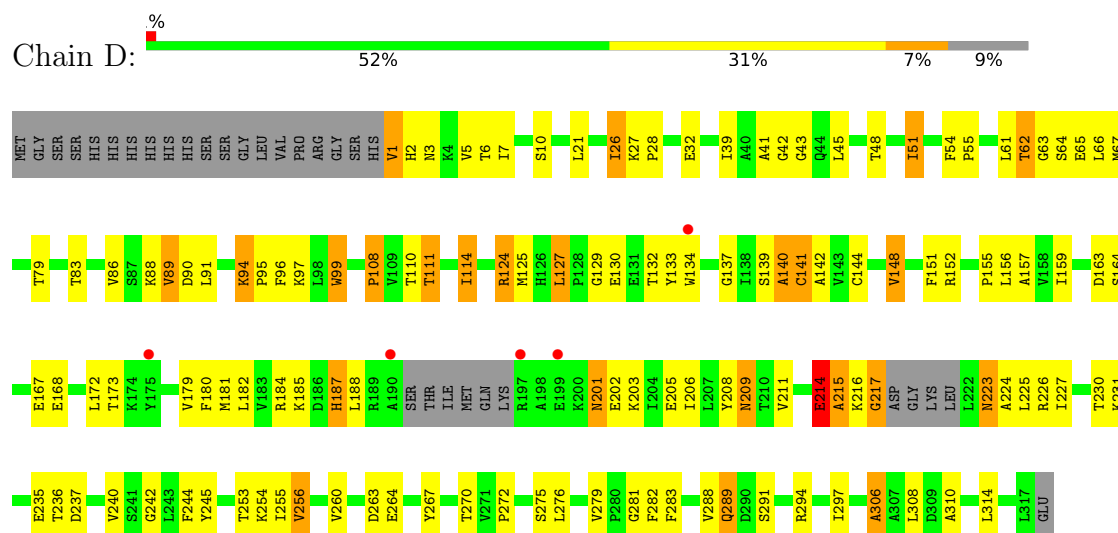
- Molecule 1: Thioredoxin reductase 1



- Molecule 1: Thioredoxin reductase 1



• Molecule 1: Thioredoxin reductase 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	127.97Å 135.41Å 75.82Å 90.00° 89.95° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.0 (50.00-2.40) 79.8 (50.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.06 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.169 , 0.194 0.199 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
Reported twinning fraction	0.783 for H, K, L 0.217 for -h,-k,l	Depositor
Outliers	0 of 40523 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9837	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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, CIT

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	1.40	10/2420 (0.4%)	1.37	17/3276 (0.5%)
1	B	1.48	11/2413 (0.5%)	1.44	26/3267 (0.8%)
1	C	1.41	10/2336 (0.4%)	1.42	21/3168 (0.7%)
1	D	1.42	9/2261 (0.4%)	1.41	19/3076 (0.6%)
All	All	1.43	40/9430 (0.4%)	1.41	83/12787 (0.6%)

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	D	0	1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	246	ALA	CA-CB	8.33	1.59	1.53
1	D	215	ALA	CA-CB	-7.74	1.41	1.53
1	A	300	ALA	CA-CB	6.96	1.64	1.53
1	B	165	ALA	CA-CB	6.88	1.64	1.53
1	C	158	VAL	CA-CB	6.82	1.62	1.54
1	A	279	VAL	CA-C	6.55	1.58	1.53
1	D	214	GLU	C-O	-6.46	1.17	1.24
1	D	159	ILE	CA-CB	6.34	1.61	1.54
1	D	209	ASN	CA-C	-6.24	1.45	1.53
1	B	57	PHE	C-O	-6.14	1.17	1.24
1	C	145	ASP	N-CA	6.09	1.53	1.45
1	B	306	ALA	CA-CB	6.04	1.62	1.53
1	D	27	LYS	C-O	-5.99	1.21	1.23
1	A	227	ILE	CA-C	-5.96	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	252	ALA	C-O	-5.96	1.17	1.23
1	A	114	ILE	CA-CB	-5.92	1.46	1.54
1	A	7	ILE	N-CA	-5.67	1.39	1.46
1	D	227	ILE	CA-C	-5.65	1.46	1.52
1	C	115	ILE	N-CA	-5.59	1.39	1.46
1	C	15	HIS	C-O	5.57	1.31	1.24
1	B	13	ALA	CA-CB	5.52	1.62	1.53
1	A	182	LEU	CA-C	-5.51	1.45	1.52
1	D	223	ASN	N-CA	5.50	1.52	1.46
1	B	234	GLU	CA-C	-5.50	1.45	1.52
1	C	22	ALA	CA-CB	-5.50	1.44	1.53
1	C	268	ILE	CA-CB	-5.44	1.47	1.54
1	B	245	TYR	CA-C	-5.42	1.46	1.52
1	C	190	ALA	N-CA	5.42	1.53	1.45
1	B	159	ILE	CA-CB	5.40	1.60	1.54
1	A	306	ALA	CA-CB	5.39	1.62	1.53
1	A	117	ALA	CA-CB	5.31	1.58	1.53
1	B	277	THR	CA-CB	-5.29	1.45	1.53
1	D	79	THR	N-CA	5.21	1.52	1.46
1	A	27	LYS	N-CA	-5.16	1.42	1.46
1	B	236	THR	N-CA	-5.09	1.39	1.45
1	A	287	ASP	CA-C	5.09	1.59	1.52
1	D	5	VAL	CA-CB	5.06	1.62	1.54
1	B	94	LYS	CA-C	-5.03	1.45	1.52
1	C	268	ILE	C-O	-5.02	1.18	1.24
1	C	284	ALA	C-O	5.01	1.30	1.24

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	214	GLU	N-CA-C	9.67	121.41	108.07
1	D	217	GLY	N-CA-C	9.06	139.56	113.30
1	B	294	ARG	N-CA-C	8.20	122.45	111.30
1	D	187	HIS	N-CA-C	7.81	121.96	110.17
1	B	107	GLU	CA-C-N	-7.72	112.74	120.31
1	B	107	GLU	C-N-CA	-7.72	112.74	120.31
1	C	169	ALA	N-CA-C	-7.65	102.88	111.14
1	B	148	VAL	CA-C-N	7.57	126.84	118.97
1	B	148	VAL	C-N-CA	7.57	126.84	118.97
1	A	37	ASN	N-CA-C	7.43	121.40	111.30
1	B	193	ILE	CB-CA-C	-7.21	102.75	111.97
1	C	224	ALA	N-CA-C	6.93	117.65	107.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	188	LEU	N-CA-C	6.91	122.89	113.21
1	B	154	LYS	CA-C-N	-6.83	112.90	120.14
1	B	154	LYS	C-N-CA	-6.83	112.90	120.14
1	A	39	ILE	N-CA-C	6.71	117.95	107.28
1	A	279	VAL	N-CA-C	6.59	115.24	107.73
1	B	298	THR	N-CA-C	-6.59	103.59	111.69
1	C	114	ILE	CG1-CB-CG2	-6.46	91.32	110.70
1	D	54	PHE	CA-C-N	6.44	126.82	119.93
1	D	54	PHE	C-N-CA	6.44	126.82	119.93
1	D	294	ARG	CG-CD-NE	-6.44	97.84	112.00
1	A	236	THR	CA-C-N	-6.43	114.48	122.84
1	A	236	THR	C-N-CA	-6.43	114.48	122.84
1	A	27	LYS	CA-C-N	-6.38	113.72	120.03
1	A	27	LYS	C-N-CA	-6.38	113.72	120.03
1	A	231	LYS	N-CA-C	-6.34	104.59	112.90
1	C	220	LYS	N-CA-C	-6.26	105.28	113.17
1	A	209	ASN	CA-C-N	-6.15	113.02	122.62
1	A	209	ASN	C-N-CA	-6.15	113.02	122.62
1	D	231	LYS	N-CA-C	-6.13	104.15	111.69
1	B	79	THR	N-CA-C	-6.05	99.79	109.96
1	C	264	GLU	N-CA-C	-5.97	105.25	112.54
1	A	256	VAL	CB-CA-C	-5.93	104.42	111.65
1	C	144	CYS	N-CA-C	5.86	117.74	111.36
1	C	18	ALA	N-CA-C	-5.82	104.94	111.28
1	B	127	LEU	CA-C-N	-5.81	113.71	119.93
1	B	127	LEU	C-N-CA	-5.81	113.71	119.93
1	D	281	GLY	N-CA-C	-5.74	107.75	115.21
1	A	32	GLU	N-CA-C	-5.69	106.34	113.28
1	D	148	VAL	CA-C-N	5.62	125.46	119.28
1	D	148	VAL	C-N-CA	5.62	125.46	119.28
1	B	136	LYS	N-CA-C	-5.54	103.79	110.44
1	B	279	VAL	CB-CA-C	-5.49	104.54	110.85
1	B	81	ILE	N-CA-C	5.48	116.66	109.21
1	C	71	ARG	CG-CD-NE	-5.48	99.95	112.00
1	B	21	LEU	N-CA-C	-5.42	105.53	111.82
1	A	17	ALA	N-CA-C	-5.41	105.28	111.07
1	C	51	ILE	CB-CA-C	5.40	118.87	110.83
1	C	110	THR	N-CA-C	-5.39	101.09	109.72
1	C	63	GLY	N-CA-C	-5.35	106.30	112.50
1	A	211	VAL	N-CA-CB	-5.34	102.69	111.45
1	C	189	ARG	N-CA-C	5.34	120.66	113.72
1	B	94	LYS	N-CA-C	-5.32	102.29	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	ASN	N-CA-C	5.32	117.94	109.81
1	C	241	SER	N-CA-C	-5.31	106.74	114.12
1	C	240	VAL	N-CA-C	-5.30	100.84	108.42
1	D	28	PRO	CB-CA-C	-5.28	104.07	110.98
1	D	41	ALA	CA-C-N	-5.27	117.72	123.30
1	D	41	ALA	C-N-CA	-5.27	117.72	123.30
1	B	131	GLU	N-CA-C	-5.26	105.96	112.38
1	B	246	ALA	N-CA-C	-5.25	102.34	109.54
1	D	279	VAL	N-CA-C	5.25	113.71	107.73
1	B	60	GLY	N-CA-C	-5.24	106.08	112.68
1	C	291	SER	N-CA-C	-5.24	106.73	113.23
1	B	247	ILE	N-CA-C	5.19	117.17	111.77
1	C	50	GLU	CA-C-N	-5.17	116.78	123.19
1	C	50	GLU	C-N-CA	-5.17	116.78	123.19
1	D	306	ALA	N-CA-C	-5.17	105.73	111.36
1	C	114	ILE	CB-CG1-CD1	-5.16	102.96	113.80
1	D	140	ALA	N-CA-C	-5.15	107.00	113.28
1	A	107	GLU	N-CA-C	-5.13	103.12	109.64
1	B	178	LYS	CA-C-N	-5.11	116.30	123.10
1	B	178	LYS	C-N-CA	-5.11	116.30	123.10
1	C	100	THR	N-CA-C	5.06	117.93	110.59
1	B	218	ASP	N-CA-C	-5.06	103.80	110.33
1	A	57	PHE	CA-C-N	5.06	124.72	119.56
1	A	57	PHE	C-N-CA	5.06	124.72	119.56
1	D	294	ARG	CB-CA-C	-5.04	105.11	111.86
1	D	141	CYS	N-CA-C	5.03	116.37	107.61
1	C	27	LYS	CA-C-N	-5.03	114.77	119.85
1	C	27	LYS	C-N-CA	-5.03	114.77	119.85
1	B	22	ALA	N-CA-C	-5.01	105.28	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	185	LYS	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	2376	0	2382	117	0
1	B	2373	0	2375	135	0
1	C	2299	0	2234	115	0
1	D	2222	0	2130	137	0
2	A	53	0	31	3	0
2	B	53	0	31	8	0
2	C	53	0	31	3	0
2	D	53	0	31	3	0
3	A	13	0	5	7	0
3	B	26	0	10	9	0
3	C	26	0	10	6	0
3	D	13	0	5	2	0
4	A	82	0	0	7	0
4	B	76	0	0	4	0
4	C	65	0	0	4	0
4	D	54	0	0	4	0
All	All	9837	0	9275	514	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 27.

