



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:22 AM UTC

PDB ID : 1NDA / pdb_00001nda
Title : THE STRUCTURE OF TRYPANOSOMA CRUZI TRYPANOTHIONE REDUCTASE IN THE OXIDIZED AND NADPH REDUCED STATE
Authors : Lantwin, C.B.; Kabsch, W.; Pai, E.F.; Schlichting, I.; Krauth-Siegel, R.L.
Deposited on : 1993-07-02
Resolution : 3.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

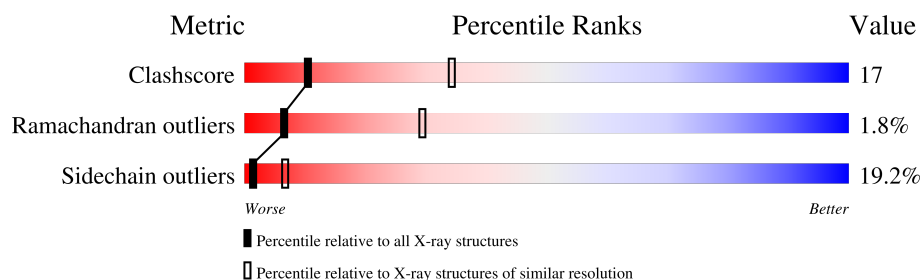
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	491	
1	B	491	
1	C	491	
1	D	491	

2 Entry composition ⓘ

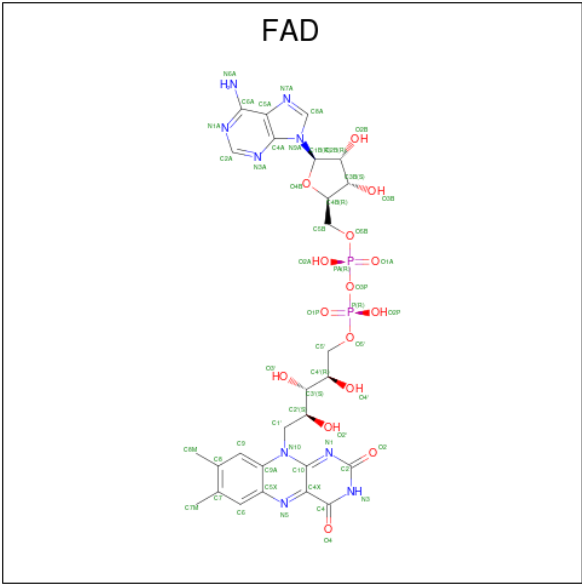
There are 2 unique types of molecules in this entry. The entry contains 15016 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3701	2352	629	699	21			
1	B	481	Total	C	N	O	S	0	0	0
			3701	2352	629	699	21			
1	C	481	Total	C	N	O	S	0	0	0
			3701	2352	629	699	21			
1	D	481	Total	C	N	O	S	0	0	0
			3701	2352	629	699	21			

- 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		

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

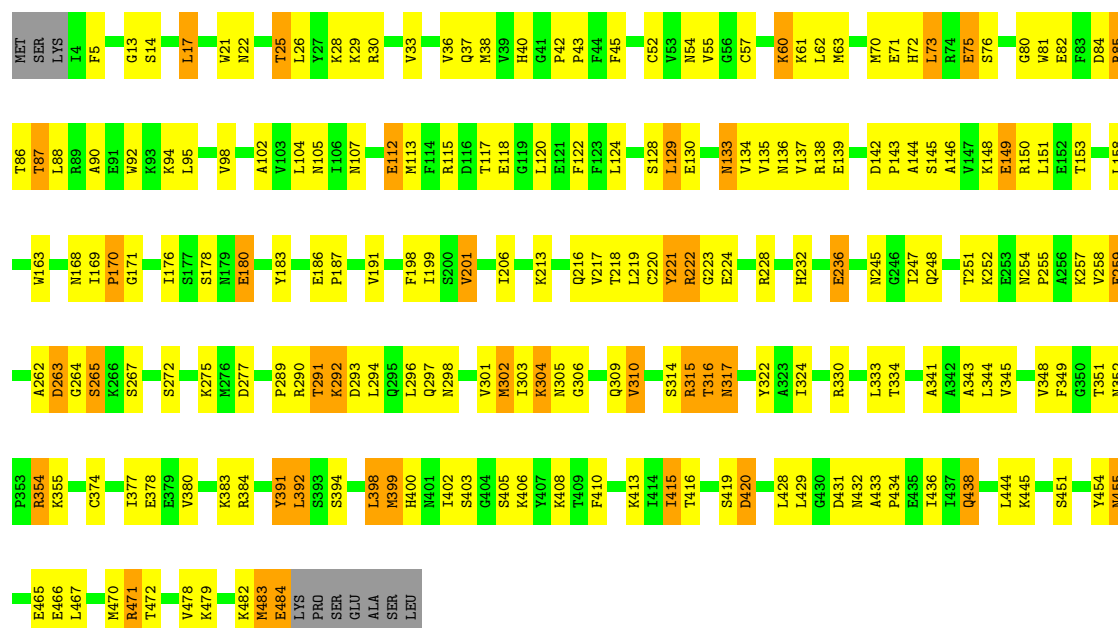
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

