



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:45 AM UTC

PDB ID : 1FEA / pdb_00001fea
Title : UNLIGANDED CRITHIDIA FASCICULATA TRYPANOTHIONE REDUC-
TASE AT 2.2 ANGSTROM RESOLUTION
Authors : Strickland, C.; Karplus, P.
Deposited on : 1995-07-12
Resolution : 2.20 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

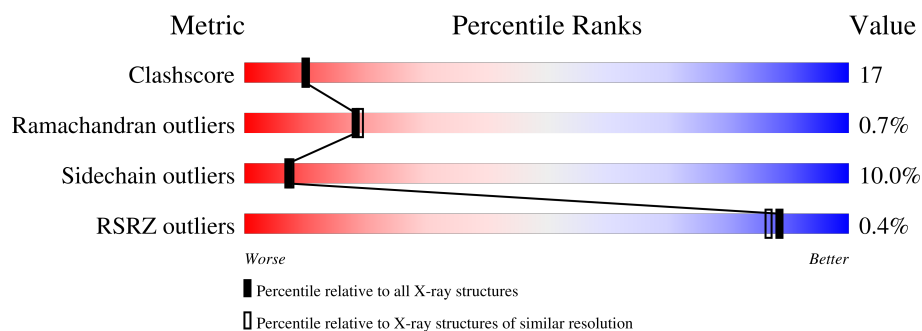
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	490	
1	B	490	
1	C	490	
1	D	490	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15364 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 TRYPANOTHIONE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3710	2334	643	713	20			
1	B	484	Total	C	N	O	S	0	0	0
			3685	2318	639	708	20			
1	C	487	Total	C	N	O	S	0	0	0
			3710	2334	643	713	20			
1	D	484	Total	C	N	O	S	0	0	0
			3685	2318	639	708	20			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	296	GLU	ASP	conflict	UNP P39040
A	478	GLU	GLN	conflict	UNP P39040
B	296	GLU	ASP	conflict	UNP P39040
B	478	GLU	GLN	conflict	UNP P39040
C	296	GLU	ASP	conflict	UNP P39040
C	478	GLU	GLN	conflict	UNP P39040
D	296	GLU	ASP	conflict	UNP P39040
D	478	GLU	GLN	conflict	UNP P39040

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



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

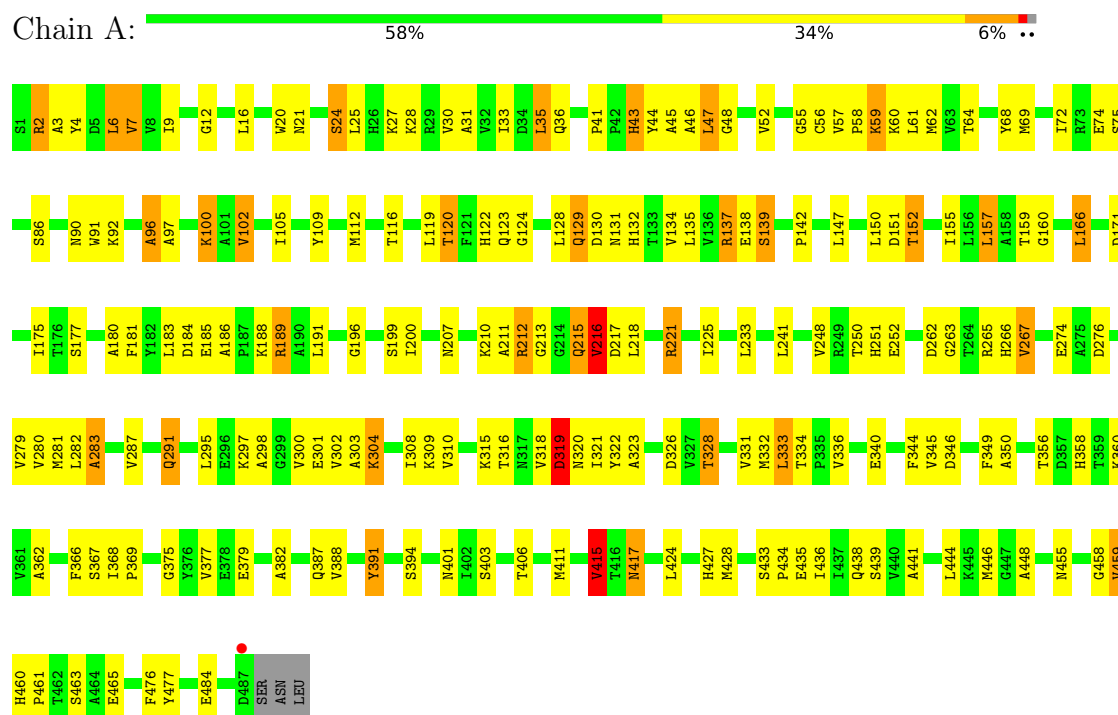
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	72	Total	O	0	0
			72	72		
3	B	94	Total	O	0	0
			94	94		
3	C	90	Total	O	0	0
			90	90		
3	D	106	Total	O	0	0
			106	106		

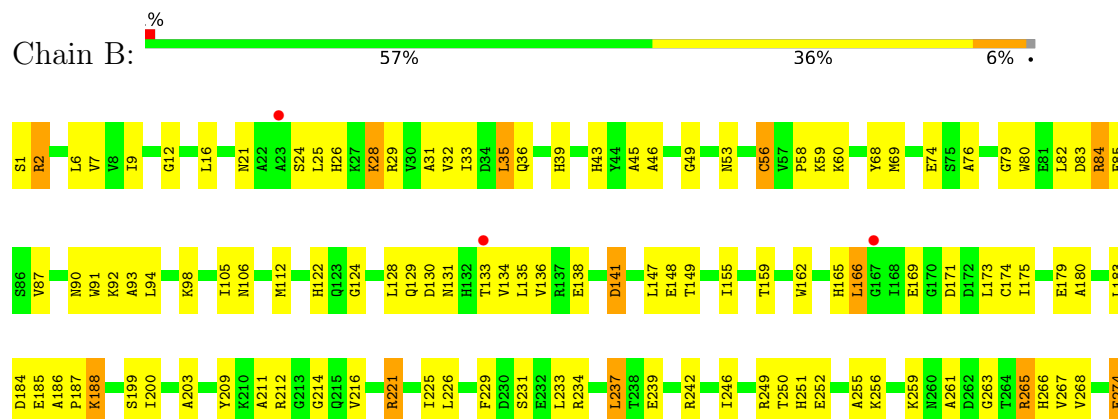
3 Residue-property plots

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: TRYPANOTHIONE REDUCTASE



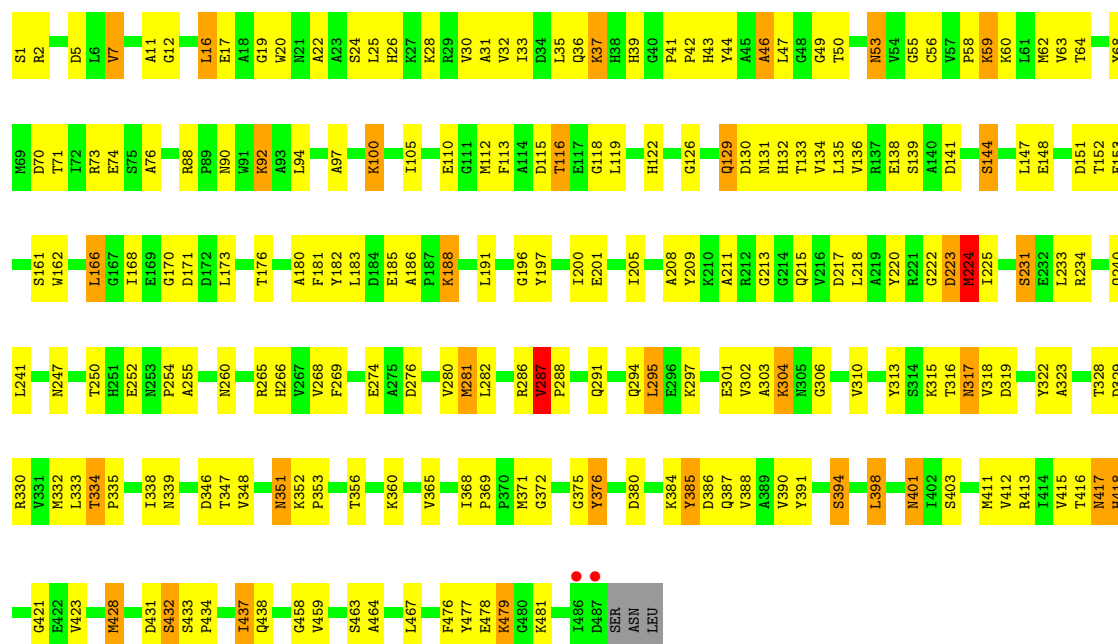
• Molecule 1: TRYPANOTHIONE REDUCTASE





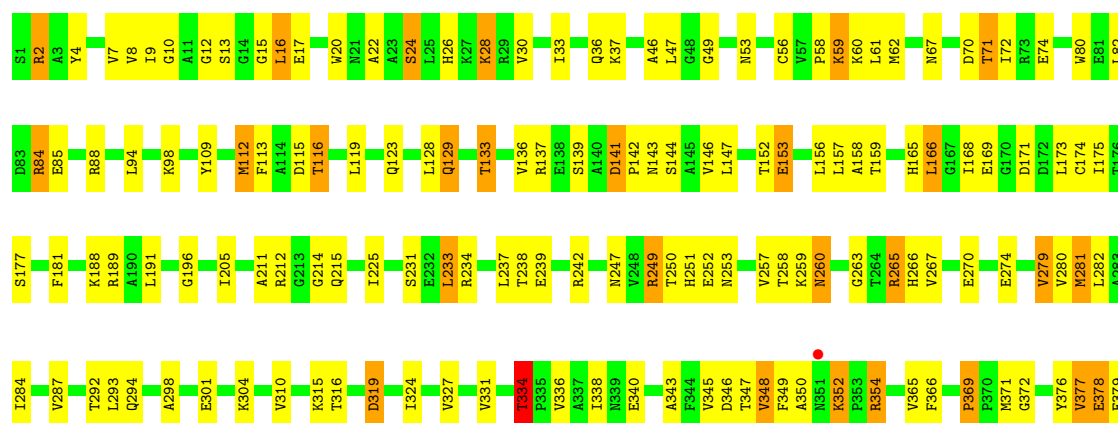
• Molecule 1: TRYPTOPHAN REDUCTASE

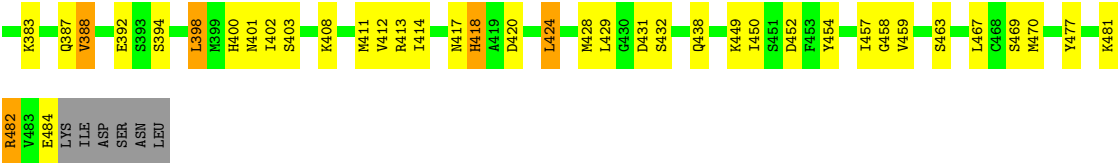
Chain C: 56% 37% 7%



• Molecule 1: TRYPTOPHAN REDUCTASE

Chain D: 60% 32% 7%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	123.00Å 160.80Å 58.50Å 90.00° 93.80° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20 8.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.20) 71.7 (8.00-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.16Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.185 , (Not available) 0.196 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15364	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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	1.03	7/3783 (0.2%)	1.27	29/5126 (0.6%)
1	B	1.03	3/3758 (0.1%)	1.29	23/5093 (0.5%)
1	C	1.07	6/3783 (0.2%)	1.31	34/5126 (0.7%)
1	D	1.07	7/3758 (0.2%)	1.33	32/5093 (0.6%)
All	All	1.05	23/15082 (0.2%)	1.30	118/20438 (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	B	0	1
1	C	0	3
All	All	0	4

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	428	MET	SD-CE	-7.94	1.59	1.79
1	D	470	MET	SD-CE	-7.74	1.60	1.79
1	C	428	MET	SD-CE	-6.73	1.62	1.79
1	A	459	VAL	CA-CB	-6.58	1.46	1.54
1	A	415	VAL	CA-CB	6.23	1.61	1.54
1	C	464	ALA	CA-CB	-6.21	1.43	1.53
1	A	62	MET	SD-CE	-6.19	1.64	1.79
1	A	102	VAL	CA-CB	-6.11	1.47	1.54
1	D	33	ILE	CA-CB	5.94	1.62	1.54
1	A	446	MET	SD-CE	-5.91	1.64	1.79
1	D	279	VAL	CA-CB	5.82	1.62	1.54
1	C	224	MET	SD-CE	5.78	1.94	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	428	MET	SD-CE	-5.65	1.65	1.79
1	A	216	VAL	CA-CB	5.60	1.60	1.54
1	A	248	VAL	CA-CB	5.48	1.59	1.53
1	B	446	MET	SD-CE	-5.46	1.65	1.79
1	D	281	MET	SD-CE	-5.41	1.66	1.79
1	D	459	VAL	CA-CB	-5.36	1.48	1.54
1	C	208	ALA	CA-CB	-5.29	1.44	1.53
1	C	390	VAL	C-O	-5.25	1.18	1.24
1	B	428	MET	CG-SD	-5.21	1.67	1.80
1	C	223	ASP	CA-C	-5.14	1.46	1.53
1	D	225	ILE	CA-CB	5.12	1.59	1.54