All (514) 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:216:LYS:CB	1:D:224:ALA:H	1.26	1.45
1:B:67:MET:CE	1:B:70:MET:HE2	1.53	1.34
1:D:201:ASN:ND2	1:D:203:LYS:H	1.37	1.20
1:C:191:SER:O	1:C:192:THR:HB	1.44	1.16
1:C:147:ALA:HB1	1:C:151:PHE:CB	1.75	1.15
1:C:249:HIS:ND1	3:C:505:CIT:O4	1.77	1.15
1:B:181:MET:HE3	1:B:204:ILE:HG21	1.30	1.14
1:D:216:LYS:CB	1:D:224:ALA:N	2.08	1.13
1:B:48:THR:HG21	2:B:401:FAD:H6	1.33	1.10
1:B:67:MET:HE1	1:B:70:MET:HE2	1.18	1.06
1:C:169:ALA:CB	1:C:181:MET:CE	2.32	1.06
1:C:169:ALA:CB	1:C:181:MET:HE2	1.86	1.05
1:B:67:MET:HE1	1:B:70:MET:CE	1.87	1.05
1:C:80:GLU:HB2	4:C:352:HOH:O	1.57	1.03
1:A:221:LEU:HD21	4:A:351:HOH:O	1.58	1.03
1:B:67:MET:SD	1:B:70:MET:HE2	1.98	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:ARG:H	1:D:124:ARG:HD2	1.20	1.02
1:B:189:ARG:HH11	3:B:502:CIT:H22	1.21	1.02
1:A:116:LEU:HD23	1:A:268:ILE:HD11	1.43	1.01
1:D:164:SER:O	1:D:168:GLU:HB2	1.61	1.00
1:D:133:TYR:OH	1:D:217:GLY:HA2	1.62	0.98
1:B:167:GLU:HG3	1:B:194:MET:HE2	1.45	0.98
1:D:51:ILE:HD11	1:D:63:GLY:HA2	1.44	0.98
1:D:201:ASN:HD22	1:D:202:GLU:N	1.60	0.98
1:B:66:LEU:HG	1:B:67:MET:HE3	1.46	0.96
1:D:181:MET:CE	1:D:206:ILE:HG12	1.98	0.93
1:B:12:PRO:HA	1:B:70:MET:HE1	1.49	0.93
1:B:48:THR:CG2	2:B:401:FAD:H6	1.98	0.93
1:C:62:THR:OG1	1:C:65:GLU:HG3	1.68	0.93
1:C:169:ALA:HB2	1:C:181:MET:HE2	1.51	0.93
1:D:201:ASN:HD22	1:D:203:LYS:H	1.15	0.92
1:C:169:ALA:HB3	1:C:181:MET:CE	1.98	0.92
1:B:48:THR:HG21	2:B:401:FAD:C6	2.00	0.91
1:A:194:MET:HE2	1:A:194:MET:HA	1.51	0.90
1:D:6:THR:OG1	1:D:111:THR:HG21	1.71	0.90
1:A:51:ILE:HD12	1:A:61:LEU:O	1.72	0.89
1:D:201:ASN:ND2	1:D:203:LYS:N	2.21	0.89
1:C:169:ALA:CB	1:C:181:MET:HE3	2.04	0.87
1:D:124:ARG:H	1:D:124:ARG:CD	1.87	0.86
1:B:67:MET:HE2	1:B:67:MET:HA	1.59	0.85
1:D:181:MET:HE2	1:D:206:ILE:HG12	1.58	0.85
1:B:189:ARG:NH1	3:B:502:CIT:H22	1.92	0.84
1:B:124:ARG:HD3	1:B:134:TRP:CZ3	2.13	0.84
1:A:116:LEU:CD2	1:A:268:ILE:HD11	2.07	0.83
1:B:66:LEU:HG	1:B:67:MET:CE	2.07	0.83
1:C:256:VAL:HG13	1:C:260:VAL:CG2	2.09	0.82
1:B:181:MET:HE1	1:B:198:ALA:HB1	1.59	0.82
1:B:12:PRO:CA	1:B:70:MET:HE1	2.08	0.82
1:D:2:HIS:HB2	1:D:110:THR:CG2	2.10	0.81
1:A:225:LEU:N	1:A:225:LEU:HD23	1.95	0.81
1:A:181:MET:HE3	1:A:206:ILE:HG12	1.61	0.81
1:B:65:GLU:O	1:B:69:ARG:HG3	1.80	0.80
1:B:48:THR:CG2	2:B:401:FAD:C6	2.57	0.80
1:A:114:ILE:HD12	1:A:282:PHE:CE1	2.17	0.79
1:C:133:TYR:CZ	1:C:217:GLY:HA3	2.17	0.79
1:A:114:ILE:HG21	1:A:282:PHE:CD1	2.18	0.79
1:A:62:THR:HG22	1:A:64:SER:H	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:ASN:HD22	1:D:201:ASN:C	1.90	0.79
1:A:116:LEU:HD23	1:A:268:ILE:CD1	2.12	0.79
1:D:201:ASN:HD21	1:D:203:LYS:H	1.28	0.78
1:C:191:SER:O	1:C:192:THR:CB	2.24	0.78
1:D:2:HIS:HB2	1:D:110:THR:HG21	1.66	0.78
1:D:2:HIS:HA	1:D:110:THR:HG23	1.66	0.78
1:A:114:ILE:CG2	1:A:282:PHE:CD1	2.66	0.78
1:C:147:ALA:HA	1:C:148:VAL:C	2.09	0.77
1:C:99:TRP:CZ3	1:C:108:PRO:HD3	2.20	0.77
1:A:164:SER:OG	3:A:501:CIT:H41	1.85	0.77
1:A:221:LEU:CD2	4:A:351:HOH:O	2.22	0.76
1:A:208:TYR:O	1:A:210:THR:HG23	1.83	0.76
1:B:67:MET:SD	1:B:70:MET:CE	2.74	0.76
3:C:503:CIT:O1	3:C:503:CIT:O7	2.01	0.76
1:A:181:MET:HE2	1:A:204:ILE:HG21	1.67	0.76
1:B:181:MET:HE3	1:B:204:ILE:CG2	2.12	0.76
3:B:506:CIT:H42	4:B:380:HOH:O	1.85	0.76
1:A:49:THR:O	1:A:62:THR:HA	1.86	0.76
1:D:201:ASN:ND2	1:D:202:GLU:N	2.35	0.75
1:A:51:ILE:HD12	1:A:51:ILE:H	1.52	0.75
1:B:167:GLU:HG3	1:B:194:MET:CE	2.17	0.74
1:C:218:ASP:CB	1:C:219:GLY:CA	2.64	0.74
1:A:181:MET:HE1	1:A:198:ALA:HB1	1.68	0.74
1:B:89:VAL:HG21	1:B:256:VAL:HG12	1.68	0.74
1:C:51:ILE:HD11	1:C:54:PHE:HB2	1.68	0.73
1:A:33:GLY:HA2	1:A:84:GLU:C	2.12	0.73
1:B:12:PRO:HA	1:B:70:MET:CE	2.19	0.73
1:D:1:VAL:O	1:D:110:THR:HG22	1.89	0.73
1:A:29:ILE:HD13	1:A:29:ILE:N	2.03	0.73
1:D:86:VAL:HG12	1:D:255:ILE:HD11	1.70	0.73
1:A:62:THR:CG2	4:A:320:HOH:O	2.36	0.73
1:B:124:ARG:HD3	1:B:134:TRP:CH2	2.23	0.73
1:A:224:ALA:C	1:A:225:LEU:HD23	2.14	0.72
1:B:67:MET:HE2	1:B:67:MET:CA	2.18	0.72
1:D:216:LYS:CB	1:D:223:ASN:H	2.03	0.72
1:C:256:VAL:HG13	1:C:260:VAL:HG23	1.71	0.72
1:A:55:PRO:HD2	1:A:297:ILE:HD13	1.72	0.72
1:C:218:ASP:CB	1:C:219:GLY:HA3	2.19	0.71
1:C:169:ALA:HB1	1:C:181:MET:HE3	1.72	0.71
1:C:249:HIS:CE1	3:C:505:CIT:O4	2.43	0.71
1:D:124:ARG:HD2	1:D:124:ARG:N	2.02	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:TYR:OH	1:C:217:GLY:HA3	1.90	0.71
1:A:114:ILE:HG21	1:A:282:PHE:HD1	1.54	0.71
1:C:218:ASP:H	1:C:219:GLY:HA3	1.55	0.71
1:D:86:VAL:O	1:D:255:ILE:CD1	2.39	0.70
1:D:86:VAL:C	1:D:255:ILE:HD11	2.17	0.70
1:D:226:ARG:HG2	1:D:237:ASP:OD1	1.92	0.70
3:A:501:CIT:O3	3:A:501:CIT:O2	2.09	0.70
1:B:67:MET:CE	1:B:70:MET:CE	2.46	0.69
1:D:45:LEU:O	1:D:48:THR:HG22	1.91	0.69
1:D:2:HIS:CB	1:D:110:THR:CG2	2.69	0.69
1:A:62:THR:HG22	4:A:320:HOH:O	1.93	0.69
1:D:96:PHE:HD2	1:D:114:ILE:HG22	1.57	0.69
3:D:504:CIT:C5	4:D:352:HOH:O	2.41	0.69
1:B:155:PRO:HD2	4:B:361:HOH:O	1.92	0.68
1:D:124:ARG:CD	1:D:124:ARG:N	2.56	0.68
1:A:33:GLY:HA2	1:A:84:GLU:O	1.93	0.68
1:D:6:THR:OG1	1:D:111:THR:CG2	2.40	0.68
1:C:181:MET:HE3	1:C:204:ILE:HD13	1.75	0.68
1:D:1:VAL:N	4:D:354:HOH:O	2.25	0.68
1:A:28:PRO:C	1:A:29:ILE:HD13	2.19	0.68
1:D:181:MET:CE	1:D:206:ILE:CG1	2.72	0.67
1:A:170:GLN:HE22	1:A:198:ALA:HA	1.59	0.67
1:C:49:THR:HG22	1:C:49:THR:O	1.95	0.67
1:D:2:HIS:HA	1:D:110:THR:CG2	2.25	0.67
1:D:2:HIS:CB	1:D:110:THR:HG23	2.25	0.66
1:D:181:MET:HE3	1:D:206:ILE:HG12	1.78	0.66
1:C:164:SER:H	3:C:505:CIT:C6	2.08	0.66
1:D:86:VAL:O	1:D:255:ILE:HD11	1.95	0.66
1:A:170:GLN:O	1:A:173:THR:OG1	2.14	0.66
1:C:213:LEU:HD23	1:C:226:ARG:NH1	2.10	0.66
1:D:157:ALA:HB1	1:D:182:LEU:HD11	1.77	0.66
1:B:10:SER:HB3	1:B:32:GLU:HA	1.77	0.65
1:D:125:MET:CB	1:D:245:TYR:CE1	2.79	0.65
1:D:182:LEU:HD12	1:D:182:LEU:H	1.62	0.65
1:B:32:GLU:OE1	1:B:71:ARG:CZ	2.44	0.65
1:D:209:ASN:HB3	1:D:230:THR:HB	1.76	0.65
1:A:240:VAL:HG13	1:A:242:GLY:H	1.60	0.65
1:A:164:SER:H	3:A:501:CIT:H21	1.61	0.65
1:D:134:TRP:CH2	1:D:140:ALA:HB2	2.31	0.65
1:A:133:TYR:CZ	1:A:217:GLY:HA3	2.32	0.65
1:C:170:GLN:HG2	1:C:197:ARG:CZ	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:LEU:HD12	1:D:182:LEU:N	2.12	0.64
1:A:3:ASN:O	1:A:111:THR:HA	1.97	0.64
1:D:264:GLU:OE2	1:D:264:GLU:N	2.31	0.64
1:C:99:TRP:N	1:C:99:TRP:CD1	2.65	0.64
1:A:194:MET:HA	1:A:194:MET:CE	2.28	0.63
1:D:2:HIS:CA	1:D:110:THR:HG23	2.28	0.63
1:D:201:ASN:HD22	1:D:203:LYS:N	1.88	0.63
1:B:169:ALA:HB3	1:B:181:MET:HE2	1.79	0.63
1:C:218:ASP:N	1:C:219:GLY:HA3	2.12	0.63
1:D:96:PHE:CD2	1:D:114:ILE:HG22	2.33	0.63
1:A:62:THR:HG22	1:A:64:SER:N	2.13	0.63
1:A:147:ALA:O	1:A:152:ARG:NH2	2.32	0.62
1:C:42:GLY:O	1:C:67:MET:HG3	1.98	0.62
1:D:157:ALA:HB1	1:D:182:LEU:CD1	2.29	0.62
1:B:66:LEU:C	1:B:67:MET:HE2	2.24	0.62
1:C:99:TRP:CH2	1:C:108:PRO:HD3	2.35	0.62
1:B:3:ASN:ND2	1:B:29:ILE:HG12	2.14	0.62
1:A:131:GLU:CD	1:A:131:GLU:H	2.08	0.61
1:D:2:HIS:CD2	1:D:110:THR:HG23	2.36	0.61
1:D:164:SER:O	1:D:168:GLU:CB	2.42	0.61
1:A:95:PRO:CG	1:A:110:THR:HG23	2.30	0.61
1:C:146:GLY:HA2	1:C:148:VAL:CB	2.31	0.61
1:A:201:ASN:HB3	1:A:204:ILE:HD12	1.81	0.61
1:B:32:GLU:OE1	1:B:71:ARG:NE	2.34	0.61
1:D:173:THR:HG21	1:D:201:ASN:OD1	2.01	0.60
1:B:49:THR:O	1:B:62:THR:HA	2.02	0.60
1:D:3:ASN:O	1:D:111:THR:HA	2.02	0.60
1:D:264:GLU:H	1:D:264:GLU:CD	2.09	0.60
1:A:166:CYS:O	1:A:170:GLN:HG2	2.01	0.60
1:D:43:GLY:HA2	2:D:403:FAD:O3B	2.00	0.60
1:D:137:GLY:O	1:D:242:GLY:HA2	2.02	0.60
1:A:30:LEU:C	1:A:30:LEU:HD23	2.27	0.60
1:D:86:VAL:HG12	1:D:255:ILE:CD1	2.32	0.60
1:B:67:MET:CE	1:B:67:MET:HA	2.31	0.60