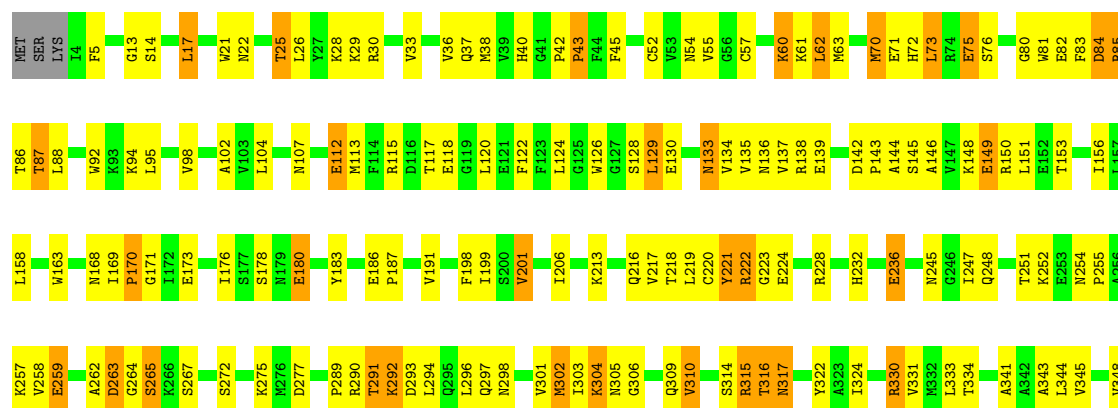
• Molecule 1: TRYPANOTHIONE OXIDOREDUCTASE

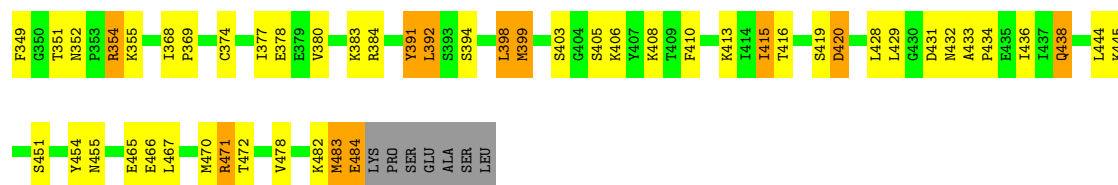
Chain A: 