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	118	GLY	N-CA-C	-10.31	101.52	114.92
1	C	348	VAL	N-CA-C	10.20	120.11	110.53
1	A	377	VAL	N-CA-C	-9.95	99.20	110.05
1	C	53	ASN	N-CA-C	9.68	121.59	111.14
1	C	166	LEU	N-CA-C	-9.00	97.54	110.59
1	A	401	ASN	N-CA-C	-8.84	101.09	112.23
1	A	123	GLN	N-CA-C	8.79	122.93	108.96
1	A	291	GLN	N-CA-C	8.61	120.67	111.28
1	D	129	GLN	N-CA-C	-8.45	102.56	113.12
1	C	401	ASN	N-CA-C	-8.32	103.26	113.41
1	A	213	GLY	N-CA-C	-8.19	104.02	115.32
1	B	401	ASN	N-CA-C	-8.14	102.49	111.36
1	D	146	VAL	N-CA-C	-7.82	99.49	109.58
1	A	217	ASP	N-CA-C	-7.75	97.62	109.95
1	D	319	ASP	N-CA-C	7.55	121.92	112.87
1	A	171	ASP	N-CA-C	-7.47	103.13	111.28
1	D	260	ASN	N-CA-C	-7.47	100.46	110.55
1	D	334	THR	CA-C-N	-7.32	112.25	119.64
1	D	334	THR	C-N-CA	-7.32	112.25	119.64
1	A	64	THR	N-CA-C	-7.25	103.31	111.14
1	D	369	PRO	CA-C-N	7.16	127.33	120.31
1	D	369	PRO	C-N-CA	7.16	127.33	120.31
1	D	112	MET	N-CA-C	-7.00	103.66	111.28
1	D	454	TYR	N-CA-C	6.79	121.42	113.20
1	D	141	ASP	CA-C-N	6.78	126.48	119.56
1	D	141	ASP	C-N-CA	6.78	126.48	119.56
1	D	53	ASN	N-CA-C	6.77	119.66	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	THR	N-CA-C	6.76	119.60	108.99
1	B	372	GLY	N-CA-C	-6.75	97.18	113.18
1	A	375	GLY	N-CA-C	6.64	121.26	111.76
1	C	116	THR	N-CA-C	-6.64	98.43	109.46
1	C	319	ASP	N-CA-C	6.63	120.47	112.38
1	B	367	SER	N-CA-C	-6.56	101.30	110.35
1	B	319	ASP	N-CA-C	6.48	124.60	110.80
1	D	72	ILE	N-CA-C	-6.42	102.83	111.44
1	A	96	ALA	N-CA-C	-6.37	104.03	110.97
1	D	401	ASN	N-CA-C	-6.37	103.86	111.69
1	B	300	VAL	N-CA-C	6.36	117.64	109.30
1	A	189	ARG	N-CA-C	-6.33	98.67	109.24
1	D	116	THR	N-CA-C	6.25	118.58	108.34
1	D	30	VAL	N-CA-C	6.19	116.83	108.17
1	D	418	HIS	N-CA-C	6.17	118.80	111.71
1	B	418	HIS	N-CA-C	6.16	120.26	112.87
1	D	463	SER	N-CA-C	-6.06	104.97	112.90
1	A	2	ARG	N-CA-C	-6.03	99.90	109.07
1	B	221	ARG	N-CA-C	6.02	117.51	111.07
1	B	141	ASP	CA-C-N	6.00	127.34	119.84
1	B	141	ASP	C-N-CA	6.00	127.34	119.84
1	C	368	ILE	N-CA-C	-5.98	102.23	108.15
1	C	162	TRP	CA-C-N	-5.94	113.85	119.85
1	C	162	TRP	C-N-CA	-5.94	113.85	119.85
1	B	188	LYS	N-CA-C	-5.92	104.17	111.40
1	B	216	VAL	CB-CA-C	5.91	117.76	110.73
1	C	385	TYR	N-CA-C	5.89	119.07	109.24
1	C	186	ALA	CA-C-N	-5.88	113.88	119.76
1	C	186	ALA	C-N-CA	-5.88	113.88	119.76
1	C	287	VAL	CA-C-N	5.88	125.90	119.90
1	C	287	VAL	C-N-CA	5.88	125.90	119.90
1	C	459	VAL	N-CA-C	-5.80	100.05	108.17
1	B	410	PHE	N-CA-C	-5.78	100.28	109.76
1	A	166	LEU	N-CA-C	-5.76	101.94	110.46
1	C	306	GLY	N-CA-C	-5.72	107.20	115.27
1	B	348	VAL	N-CA-C	5.72	120.42	112.35
1	A	43	HIS	N-CA-C	5.70	120.29	113.23
1	B	384	LYS	N-CA-CB	-5.70	103.42	111.00
1	C	88	ARG	CA-C-N	5.62	126.06	119.99
1	C	88	ARG	C-N-CA	5.62	126.06	119.99
1	A	459	VAL	N-CA-C	-5.60	100.35	108.36
1	D	123	GLN	N-CA-C	5.59	118.35	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	352	LYS	CA-C-N	5.58	126.81	119.84
1	B	352	LYS	C-N-CA	5.58	126.81	119.84
1	D	365	VAL	N-CA-C	-5.57	98.43	107.28
1	A	129	GLN	N-CA-C	-5.56	104.03	112.04
1	B	301	GLU	N-CA-C	5.55	118.97	110.20
1	C	129	GLN	N-CA-C	-5.55	99.79	110.56
1	D	459	VAL	N-CA-C	-5.54	100.42	108.17
1	C	152	THR	N-CA-C	5.53	117.38	109.14
1	B	463	SER	N-CA-C	-5.53	105.34	111.36
1	D	13	SER	N-CA-C	5.50	116.96	111.07
1	C	368	ILE	CB-CA-C	-5.50	105.86	111.08
1	C	463	SER	N-CA-C	-5.49	105.45	111.82
1	C	173	LEU	N-CA-C	-5.43	106.50	113.23
1	A	417	ASN	N-CA-C	-5.42	99.69	108.41
1	C	255	ALA	N-CA-C	-5.42	106.35	113.12
1	C	64	THR	N-CA-C	-5.41	105.39	111.28
1	A	458	GLY	N-CA-C	5.40	119.92	112.37
1	A	319	ASP	N-CA-C	5.39	122.28	110.80
1	A	45	ALA	N-CA-C	-5.38	103.28	110.55
1	D	352	LYS	CA-C-N	5.38	126.57	119.84
1	D	352	LYS	C-N-CA	5.38	126.57	119.84
1	D	168	ILE	N-CA-C	-5.37	100.61	108.99
1	B	459	VAL	N-CA-C	-5.33	100.74	108.36
1	B	35	LEU	N-CA-C	5.30	119.00	112.54
1	D	408	LYS	N-CA-C	5.28	117.79	109.39
1	A	139	SER	N-CA-C	5.28	115.10	108.45
1	B	32	VAL	N-CA-C	-5.26	100.89	108.89
1	C	116	THR	CA-C-N	-5.26	114.40	122.87
1	C	116	THR	C-N-CA	-5.26	114.40	122.87
1	A	328	THR	N-CA-C	-5.24	106.73	113.23
1	D	153	GLU	N-CA-C	-5.23	105.23	111.03
1	B	365	VAL	N-CA-C	-5.23	100.22	107.80
1	A	30	VAL	N-CA-C	5.21	115.46	108.17
1	C	418	HIS	N-CA-C	5.20	117.69	111.71
1	A	387	GLN	N-CA-C	5.19	117.10	108.02
1	A	241	LEU	N-CA-C	-5.19	105.07	111.40
1	C	213	GLY	N-CA-C	-5.18	108.47	115.36
1	C	351	ASN	N-CA-C	-5.17	105.61	112.24
1	D	347	THR	N-CA-C	5.15	117.28	111.11
1	A	48	GLY	N-CA-C	-5.12	107.80	113.79
1	B	203	ALA	N-CA-C	-5.12	105.78	111.36
1	A	448	ALA	N-CA-C	5.12	117.65	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	352	LYS	CA-C-N	5.11	126.23	119.84
1	C	352	LYS	C-N-CA	5.11	126.23	119.84
1	D	15	GLY	N-CA-C	5.07	118.77	112.64
1	D	196	GLY	N-CA-C	5.05	120.85	112.66
1	D	372	GLY	N-CA-C	-5.05	101.22	113.18
1	A	283	ALA	N-CA-C	-5.04	100.28	109.56
1	C	412	VAL	CB-CA-C	-5.03	102.98	110.33

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	475	TYR	Sidechain
1	C	182	TYR	Sidechain
1	C	313	TYR	Sidechain
1	C	376	TYR	Sidechain

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	3710	0	3652	130	0
1	B	3685	0	3624	138	1
1	C	3710	0	3652	142	0
1	D	3685	0	3624	113	1
2	A	53	0	31	2	0
2	B	53	0	30	2	0
2	C	53	0	30	4	0
2	D	53	0	30	0	0
3	A	72	0	0	5	0
3	B	94	0	0	8	0
3	C	90	0	0	7	0
3	D	106	0	0	5	0
All	All	15364	0	14673	512	1

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 17.