1:B:181:MET:CE	1:B:204:ILE:HD13	2.32	0.60
1:D:156:LEU:HA	1:D:240:VAL:CG2	2.32	0.59
1:A:315:THR:HG22	1:A:315:THR:O	2.02	0.59
1:B:313:TYR:O	1:B:316:SER:OG	2.21	0.59
1:A:287:ASP:OD1	1:A:294:ARG:HA	2.02	0.59
1:B:67:MET:HE2	1:B:67:MET:N	2.17	0.59
1:A:41:ALA:HB3	4:A:322:HOH:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:GLY:O	1:A:189:ARG:HG2	2.03	0.59
1:C:91:LEU:H	1:C:259:GLN:NE2	2.00	0.59
1:B:71:ARG:O	1:B:75:THR:HG23	2.03	0.59
1:B:169:ALA:O	1:B:173:THR:HG23	2.02	0.59
1:B:89:VAL:HG23	1:B:89:VAL:O	2.02	0.58
1:C:87:SER:HA	1:C:255:ILE:HD11	1.85	0.58
1:C:216:LYS:O	1:C:222:LEU:HD12	2.03	0.58
1:C:256:VAL:CG1	1:C:260:VAL:CG2	2.81	0.58
1:D:10:SER:HB3	1:D:32:GLU:HA	1.84	0.58
1:C:91:LEU:H	1:C:259:GLN:HE22	1.50	0.58
1:C:140:ALA:HB1	4:C:341:HOH:O	2.03	0.58
1:C:206:ILE:HD12	4:C:374:HOH:O	2.04	0.58
1:B:181:MET:HE1	1:B:198:ALA:CB	2.32	0.58
1:A:124:ARG:NH1	1:A:130:GLU:OE2	2.35	0.57
1:B:2:HIS:CD2	1:B:110:THR:HG22	2.39	0.57
1:B:2:HIS:HD2	1:B:110:THR:HG22	1.68	0.57
1:C:44:GLN:OE1	1:C:122:ALA:N	2.24	0.57
1:A:10:SER:HB3	1:A:32:GLU:HA	1.85	0.57
1:D:155:PRO:O	1:D:240:VAL:HG23	2.05	0.57
1:A:55:PRO:CD	1:A:297:ILE:HD13	2.35	0.57
1:A:178:LYS:HD3	1:A:180:PHE:CZ	2.40	0.57
1:D:181:MET:CE	1:D:206:ILE:CD1	2.82	0.57
1:C:133:TYR:OH	1:C:217:GLY:CA	2.53	0.57
1:D:267:TYR:CE1	1:D:291:SER:HB3	2.39	0.57
1:C:184:ARG:HH21	3:C:503:CIT:C2	2.18	0.56
1:A:32:GLU:OE2	1:A:71:ARG:NH2	2.38	0.56
1:D:156:LEU:HA	1:D:240:VAL:HG23	1.87	0.56
1:C:186:ASP:HB3	1:C:209:ASN:OD1	2.06	0.56
1:A:95:PRO:HG2	1:A:110:THR:HG23	1.88	0.56
1:A:164:SER:O	1:A:168:GLU:HG3	2.05	0.56
1:B:95:PRO:HB2	1:B:110:THR:HG23	1.86	0.56
1:D:216:LYS:CB	1:D:224:ALA:O	2.53	0.56
1:B:66:LEU:CG	1:B:67:MET:HE3	2.28	0.56
1:A:169:ALA:O	1:A:173:THR:HG23	2.06	0.55
1:D:130:GLU:C	1:D:132:THR:H	2.13	0.55
1:D:45:LEU:O	1:D:63:GLY:HA3	2.06	0.55
1:A:44:GLN:NE2	2:A:400:FAD:H9	2.21	0.55
1:C:147:ALA:CB	1:C:151:PHE:CB	2.68	0.55
1:C:90:ASP:HB3	1:C:97:LYS:HB2	1.88	0.55
3:A:501:CIT:O3	3:A:501:CIT:C1	2.55	0.55
1:C:222:LEU:HD11	1:C:224:ALA:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:ARG:O	1:C:209:ASN:HA	2.06	0.55
1:D:99:TRP:CH2	1:D:108:PRO:HD3	2.42	0.55
1:D:51:ILE:HD13	1:D:66:LEU:HD23	1.89	0.55
1:A:171:PHE:O	1:A:174:LYS:HG3	2.08	0.54
1:B:51:ILE:HD11	1:B:54:PHE:HB2	1.89	0.54
1:C:133:TYR:CE2	1:C:217:GLY:HA3	2.41	0.54
1:D:83:THR:O	1:D:83:THR:HG22	2.07	0.54
1:B:45:LEU:HD12	4:B:327:HOH:O	2.06	0.54
1:D:156:LEU:CA	1:D:240:VAL:HG23	2.38	0.54
3:B:502:CIT:C6	3:B:502:CIT:O2	2.51	0.54
1:A:2:HIS:ND1	1:A:110:THR:HG22	2.22	0.54
1:D:2:HIS:CA	1:D:110:THR:CG2	2.85	0.54
1:B:37:ASN:HD21	1:B:39:ILE:HD13	1.73	0.54
1:C:124:ARG:HD3	1:C:134:TRP:CH2	2.43	0.53
1:D:99:TRP:CD2	1:D:108:PRO:HB3	2.43	0.53
1:A:114:ILE:CG2	1:A:282:PHE:HD1	2.15	0.53
1:A:29:ILE:HD12	1:A:80:GLU:HB3	1.88	0.53
1:B:148:VAL:HG22	1:B:151:PHE:CD2	2.43	0.53
1:D:163:ASP:O	1:D:167:GLU:HB2	2.08	0.53
1:C:223:ASN:O	1:C:224:ALA:HB2	2.08	0.53
1:D:61:LEU:HD23	1:D:66:LEU:HB2	1.91	0.53
1:D:99:TRP:CZ3	1:D:108:PRO:HD3	2.43	0.53
1:B:33:GLY:HA2	1:B:84:GLU:C	2.34	0.53
1:D:42:GLY:O	1:D:67:MET:HG3	2.08	0.53
1:B:94:LYS:HE3	1:B:96:PHE:CZ	2.45	0.52
1:B:240:VAL:HG13	1:B:242:GLY:O	2.09	0.52
1:C:145:ASP:CB	1:C:146:GLY:HA2	2.39	0.52
1:D:62:THR:HG22	1:D:65:GLU:H	1.75	0.52
1:C:139:SER:O	1:C:244:PHE:HA	2.10	0.52
1:D:129:GLY:HA3	1:D:215:ALA:HB2	1.92	0.52
1:B:67:MET:HE1	1:B:70:MET:SD	2.50	0.52
1:B:178:LYS:HE3	1:B:205:GLU:HB2	1.92	0.52
1:A:55:PRO:CG	1:A:297:ILE:HD13	2.39	0.52
1:B:263:ASP:OD1	1:B:263:ASP:C	2.52	0.51
1:D:124:ARG:O	1:D:124:ARG:HD3	2.11	0.51
1:B:186:ASP:OD1	1:B:186:ASP:C	2.54	0.51
1:D:7:ILE:HD11	1:D:21:LEU:HD12	1.92	0.51
1:D:275:SER:OG	1:D:306:ALA:HA	2.10	0.51
1:D:62:THR:HB	1:D:65:GLU:CD	2.35	0.51
1:D:89:VAL:HG21	1:D:256:VAL:HG23	1.91	0.51
1:B:134:TRP:O	1:B:135:GLN:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:TYR:O	1:C:138:ILE:HG13	2.11	0.51
1:C:169:ALA:O	1:C:173:THR:HG23	2.11	0.51
1:C:184:ARG:HH21	3:C:503:CIT:H21	1.76	0.51
1:C:49:THR:O	1:C:49:THR:CG2	2.59	0.51
1:B:181:MET:HE3	1:B:204:ILE:HD13	1.93	0.51
1:C:128:PRO:HD2	1:C:213:LEU:O	2.11	0.51
1:C:45:LEU:O	1:C:63:GLY:HA3	2.11	0.50
1:C:45:LEU:O	1:C:48:THR:HG22	2.11	0.50
1:D:86:VAL:O	1:D:255:ILE:HD12	2.11	0.50
1:A:170:GLN:HE22	1:A:198:ALA:CA	2.23	0.50
1:A:24:ALA:O	1:A:25:GLU:CB	2.59	0.50
1:A:208:TYR:O	1:A:210:THR:CG2	2.55	0.50
1:C:169:ALA:HB3	1:C:181:MET:HE2	1.69	0.50
1:D:91:LEU:HD11	1:D:256:VAL:CG2	2.42	0.50
1:D:88:LYS:HA	4:D:337:HOH:O	2.12	0.50
1:D:99:TRP:CE2	1:D:108:PRO:HB3	2.45	0.50
1:A:24:ALA:HB3	1:A:26:ILE:HD12	1.93	0.50
1:D:181:MET:HE1	1:D:206:ILE:CD1	2.41	0.50
1:D:270:THR:OG1	1:D:289:GLN:NE2	2.44	0.50
1:C:147:ALA:HA	1:C:148:VAL:CB	2.40	0.50
1:A:164:SER:O	1:A:168:GLU:CG	2.59	0.50
1:B:240:VAL:CG1	1:B:242:GLY:O	2.59	0.50
1:C:130:GLU:HA	1:C:138:ILE:HD12	1.94	0.50
1:A:299:SER:OG	2:A:400:FAD:H5'2	2.11	0.50
1:B:169:ALA:CB	1:B:181:MET:HE2	2.41	0.50
1:C:5:VAL:HG22	1:C:113:ALA:HB3	1.93	0.49
1:A:88:LYS:O	1:A:99:TRP:HD1	1.95	0.49
1:D:133:TYR:OH	1:D:217:GLY:CA	2.49	0.49
1:B:193:ILE:N	1:B:193:ILE:HD13	2.28	0.49
1:C:214:GLU:O	1:C:225:LEU:HD12	2.11	0.49
1:B:57:PHE:HE2	1:B:69:ARG:NH1	2.11	0.49
1:B:155:PRO:O	1:B:156:LEU:HD23	2.13	0.49
1:C:297:ILE:HG23	1:C:298:THR:N	2.28	0.49
1:D:263:ASP:C	1:D:263:ASP:OD1	2.55	0.49
1:D:267:TYR:CZ	1:D:291:SER:HB3	2.46	0.49
1:C:264:GLU:HG2	4:C:369:HOH:O	2.12	0.49
1:B:137:GLY:O	1:B:242:GLY:HA2	2.12	0.49
1:A:31:TYR:OH	1:A:109:VAL:HG21	2.13	0.48
1:B:263:ASP:O	4:B:344:HOH:O	2.20	0.48
1:B:285:ALA:HB2	1:B:306:ALA:HB2	1.95	0.48
1:B:116:LEU:O	1:B:284:ALA:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ILE:HD12	1:A:51:ILE:N	2.25	0.48
1:B:94:LYS:HA	1:B:95:PRO:C	2.38	0.48
1:D:62:THR:HG22	1:D:64:SER:N	2.28	0.48
1:B:186:ASP:OD1	1:B:187:HIS:ND1	2.35	0.48
1:D:21:LEU:HD22	1:D:26:ILE:HG21	1.96	0.48
1:D:133:TYR:CE2	1:D:215:ALA:HB1	2.49	0.48
1:C:130:GLU:O	1:C:130:GLU:HG2	2.14	0.48
1:D:2:HIS:CG	1:D:110:THR:HG23	2.48	0.48
1:B:89:VAL:O	1:B:89:VAL:CG2	2.62	0.48
1:A:10:SER:HB3	1:A:32:GLU:CA	2.43	0.47
1:C:132:THR:HG22	1:C:132:THR:O	2.14	0.47
1:D:263:ASP:HB2	1:D:264:GLU:OE2	2.14	0.47
1:A:137:GLY:O	1:A:242:GLY:HA2	2.13	0.47
1:B:37:ASN:O	1:B:37:ASN:ND2	2.46	0.47
1:B:67:MET:CE	1:B:67:MET:CA	2.87	0.47
1:B:274:SER:HA	1:B:305:MET:HE2	1.95	0.47
1:C:96:PHE:O	1:C:110:THR:HA	2.14	0.47
1:B:48:THR:HG23	2:B:401:FAD:C6	2.41	0.47
1:D:96:PHE:O	1:D:110:THR:HA	2.14	0.47
1:C:26:ILE:HG22	1:C:26:ILE:O	2.15	0.47
1:D:214:GLU:HB2	1:D:226:ARG:HB2	1.96	0.47
1:B:89:VAL:HG21	1:B:256:VAL:CG1	2.40	0.47
1:C:114:ILE:HG13	1:C:282:PHE:CD1	2.49	0.47
1:B:184:ARG:HG3	1:B:211:VAL:CG2	2.44	0.47
1:C:15:HIS:O	1:C:19:ILE:N	2.44	0.47
1:A:19:ILE:O	1:A:23:ARG:HG3	2.14	0.47
1:A:114:ILE:HD13	1:A:114:ILE:C	2.39	0.47
1:A:181:MET:CE	1:A:198:ALA:HB1	2.43	0.47
1:C:120:ALA:HA	1:C:250:THR:O	2.15	0.47
1:B:51:ILE:CD1	1:B:54:PHE:HB2	2.45	0.47
1:B:133:TYR:CE2	1:B:218:ASP:O	2.67	0.47
1:D:10:SER:HB3	1:D:32:GLU:CA	2.45	0.47
1:B:99:TRP:CE2	1:B:108:PRO:HB3	2.49	0.47
1:C:213:LEU:HD23	1:C:226:ARG:HH12	1.80	0.47
1:D:156:LEU:O	1:D:179:VAL:HA	2.15	0.47
1:D:288:VAL:O	1:D:288:VAL:HG22	2.14	0.46
1:B:3:ASN:O	1:B:111:THR:HA	2.16	0.46
1:B:152:ARG:HD3	1:B:152:ARG:HA	1.75	0.46
1:A:101:GLU:O	1:A:102:PHE:HB2	2.15	0.46
1:C:134:TRP:O	1:C:135:GLN:HB2	2.15	0.46
1:C:240:VAL:HG13	1:C:242:GLY:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:MET:HE3	1:D:206:ILE:CG1	2.43	0.46
1:A:99:TRP:CD1	1:A:99:TRP:N	2.84	0.46
1:A:114:ILE:O	1:A:114:ILE:HG23	2.15	0.46