• Molecule 1: TRYPANOTHIONE OXIDOREDUCTASE

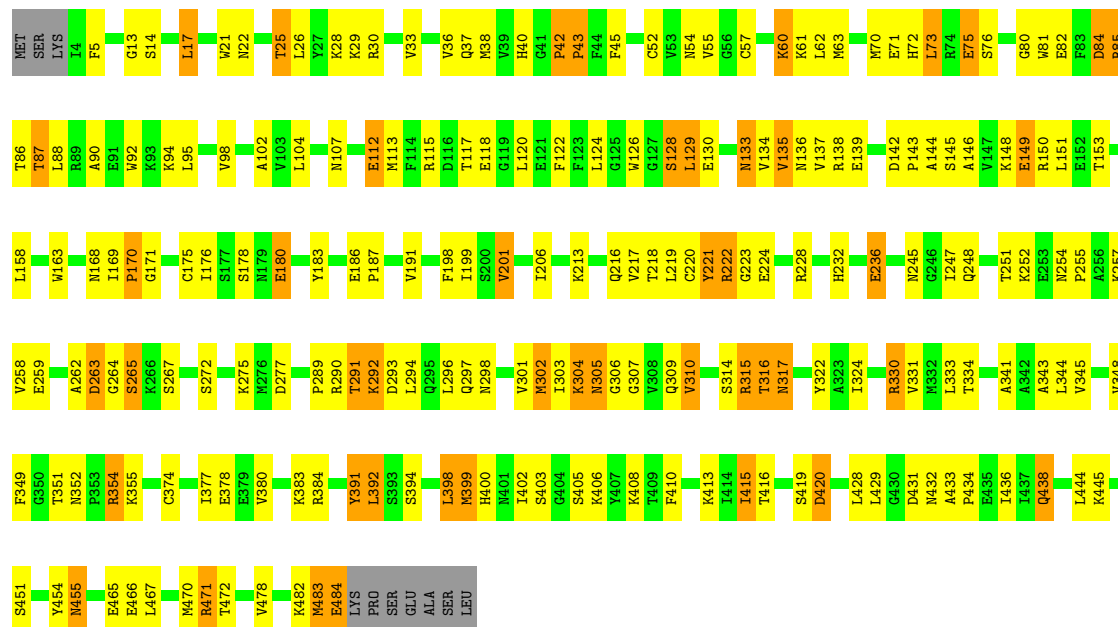
Chain B: 





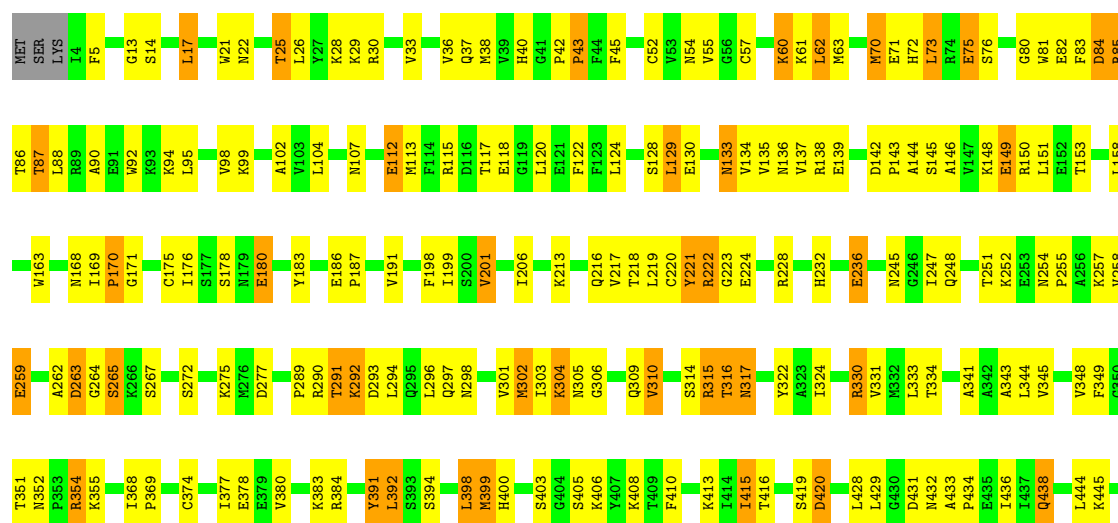
• Molecule 1: TRYPANOTHIONE OXIDOREDUCTASE

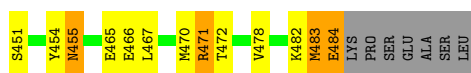
Chain C: 55% 34% 9% .



• Molecule 1: TRYPANOTHIONE OXIDOREDUCTASE

Chain D: 55% 34% 9% .