All (512) 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:200:ILE:HD11	1:B:225:ILE:HD12	1.31	1.09
1:B:199:SER:HB2	1:B:283:ALA:HB3	1.47	0.96
1:C:138:GLU:HB2	1:C:147:LEU:HD21	1.49	0.92
1:B:76:ALA:HB2	1:B:84:ARG:NH1	1.89	0.88
1:B:188:LYS:HG3	1:B:211:ALA:HB3	1.57	0.87
1:A:394:SER:HB3	1:A:411:MET:HE3	1.58	0.86
1:D:388:VAL:HG22	1:D:477:TYR:HB2	1.58	0.84
1:C:301:GLU:HB2	1:C:317:ASN:OD1	1.78	0.83
1:A:74:GLU:HB3	1:A:403:SER:HB2	1.61	0.82
1:A:3:ALA:HB3	1:A:151:ASP:O	1.79	0.82
1:D:74:GLU:HG2	1:D:403:SER:HB2	1.59	0.82
1:A:137:ARG:HH21	1:A:142:PRO:HA	1.43	0.82
1:C:100:LYS:N	1:C:100:LYS:HD2	1.94	0.81
1:B:200:ILE:CD1	1:B:225:ILE:HD12	2.10	0.81
1:A:388:VAL:HG22	1:A:477:TYR:HB2	1.64	0.79
1:C:260:ASN:HD21	1:C:266:HIS:HB2	1.48	0.78
1:B:360:LYS:HD2	1:B:444:LEU:HB3	1.65	0.78
1:C:92:LYS:HE3	1:C:92:LYS:H	1.50	0.77
1:A:2:ARG:HG3	1:A:151:ASP:OD2	1.85	0.76
1:B:398:LEU:HA	1:B:401:ASN:HD22	1.51	0.76
1:A:157:LEU:HD23	1:A:308:ILE:HD13	1.70	0.74
1:B:237:LEU:HD23	1:B:429:LEU:HD11	1.69	0.74
1:B:33:ILE:HG22	2:B:499:FAD:H2A	1.69	0.73
1:A:196:GLY:O	1:A:200:ILE:HG12	1.88	0.73
1:A:6:LEU:HD11	1:A:344:PHE:HE2	1.54	0.73
1:D:177:SER:O	1:D:181:PHE:HD2	1.72	0.72
1:A:166:LEU:HD11	1:A:282:LEU:HD22	1.72	0.72
1:A:180:ALA:HA	1:A:183:LEU:HG	1.71	0.71
1:B:310:VAL:HB	1:B:314:SER:HA	1.73	0.71
1:B:199:SER:HB2	1:B:283:ALA:CB	2.20	0.71
1:B:388:VAL:HG22	1:B:477:TYR:HB2	1.74	0.70
1:A:4:TYR:CE1	1:A:150:LEU:HD22	2.26	0.70
1:B:26:HIS:O	1:B:28:LYS:HD2	1.91	0.70
1:A:331:VAL:HG12	1:A:333:LEU:HD22	1.72	0.69
1:C:394:SER:HB3	1:C:411:MET:HG3	1.75	0.69
1:D:156:LEU:HD11	1:D:324:ILE:HG23	1.75	0.69
1:A:96:ALA:O	1:A:100:LYS:HD2	1.92	0.69
1:A:310:VAL:HG11	1:A:323:ALA:HB3	1.76	0.67
1:A:281:MET:HE2	1:A:283:ALA:HB2	1.77	0.67
1:B:261:ALA:HB3	3:B:584:HOH:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:ASP:O	1:C:384:LYS:HG3	1.95	0.66
1:A:207:ASN:HB2	1:A:216:VAL:HG11	1.78	0.66
1:C:11:ALA:HB1	1:C:16:LEU:HD13	1.78	0.66
1:B:21:ASN:O	1:B:25:LEU:HB2	1.96	0.65
1:A:295:LEU:HB3	1:A:300:VAL:HB	1.78	0.65
1:A:310:VAL:CG1	1:A:323:ALA:HB3	2.26	0.65
1:A:112:MET:HE3	1:A:119:LEU:HD21	1.78	0.65
1:C:188:LYS:HG3	1:C:211:ALA:HB3	1.79	0.65
1:B:76:ALA:HB2	1:B:84:ARG:HH12	1.59	0.65
1:A:75:SER:HB3	1:B:68:TYR:CD1	2.31	0.64
1:B:291:GLN:CD	1:B:291:GLN:H	2.06	0.64
1:A:267:VAL:O	1:A:274:GLU:HA	1.99	0.63
1:D:20:TRP:HZ3	1:D:116:THR:HG1	1.45	0.63
1:C:315:LYS:HB2	1:C:322:TYR:CE2	2.33	0.63
1:A:281:MET:CE	1:A:283:ALA:HB2	2.29	0.63
1:C:94:LEU:HD22	1:C:209:TYR:CZ	2.34	0.63
1:B:300:VAL:HG21	1:B:321:ILE:HG21	1.79	0.63
1:C:388:VAL:HG22	1:C:477:TYR:HB2	1.81	0.63
1:C:268:VAL:HG22	1:C:274:GLU:HG2	1.81	0.62
1:C:304:LYS:HE2	1:C:304:LYS:O	1.99	0.62
1:D:231:SER:HA	1:D:234:ARG:HD3	1.81	0.62
1:C:339:ASN:OD1	1:C:356:THR:HG23	1.98	0.62
1:C:431:ASP:O	1:C:432:SER:HB2	1.99	0.62
1:B:59:LYS:HD2	1:B:59:LYS:C	2.25	0.62
1:B:129:GLN:OE1	1:B:133:THR:HG21	1.99	0.62
1:D:7:VAL:HG23	1:D:152:THR:HB	1.81	0.62
1:A:92:LYS:HE2	1:A:185:GLU:OE1	1.99	0.62
1:C:438:GLN:OE1	1:D:458:GLY:HA2	2.00	0.62
1:C:260:ASN:ND2	1:C:266:HIS:HB2	2.12	0.61
1:C:116:THR:HB	1:C:119:LEU:HD23	1.81	0.61
1:C:130:ASP:O	1:C:132:HIS:N	2.34	0.61
1:A:189:ARG:HA	1:A:215:GLN:O	2.01	0.61
1:C:372:GLY:O	1:C:437:ILE:HD13	2.00	0.61
1:B:9:ILE:HG22	1:B:159:THR:CG2	2.31	0.61
1:C:59:LYS:HD3	1:C:60:LYS:N	2.15	0.60
1:B:58:PRO:HB3	1:B:98:LYS:HD3	1.82	0.60
1:B:129:GLN:HB3	1:B:133:THR:CG2	2.32	0.60
1:B:94:LEU:HD22	1:B:209:TYR:CZ	2.36	0.60
1:B:398:LEU:HD23	1:B:401:ASN:HD22	1.66	0.60
1:C:7:VAL:HG22	1:C:31:ALA:HB3	1.84	0.60
1:B:398:LEU:HA	1:B:401:ASN:ND2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LEU:CD1	1:A:282:LEU:HD22	2.32	0.59
1:D:166:LEU:HD22	1:D:282:LEU:HD22	1.84	0.59
1:A:199:SER:HB2	1:A:283:ALA:HB3	1.84	0.59
1:D:10:GLY:HA3	1:D:158:ALA:O	2.03	0.59
1:A:394:SER:CB	1:A:411:MET:HE3	2.32	0.59
1:C:197:TYR:O	1:C:201:GLU:HG3	2.03	0.59
1:D:343:ALA:HB2	1:D:354:ARG:NH1	2.18	0.59
1:C:12:GLY:HA2	1:C:49:GLY:CA	2.33	0.59
1:D:20:TRP:HZ3	1:D:116:THR:OG1	1.85	0.59
1:D:331:VAL:CG1	1:D:336:VAL:HG21	2.33	0.58
1:C:317:ASN:ND2	1:C:318:VAL:HG23	2.18	0.58
1:D:191:LEU:HD23	1:D:280:VAL:HG23	1.86	0.58
1:D:249:ARG:HB3	1:D:252:GLU:HG3	1.85	0.58
1:A:137:ARG:HH21	1:A:142:PRO:CA	2.16	0.58
1:A:155:ILE:HD12	1:A:321:ILE:CD1	2.34	0.58
1:D:7:VAL:HG23	1:D:152:THR:CB	2.33	0.58
1:B:323:ALA:O	1:B:328:THR:HG21	2.03	0.58
1:D:58:PRO:HB2	1:D:181:PHE:CE1	2.37	0.58
1:A:200:ILE:HD13	1:A:218:LEU:HD11	1.84	0.58
1:C:417:ASN:C	1:C:417:ASN:HD22	2.09	0.58
1:C:33:ILE:HG22	2:C:499:FAD:H2A	1.86	0.57
1:C:398:LEU:HD23	1:C:401:ASN:HD22	1.69	0.57
1:D:259:LYS:HE2	1:D:263:GLY:HA2	1.87	0.57
1:D:398:LEU:HB2	3:D:514:HOH:O	2.03	0.57
1:B:231:SER:HA	1:B:234:ARG:HD3	1.86	0.57
1:C:188:LYS:CG	1:C:211:ALA:HB3	2.34	0.57
1:A:3:ALA:CB	1:A:151:ASP:HB3	2.34	0.57
1:B:12:GLY:HA2	1:B:49:GLY:HA3	1.85	0.57
1:B:129:GLN:HB2	1:B:135:LEU:HD11	1.87	0.57
1:A:394:SER:HB3	1:A:411:MET:CE	2.32	0.57
1:B:173:LEU:O	1:B:265:ARG:HD2	2.04	0.57
1:B:389:ALA:HB1	1:B:473:PRO:HB3	1.87	0.57
1:A:3:ALA:HB2	1:A:151:ASP:HB3	1.87	0.57
1:A:112:MET:HE3	1:A:119:LEU:CD2	2.34	0.57
1:D:28:LYS:HD2	1:D:28:LYS:N	2.19	0.57
1:C:138:GLU:CB	1:C:147:LEU:HD21	2.30	0.56
1:A:155:ILE:HD12	1:A:321:ILE:HD11	1.87	0.56
1:C:58:PRO:HB2	1:C:181:PHE:CE1	2.41	0.56
1:C:136:VAL:HB	1:C:148:GLU:HG2	1.86	0.56
1:C:20:TRP:O	1:C:24:SER:HB3	2.06	0.56
1:C:141:ASP:O	1:C:144:SER:OG	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:GLN:O	1:A:297:LYS:HB3	2.06	0.56
1:B:36:GLN:HG3	1:B:46:ALA:HB2	1.88	0.56
1:D:67:ASN:O	1:D:71:THR:HG23	2.05	0.56
1:D:331:VAL:HB	1:D:336:VAL:HG21	1.88	0.56
1:A:55:GLY:O	1:A:59:LYS:HB3	2.06	0.56
1:C:351:ASN:C	1:C:353:PRO:HD3	2.31	0.56
1:C:12:GLY:HA2	1:C:49:GLY:HA3	1.88	0.56
1:A:216:VAL:HB	3:A:512:HOH:O	2.06	0.55
1:D:16:LEU:HG	1:D:112:MET:HE1	1.88	0.55
1:D:36:GLN:HG3	1:D:46:ALA:HB2	1.88	0.55
1:A:57:VAL:HB	1:A:58:PRO:CD	2.35	0.55
1:A:61:LEU:HD11	1:B:398:LEU:HD13	1.89	0.55
1:B:283:ALA:HA	3:B:575:HOH:O	2.07	0.55
1:D:88:ARG:NH2	1:D:212:ARG:HH21	2.03	0.55
1:A:315:LYS:HG2	1:A:316:THR:O	2.05	0.55
1:B:302:VAL:HG12	1:B:303:ALA:O	2.07	0.55
1:A:218:LEU:HD23	1:A:218:LEU:C	2.32	0.55
1:B:175:ILE:HB	1:B:179:GLU:HB2	1.89	0.55
1:B:200:ILE:HD12	1:B:226:LEU:HG	1.88	0.55
1:A:303:ALA:HA	1:A:309:LYS:HE3	1.88	0.54
1:A:461:PRO:HD3	1:B:56:CYS:HB3	1.89	0.54
1:B:90:ASN:ND2	1:B:93:ALA:HB2	2.21	0.54
1:C:41:PRO:HG3	1:C:44:TYR:CE1	2.42	0.54
1:B:84:ARG:O	1:B:87:VAL:HG23	2.06	0.54
1:D:334:THR:O	1:D:338:ILE:HG13	2.08	0.54
1:A:12:GLY:O	1:A:16:LEU:HB2	2.07	0.54
1:D:233:LEU:HG	1:D:429:LEU:HB2	1.88	0.54
1:D:177:SER:O	1:D:181:PHE:CD2	2.57	0.54
1:A:6:LEU:HD11	1:A:344:PHE:CE2	2.39	0.54
1:A:138:GLU:HB2	1:A:147:LEU:HD21	1.90	0.54
1:B:259:LYS:HE3	1:B:263:GLY:HA2	1.88	0.54
1:B:330:ARG:HB2	3:B:526:HOH:O	2.07	0.54
1:D:346:ASP:HA	1:D:350:ALA:HB3	1.90	0.54
1:C:92:LYS:H	1:C:92:LYS:CE	2.19	0.54
1:A:175:ILE:HD11	1:A:279:VAL:CG1	2.38	0.54
1:C:130:ASP:C	1:C:132:HIS:H	2.15	0.53
1:A:212:ARG:HA	1:A:212:ARG:NE	2.23	0.53
1:B:9:ILE:HG22	1:B:159:THR:HG22	1.90	0.53
1:C:398:LEU:HD13	1:D:61:LEU:HD11	1.91	0.53
1:C:2:ARG:HB3	1:C:151:ASP:OD2	2.09	0.53
1:C:35:LEU:HD13	2:C:499:FAD:N3A	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LYS:HE3	1:A:366:PHE:CE1	2.43	0.53
1:B:36:GLN:OE1	1:B:43:HIS:HB2	2.08	0.53
1:C:74:GLU:HB3	1:C:403:SER:HB2	1.90	0.53
1:D:137:ARG:HH12	1:D:294:GLN:NE2	2.06	0.53
1:A:188:LYS:HG3	1:A:211:ALA:HB3	1.90	0.53
1:D:59:LYS:HD2	1:D:59:LYS:C	2.34	0.53