1:A:150:ILE:HD12	1:A:150:ILE:HG23	1.72	0.46
1:B:67:MET:CE	1:B:67:MET:N	2.77	0.46
1:B:179:VAL:O	1:B:204:ILE:HA	2.16	0.46
1:B:189:ARG:NH1	3:B:502:CIT:H41	2.30	0.46
1:C:276:LEU:HD23	1:C:283:PHE:CE2	2.51	0.46
1:D:139:SER:HB3	1:D:244:PHE:CD2	2.51	0.46
1:A:95:PRO:CG	1:A:110:THR:CG2	2.94	0.46
1:A:114:ILE:HD12	1:A:282:PHE:HE1	1.78	0.46
1:D:133:TYR:CD2	1:D:215:ALA:HB1	2.50	0.46
3:A:501:CIT:O3	3:A:501:CIT:C2	2.60	0.45
1:B:125:MET:CG	1:B:245:TYR:CE1	2.99	0.45
1:A:51:ILE:HD11	1:A:63:GLY:HA2	1.97	0.45
1:B:262:THR:HA	1:B:267:TYR:O	2.16	0.45
1:C:134:TRP:C	1:C:136:LYS:H	2.24	0.45
1:D:94:LYS:HA	1:D:94:LYS:HD3	1.78	0.45
1:D:141:CYS:HB3	1:D:144:CYS:HB2	1.84	0.45
1:D:201:ASN:ND2	1:D:201:ASN:C	2.61	0.45
1:A:114:ILE:HD13	1:A:114:ILE:HG23	1.36	0.45
1:B:167:GLU:CG	1:B:194:MET:CE	2.92	0.45
1:D:95:PRO:CG	1:D:110:THR:OG1	2.65	0.45
1:B:29:ILE:N	1:B:29:ILE:CD1	2.80	0.45
1:B:213:LEU:HD11	1:B:228:LYS:HB2	1.98	0.45
1:C:91:LEU:HD11	1:C:256:VAL:HG21	1.97	0.45
1:A:66:LEU:O	1:A:69:ARG:HB2	2.17	0.45
1:B:104:GLU:H	1:B:104:GLU:HG2	1.46	0.45
1:B:139:SER:O	1:B:244:PHE:HA	2.16	0.45
1:C:91:LEU:HD11	1:C:256:VAL:CG2	2.47	0.45
1:B:6:THR:HG21	1:B:98:LEU:HD22	1.98	0.45
1:C:287:ASP:OD1	1:C:294:ARG:HA	2.16	0.45
1:D:155:PRO:C	1:D:240:VAL:HG23	2.42	0.45
1:A:114:ILE:HD12	1:A:282:PHE:CD1	2.52	0.45
1:B:133:TYR:OH	1:B:218:ASP:O	2.33	0.45
1:B:182:LEU:CD2	1:B:207:LEU:HD12	2.47	0.45
1:D:62:THR:HG22	1:D:64:SER:H	1.81	0.45
1:A:133:TYR:CE2	1:A:217:GLY:HA3	2.51	0.45
1:B:144:CYS:SG	2:B:401:FAD:C4X	3.05	0.45
1:A:114:ILE:HD12	1:A:114:ILE:HG21	1.56	0.44
1:C:118:THR:HB	1:C:252:ALA:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ASP:HB3	1:A:97:LYS:HB2	1.98	0.44
2:B:401:FAD:HM71	2:B:401:FAD:HM83	1.82	0.44
1:C:147:ALA:CA	1:C:148:VAL:C	2.78	0.44
1:D:142:ALA:HA	1:D:244:PHE:CD2	2.52	0.44
1:C:83:THR:HG22	1:C:83:THR:O	2.18	0.44
1:C:256:VAL:CG1	1:C:260:VAL:HG21	2.46	0.44
1:B:17:ALA:HA	1:B:307:ALA:HB2	1.97	0.44
1:A:155:PRO:O	1:A:156:LEU:HD23	2.17	0.44
1:B:130:GLU:OE1	1:B:245:TYR:OH	2.29	0.44
1:B:168:GLU:O	1:B:172:LEU:HG	2.18	0.44
1:B:125:MET:HB2	1:B:245:TYR:CE1	2.52	0.44
1:B:217:GLY:HA2	1:B:223:ASN:CG	2.42	0.44
1:C:6:THR:HB	1:C:114:ILE:HG22	2.00	0.44
1:D:187:HIS:ND1	1:D:208:TYR:HE2	2.16	0.44
1:B:57:PHE:CD2	1:B:61:LEU:HD22	2.53	0.44
1:B:163:ASP:OD2	3:B:506:CIT:O1	2.36	0.44
1:D:43:GLY:O	1:D:45:LEU:N	2.51	0.44
1:D:235:GLU:C	1:D:236:THR:HG23	2.43	0.44
1:B:67:MET:HE2	1:B:70:MET:HE2	1.79	0.43
1:A:114:ILE:CD1	1:A:282:PHE:CE1	2.97	0.43
1:A:234:GLU:OE1	1:C:125:MET:HE2	2.17	0.43
1:C:119:GLY:HA3	2:C:402:FAD:O1A	2.18	0.43
1:C:213:LEU:HD12	1:C:213:LEU:HA	1.70	0.43
2:C:402:FAD:H9	2:C:402:FAD:H1'1	1.85	0.43
1:D:180:PHE:HE1	1:D:205:GLU:OE2	2.01	0.43
1:A:172:LEU:HD11	1:A:244:PHE:CG	2.54	0.43
1:B:62:THR:OG1	1:B:65:GLU:HG3	2.18	0.43
1:D:91:LEU:HA	1:D:96:PHE:CD1	2.53	0.43
1:D:310:ALA:O	1:D:314:LEU:HG	2.17	0.43
1:A:57:PHE:CG	1:A:61:LEU:HD22	2.53	0.43
1:A:240:VAL:CG1	1:A:242:GLY:O	2.67	0.43
1:B:66:LEU:O	1:B:67:MET:HE2	2.18	0.43
1:A:115:ILE:HG12	1:A:283:PHE:HB2	2.00	0.43
1:A:62:THR:HB	1:A:65:GLU:HB2	2.01	0.43
1:C:184:ARG:HB2	1:C:211:VAL:HG22	2.01	0.43
1:C:211:VAL:HG12	1:C:212:ALA:O	2.19	0.43
1:A:315:THR:O	1:A:315:THR:CG2	2.67	0.43
1:B:240:VAL:HG13	1:B:242:GLY:H	1.84	0.43
1:C:34:MET:O	1:C:35:MET:HB2	2.19	0.43
1:D:114:ILE:C	1:D:114:ILE:HD13	2.44	0.43
1:C:114:ILE:HG23	1:C:114:ILE:HD13	1.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ASN:ND2	4:A:348:HOH:O	2.48	0.43
1:B:37:ASN:ND2	1:B:39:ILE:HD13	2.34	0.43
1:B:90:ASP:OD1	1:B:92:SER:OG	2.30	0.43
1:A:6:THR:O	1:A:114:ILE:HA	2.18	0.42
1:D:55:PRO:HG2	1:D:297:ILE:HD13	2.00	0.42
3:D:504:CIT:C4	4:D:352:HOH:O	2.67	0.42
1:B:225:LEU:HD11	1:B:243:LEU:HD13	2.00	0.42
1:B:164:SER:OG	3:B:506:CIT:O5	2.27	0.42
1:C:45:LEU:HA	1:C:45:LEU:HD12	1.63	0.42
1:B:94:LYS:HE3	1:B:96:PHE:CE2	2.54	0.42
1:B:159:ILE:HG22	1:B:247:ILE:CG2	2.50	0.42
1:D:55:PRO:CG	1:D:297:ILE:HD13	2.49	0.42
1:D:90:ASP:N	1:D:97:LYS:O	2.36	0.42
1:B:256:VAL:O	1:B:257:ALA:C	2.61	0.42
1:B:270:THR:OG1	1:B:289:GLN:NE2	2.50	0.42
1:A:59:ASP:HB2	4:A:324:HOH:O	2.19	0.42
1:C:34:MET:O	1:C:34:MET:HG2	2.20	0.42
1:C:35:MET:O	1:C:36:ALA:C	2.60	0.42
1:C:62:THR:HG1	1:C:65:GLU:HG3	1.80	0.42
1:C:88:LYS:O	1:C:99:TRP:HD1	2.02	0.42
2:C:402:FAD:HM71	2:C:402:FAD:HM83	1.81	0.42
1:B:12:PRO:CB	1:B:70:MET:HE1	2.50	0.42
1:B:26:ILE:CD1	1:B:311:GLU:HG2	2.50	0.42
1:B:144:CYS:SG	2:B:401:FAD:C10	3.08	0.42
1:B:173:THR:HB	1:B:203:LYS:HE3	2.01	0.42
1:C:6:THR:OG1	1:C:111:THR:HG21	2.19	0.42
1:C:186:ASP:HA	1:C:208:TYR:HB3	2.00	0.42
1:A:164:SER:HB2	3:A:501:CIT:H22	2.02	0.42
1:B:10:SER:O	1:B:42:GLY:HA2	2.20	0.42
1:B:69:ARG:HB3	1:C:58:PRO:HG3	2.02	0.42
1:D:99:TRP:CE3	1:D:108:PRO:HB3	2.55	0.42
1:D:134:TRP:CZ2	1:D:140:ALA:HB2	2.55	0.42
1:D:214:GLU:O	1:D:225:LEU:HD12	2.19	0.42
1:B:57:PHE:CG	1:B:61:LEU:HD22	2.55	0.42
1:B:90:ASP:CG	1:B:92:SER:HG	2.26	0.42
1:C:170:GLN:HG2	1:C:197:ARG:NH2	2.34	0.42
1:A:45:LEU:O	1:A:63:GLY:HA3	2.20	0.42
1:C:213:LEU:HB2	1:C:226:ARG:O	2.20	0.42
1:C:276:LEU:CD2	1:C:283:PHE:HE2	2.33	0.42
1:C:223:ASN:OD1	1:C:223:ASN:C	2.63	0.41
1:A:160:GLY:O	1:A:183:VAL:HG22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LYS:HA	1:A:200:LYS:HD3	1.79	0.41
2:D:403:FAD:H9	2:D:403:FAD:H1'1	1.72	0.41
1:D:91:LEU:HD11	1:D:256:VAL:HG21	2.03	0.41
1:D:151:PHE:O	1:D:152:ARG:C	2.64	0.41
1:D:184:ARG:O	1:D:209:ASN:HA	2.20	0.41
1:A:181:MET:CE	1:A:204:ILE:HG21	2.46	0.41
1:A:240:VAL:HG13	1:A:242:GLY:O	2.21	0.41
1:D:127:LEU:HD22	1:D:127:LEU:HA	1.64	0.41
1:B:28:PRO:C	1:B:29:ILE:HD12	2.46	0.41
1:B:66:LEU:C	1:B:67:MET:CE	2.93	0.41
1:B:215:ALA:HB1	1:B:222:LEU:CD1	2.50	0.41
1:C:122:ALA:HA	1:C:249:HIS:CD2	2.55	0.41
1:A:127:LEU:HD23	1:A:127:LEU:HA	1.90	0.41
1:A:164:SER:OG	3:A:501:CIT:C4	2.63	0.41
1:A:270:THR:OG1	1:A:289:GLN:NE2	2.53	0.41
1:B:206:ILE:HG21	1:B:208:TYR:CZ	2.56	0.41
1:C:262:THR:HA	1:C:267:TYR:O	2.21	0.41
1:A:57:PHE:HA	1:A:58:PRO:HD2	1.88	0.41
1:A:144:CYS:SG	2:A:400:FAD:C4X	3.09	0.41
1:B:178:LYS:HA	1:B:178:LYS:HD3	1.84	0.41
1:C:124:ARG:HD3	1:C:134:TRP:CZ3	2.55	0.41
1:C:168:GLU:O	1:C:172:LEU:HG	2.21	0.41
1:D:43:GLY:HA2	2:D:403:FAD:HO3A	1.84	0.41
1:D:172:LEU:HD23	1:D:172:LEU:HA	1.94	0.41
1:D:235:GLU:C	1:D:236:THR:CG2	2.93	0.41
1:D:240:VAL:HG22	1:D:242:GLY:H	1.85	0.41
1:A:133:TYR:HB2	1:A:138:ILE:HD12	2.03	0.41
1:B:227:ILE:HD11	1:B:236:THR:HG23	2.03	0.41
1:C:225:LEU:HD12	1:C:225:LEU:HA	1.78	0.41
1:D:114:ILE:HD12	1:D:282:PHE:CE1	2.56	0.41
1:B:189:ARG:NH2	3:B:506:CIT:O6	2.53	0.40
1:A:109:VAL:HG12	1:A:110:THR:N	2.37	0.40
1:A:178:LYS:NZ	1:A:205:GLU:OE1	2.54	0.40
1:A:181:MET:HE1	1:A:198:ALA:CB	2.44	0.40
1:B:164:SER:CB	3:B:506:CIT:O5	2.69	0.40
1:B:227:ILE:CG1	1:B:236:THR:HG23	2.51	0.40
1:C:172:LEU:HB2	1:C:179:VAL:HG21	2.03	0.40
1:A:122:ALA:HA	1:A:249:HIS:CD2	2.56	0.40
1:B:178:LYS:HD3	1:B:203:LYS:O	2.21	0.40
1:C:109:VAL:H	1:C:109:VAL:HG23	1.57	0.40
1:C:133:TYR:CZ	1:C:217:GLY:CA	2.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:ALA:CA	1:C:148:VAL:CB	2.98	0.40
1:A:161:GLY:C	1:A:189:ARG:HG2	2.46	0.40
1:D:253:THR:O	1:D:254:LYS:C	2.65	0.40
1:D:276:LEU:HD23	1:D:283:PHE:HE2	1.87	0.40
1:D:130:GLU:C	1:D:132:THR:N	2.78	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	316/338 (94%)	300 (95%)	15 (5%)	1 (0%)	36	50
1	B	317/338 (94%)	301 (95%)	16 (5%)	0	100	100
1	C	308/338 (91%)	296 (96%)	12 (4%)	0	100	100
1	D	301/338 (89%)	280 (93%)	21 (7%)	0	100	100
All	All	1242/1352 (92%)	1177 (95%)	64 (5%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ALA