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.30Å 91.10Å 126.00Å 90.00° 94.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.206 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15016	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.55	0/3776	0.85	0/5116
1	B	0.55	0/3776	0.85	0/5116
1	C	0.55	0/3776	0.85	0/5116
1	D	0.55	0/3776	0.85	0/5116
All	All	0.55	0/15104	0.85	0/20464

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	4
1	C	0	4
1	D	0	4
All	All	0	16

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	183	TYR	Sidechain
1	A	221	TYR	Sidechain
1	A	352	ASN	Peptide
1	A	42	PRO	Peptide
1	B	183	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	B	221	TYR	Sidechain
1	B	352	ASN	Peptide
1	B	42	PRO	Peptide
1	C	183	TYR	Sidechain
1	C	221	TYR	Sidechain
1	C	352	ASN	Peptide
1	C	42	PRO	Peptide
1	D	183	TYR	Sidechain
1	D	221	TYR	Sidechain
1	D	352	ASN	Peptide
1	D	42	PRO	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	3701	0	3705	138	0
1	B	3701	0	3705	133	1
1	C	3701	0	3705	139	1
1	D	3701	0	3705	138	0
2	A	53	0	25	0	0
2	B	53	0	25	0	0
2	C	53	0	25	0	0
2	D	53	0	25	0	0
All	All	15016	0	14920	503	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 (503) 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:A:479:LYS:HG2	1:C:42:PRO:O	1.60	1.00
1:A:479:LYS:CG	1:C:42:PRO:O	2.18	0.90
1:B:267:SER:HB3	1:B:275:LYS:HE3	1.60	0.83
1:A:267:SER:HB3	1:A:275:LYS:HE3	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:LYS:HE3	1:D:80:GLY:HA2	1.60	0.82
1:A:94:LYS:HE3	1:B:80:GLY:HA2	1.60	0.81
1:C:267:SER:HB3	1:C:275:LYS:HE3	1.60	0.81
1:D:267:SER:HB3	1:D:275:LYS:HE3	1.60	0.81
1:B:176:ILE:HB	1:B:180:GLU:HG3	1.67	0.77
1:A:176:ILE:HB	1:A:180:GLU:HG3	1.67	0.76
1:C:176:ILE:HB	1:C:180:GLU:HG3	1.67	0.76
1:D:22:ASN:HB3	1:D:345:VAL:HG21	1.68	0.75
1:D:301:VAL:HG13	1:D:316:THR:HG21	1.69	0.75
1:B:22:ASN:HB3	1:B:345:VAL:HG21	1.68	0.75
1:B:301:VAL:HG13	1:B:316:THR:HG21	1.69	0.74
1:C:22:ASN:HB3	1:C:345:VAL:HG21	1.68	0.74
1:A:22:ASN:HB3	1:A:345:VAL:HG21	1.68	0.74
1:D:176:ILE:HB	1:D:180:GLU:HG3	1.67	0.74
1:A:130:GLU:HB3	1:A:134:VAL:HG13	1.70	0.73
1:B:130:GLU:HB3	1:B:134:VAL:HG13	1.70	0.73
1:D:130:GLU:HB3	1:D:134:VAL:HG13	1.70	0.73
1:A:391:TYR:HE2	1:A:471:ARG:O	1.72	0.72
1:C:301:VAL:HG13	1:C:316:THR:HG21	1.69	0.72
1:A:301:VAL:HG13	1:A:316:THR:HG21	1.69	0.72