1:C:59:LYS:HE2	2:C:499:FAD:O4	2.09	0.52
1:D:165:HIS:HB3	1:D:171:ASP:OD2	2.09	0.52
1:D:418:HIS:HA	3:D:603:HOH:O	2.09	0.52
1:B:183:LEU:HD13	1:B:187:PRO:HD3	1.91	0.52
1:B:462:THR:O	1:B:465:GLU:HG2	2.09	0.52
1:D:284:ILE:N	1:D:284:ILE:HD13	2.25	0.52
1:A:24:SER:O	1:A:25:LEU:HD23	2.08	0.52
1:C:240:GLN:OE1	1:C:369:PRO:HG3	2.08	0.52
1:D:378:GLU:HB2	3:D:543:HOH:O	2.09	0.52
1:B:166:LEU:HD21	1:B:282:LEU:HD22	1.91	0.52
1:B:414:ILE:HD12	1:B:470:MET:SD	2.50	0.52
1:D:215:GLN:NE2	1:D:247:ASN:HB2	2.25	0.52
1:C:168:ILE:CD1	1:C:254:PRO:HB2	2.39	0.52
1:C:477:TYR:HA	1:C:481:LYS:O	2.10	0.52
1:A:7:VAL:HG11	1:A:134:VAL:HG21	1.91	0.52
1:D:165:HIS:HD2	1:D:171:ASP:OD1	1.92	0.52
1:C:428:MET:HE2	1:C:437:ILE:HD12	1.91	0.52
1:B:267:VAL:O	1:B:274:GLU:HA	2.10	0.52
1:A:302:VAL:HG12	1:A:303:ALA:O	2.09	0.52
1:A:28:LYS:HD2	1:A:349:PHE:CD1	2.45	0.51
1:D:17:GLU:HG2	1:D:338:ILE:HG23	1.93	0.51
1:B:35:LEU:HD23	1:B:124:GLY:O	2.10	0.51
1:C:94:LEU:HD22	1:C:209:TYR:CE2	2.46	0.51
1:C:384:LYS:HB2	1:C:385:TYR:CD1	2.45	0.51
1:D:336:VAL:O	1:D:340:GLU:HG3	2.10	0.51
1:A:331:VAL:HB	1:A:336:VAL:HG21	1.92	0.51
1:C:92:LYS:HE2	1:C:185:GLU:CD	2.34	0.51
1:C:294:GLN:HB3	1:C:297:LYS:CG	2.40	0.51
1:D:378:GLU:OE1	1:D:413:ARG:NH2	2.44	0.51
1:A:7:VAL:HG11	1:A:134:VAL:HG11	1.91	0.51
1:B:249:ARG:HB3	1:B:252:GLU:HG3	1.93	0.51
1:B:329:ASP:OD1	1:B:332:MET:HE3	2.11	0.51
1:A:90:ASN:N	1:B:79:GLY:O	2.43	0.51
1:A:16:LEU:CD2	1:A:112:MET:HE1	2.40	0.51
1:D:331:VAL:HB	1:D:336:VAL:HG11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:GLU:HB3	1:B:436:ILE:HG12	1.92	0.51
1:C:286:ARG:NH2	3:C:537:HOH:O	2.42	0.51
1:C:351:ASN:O	1:C:353:PRO:HD3	2.11	0.51
1:C:416:THR:HG22	1:C:423:VAL:HA	1.93	0.51
1:D:189:ARG:HA	1:D:215:GLN:O	2.11	0.51
1:C:5:ASP:O	1:C:153:GLU:HB3	2.11	0.51
1:D:4:TYR:O	1:D:152:THR:HA	2.10	0.51
1:B:221:ARG:O	1:B:251:HIS:HA	2.12	0.50
1:C:294:GLN:O	1:C:297:LYS:HB2	2.11	0.50
1:B:242:ARG:HA	1:B:246:ILE:O	2.11	0.50
1:B:387:GLN:CD	3:B:523:HOH:O	2.54	0.50
1:B:477:TYR:HA	1:B:481:LYS:O	2.11	0.50
1:A:263:GLY:O	1:A:265:ARG:NH1	2.44	0.50
1:D:400:HIS:HA	1:D:403:SER:OG	2.12	0.50
1:A:35:LEU:HD12	1:A:124:GLY:O	2.12	0.50
1:D:250:THR:O	1:D:251:HIS:HB2	2.11	0.50
1:B:432:SER:O	1:B:436:ILE:HG13	2.11	0.50
1:A:120:THR:OG1	1:A:122:HIS:NE2	2.45	0.50
1:C:196:GLY:O	1:C:200:ILE:HG12	2.12	0.50
1:B:165:HIS:HB3	1:B:171:ASP:OD2	2.12	0.49
1:B:440:VAL:O	1:B:443:CYS:HB2	2.11	0.49
1:C:17:GLU:HG2	1:C:338:ILE:O	2.11	0.49
1:D:412:VAL:HG11	1:D:467:LEU:HD23	1.95	0.49
1:C:387:GLN:HA	1:C:477:TYR:O	2.12	0.49
1:A:346:ASP:HA	1:A:350:ALA:HB3	1.93	0.49
1:C:92:LYS:HE3	1:C:92:LYS:N	2.24	0.49
1:D:267:VAL:O	1:D:274:GLU:HA	2.13	0.49
1:A:138:GLU:HA	1:A:147:LEU:HD11	1.94	0.49
1:A:160:GLY:HA2	1:A:326:ASP:HB2	1.94	0.49
1:A:91:TRP:HB2	1:A:186:ALA:HB2	1.95	0.49
1:C:70:ASP:HA	1:C:73:ARG:NH1	2.28	0.49
1:C:90:ASN:OD1	1:C:92:LYS:HD2	2.13	0.49
1:D:7:VAL:CG2	1:D:152:THR:HB	2.42	0.49
1:B:7:VAL:HG11	1:B:134:VAL:HG11	1.94	0.49
1:D:36:GLN:O	1:D:46:ALA:HB1	2.12	0.49
1:A:340:GLU:HA	1:A:356:THR:OG1	2.13	0.48
1:B:322:TYR:CD2	1:B:344:PHE:HD2	2.30	0.48
1:D:348:VAL:CG2	1:D:349:PHE:CE2	2.96	0.48
1:A:7:VAL:HG22	1:A:31:ALA:HB3	1.95	0.48
1:B:162:TRP:HB2	1:B:289:ARG:HD2	1.94	0.48
1:C:386:ASP:O	1:C:479:LYS:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:GLN:HB3	1:D:133:THR:HB	1.94	0.48
1:D:238:THR:O	1:D:242:ARG:HG3	2.13	0.48
1:A:433:SER:OG	1:A:434:PRO:HD3	2.14	0.48
1:A:21:ASN:O	1:A:25:LEU:HB2	2.13	0.48
1:A:96:ALA:HB1	1:A:100:LYS:HE2	1.96	0.48
1:B:237:LEU:HD23	1:B:429:LEU:CD1	2.39	0.48
1:B:310:VAL:HB	1:B:314:SER:CA	2.43	0.48
1:A:323:ALA:O	1:A:328:THR:HG21	2.14	0.48
1:B:135:LEU:HD23	1:B:149:THR:HG23	1.95	0.48
1:B:324:ILE:CD1	1:B:341:GLY:HA2	2.43	0.48
1:B:378:GLU:H	1:B:378:GLU:HG3	1.45	0.48
1:B:233:LEU:HD23	1:B:371:MET:HE3	1.96	0.48
1:C:231:SER:HA	1:C:234:ARG:HD3	1.96	0.48
1:B:80:TRP:O	1:B:84:ARG:NH2	2.47	0.48
1:B:301:GLU:HG3	1:B:317:ASN:ND2	2.29	0.48
1:B:377:VAL:O	1:B:378:GLU:C	2.57	0.48
1:A:175:ILE:HD11	1:A:279:VAL:HG11	1.96	0.47
1:C:295:LEU:HD23	1:C:302:VAL:HG21	1.96	0.47
1:A:20:TRP:CZ3	1:A:116:THR:OG1	2.63	0.47
1:B:2:ARG:CD	1:B:2:ARG:H	2.27	0.47
1:B:12:GLY:HA2	1:B:49:GLY:CA	2.45	0.47
1:C:35:LEU:HD13	2:C:499:FAD:C4A	2.45	0.47
1:C:376:TYR:CE1	1:C:384:LYS:HE3	2.49	0.47
1:A:340:GLU:OE2	1:A:358:HIS:NE2	2.45	0.47
1:B:315:LYS:HG3	1:B:322:TYR:CE1	2.48	0.47
1:B:412:VAL:HG11	1:B:467:LEU:HD13	1.96	0.47
1:B:281:MET:HE2	1:B:281:MET:HB3	1.78	0.47
1:C:7:VAL:HG11	1:C:134:VAL:HG21	1.97	0.47
1:A:41:PRO:HG3	1:A:44:TYR:CE1	2.50	0.47
1:A:379:GLU:O	1:A:382:ALA:HB3	2.14	0.47
1:C:200:ILE:HG23	1:C:241:LEU:HD11	1.97	0.47
1:D:345:VAL:O	1:D:346:ASP:C	2.58	0.47
1:D:394:SER:HB2	1:D:411:MET:HE3	1.97	0.47
1:A:43:HIS:O	1:A:44:TYR:HB2	2.14	0.47
1:C:428:MET:HB2	1:C:428:MET:HE3	1.68	0.47
1:D:98:LYS:C	1:D:98:LYS:HD2	2.39	0.47
1:A:129:GLN:HB2	1:A:135:LEU:HD13	1.97	0.47
1:B:74:GLU:HB3	1:B:403:SER:HB2	1.97	0.47
1:B:296:GLU:HG2	1:B:297:LYS:N	2.29	0.47
1:B:304:LYS:O	1:B:304:LYS:HG2	2.15	0.47
1:C:360:LYS:HD3	1:C:375:GLY:HA2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:GLU:CD	1:D:413:ARG:HH11	2.23	0.47
1:A:391:TYR:CD1	1:A:391:TYR:N	2.83	0.47
1:B:388:VAL:CG2	1:B:477:TYR:HB2	2.45	0.46
1:A:33:ILE:HA	1:A:122:HIS:O	2.15	0.46
1:A:166:LEU:N	1:A:166:LEU:HD12	2.30	0.46
1:A:315:LYS:NZ	1:A:322:TYR:OH	2.46	0.46
1:B:412:VAL:HG11	1:B:467:LEU:CD1	2.46	0.46
1:C:217:ASP:HA	1:C:247:ASN:HB3	1.97	0.46
1:C:294:GLN:HB3	1:C:297:LYS:HG3	1.98	0.46
1:C:417:ASN:C	1:C:417:ASN:ND2	2.70	0.46
1:B:296:GLU:HG2	1:B:297:LYS:H	1.79	0.46
1:C:458:GLY:HA2	1:D:438:GLN:OE1	2.15	0.46
1:D:88:ARG:NH2	1:D:212:ARG:NH2	2.63	0.46
1:A:47:LEU:HD13	1:A:109:TYR:HB3	1.97	0.46
1:A:332:MET:O	1:A:333:LEU:HD13	2.15	0.46
1:C:265:ARG:O	1:C:276:ASP:HA	2.16	0.46
1:D:310:VAL:HG12	1:D:316:THR:HG22	1.96	0.46
1:A:52:VAL:HG13	1:A:105:ILE:HG21	1.97	0.46
1:D:166:LEU:HD23	1:D:166:LEU:H	1.80	0.46
1:B:324:ILE:HD12	1:B:341:GLY:HA2	1.98	0.46
1:C:43:HIS:HD2	3:C:530:HOH:O	1.97	0.46
1:C:129:GLN:HB3	1:C:133:THR:HB	1.98	0.45
1:B:43:HIS:O	1:B:45:ALA:N	2.49	0.45
1:A:177:SER:O	1:A:181:PHE:CD2	2.69	0.45
1:A:291:GLN:CD	1:A:291:GLN:H	2.24	0.45
1:A:336:VAL:O	1:A:340:GLU:HG3	2.16	0.45
1:C:191:LEU:HD23	1:C:280:VAL:HG13	1.98	0.45
1:C:316:THR:HB	3:C:573:HOH:O	2.16	0.45
1:C:176:THR:HB	3:C:528:HOH:O	2.16	0.45
1:C:334:THR:HB	1:C:335:PRO:HD3	1.99	0.45
1:D:62:MET:HB3	1:D:205:ILE:HD12	1.98	0.45
1:D:482:ARG:NH2	3:D:605:HOH:O	2.49	0.45
1:A:304:LYS:HB3	1:A:304:LYS:HE2	1.71	0.45
1:B:31:ALA:HB1	1:B:122:HIS:CD2	2.52	0.45
1:C:36:GLN:OE1	1:C:43:HIS:HB2	2.17	0.45
2:A:499:FAD:H9	2:A:499:FAD:H1'1	1.80	0.45
1:D:188:LYS:O	1:D:214:GLY:HA3	2.17	0.45
1:C:417:ASN:HD22	1:C:418:HIS:N	2.15	0.45
1:C:417:ASN:O	1:C:421:GLY:N	2.49	0.45
1:D:253:ASN:HB3	1:D:270:GLU:HG3	1.98	0.45
1:B:135:LEU:CD2	1:B:149:THR:HG23	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:ALA:O	1:C:26:HIS:HB2	2.16	0.44
1:C:332:MET:O	1:C:333:LEU:HD23	2.16	0.44
1:D:331:VAL:CB	1:D:336:VAL:HG21	2.46	0.44
2:B:499:FAD:H1'1	2:B:499:FAD:H9	1.71	0.44
1:C:113:PHE:C	1:C:115:ASP:N	2.75	0.44
1:D:137:ARG:HH22	1:D:294:GLN:HE22	1.65	0.44
1:D:450:ILE:O	1:D:450:ILE:HG13	2.16	0.44
1:C:11:ALA:HB2	1:C:32:VAL:CG1	2.48	0.44
1:D:9:ILE:HD12	1:D:157:LEU:CD2	2.48	0.44
1:D:233:LEU:HD23	1:D:371:MET:HE3	1.99	0.44
1:A:21:ASN:HB2	1:A:345:VAL:HG21	2.00	0.44
1:A:225:ILE:HG12	3:A:527:HOH:O	2.17	0.44
1:A:315:LYS:HG2	1:A:316:THR:N	2.33	0.44
1:B:334:THR:HB	1:B:335:PRO:HD3	2.00	0.44