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	249/270 (92%)	230 (92%)	19 (8%)	12	21
1	B	247/270 (92%)	230 (93%)	17 (7%)	14	24
1	C	232/270 (86%)	214 (92%)	18 (8%)	11	20
1	D	222/270 (82%)	200 (90%)	22 (10%)	7	11
All	All	950/1080 (88%)	874 (92%)	76 (8%)	11	19

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ILE
1	A	45	LEU
1	A	51	ILE
1	A	59	ASP
1	A	98	LEU
1	A	99	TRP
1	A	110	THR
1	A	114	ILE
1	A	125	MET
1	A	168	GLU
1	A	194	MET
1	A	200	LYS
1	A	203	LYS
1	A	221	LEU
1	A	225	LEU
1	A	240	VAL
1	A	260	VAL
1	A	276	LEU
1	A	289	GLN
1	B	27	LYS
1	B	29	ILE
1	B	37	ASN
1	B	45	LEU
1	B	104	GLU
1	B	110	THR
1	B	170	GLN
1	B	178	LYS
1	B	189	ARG
1	B	202	GLU
1	B	221	LEU
1	B	230	THR
1	B	236	THR
1	B	240	VAL

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Mol	Chain	Res	Type
1	B	289	GLN
1	B	292	LYS
1	B	297	ILE
1	C	45	LEU
1	C	51	ILE
1	C	52	GLU
1	C	64	SER
1	C	99	TRP
1	C	109	VAL
1	C	111	THR
1	C	114	ILE
1	C	153	ASN
1	C	178	LYS
1	C	213	LEU
1	C	240	VAL
1	C	255	ILE
1	C	256	VAL
1	C	260	VAL
1	C	289	GLN
1	C	291	SER
1	C	314	LEU
1	D	1	VAL
1	D	26	ILE
1	D	39	ILE
1	D	51	ILE
1	D	62	THR
1	D	89	VAL
1	D	94	LYS
1	D	99	TRP
1	D	108	PRO
1	D	111	THR
1	D	114	ILE
1	D	124	ARG
1	D	127	LEU
1	D	148	VAL
1	D	201	ASN
1	D	211	VAL
1	D	214	GLU
1	D	256	VAL
1	D	260	VAL
1	D	272	PRO
1	D	289	GLN

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Mol	Chain	Res	Type
1	D	308	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	289	GLN
1	A	295	GLN
1	B	2	HIS
1	B	3	ASN
1	B	37	ASN
1	B	170	GLN
1	B	289	GLN
1	C	103	ASN
1	C	126	HIS
1	C	259	GLN
1	C	289	GLN
1	D	3	ASN
1	D	201	ASN
1	D	289	GLN

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](#)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CIT	C	503	-	12,12,12	1.56	2 (16%)	17,17,17	2.25	7 (41%)
2	FAD	B	401	-	58,58,58	1.20	7 (12%)	85,89,89	1.96	20 (23%)
2	FAD	A	400	-	58,58,58	1.45	6 (10%)	85,89,89	1.76	21 (24%)
3	CIT	B	506	-	12,12,12	1.93	3 (25%)	17,17,17	2.60	10 (58%)
3	CIT	C	505	-	12,12,12	2.72	2 (16%)	17,17,17	3.71	12 (70%)
3	CIT	B	502	-	12,12,12	1.28	2 (16%)	17,17,17	2.12	6 (35%)
3	CIT	A	501	-	12,12,12	1.45	2 (16%)	17,17,17	2.81	9 (52%)
2	FAD	C	402	-	58,58,58	1.46	8 (13%)	85,89,89	1.74	22 (25%)
2	FAD	D	403	-	58,58,58	1.19	6 (10%)	85,89,89	1.82	26 (30%)
3	CIT	D	504	-	12,12,12	1.31	1 (8%)	17,17,17	2.04	7 (41%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CIT	C	503	-	-	7/16/16/16	-
2	FAD	B	401	-	-	5/34/50/50	0/6/6/6
2	FAD	A	400	-	-	9/34/50/50	0/6/6/6
3	CIT	B	506	-	-	10/16/16/16	-
3	CIT	C	505	-	-	0/16/16/16	-
3	CIT	B	502	-	-	5/16/16/16	-
3	CIT	A	501	-	-	5/16/16/16	-
2	FAD	C	402	-	-	6/34/50/50	0/6/6/6
2	FAD	D	403	-	-	5/34/50/50	0/6/6/6
3	CIT	D	504	-	-	6/16/16/16	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	505	CIT	C3-C6	-8.52	1.44	1.53
2	C	402	FAD	P-O3P	-6.48	1.52	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	506	CIT	C3-C6	-4.73	1.48	1.53
2	A	400	FAD	C2A-N1A	4.28	1.41	1.33
3	C	503	CIT	C3-C6	4.05	1.57	1.53
2	D	403	FAD	C8A-N7A	3.97	1.39	1.31
2	A	400	FAD	C8A-N7A	3.85	1.39	1.31
2	A	400	FAD	C4X-N5	3.61	1.38	1.30
2	A	400	FAD	C5A-N7A	-3.33	1.33	1.39
3	B	506	CIT	C2-C3	-3.09	1.50	1.54
2	C	402	FAD	C4X-N5	3.01	1.37	1.30
2	B	401	FAD	C2A-N1A	2.98	1.39	1.33
2	B	401	FAD	C4X-N5	2.89	1.37	1.30
2	D	403	FAD	C4'-C3'	-2.68	1.48	1.53
2	D	403	FAD	C2A-N3A	2.64	1.38	1.33
2	A	400	FAD	O4B-C4B	-2.62	1.39	1.45
3	D	504	CIT	C3-C6	-2.61	1.50	1.53
2	D	403	FAD	C4X-N5	2.50	1.36	1.30
3	A	501	CIT	C4-C3	-2.46	1.50	1.54
2	B	401	FAD	P-O3P	2.45	1.62	1.59
2	B	401	FAD	C5A-N7A	-2.38	1.34	1.39
3	B	502	CIT	C3-C6	-2.37	1.51	1.53
2	C	402	FAD	C2A-N1A	2.29	1.38	1.33
2	D	403	FAD	C2A-N1A	2.27	1.38	1.33
3	C	503	CIT	O7-C3	2.26	1.47	1.43
3	A	501	CIT	O7-C3	2.20	1.47	1.43
2	C	402	FAD	C8A-N7A	2.18	1.35	1.31
2	C	402	FAD	C10-N1	2.17	1.37	1.33
2	A	400	FAD	PA-O3P	2.17	1.61	1.59
2	D	403	FAD	C4X-C4	-2.16	1.36	1.44
3	B	502	CIT	C4-C3	-2.15	1.51	1.54
2	B	401	FAD	C4X-C4	-2.14	1.36	1.44
2	C	402	FAD	O2-C2	-2.14	1.20	1.24
2	C	402	FAD	C5X-N5	-2.13	1.35	1.39
3	C	505	CIT	O2-C1	-2.11	1.23	1.30
2	B	401	FAD	C9A-N10	-2.04	1.37	1.41
2	C	402	FAD	C4X-C10	-2.03	1.38	1.44
3	B	506	CIT	O2-C1	-2.02	1.24	1.30
2	B	401	FAD	C4X-C10	-2.02	1.38	1.44