1:B:391:TYR:HE2	1:B:471:ARG:O	1.72	0.72
1:A:317:ASN:H	1:A:317:ASN:ND2	1.87	0.72
1:C:317:ASN:H	1:C:317:ASN:ND2	1.87	0.71
1:D:391:TYR:HE2	1:D:471:ARG:O	1.72	0.71
1:C:130:GLU:HB3	1:C:134:VAL:HG13	1.70	0.71
1:C:73:LEU:HD12	1:D:73:LEU:HD12	1.71	0.71
1:A:73:LEU:HD12	1:B:73:LEU:HD12	1.72	0.71
1:C:391:TYR:HE2	1:C:471:ARG:O	1.72	0.71
1:C:310:VAL:HG13	1:C:314:SER:HA	1.74	0.70
1:D:317:ASN:H	1:D:317:ASN:ND2	1.87	0.70
1:B:317:ASN:ND2	1:B:317:ASN:H	1.87	0.70
1:B:310:VAL:HG13	1:B:314:SER:HA	1.74	0.70
1:C:171:GLY:HA3	1:C:258:VAL:O	1.92	0.70
1:A:171:GLY:HA3	1:A:258:VAL:O	1.92	0.69
1:A:310:VAL:HG13	1:A:314:SER:HA	1.74	0.69
1:D:310:VAL:HG13	1:D:314:SER:HA	1.74	0.69
1:D:171:GLY:HA3	1:D:258:VAL:O	1.92	0.69
1:B:171:GLY:HA3	1:B:258:VAL:O	1.92	0.69
1:C:133:ASN:N	1:C:133:ASN:HD22	1.92	0.68
1:A:133:ASN:N	1:A:133:ASN:HD22	1.92	0.68
1:C:402:ILE:CD1	1:D:62:LEU:HG	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ILE:CD1	1:B:62:LEU:HG	2.23	0.68
1:D:133:ASN:N	1:D:133:ASN:HD22	1.92	0.67
1:B:133:ASN:N	1:B:133:ASN:HD22	1.92	0.67
1:D:315:ARG:HB3	1:D:322:TYR:HD2	1.61	0.66
1:A:315:ARG:HB3	1:A:322:TYR:HD2	1.60	0.66
1:B:315:ARG:HB3	1:B:322:TYR:HD2	1.60	0.65
1:C:315:ARG:HB3	1:C:322:TYR:HD2	1.61	0.65
1:C:465:GLU:HA	1:D:438:GLN:OE1	1.98	0.64
1:A:465:GLU:HA	1:B:438:GLN:OE1	1.98	0.64
1:A:84:ASP:H	1:B:87:THR:CG2	2.11	0.63
1:C:84:ASP:H	1:D:87:THR:CG2	2.11	0.63
1:C:302:MET:HB2	1:C:317:ASN:ND2	2.15	0.62
1:D:22:ASN:O	1:D:26:LEU:HB2	2.00	0.62
1:B:22:ASN:O	1:B:26:LEU:HB2	2.00	0.61
1:D:302:MET:HB2	1:D:317:ASN:ND2	2.15	0.61
1:C:22:ASN:O	1:C:26:LEU:HB2	2.00	0.61
1:B:302:MET:HB2	1:B:317:ASN:ND2	2.15	0.61
1:A:22:ASN:O	1:A:26:LEU:HB2	2.00	0.61
1:B:483:MET:SD	1:B:483:MET:C	2.84	0.61
1:D:136:ASN:HD22	1:D:150:ARG:HG2	1.66	0.61
1:A:302:MET:HB2	1:A:317:ASN:ND2	2.15	0.61
1:A:483:MET:SD	1:A:483:MET:C	2.84	0.61
1:B:136:ASN:HD22	1:B:150:ARG:HG2	1.66	0.61
1:A:136:ASN:HD22	1:A:150:ARG:HG2	1.66	0.61
1:C:483:MET:SD	1:C:483:MET:C	2.84	0.60
1:A:133:ASN:HB2	1:A:153:THR:O	2.02	0.60
1:C:296:LEU:HD12	1:C:303:ILE:HD11	1.84	0.60
1:D:296:LEU:HD12	1:D:303:ILE:HD11	1.84	0.60
1:D:483:MET:C	1:D:483:MET:SD	2.84	0.60
1:B:5:PHE:CD1	1:B:30:ARG:HG2	2.37	0.60
1:B:296:LEU:HD12	1:B:303:ILE:HD11	1.84	0.60
1:C:136:ASN:HD22	1:C:150:ARG:HG2	1.66	0.60
1:D:133:ASN:HB2	1:D:153:THR:O	2.02	0.60