1:C:31:ALA:HB1	1:C:122:HIS:CD2	2.53	0.44
1:C:92:LYS:HE2	1:C:185:GLU:OE2	2.18	0.44
1:D:58:PRO:HB2	1:D:181:PHE:CD1	2.51	0.44
1:B:2:ARG:O	1:B:29:ARG:NH1	2.50	0.44
1:B:377:VAL:HG23	3:B:516:HOH:O	2.17	0.44
1:C:317:ASN:HD22	1:C:318:VAL:N	2.14	0.44
1:D:159:THR:HG21	1:D:293:LEU:HD21	1.99	0.44
3:A:511:HOH:O	1:B:333:LEU:HD13	2.16	0.44
1:D:377:VAL:O	1:D:378:GLU:C	2.59	0.44
1:D:383:LYS:HB2	1:D:383:LYS:HE3	1.74	0.44
1:A:318:VAL:O	1:A:320:ASN:N	2.51	0.43
1:C:224:MET:HE3	1:C:234:ARG:CZ	2.48	0.43
1:B:290:SER:HA	1:B:293:LEU:HD12	2.00	0.43
1:B:384:LYS:HB3	1:B:385:TYR:CD1	2.54	0.43
1:C:19:GLY:HA2	1:C:30:VAL:HG11	2.00	0.43
1:A:20:TRP:HZ3	1:A:116:THR:HG1	1.59	0.43
1:C:112:MET:HE3	1:C:119:LEU:HD21	2.00	0.43
1:D:88:ARG:HG2	1:D:88:ARG:HH11	1.83	0.43
1:C:200:ILE:HD12	1:C:225:ILE:HD12	2.00	0.43
1:D:352:LYS:O	1:D:352:LYS:HG3	2.19	0.43
1:A:9:ILE:HG22	1:A:159:THR:HG22	1.99	0.43
1:A:68:TYR:O	1:A:69:MET:C	2.59	0.43
1:B:174:CYS:HA	1:B:280:VAL:HG13	2.00	0.43
1:B:266:HIS:HA	1:B:276:ASP:OD1	2.19	0.43
1:B:314:SER:HB3	1:B:323:ALA:O	2.18	0.43
1:D:9:ILE:HG22	1:D:159:THR:CG2	2.49	0.43
1:D:47:LEU:HD11	1:D:113:PHE:HE2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:VAL:HG13	1:B:280:VAL:O	2.17	0.43
1:B:305:ASN:C	1:B:305:ASN:OD1	2.60	0.43
1:C:317:ASN:HD22	1:C:317:ASN:C	2.26	0.43
1:D:12:GLY:HA2	1:D:49:GLY:CA	2.48	0.43
1:D:28:LYS:HE3	1:D:349:PHE:CD1	2.54	0.43
1:D:80:TRP:O	1:D:84:ARG:NH2	2.51	0.43
1:A:130:ASP:O	1:A:132:HIS:N	2.51	0.43
1:B:136:VAL:HB	1:B:148:GLU:HB2	2.00	0.43
1:B:417:ASN:HB2	1:B:424:LEU:HD11	2.00	0.43
1:C:39:HIS:HB3	1:C:53:ASN:OD1	2.18	0.43
1:A:36:GLN:O	1:A:46:ALA:HB1	2.19	0.43
1:C:105:ILE:HD11	1:D:398:LEU:HD11	2.01	0.43
1:C:329:ASP:O	1:C:329:ASP:CG	2.62	0.43
1:C:346:ASP:O	1:C:347:THR:C	2.60	0.43
1:D:139:SER:OG	1:D:144:SER:HB3	2.19	0.43
1:A:68:TYR:O	1:A:72:ILE:HG13	2.19	0.43
1:A:128:LEU:HD13	1:A:298:ALA:HB3	2.01	0.43
1:C:180:ALA:HA	1:C:183:LEU:HG	2.01	0.43
1:D:315:LYS:HG2	1:D:316:THR:O	2.18	0.43
1:D:60:LYS:HE3	1:D:366:PHE:CE1	2.54	0.43
1:D:281:MET:HB3	1:D:281:MET:HE2	1.68	0.43
1:B:398:LEU:O	1:B:401:ASN:HB2	2.18	0.42
1:C:70:ASP:HA	1:C:73:ARG:HH12	1.84	0.42
1:D:270:GLU:HB2	3:D:529:HOH:O	2.19	0.42
1:D:387:GLN:HA	1:D:477:TYR:O	2.19	0.42
1:B:2:ARG:H	1:B:2:ARG:HD2	1.84	0.42
1:B:212:ARG:HG3	3:B:502:HOH:O	2.19	0.42
1:D:136:VAL:O	1:D:147:LEU:HB2	2.19	0.42
1:D:166:LEU:CD2	1:D:282:LEU:HD22	2.49	0.42
1:A:20:TRP:HZ3	1:A:116:THR:OG1	2.02	0.42
1:C:170:GLY:O	1:C:171:ASP:C	2.63	0.42
1:A:191:LEU:HB3	1:A:280:VAL:HG13	2.01	0.42
1:A:233:LEU:HD22	1:A:427:HIS:HB3	2.01	0.42
1:A:367:SER:OG	1:A:369:PRO:O	2.35	0.42
1:B:417:ASN:C	1:B:417:ASN:ND2	2.76	0.42
1:C:73:ARG:NH1	3:C:583:HOH:O	2.51	0.42
1:D:12:GLY:O	1:D:16:LEU:HB2	2.19	0.42
1:D:175:ILE:HG13	1:D:281:MET:HA	2.01	0.42
1:C:36:GLN:HG3	1:C:46:ALA:HB2	2.02	0.42
1:C:281:MET:HE2	1:C:281:MET:HB3	1.74	0.42
1:B:60:LYS:HE3	1:B:366:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:HIS:HB2	1:C:28:LYS:HG2	2.02	0.42
1:C:28:LYS:HA	1:C:28:LYS:HD3	1.68	0.42
1:C:310:VAL:HA	1:C:315:LYS:O	2.19	0.42
1:D:188:LYS:HG3	1:D:211:ALA:HB3	2.00	0.42
1:C:334:THR:O	1:C:338:ILE:HG13	2.20	0.42
1:D:260:ASN:OD1	1:D:266:HIS:HB2	2.20	0.42
1:B:36:GLN:HG3	1:B:46:ALA:CB	2.50	0.42
1:C:37:LYS:H	1:C:37:LYS:HG2	1.72	0.42
1:C:92:LYS:H	1:C:92:LYS:CD	2.32	0.42
1:C:113:PHE:C	1:C:115:ASP:H	2.27	0.42
1:D:431:ASP:O	1:D:432:SER:HB2	2.20	0.42
1:A:315:LYS:HD3	1:A:319:ASP:HA	2.02	0.42
1:A:362:ALA:HB2	1:A:441:ALA:HB2	2.02	0.42
1:B:90:ASN:O	1:B:93:ALA:HB3	2.19	0.42
1:B:255:ALA:HB3	1:B:268:VAL:O	2.20	0.42
1:C:220:TYR:CE2	1:C:222:GLY:HA3	2.54	0.42
1:D:109:TYR:HD1	1:D:109:TYR:HA	1.73	0.42
1:A:207:ASN:HA	1:A:210:LYS:HD3	2.01	0.42
1:A:476:PHE:CD1	1:A:476:PHE:N	2.87	0.42
1:B:92:LYS:HE3	1:B:92:LYS:HB3	1.81	0.42
1:B:295:LEU:HD23	1:B:302:VAL:CG2	2.50	0.42
1:C:68:TYR:HA	1:C:71:THR:HB	2.02	0.42
1:C:129:GLN:O	1:C:297:LYS:HB3	2.20	0.42
1:C:252:GLU:HG3	1:C:269:PHE:CD1	2.55	0.42
1:C:330:ARG:HB2	3:C:556:HOH:O	2.20	0.42
1:B:105:ILE:O	1:B:106:ASN:C	2.63	0.41
1:B:233:LEU:CD1	1:B:413:ARG:HG3	2.50	0.41
1:C:62:MET:HE2	1:C:205:ILE:HG21	2.02	0.41
1:C:287:VAL:HA	1:C:288:PRO:HD3	1.84	0.41
1:C:291:GLN:CD	1:C:291:GLN:H	2.27	0.41
1:D:376:TYR:HD2	1:D:424:LEU:HG	1.86	0.41
1:B:112:MET:O	1:B:112:MET:HG2	2.19	0.41
1:C:37:LYS:HE2	1:C:110:GLU:HG2	2.01	0.41
1:C:50:THR:O	1:C:55:GLY:N	2.53	0.41
1:D:141:ASP:HA	1:D:142:PRO:HD3	1.81	0.41
1:B:229:PHE:O	1:B:234:ARG:HD2	2.20	0.41
1:B:373:VAL:HG11	3:B:551:HOH:O	2.20	0.41
1:C:433:SER:OG	1:C:434:PRO:HD3	2.21	0.41
1:D:128:LEU:HD13	1:D:298:ALA:CB	2.51	0.41
1:A:212:ARG:HA	1:A:212:ARG:HE	1.85	0.41
1:A:438:GLN:OE1	1:B:465:GLU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:GLY:HA2	3:B:540:HOH:O	2.19	0.41
1:C:100:LYS:N	1:C:100:LYS:CD	2.77	0.41
1:C:130:ASP:C	1:C:132:HIS:N	2.77	0.41
1:A:35:LEU:CD1	2:A:499:FAD:C2A	2.98	0.41
1:B:68:TYR:O	1:B:69:MET:C	2.62	0.41
1:C:76:ALA:HB3	3:C:589:HOH:O	2.21	0.41
1:D:392:GLU:HG3	1:D:413:ARG:HD2	2.03	0.41
1:A:157:LEU:HD23	1:A:308:ILE:CD1	2.46	0.41
1:A:191:LEU:HA	1:A:191:LEU:HD12	1.78	0.41
1:A:433:SER:N	1:A:434:PRO:CD	2.84	0.41
1:C:398:LEU:HD23	1:C:398:LEU:HA	1.90	0.41
1:A:128:LEU:HD13	1:A:298:ALA:CB	2.50	0.41
3:A:502:HOH:O	1:B:456:THR:HG23	2.19	0.41
1:B:313:TYR:CD1	1:B:313:TYR:N	2.88	0.41
1:C:126:GLY:HA2	1:C:135:LEU:O	2.20	0.41
1:D:315:LYS:HD2	1:D:319:ASP:HA	2.01	0.41
1:C:241:LEU:HD23	1:C:241:LEU:HA	1.77	0.41
1:D:22:ALA:O	1:D:26:HIS:HB2	2.21	0.41
1:D:58:PRO:HB3	1:D:98:LYS:HD3	2.03	0.41
1:A:459:VAL:O	1:A:465:GLU:HB3	2.20	0.41
1:B:39:HIS:HB3	1:B:53:ASN:OD1	2.20	0.41
1:B:91:TRP:CD2	1:B:186:ALA:HB2	2.56	0.41
1:B:314:SER:CB	1:B:330:ARG:HH22	2.34	0.41
1:B:411:MET:O	1:B:428:MET:HA	2.21	0.41
1:D:16:LEU:HD12	1:D:16:LEU:HA	1.84	0.41
1:D:20:TRP:O	1:D:24:SER:HB2	2.20	0.41
1:D:74:GLU:HG2	1:D:403:SER:CB	2.41	0.41
1:D:173:LEU:HB3	1:D:265:ARG:HH11	1.85	0.41
1:D:449:LYS:O	1:D:452:ASP:HB2	2.20	0.41
1:B:138:GLU:HB3	1:B:147:LEU:HD21	2.02	0.41
1:D:417:ASN:HB3	1:D:420:ASP:OD1	2.21	0.41
1:A:102:VAL:O	1:A:105:ILE:HB	2.21	0.40
1:B:318:VAL:O	1:B:320:ASN:N	2.54	0.40
1:B:395:PHE:CD1	1:B:395:PHE:N	2.89	0.40
1:B:451:SER:O	1:B:455:ASN:ND2	2.45	0.40
1:B:479:LYS:HB2	1:B:479:LYS:HE2	1.84	0.40
1:C:36:GLN:O	1:C:46:ALA:HB1	2.22	0.40
1:C:97:ALA:HB1	1:D:402:ILE:HG23	2.03	0.40
1:C:323:ALA:O	1:C:328:THR:HG21	2.21	0.40
1:D:398:LEU:HD23	1:D:398:LEU:HA	1.87	0.40
1:A:135:LEU:HD23	1:A:137:ARG:HH11	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:HIS:ND1	1:A:276:ASP:OD1	2.55	0.40
1:A:439:SER:HB2	3:A:567:HOH:O	2.20	0.40
1:B:412:VAL:HG13	1:B:428:MET:HG2	2.03	0.40
1:C:478:GLU:O	1:C:479:LYS:C	2.63	0.40
1:A:86:SER:OG	1:B:83:ASP:N	2.45	0.40
1:A:415:VAL:HG22	1:A:424:LEU:HB2	2.03	0.40
1:A:455:ASN:O	1:B:445:LYS:HE2	2.21	0.40
1:A:460:HIS:HA	1:A:461:PRO:HA	1.73	0.40
1:B:129:GLN:HB3	1:B:133:THR:HG22	1.99	0.40
1:C:391:TYR:O	1:C:413:ARG:HA	2.22	0.40
1:A:96:ALA:O	1:A:97:ALA:C	2.64	0.40
1:A:221:ARG:NH2	1:A:251:HIS:O	2.55	0.40
1:A:428:MET:HE1	1:A:436:ILE:HB	2.03	0.40
1:C:365:VAL:HB	1:C:371:MET:HB2	2.04	0.40
1:D:119:LEU:HD12	1:D:119:LEU:HA	1.86	0.40
1:B:128:LEU:CD2	1:B:155:ILE:HD13	2.52	0.40
1:B:250:THR:O	1:B:251:HIS:HB2	2.22	0.40
1:C:41:PRO:HA	1:C:42:PRO:HA	1.74	0.40
1:C:183:LEU:HD23	1:C:183:LEU:HA	1.83	0.40
1:C:476:PHE:CD1	1:C:476:PHE:N	2.90	0.40
1:D:174:CYS:HB3	1:D:282:LEU:HG	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:LYS:NZ	1:D:113:PHE:O[2_656]	2.14	0.06