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	505	CIT	O7-C3-C6	-8.25	97.26	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	503	CIT	O6-C6-C3	6.85	126.28	113.14
2	C	402	FAD	N3A-C2A-N1A	-6.11	119.33	128.58
2	D	403	FAD	N3A-C2A-N1A	-6.09	119.37	128.58
2	B	401	FAD	N3A-C2A-N1A	-5.81	119.79	128.58
3	B	506	CIT	C2-C3-C6	-5.40	98.08	110.03
3	C	505	CIT	O2-C1-C2	5.36	131.34	114.35
2	A	400	FAD	N9A-C8A-N7A	-5.17	106.61	113.94
3	A	501	CIT	O6-C6-C3	5.15	123.03	113.14
3	A	501	CIT	C4-C3-C2	-5.14	96.13	109.31
3	B	502	CIT	O6-C6-C3	4.89	122.51	113.14
3	D	504	CIT	O7-C3-C6	-4.86	102.06	108.96
3	C	505	CIT	C4-C3-C6	-4.48	100.12	110.03
2	B	401	FAD	N9A-C8A-N7A	-4.46	107.61	113.94
3	A	501	CIT	O1-C1-C2	-4.41	110.46	122.95
2	B	401	FAD	C5A-C4A-N3A	-4.37	120.70	126.72
2	D	403	FAD	O3P-PA-O1A	-4.29	97.80	110.70
3	B	506	CIT	O2-C1-C2	4.26	127.84	114.35
3	C	505	CIT	O2-C1-O1	-4.22	112.48	123.33
3	B	502	CIT	O5-C6-C3	-4.21	113.93	122.09
2	A	400	FAD	N3A-C2A-N1A	-4.18	122.25	128.58
2	C	402	FAD	C9A-C5X-N5	-4.14	118.06	122.45
2	B	401	FAD	C4X-C10-N10	4.13	122.40	116.48
2	B	401	FAD	C4-N3-C2	-4.09	118.37	125.64
2	B	401	FAD	O2A-PA-O3P	4.05	118.21	107.27
2	B	401	FAD	C2B-C1B-N9A	-4.03	103.28	113.30
2	B	401	FAD	C5A-N7A-C8A	4.00	109.74	103.45
3	C	505	CIT	C2-C3-C6	-3.98	101.23	110.03
3	C	505	CIT	O5-C6-C3	-3.94	114.46	122.09
2	B	401	FAD	O3P-PA-O1A	-3.90	98.97	110.70
3	A	501	CIT	C3-C4-C5	-3.77	103.62	113.92
2	A	400	FAD	O2A-PA-O3P	3.74	117.39	107.27
3	C	505	CIT	O7-C3-C4	3.73	117.88	109.38
3	C	505	CIT	C4-C3-C2	3.68	118.76	109.31
2	D	403	FAD	C4X-C10-N10	3.67	121.74	116.48
2	B	401	FAD	C2A-N3A-C4A	3.62	120.66	111.83
3	A	501	CIT	C3-C2-C1	-3.60	104.08	113.92
2	A	400	FAD	C5A-N7A-C8A	3.48	108.93	103.45
2	B	401	FAD	O2P-P-O3P	-3.45	97.96	107.27
2	B	401	FAD	C4X-C4-N3	3.44	122.02	113.25
2	C	402	FAD	C2A-N1A-C6A	3.36	124.25	118.73
2	C	402	FAD	C5'-C4'-C3'	-3.28	106.02	112.22
2	D	403	FAD	C9A-C5X-N5	-3.26	118.99	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	403	FAD	O5'-C5'-C4'	-3.25	100.68	109.36
2	A	400	FAD	C4A-N9A-C8A	3.25	109.15	105.74
2	A	400	FAD	O4-C4-C4X	-3.24	117.99	126.53
2	D	403	FAD	N9A-C8A-N7A	-3.23	109.35	113.94
3	B	506	CIT	O4-C5-O3	-3.23	115.03	123.33
3	C	505	CIT	O3-C5-C4	-3.21	113.86	122.95
2	A	400	FAD	C4-N3-C2	-3.19	119.98	125.64
2	B	401	FAD	C4X-C10-N1	-3.16	116.85	124.59
2	B	401	FAD	O3P-P-O1P	3.15	120.17	110.70
2	C	402	FAD	O3'-C3'-C2'	3.09	115.94	108.93
2	D	403	FAD	O2P-P-O3P	-3.05	99.03	107.27
3	C	505	CIT	O4-C5-C4	3.05	124.00	114.35
2	D	403	FAD	C2A-N1A-C6A	3.04	123.73	118.73
2	A	400	FAD	C4'-C3'-C2'	-3.04	108.52	113.57
2	A	400	FAD	O3P-PA-O1A	-3.04	101.57	110.70
2	C	402	FAD	O2'-C2'-C3'	-3.01	102.21	109.25
2	C	402	FAD	O5'-C5'-C4'	-3.00	101.34	109.36
2	A	400	FAD	C4X-C4-N3	2.99	120.86	113.25
2	A	400	FAD	C9A-C5X-N5	-2.98	119.30	122.45
2	D	403	FAD	C10-C4X-N5	-2.96	118.76	124.81
3	B	506	CIT	O5-C6-C3	-2.95	116.39	122.09
2	D	403	FAD	C5A-C4A-N3A	-2.95	122.66	126.72
2	C	402	FAD	C4-N3-C2	-2.91	120.47	125.64
2	C	402	FAD	C5A-C4A-N3A	-2.90	122.72	126.72
2	C	402	FAD	O4'-C4'-C3'	2.90	116.04	109.25
3	D	504	CIT	O4-C5-C4	2.88	123.47	114.35
2	D	403	FAD	C10-N1-C2	2.88	123.08	116.85
2	D	403	FAD	C5X-C9A-N10	2.87	120.56	117.97
3	B	506	CIT	O4-C5-C4	2.84	123.36	114.35
3	B	502	CIT	C3-C2-C1	-2.79	106.28	113.92
2	B	401	FAD	C10-C4X-N5	-2.78	119.12	124.81
3	B	506	CIT	O1-C1-C2	-2.78	115.07	122.95
3	A	501	CIT	O2-C1-C2	2.75	123.07	114.35
3	D	504	CIT	O4-C5-O3	-2.75	116.26	123.33
2	A	400	FAD	C4X-C10-N10	2.73	120.39	116.48
3	B	506	CIT	O6-C6-C3	2.69	118.29	113.14
2	B	401	FAD	C4A-C5A-N7A	-2.68	107.52	110.58
3	A	501	CIT	O6-C6-O5	-2.68	115.30	123.86
2	B	401	FAD	N3A-C4A-N9A	2.67	131.71	127.17
3	A	501	CIT	C2-C3-C6	2.67	115.94	110.03
2	A	400	FAD	O5B-C5B-C4B	-2.61	100.09	108.99
2	A	400	FAD	C5A-C4A-N3A	-2.60	123.14	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	504	CIT	O2-C1-C2	2.59	122.56	114.35
3	A	501	CIT	O7-C3-C2	2.59	115.28	109.38
3	C	505	CIT	O7-C3-C2	2.58	115.26	109.38
2	C	402	FAD	O3P-P-O1P	-2.57	102.97	110.70
2	C	402	FAD	C2A-N3A-C4A	2.56	118.08	111.83
3	D	504	CIT	C4-C3-C2	2.55	115.84	109.31
2	A	400	FAD	O3P-P-O1P	2.54	118.34	110.70
3	B	502	CIT	C4-C3-C6	-2.52	104.47	110.03
2	B	401	FAD	C10-N1-C2	2.52	122.30	116.85
2	D	403	FAD	C4-N3-C2	-2.52	121.17	125.64
3	B	506	CIT	O2-C1-O1	-2.49	116.94	123.33
3	C	503	CIT	O6-C6-O5	-2.46	115.99	123.86
2	D	403	FAD	C5A-C4A-N9A	2.46	108.49	105.81
2	C	402	FAD	C6-C5X-C9A	2.45	122.42	119.05
2	A	400	FAD	C1'-N10-C9A	2.45	125.39	120.63
2	A	400	FAD	O3'-C3'-C4'	-2.45	103.37	108.93
3	C	503	CIT	O1-C1-C2	-2.43	116.06	122.95
2	A	400	FAD	C6-C5X-C9A	2.39	122.34	119.05
3	C	505	CIT	O1-C1-C2	-2.39	116.17	122.95
3	C	503	CIT	O2-C1-C2	2.39	121.90	114.35
2	D	403	FAD	C4X-C10-N1	-2.36	118.80	124.59
2	B	401	FAD	O4-C4-C4X	-2.31	120.43	126.53
3	D	504	CIT	O2-C1-O1	-2.31	117.39	123.33
3	B	502	CIT	O7-C3-C6	-2.31	105.68	108.96
2	D	403	FAD	C2A-N3A-C4A	2.29	117.43	111.83
2	D	403	FAD	O2A-PA-O3P	2.28	113.45	107.27
3	D	504	CIT	C3-C2-C1	-2.28	107.68	113.92
2	D	403	FAD	C4A-N9A-C1B	-2.26	121.34	126.63
2	C	402	FAD	C5A-N7A-C8A	2.26	107.00	103.45
3	C	503	CIT	O5-C6-C3	-2.26	117.72	122.09
2	C	402	FAD	C5X-C9A-N10	2.25	120.00	117.97
2	D	403	FAD	C2B-C1B-N9A	-2.25	107.72	113.30
2	C	402	FAD	N9A-C8A-N7A	-2.24	110.76	113.94
2	A	400	FAD	C10-N1-C2	2.24	121.69	116.85
2	C	402	FAD	C5X-N5-C4X	2.24	121.71	118.09
2	C	402	FAD	C5B-C4B-C3B	-2.23	107.17	115.21
2	D	403	FAD	C4A-C5A-N7A	-2.19	108.08	110.58
2	A	400	FAD	O2'-C2'-C3'	-2.17	104.17	109.25
2	C	402	FAD	C4A-C5A-N7A	-2.16	108.11	110.58
2	D	403	FAD	C5A-N7A-C8A	2.15	106.83	103.45
3	B	506	CIT	C4-C3-C6	2.14	114.77	110.03
3	C	503	CIT	C3-C2-C1	-2.13	108.10	113.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	402	FAD	C5A-C4A-N9A	2.12	108.12	105.81
2	D	403	FAD	C5X-N5-C4X	2.11	121.50	118.09
3	C	503	CIT	O4-C5-C4	2.10	120.99	114.35
2	C	402	FAD	C4'-C3'-C2'	-2.09	110.10	113.57
2	D	403	FAD	C4-C4X-C10	2.05	120.45	116.93
2	D	403	FAD	O4'-C4'-C5'	-2.05	105.47	109.99
3	B	502	CIT	O7-C3-C4	2.04	114.03	109.38
2	B	401	FAD	C4'-C3'-C2'	-2.03	110.19	113.57
2	D	403	FAD	C1'-C2'-C3'	-2.03	104.16	109.66
2	D	403	FAD	C4X-C4-N3	2.02	118.40	113.25
2	C	402	FAD	C4X-C10-N10	2.02	119.37	116.48
3	B	506	CIT	C3-C2-C1	-2.00	108.44	113.92
2	A	400	FAD	C6A-C5A-C4A	2.00	119.92	117.18