1:D:73:LEU:HD23	1:D:88:LEU:HD11	1.84	0.60
1:D:5:PHE:CD1	1:D:30:ARG:HG2	2.37	0.60
1:D:315:ARG:HB3	1:D:322:TYR:CD2	2.37	0.60
1:B:133:ASN:HB2	1:B:153:THR:O	2.02	0.60
1:C:133:ASN:HB2	1:C:153:THR:O	2.02	0.60
1:B:73:LEU:HD23	1:B:88:LEU:HD11	1.84	0.59
1:A:315:ARG:HB3	1:A:322:TYR:CD2	2.37	0.59
1:C:5:PHE:CD1	1:C:30:ARG:HG2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:PHE:CD1	1:A:30:ARG:HG2	2.37	0.59
1:A:72:HIS:O	1:A:76:SER:HB3	2.03	0.59
1:C:73:LEU:HD23	1:C:88:LEU:HD11	1.83	0.59
1:B:315:ARG:HB3	1:B:322:TYR:CD2	2.37	0.59
1:C:315:ARG:HB3	1:C:322:TYR:CD2	2.37	0.59
1:B:72:HIS:O	1:B:76:SER:HB3	2.03	0.59
1:C:72:HIS:O	1:C:76:SER:HB3	2.03	0.59
1:A:87:THR:CG2	1:B:84:ASP:H	2.16	0.58
1:D:72:HIS:O	1:D:76:SER:HB3	2.03	0.58
1:A:296:LEU:HD12	1:A:303:ILE:HD11	1.84	0.58
1:A:73:LEU:HD23	1:A:88:LEU:HD11	1.84	0.58
1:C:87:THR:CG2	1:D:84:ASP:H	2.16	0.58
1:D:136:ASN:ND2	1:D:150:ARG:HG2	2.19	0.58
1:C:136:ASN:ND2	1:C:150:ARG:HG2	2.19	0.58
1:A:71:GLU:O	1:A:75:GLU:HG2	2.04	0.57
1:B:136:ASN:ND2	1:B:150:ARG:HG2	2.19	0.57
1:C:71:GLU:O	1:C:75:GLU:HG2	2.04	0.57
1:A:136:ASN:ND2	1:A:150:ARG:HG2	2.19	0.57
1:B:71:GLU:O	1:B:75:GLU:HG2	2.04	0.57
1:A:392:LEU:HD23	1:A:413:LYS:HG3	1.87	0.57
1:B:392:LEU:HD23	1:B:413:LYS:HG3	1.87	0.57
1:D:71:GLU:O	1:D:75:GLU:HG2	2.04	0.57
1:C:392:LEU:HD23	1:C:413:LYS:HG3	1.87	0.57
1:A:84:ASP:H	1:B:87:THR:HG21	1.69	0.56
1:C:87:THR:HG21	1:D:84:ASP:H	1.70	0.56
1:A:87:THR:HG21	1:B:84:ASP:H	1.70	0.56
1:A:73:LEU:CD1	1:B:73:LEU:HD12	2.35	0.56
1:C:87:THR:CG2	1:D:83:PHE:HB2	2.36	0.56
1:D:392:LEU:HD23	1:D:413:LYS:HG3	1.87	0.56
1:C:73:LEU:CD1	1:D:73:LEU:HD12	2.35	0.56
1:C:84:ASP:H	1:D:87:THR:HG21	1.69	0.56
1:A:73:LEU:HD12	1:B:73:LEU:CD1	2.36	0.56
1:A:87:THR:CG2	1:B:83:PHE:HB2	2.36	0.56
1:A:402:ILE:HD11	1:B:62:LEU:HG	1.88	0.55
1:B:438:GLN:HE21	1:B:438:GLN:HA	1.72	0.55
1:A:301:VAL:CG1	1:A:316:THR:HG21	2.37	0.55
1:D:438:GLN:HE21	1:D:438:GLN:HA	1.72	0.55
1:A:45:PHE:HB3	1:A:55:VAL:HG11	1.89	0.55
1:C:301:VAL:CG1	1:C:316:THR:HG21	2.37	0.55
1:C:402:ILE:HD11	1:D:62:LEU:HG	1.88	0.55
1:D:301:VAL:CG1	1:D:316:THR:HG21	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLY:HA2	1:B:94:LYS:HE3	1.88	0.55
1:B:301:VAL:CG1	1:B:316:THR:HG21	2.37	0.54
1:A:438:GLN:HE21	1:A:438:GLN:HA	1.72	0.54
1:D:45:PHE:HB3	1:D:55:VAL:HG11	1.89	0.54
1:A:90:ALA:HB2	1:B:81:TRP:CZ3	2.43	0.54