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	485/490 (99%)	436 (90%)	46 (10%)	3 (1%)	21	23
1	B	482/490 (98%)	446 (92%)	30 (6%)	6 (1%)	10	8
1	C	485/490 (99%)	454 (94%)	28 (6%)	3 (1%)	21	23
1	D	482/490 (98%)	452 (94%)	28 (6%)	2 (0%)	30	34
All	All	1934/1960 (99%)	1788 (92%)	132 (7%)	14 (1%)	18	19

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	ASP
1	B	2	ARG
1	B	319	ASP
1	C	131	ASN
1	D	378	GLU
1	A	131	ASN
1	B	131	ASN
1	B	180	ALA
1	B	291	GLN
1	D	2	ARG
1	A	262	ASP
1	C	46	ALA
1	C	303	ALA
1	B	214	GLY

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	390/393 (99%)	354 (91%)	36 (9%)	8	9
1	B	387/393 (98%)	353 (91%)	34 (9%)	9	10
1	C	390/393 (99%)	352 (90%)	38 (10%)	8	8
1	D	387/393 (98%)	339 (88%)	48 (12%)	4	4
All	All	1554/1572 (99%)	1398 (90%)	156 (10%)	7	7

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	7	VAL
1	A	24	SER
1	A	27	LYS
1	A	35	LEU
1	A	47	LEU
1	A	56	CYS
1	A	59	LYS
1	A	100	LYS
1	A	120	THR
1	A	137	ARG
1	A	139	SER
1	A	152	THR
1	A	157	LEU
1	A	184	ASP
1	A	212	ARG
1	A	215	GLN
1	A	216	VAL
1	A	221	ARG
1	A	250	THR
1	A	252	GLU
1	A	267	VAL
1	A	287	VAL
1	A	301	GLU
1	A	304	LYS
1	A	333	LEU
1	A	334	THR
1	A	360	LYS
1	A	368	ILE
1	A	391	TYR
1	A	406	THR
1	A	415	VAL
1	A	417	ASN
1	A	444	LEU
1	A	463	SER
1	A	484	GLU
1	B	1	SER
1	B	6	LEU
1	B	16	LEU
1	B	24	SER
1	B	28	LYS
1	B	56	CYS

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Mol	Chain	Res	Type
1	B	82	LEU
1	B	84	ARG
1	B	85	GLU
1	B	130	ASP
1	B	141	ASP
1	B	166	LEU
1	B	169	GLU
1	B	184	ASP
1	B	185	GLU
1	B	237	LEU
1	B	239	GLU
1	B	256	LYS
1	B	265	ARG
1	B	274	GLU
1	B	295	LEU
1	B	314	SER
1	B	334	THR
1	B	348	VAL
1	B	354	ARG
1	B	378	GLU
1	B	387	GLN
1	B	398	LEU
1	B	411	MET
1	B	417	ASN
1	B	444	LEU
1	B	445	LYS
1	B	467	LEU
1	B	482	ARG
1	C	1	SER
1	C	7	VAL
1	C	16	LEU
1	C	25	LEU
1	C	37	LYS
1	C	47	LEU
1	C	56	CYS
1	C	59	LYS
1	C	63	VAL
1	C	92	LYS
1	C	100	LYS
1	C	139	SER
1	C	144	SER
1	C	161	SER

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Mol	Chain	Res	Type
1	C	166	LEU
1	C	188	LYS
1	C	215	GLN
1	C	218	LEU
1	C	223	ASP
1	C	224	MET
1	C	231	SER
1	C	233	LEU
1	C	250	THR
1	C	281	MET
1	C	282	LEU
1	C	287	VAL
1	C	295	LEU
1	C	304	LYS
1	C	317	ASN
1	C	334	THR
1	C	394	SER
1	C	398	LEU
1	C	415	VAL
1	C	417	ASN
1	C	432	SER
1	C	437	ILE
1	C	467	LEU
1	C	479	LYS
1	D	2	ARG
1	D	8	VAL
1	D	16	LEU
1	D	24	SER
1	D	28	LYS
1	D	37	LYS
1	D	56	CYS
1	D	59	LYS
1	D	70	ASP
1	D	71	THR
1	D	82	LEU
1	D	84	ARG
1	D	85	GLU
1	D	94	LEU
1	D	115	ASP
1	D	133	THR
1	D	143	ASN
1	D	153	GLU

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Mol	Chain	Res	Type
1	D	166	LEU
1	D	169	GLU
1	D	233	LEU
1	D	237	LEU
1	D	239	GLU
1	D	249	ARG
1	D	257	VAL
1	D	258	THR
1	D	265	ARG
1	D	279	VAL
1	D	287	VAL
1	D	292	THR
1	D	301	GLU
1	D	304	LYS
1	D	327	VAL
1	D	334	THR
1	D	348	VAL
1	D	354	ARG
1	D	369	PRO
1	D	377	VAL
1	D	379	GLU
1	D	388	VAL
1	D	398	LEU
1	D	414	ILE
1	D	424	LEU
1	D	457	ILE
1	D	469	SER
1	D	481	LYS
1	D	482	ARG
1	D	484	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	417	ASN
1	B	26	HIS
1	B	43	HIS
1	B	90	ASN
1	B	106	ASN
1	B	123	GLN
1	B	132	HIS

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Mol	Chain	Res	Type
1	B	401	ASN
1	B	417	ASN
1	C	26	HIS
1	C	43	HIS
1	C	129	GLN
1	C	260	ASN
1	C	401	ASN
1	C	417	ASN
1	D	123	GLN
1	D	165	HIS
1	D	207	ASN
1	D	236	GLN
1	D	247	ASN
1	D	251	HIS
1	D	294	GLN
1	D	339	ASN
1	D	387	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](#)

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	D	499	-	58,58,58	2.20	14 (24%)	85,89,89	0.96	3 (3%)
2	FAD	B	499	-	58,58,58	2.40	18 (31%)	85,89,89	0.91	1 (1%)
2	FAD	C	499	-	58,58,58	2.62	24 (41%)	85,89,89	0.98	3 (3%)
2	FAD	A	499	-	58,58,58	2.02	13 (22%)	85,89,89	1.01	6 (7%)

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	D	499	-	-	4/34/50/50	0/6/6/6
2	FAD	B	499	-	-	7/34/50/50	0/6/6/6
2	FAD	C	499	-	-	4/34/50/50	0/6/6/6
2	FAD	A	499	-	-	2/34/50/50	0/6/6/6

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	499	FAD	PA-O3P	11.76	1.72	1.59
2	D	499	FAD	P-O3P	11.63	1.72	1.59
2	B	499	FAD	C1'-C2'	-8.56	1.40	1.52
2	A	499	FAD	P-O3P	7.34	1.67	1.59
2	B	499	FAD	C8M-C8	-7.22	1.37	1.51
2	C	499	FAD	P-O3P	6.45	1.66	1.59
2	B	499	FAD	C4'-C3'	-6.15	1.42	1.53
2	A	499	FAD	C4'-C3'	-5.76	1.43	1.53
2	B	499	FAD	C5X-N5	-5.15	1.30	1.39
2	A	499	FAD	C8M-C8	-4.54	1.42	1.51
2	B	499	FAD	O4'-C4'	-4.20	1.34	1.43
2	D	499	FAD	PA-O5B	-4.11	1.43	1.59
2	C	499	FAD	C4A-N3A	4.11	1.42	1.34
2	A	499	FAD	C4X-N5	3.90	1.39	1.30
2	C	499	FAD	C2'-C3'	3.84	1.60	1.53
2	C	499	FAD	C2A-N3A	-3.62	1.27	1.33
2	C	499	FAD	C5X-N5	-3.61	1.32	1.39
2	A	499	FAD	C10-N10	3.61	1.45	1.37
2	B	499	FAD	C1'-N10	-3.42	1.39	1.47
2	A	499	FAD	PA-O5B	-3.25	1.46	1.59
2	D	499	FAD	C1B-N9A	-3.24	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	499	FAD	C4-N3	-3.21	1.32	1.38
2	C	499	FAD	O4'-C4'	-3.13	1.36	1.43
2	C	499	FAD	C4X-N5	3.06	1.37	1.30
2	C	499	FAD	O2B-C2B	3.04	1.50	1.43
2	C	499	FAD	C6-C7	-2.99	1.35	1.39
2	B	499	FAD	PA-O1A	-2.97	1.40	1.50
2	D	499	FAD	C1'-N10	-2.97	1.40	1.47
2	A	499	FAD	C2B-C1B	-2.91	1.44	1.53
2	B	499	FAD	C9-C9A	-2.89	1.35	1.39
2	D	499	FAD	C2B-C1B	-2.89	1.44	1.53
2	B	499	FAD	C4X-N5	2.86	1.36	1.30
2	C	499	FAD	C7M-C7	-2.79	1.45	1.51
2	C	499	FAD	C4'-C3'	-2.77	1.48	1.53
2	D	499	FAD	C5A-N7A	-2.72	1.34	1.39
2	A	499	FAD	C5A-C4A	2.67	1.43	1.39
2	C	499	FAD	C1B-N9A	-2.65	1.39	1.46
2	C	499	FAD	C5A-C6A	-2.62	1.33	1.41
2	C	499	FAD	C6-C5X	-2.61	1.36	1.40
2	A	499	FAD	C8A-N9A	2.61	1.42	1.37
2	B	499	FAD	C4-N3	-2.60	1.34	1.38
2	B	499	FAD	PA-O3P	2.52	1.62	1.59
2	B	499	FAD	C2B-C3B	-2.52	1.46	1.53
2	B	499	FAD	O4B-C1B	-2.50	1.36	1.42
2	C	499	FAD	PA-O2A	-2.48	1.43	1.55
2	A	499	FAD	P-O5'	-2.48	1.49	1.59
2	C	499	FAD	P-O5'	-2.48	1.49	1.59
2	D	499	FAD	O2B-C2B	-2.47	1.36	1.43
2	D	499	FAD	C4X-N5	2.45	1.36	1.30
2	A	499	FAD	C4X-C4	2.42	1.53	1.44
2	C	499	FAD	P-O2P	-2.40	1.44	1.55
2	B	499	FAD	PA-O5B	-2.37	1.50	1.59
2	D	499	FAD	P-O2P	-2.34	1.44	1.55
2	C	499	FAD	P-O1P	-2.33	1.42	1.50
2	A	499	FAD	C5B-C4B	-2.27	1.44	1.51
2	B	499	FAD	C5A-N7A	-2.26	1.35	1.39
2	D	499	FAD	P-O1P	-2.25	1.43	1.50
2	D	499	FAD	C5'-C4'	2.21	1.54	1.51
2	C	499	FAD	O4B-C4B	-2.21	1.40	1.45
2	C	499	FAD	C2B-C3B	-2.21	1.47	1.53
2	B	499	FAD	C2-N3	-2.16	1.34	1.39
2	D	499	FAD	O4'-C4'	-2.15	1.38	1.43
2	B	499	FAD	C8A-N7A	-2.14	1.27	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	499	FAD	C6-C7	-2.13	1.36	1.39
2	C	499	FAD	O5B-C5B	2.13	1.52	1.44
2	C	499	FAD	O4B-C1B	-2.11	1.37	1.42
2	D	499	FAD	C9A-N10	-2.05	1.37	1.41
2	D	499	FAD	PA-O2A	-2.03	1.45	1.55
2	C	499	FAD	C8M-C8	2.01	1.54	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	499	FAD	C5A-N7A-C8A	3.44	108.86	103.45
2	C	499	FAD	C5A-N7A-C8A	3.29	108.61	103.45
2	B	499	FAD	C5A-N7A-C8A	3.06	108.26	103.45
2	A	499	FAD	C5A-N7A-C8A	2.60	107.53	103.45
2	D	499	FAD	C4-N3-C2	-2.55	121.12	125.64
2	C	499	FAD	C4-N3-C2	-2.52	121.17	125.64
2	D	499	FAD	C4A-C5A-N7A	-2.41	107.83	110.58
2	A	499	FAD	C4X-C10-N1	-2.14	119.34	124.59
2	C	499	FAD	C4X-C10-N10	2.11	119.50	116.48
2	A	499	FAD	C4A-C5A-N7A	-2.02	108.27	110.58
2	A	499	FAD	C4-N3-C2	-2.02	122.05	125.64
2	A	499	FAD	C10-N1-C2	2.02	121.21	116.85
2	A	499	FAD	C4X-C10-N10	2.00	119.35	116.48

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	499	FAD	C5'-O5'-P-O2P
2	B	499	FAD	C5'-O5'-P-O3P
2	B	499	FAD	PA-O3P-P-O5'
2	D	499	FAD	C3B-C4B-C5B-O5B
2	B	499	FAD	C3B-C4B-C5B-O5B
2	D	499	FAD	O4B-C4B-C5B-O5B
2	A	499	FAD	PA-O3P-P-O5'
2	C	499	FAD	PA-O3P-P-O5'
2	D	499	FAD	PA-O3P-P-O5'
2	B	499	FAD	O4B-C4B-C5B-O5B
2	C	499	FAD	O4B-C4B-C5B-O5B
2	B	499	FAD	C5'-O5'-P-O1P
2	B	499	FAD	C2B-C1B-N9A-C8A
2	C	499	FAD	PA-O3P-P-O1P