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	FAD	O4'-C4'-C5'-O5'
2	B	401	FAD	O4B-C4B-C5B-O5B
2	C	402	FAD	C5'-O5'-P-O2P
2	C	402	FAD	C5'-O5'-P-O3P
3	A	501	CIT	C1-C2-C3-O7
3	A	501	CIT	C1-C2-C3-C6
3	B	502	CIT	C2-C3-C4-C5
3	B	502	CIT	C6-C3-C4-C5
3	C	503	CIT	C2-C3-C6-O5
3	C	503	CIT	C2-C3-C6-O6
3	C	503	CIT	O7-C3-C6-O5
3	C	503	CIT	O7-C3-C6-O6
3	D	504	CIT	C1-C2-C3-C6
3	D	504	CIT	C2-C3-C6-O5
3	D	504	CIT	C2-C3-C6-O6
3	D	504	CIT	O7-C3-C6-O5
3	D	504	CIT	O7-C3-C6-O6
2	B	401	FAD	C3B-C4B-C5B-O5B
3	A	501	CIT	C1-C2-C3-C4
2	A	400	FAD	O4B-C4B-C5B-O5B
2	C	402	FAD	O4B-C4B-C5B-O5B
2	C	402	FAD	C3B-C4B-C5B-O5B
2	D	403	FAD	O4B-C4B-C5B-O5B
3	B	506	CIT	O7-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	D	504	CIT	C1-C2-C3-C4
2	D	403	FAD	C3B-C4B-C5B-O5B
2	A	400	FAD	O2'-C2'-C3'-C4'
2	A	400	FAD	C3B-C4B-C5B-O5B
3	C	503	CIT	C1-C2-C3-O7
3	C	503	CIT	C1-C2-C3-C6
3	B	506	CIT	C2-C3-C4-C5
3	B	506	CIT	C6-C3-C4-C5
3	B	506	CIT	C1-C2-C3-O7
2	B	401	FAD	P-O3P-PA-O1A
2	C	402	FAD	PA-O3P-P-O1P
3	B	502	CIT	O7-C3-C4-C5
3	C	503	CIT	C1-C2-C3-C4
2	A	400	FAD	PA-O3P-P-O5'
2	B	401	FAD	PA-O3P-P-O5'
2	C	402	FAD	PA-O3P-P-O5'
2	A	400	FAD	P-O3P-PA-O2A
2	A	400	FAD	C5'-O5'-P-O1P
2	D	403	FAD	P-O3P-PA-O2A
3	A	501	CIT	C2-C3-C6-O6
2	D	403	FAD	PA-O3P-P-O5'
3	A	501	CIT	C2-C3-C6-O5
3	B	506	CIT	C4-C3-C6-O5
3	B	502	CIT	O2-C1-C2-C3
2	A	400	FAD	O2'-C2'-C3'-O3'
3	B	502	CIT	O1-C1-C2-C3
3	B	506	CIT	O1-C1-C2-C3
2	A	400	FAD	PA-O3P-P-O2P
2	B	401	FAD	P-O3P-PA-O2A
3	B	506	CIT	O7-C3-C6-O5
3	B	506	CIT	C3-C4-C5-O3
3	B	506	CIT	O2-C1-C2-C3
3	B	506	CIT	C3-C4-C5-O4
2	D	403	FAD	PA-O3P-P-O2P

There are no ring outliers.

10 monomers are involved in 41 short contacts:

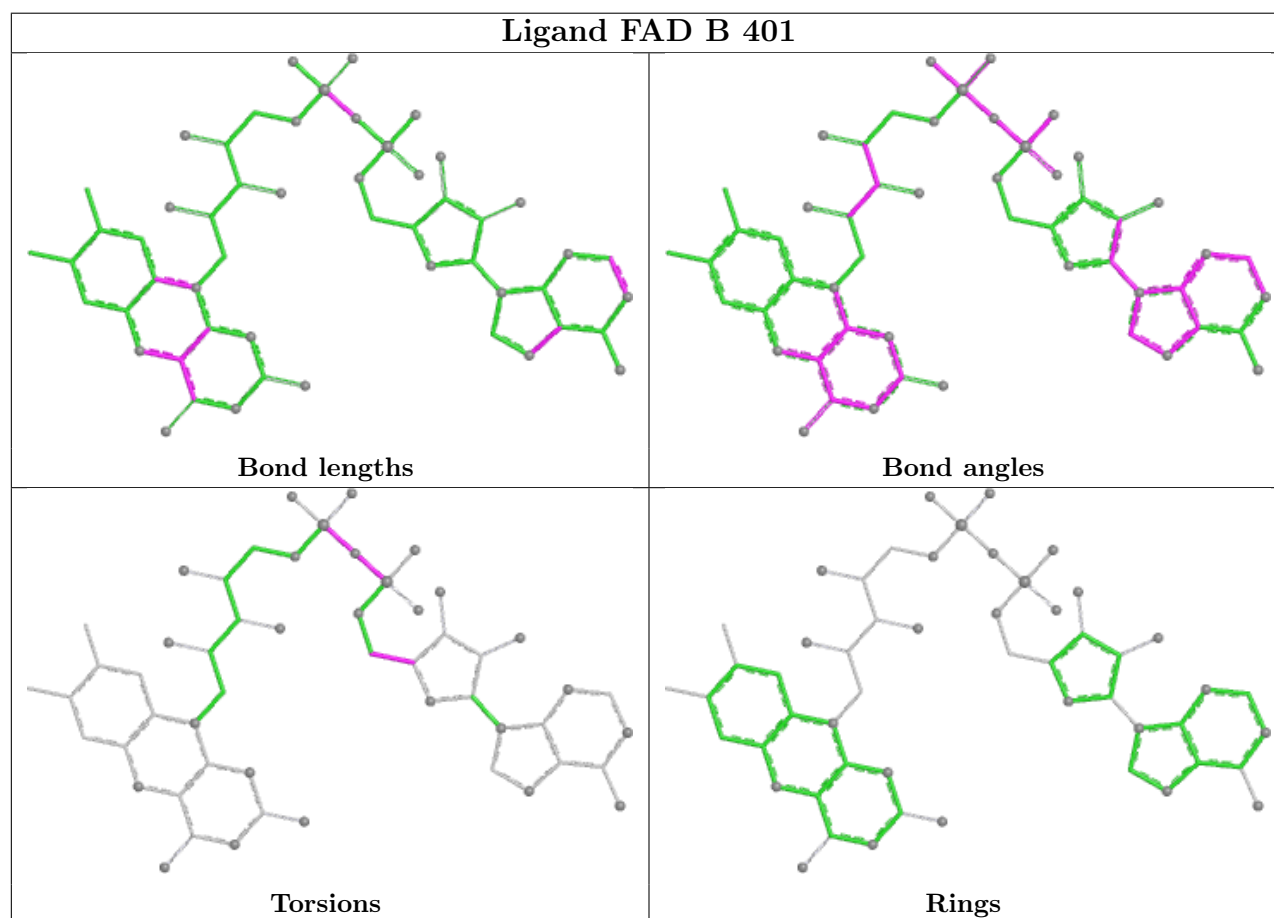
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	503	CIT	3	0
2	B	401	FAD	8	0
2	A	400	FAD	3	0

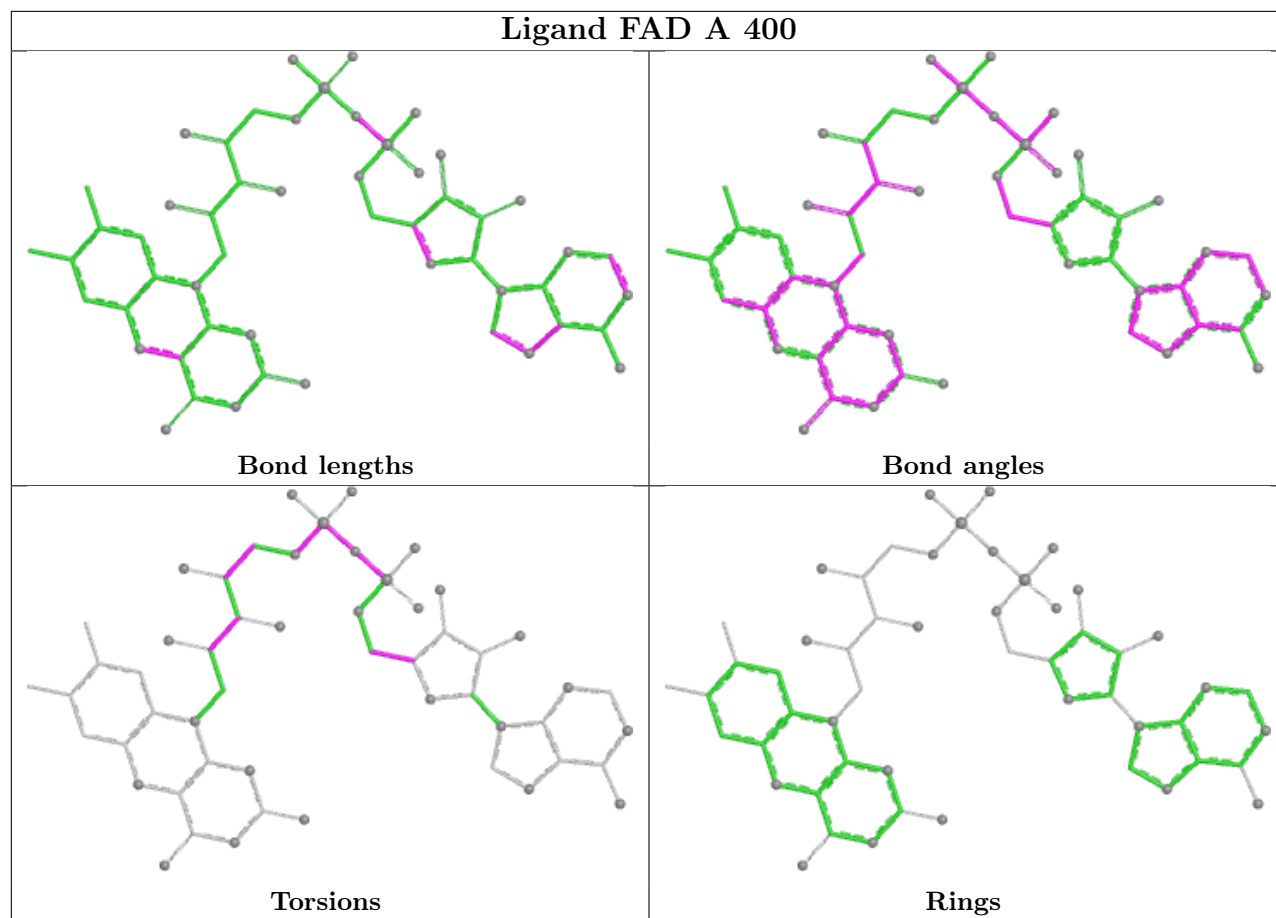
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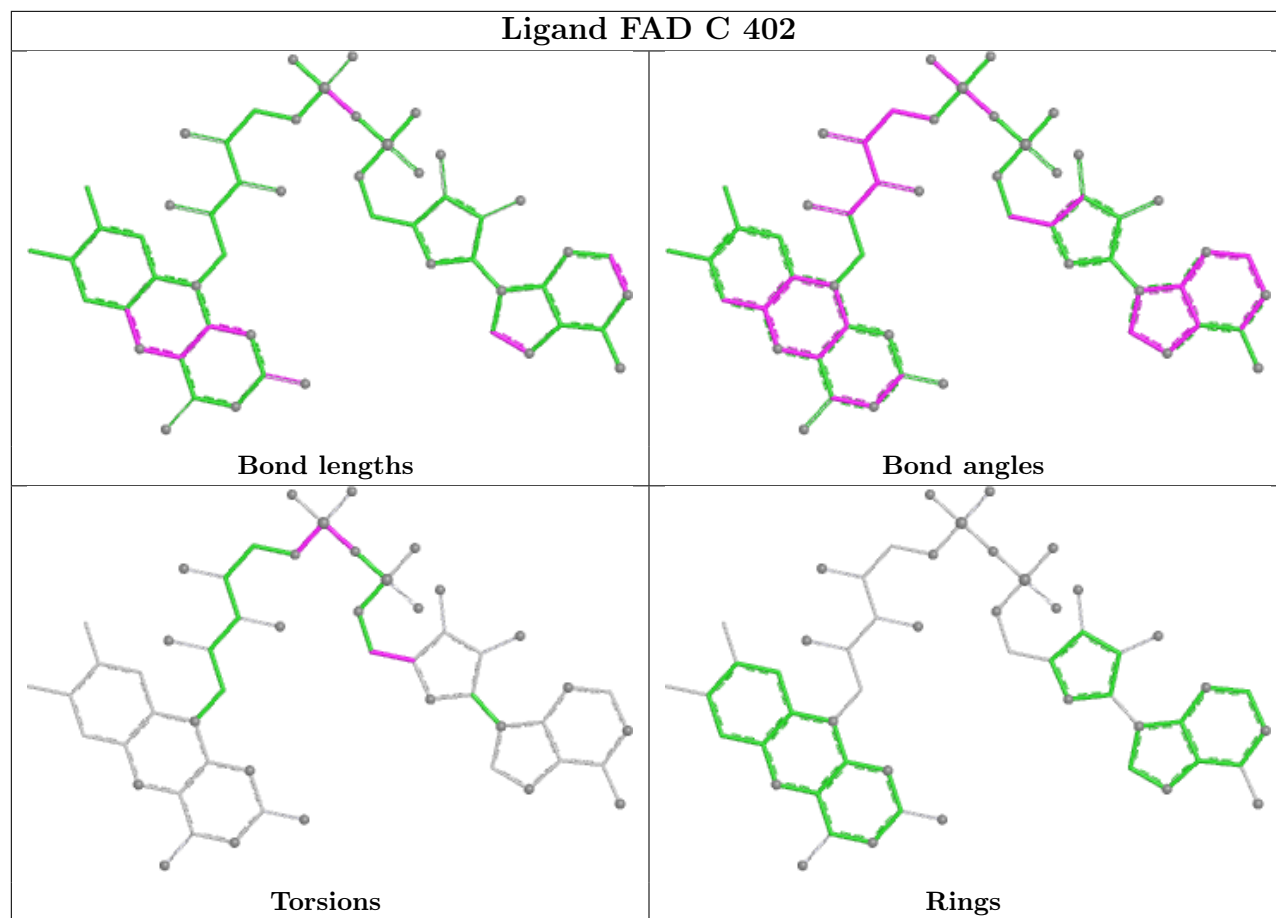
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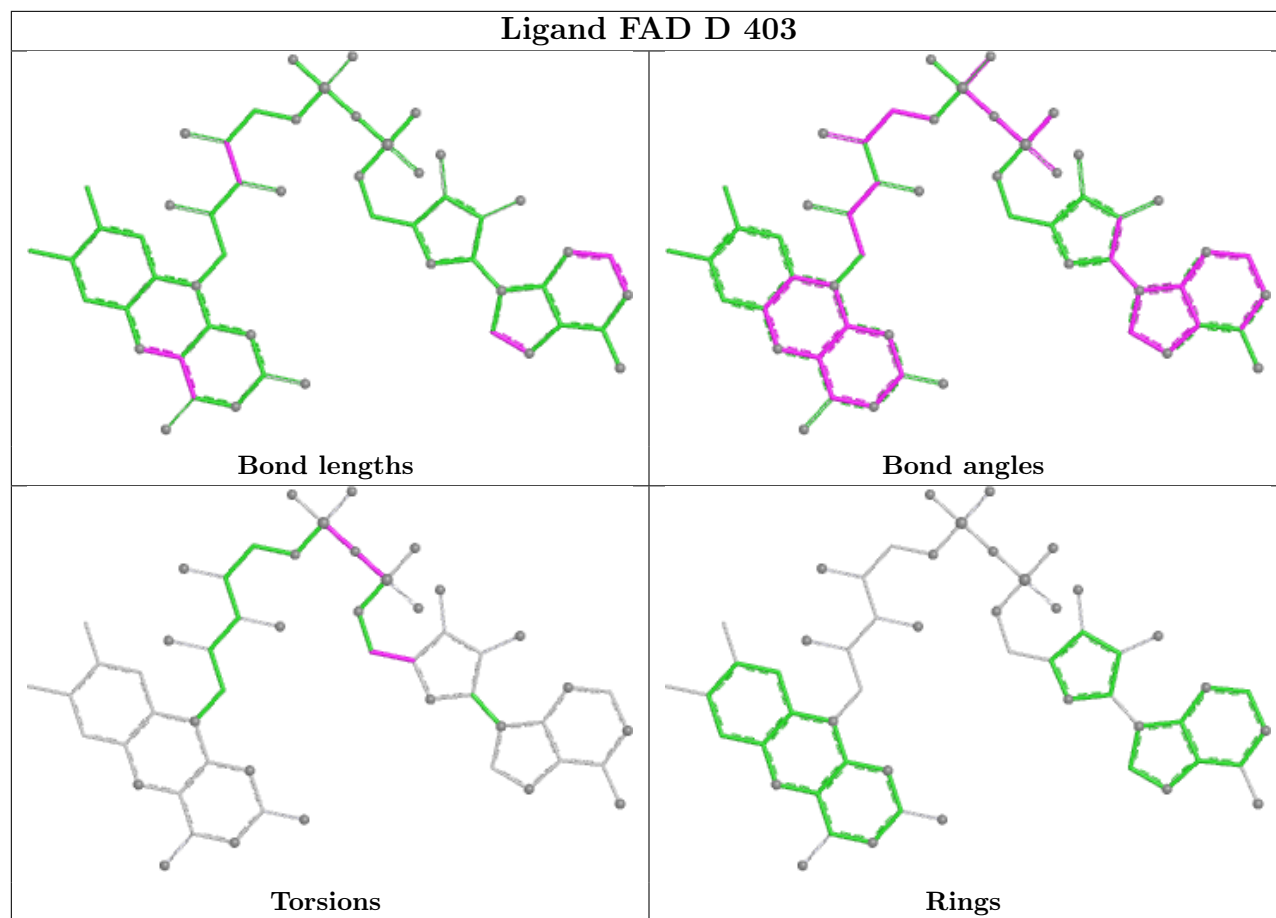
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	506	CIT	5	0
3	C	505	CIT	3	0
3	B	502	CIT	4	0
3	A	501	CIT	7	0
2	C	402	FAD	3	0
2	D	403	FAD	3	0
3	D	504	CIT	2	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	317/338 (93%)	-0.13	0 100 100	9, 19, 31, 41	1 (0%)
1	B	319/338 (94%)	-0.13	3 (0%) 81 78	10, 19, 31, 38	0
1	C	314/338 (92%)	0.03	9 (2%) 53 50	10, 20, 33, 46	0
1	D	307/338 (90%)	0.11	5 (1%) 70 66	9, 19, 32, 40	0
All	All	1257/1352 (92%)	-0.03	17 (1%) 73 69	9, 19, 33, 46	1 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	37	ASN	4.0
1	C	49	THR	4.0
1	C	190	ALA	3.4
1	D	197	ARG	3.3
1	D	190	ALA	2.8
1	C	-1	SER	2.7
1	C	148	VAL	2.6
1	B	1	VAL	2.5
1	C	0	HIS	2.5
1	C	37	ASN	2.5
1	D	199	GLU	2.4
1	C	219	GLY	2.3
1	D	175	TYR	2.1
1	C	151	PHE	2.1
1	D	134	TRP	2.1
1	C	198	ALA	2.1
1	B	0	HIS	2.1