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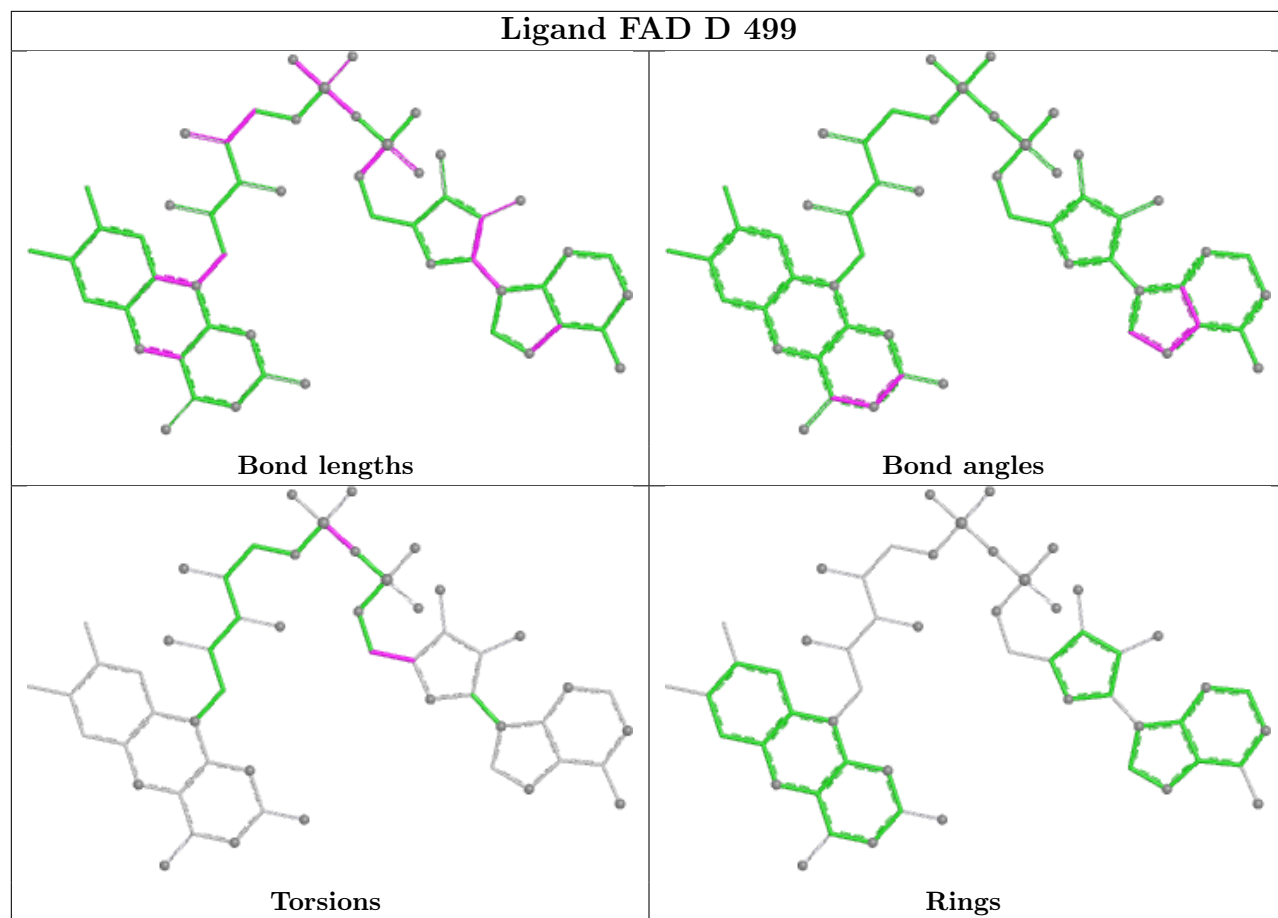
Mol	Chain	Res	Type	Atoms
2	A	499	FAD	O4B-C4B-C5B-O5B
2	C	499	FAD	C3B-C4B-C5B-O5B
2	D	499	FAD	PA-O3P-P-O2P

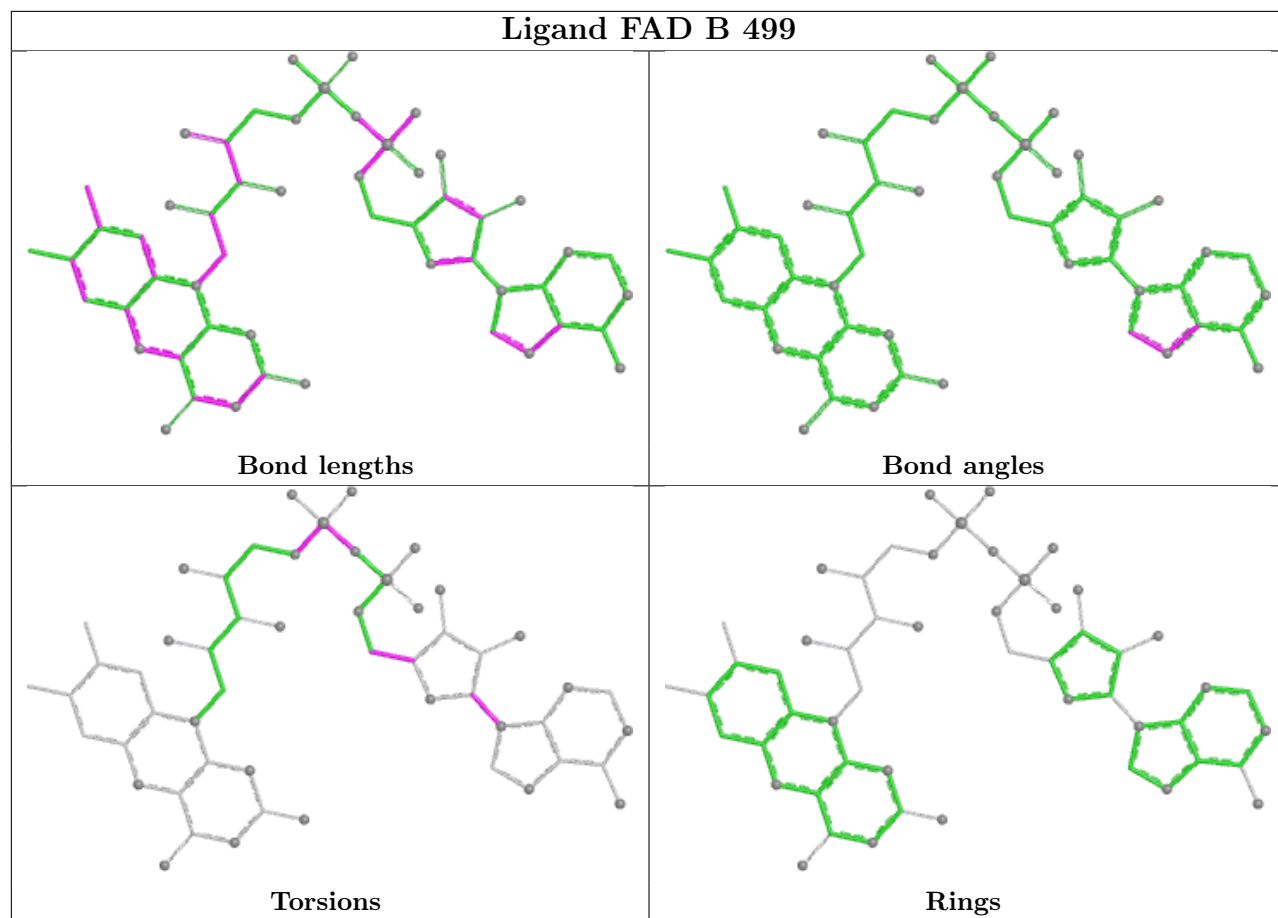
There are no ring outliers.

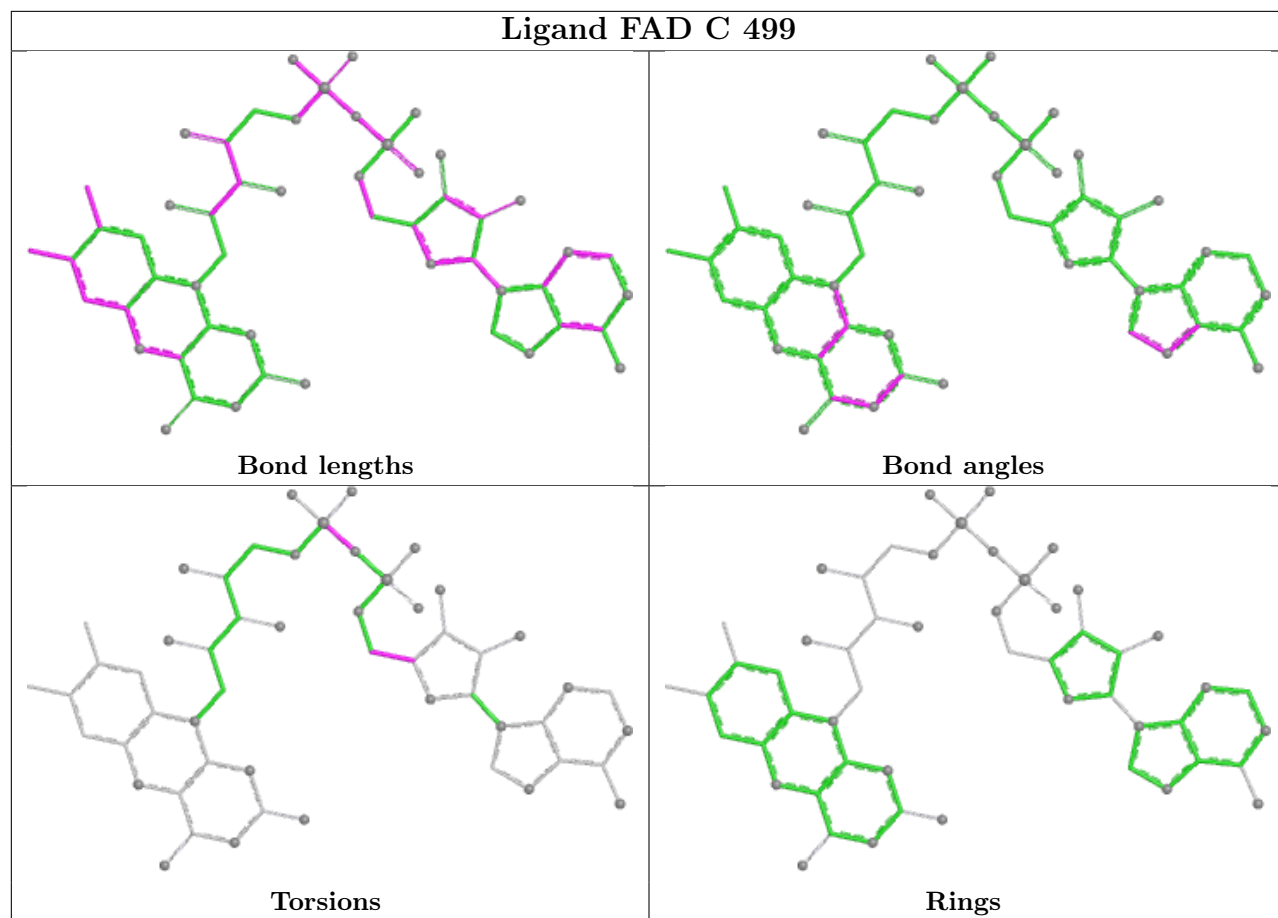
3 monomers are involved in 8 short contacts:

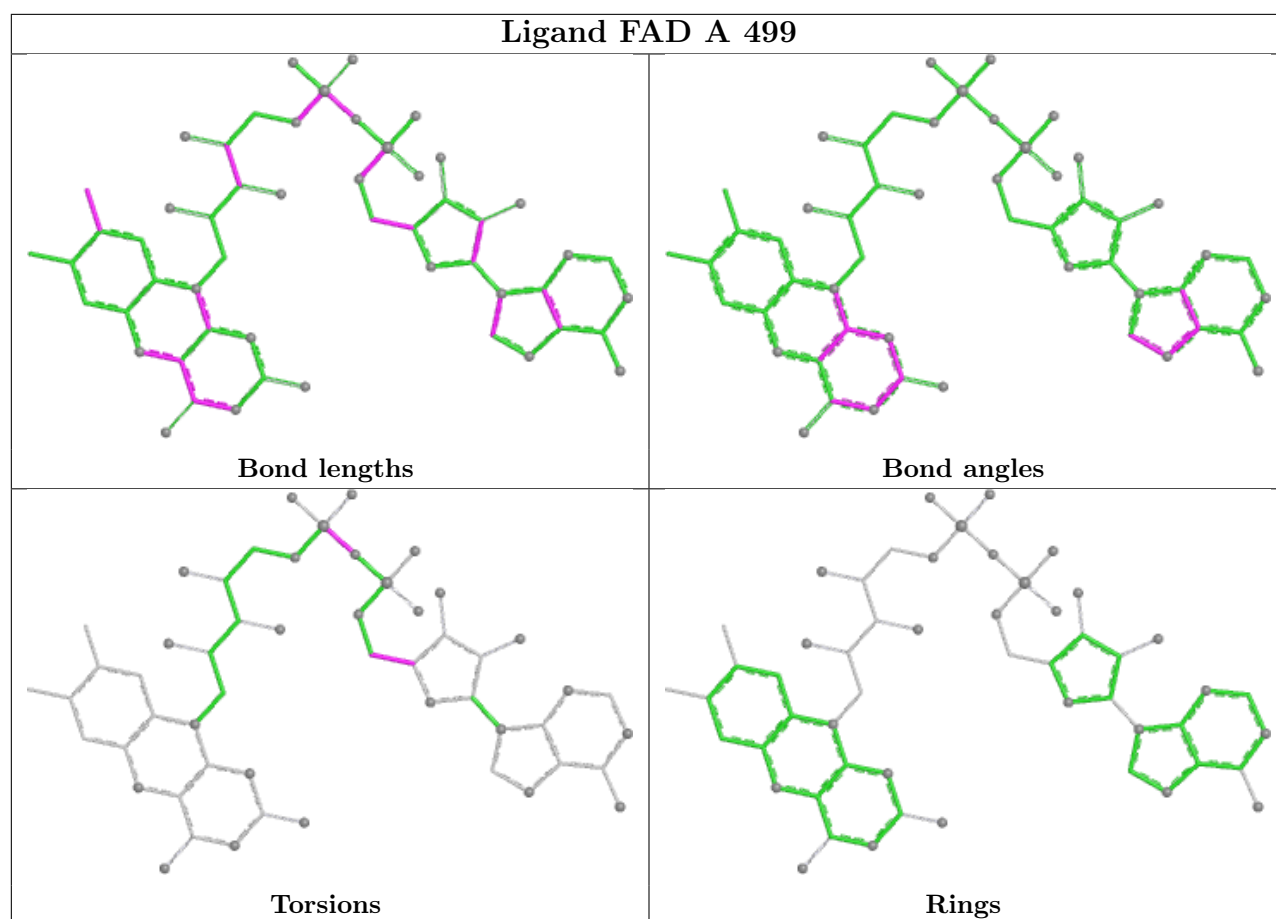
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	499	FAD	2	0
2	C	499	FAD	4	0
2	A	499	FAD	2	0

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	487/490 (99%)	-0.42	1 (0%) 91 90	4, 19, 56, 103	0
1	B	484/490 (98%)	-0.18	4 (0%) 82 80	3, 21, 58, 93	0
1	C	487/490 (99%)	-0.61	2 (0%) 88 87	2, 17, 43, 95	0
1	D	484/490 (98%)	-0.68	1 (0%) 91 90	3, 16, 40, 70	0
All	All	1942/1960 (99%)	-0.47	8 (0%) 88 87	2, 18, 52, 103	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	386	ASP	3.5
1	C	486	ILE	3.2
1	C	487	ASP	3.0
1	B	23	ALA	2.6
1	A	487	ASP	2.6
1	B	167	GLY	2.6
1	D	351	ASN	2.4
1	B	133	THR	2.2

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](#)

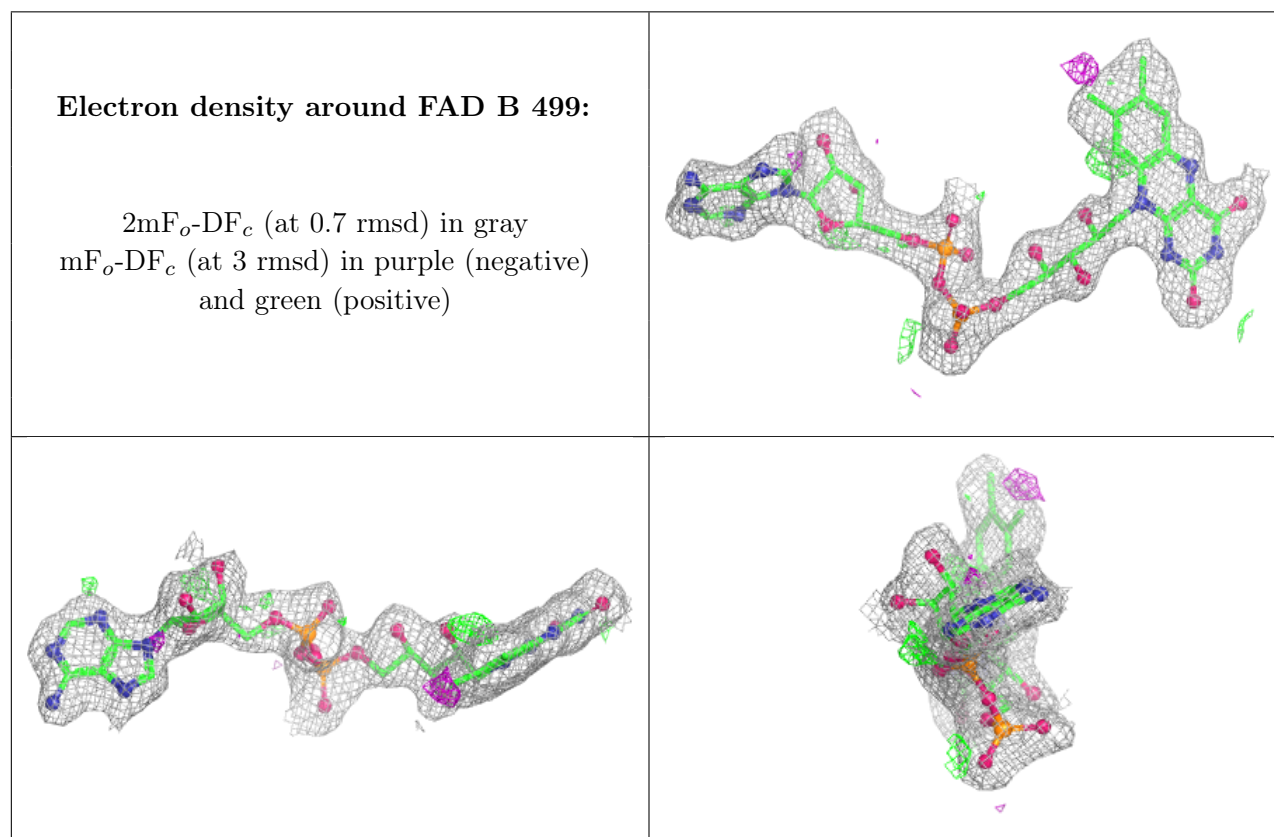
There are no oligosaccharides in this entry.

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.

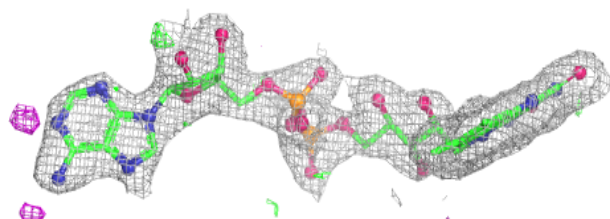
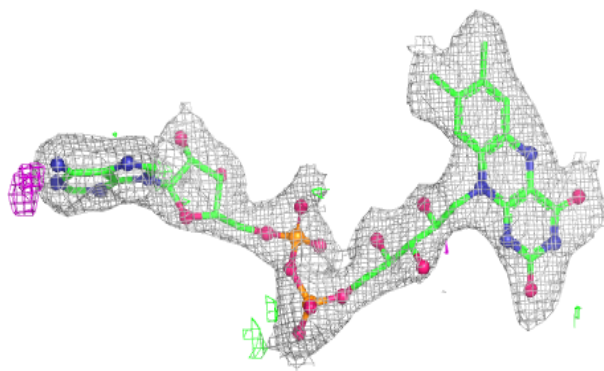
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	B	499	53/53	0.96	0.06	2,15,21,23	0
2	FAD	A	499	53/53	0.97	0.05	2,12,29,30	0
2	FAD	C	499	53/53	0.98	0.04	2,10,15,18	0
2	FAD	D	499	53/53	0.98	0.05	2,14,18,20	0

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.

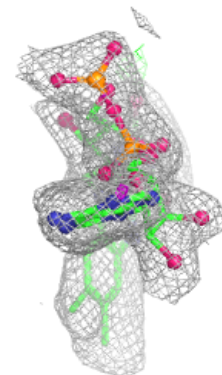
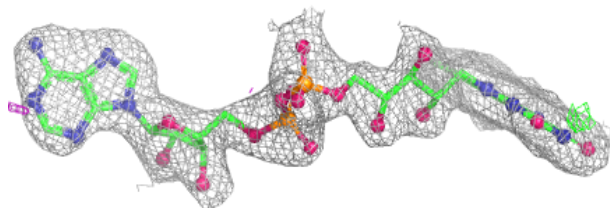
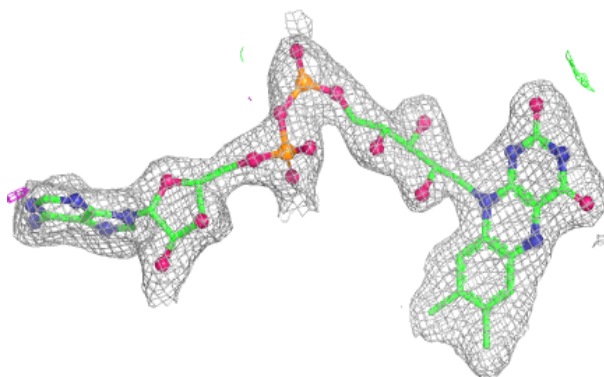


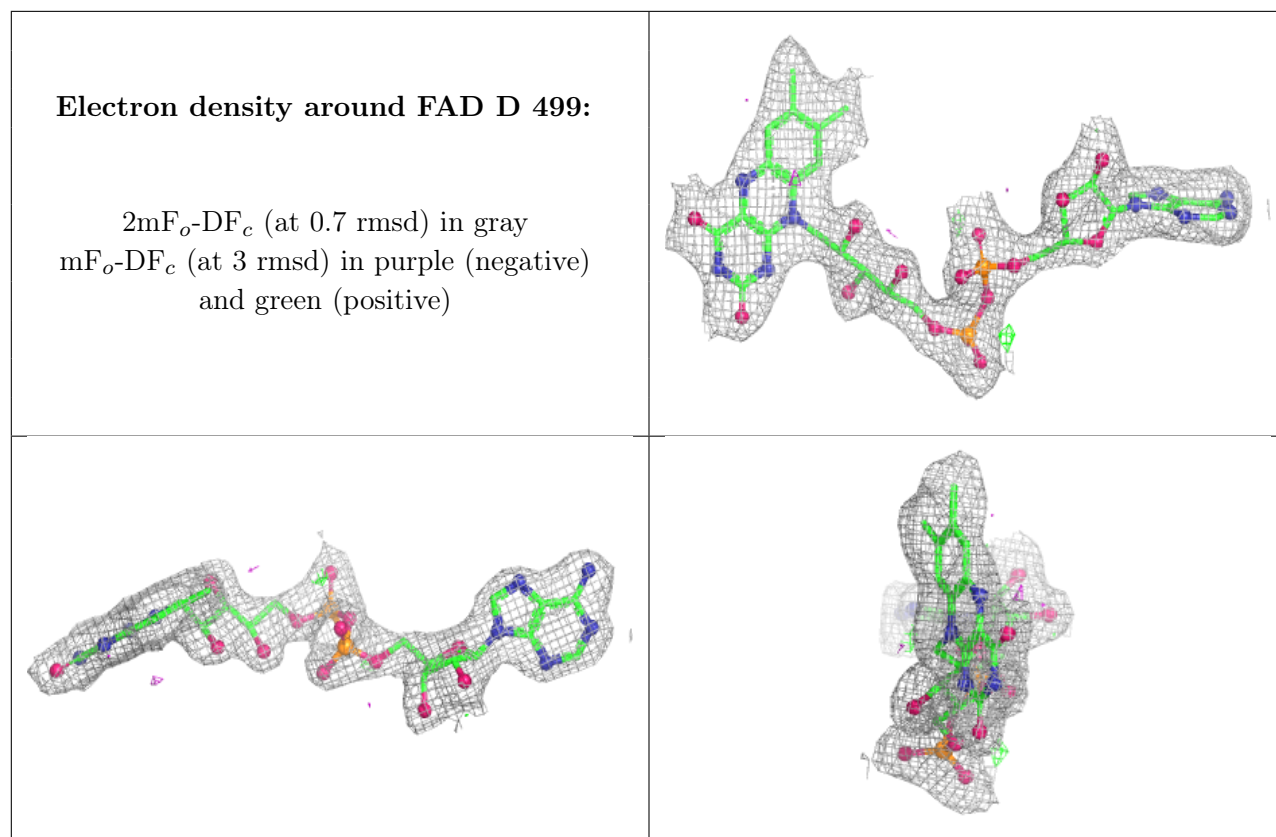
Electron density around FAD A 499:

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

**Electron density around FAD C 499:**

$2mF_o-DF_c$ (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.