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](#)

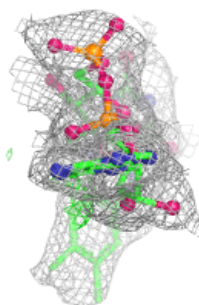
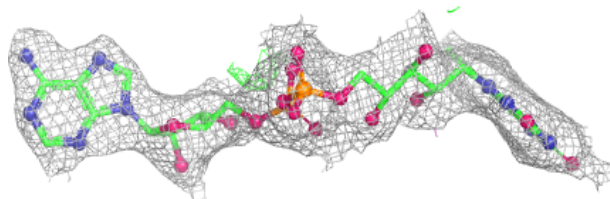
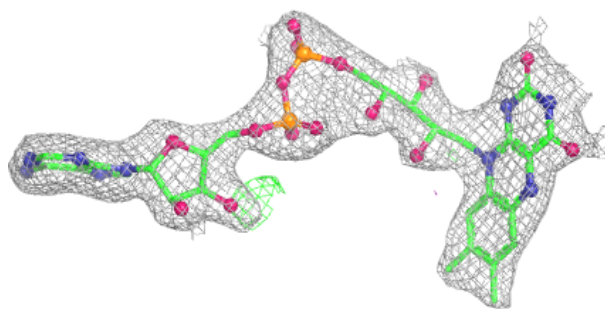
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CIT	C	503	13/13	0.71	0.18	44,49,52,56	0
3	CIT	D	504	13/13	0.76	0.14	55,58,64,65	0
3	CIT	C	505	13/13	0.79	0.16	31,39,46,50	0
3	CIT	A	501	13/13	0.86	0.12	26,39,49,51	0
3	CIT	B	502	13/13	0.88	0.10	33,37,40,40	0
3	CIT	B	506	13/13	0.93	0.08	28,35,40,44	0
2	FAD	C	402	53/53	0.96	0.07	12,23,29,35	1
2	FAD	D	403	53/53	0.96	0.08	11,22,28,31	1
2	FAD	A	400	53/53	0.96	0.07	5,19,27,30	1
2	FAD	B	401	53/53	0.96	0.07	7,22,31,35	1

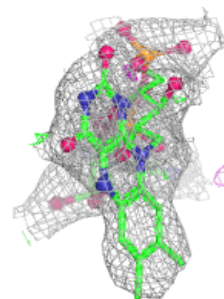
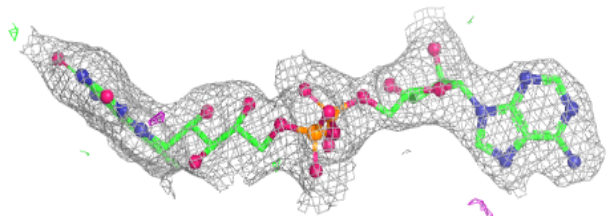
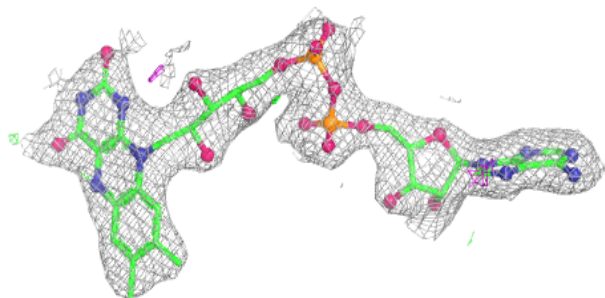
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD C 402:

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

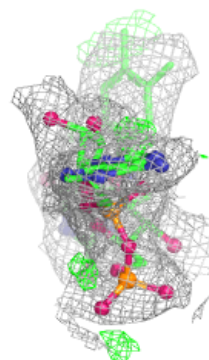
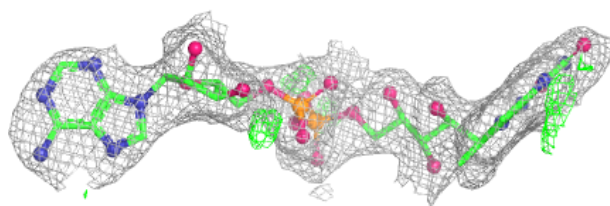
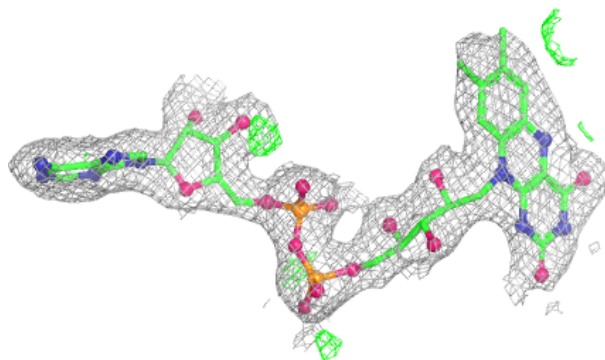
**Electron density around FAD D 403:**

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

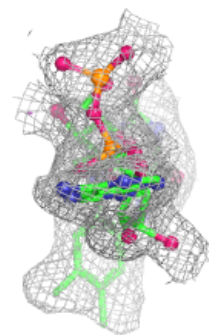
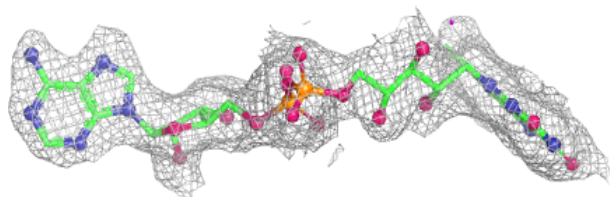
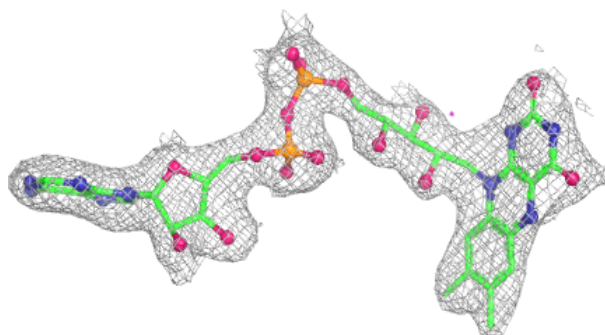


Electron density around FAD A 400:

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

**Electron density around FAD B 401:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.