1:C:73:LEU:HD12	1:D:73:LEU:CD1	2.36	0.54
1:C:80:GLY:HA2	1:D:94:LYS:HE3	1.88	0.54
1:C:438:GLN:HE21	1:C:438:GLN:HA	1.72	0.54
1:D:302:MET:HB2	1:D:317:ASN:HD21	1.73	0.54
1:C:90:ALA:HB2	1:D:81:TRP:CZ3	2.43	0.54
1:A:60:LYS:HD3	1:A:60:LYS:C	2.33	0.54
1:A:302:MET:HB2	1:A:317:ASN:HD21	1.72	0.54
1:C:60:LYS:HD3	1:C:60:LYS:C	2.33	0.54
1:D:84:ASP:O	1:D:87:THR:HG22	2.08	0.54
1:B:45:PHE:HB3	1:B:55:VAL:HG11	1.89	0.53
1:C:343:ALA:HB1	1:C:354:ARG:HB3	1.90	0.53
1:D:343:ALA:HB1	1:D:354:ARG:HB3	1.90	0.53
1:B:84:ASP:O	1:B:87:THR:HG22	2.08	0.53
1:C:45:PHE:HB3	1:C:55:VAL:HG11	1.89	0.53
1:C:84:ASP:O	1:C:87:THR:HG22	2.08	0.53
1:A:84:ASP:O	1:A:87:THR:HG22	2.08	0.53
1:B:60:LYS:HD3	1:B:60:LYS:C	2.33	0.53
1:C:302:MET:HB2	1:C:317:ASN:HD21	1.73	0.53
1:D:60:LYS:HD3	1:D:60:LYS:C	2.33	0.53
1:A:232:HIS:O	1:A:236:GLU:HG2	2.09	0.53
1:B:232:HIS:O	1:B:236:GLU:HG2	2.09	0.53
1:D:232:HIS:O	1:D:236:GLU:HG2	2.09	0.53
1:A:482:LYS:HE3	1:A:484:GLU:HB2	1.91	0.52
1:C:232:HIS:O	1:C:236:GLU:HG2	2.09	0.52
1:D:482:LYS:HE3	1:D:484:GLU:HB2	1.91	0.52
1:A:343:ALA:HB1	1:A:354:ARG:HB3	1.90	0.52
1:B:317:ASN:H	1:B:317:ASN:HD22	1.57	0.52
1:C:88:LEU:HG	1:C:88:LEU:O	2.10	0.52
1:A:479:LYS:HG3	1:C:42:PRO:O	2.05	0.52
1:D:38:MET:SD	1:D:124:LEU:HD13	2.50	0.52
1:A:38:MET:SD	1:A:124:LEU:HD13	2.50	0.52
1:A:224:GLU:HG2	1:A:252:LYS:HE3	1.92	0.52
1:C:482:LYS:HE3	1:C:484:GLU:HB2	1.91	0.52
1:B:38:MET:SD	1:B:124:LEU:HD13	2.50	0.51
1:B:88:LEU:O	1:B:88:LEU:HG	2.10	0.51
1:A:471:ARG:NH1	1:A:472:THR:HA	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:ARG:NH1	1:B:472:THR:HA	2.26	0.51
1:B:482:LYS:HE3	1:B:484:GLU:HB2	1.91	0.51
1:C:224:GLU:HG2	1:C:252:LYS:HE3	1.92	0.51
1:B:343:ALA:HB1	1:B:354:ARG:HB3	1.90	0.51
1:C:102:ALA:HB1	1:D:398:LEU:HD11	1.92	0.51
1:D:391:TYR:CE2	1:D:471:ARG:O	2.61	0.51
1:C:38:MET:SD	1:C:124:LEU:HD13	2.50	0.51
1:C:75:GLU:HB2	1:C:403:SER:HB2	1.93	0.51
1:C:317:ASN:H	1:C:317:ASN:HD22	1.57	0.51
1:C:471:ARG:NH1	1:C:472:THR:HA	2.25	0.51
1:A:317:ASN:H	1:A:317:ASN:HD22	1.57	0.51
1:B:302:MET:HB2	1:B:317:ASN:HD21	1.73	0.51
1:D:88:LEU:O	1:D:88:LEU:HG	2.10	0.51
1:B:75:GLU:HB2	1:B:403:SER:HB2	1.93	0.51
1:D:75:GLU:HB2	1:D:403:SER:HB2	1.93	0.51
1:B:391:TYR:CE2	1:B:471:ARG:O	2.61	0.51
1:A:438:GLN:HE21	1:A:438:GLN:CA	2.25	0.50
1:D:471:ARG:NH1	1:D:472:THR:HA	2.25	0.50
1:B:224:GLU:HG2	1:B:252:LYS:HE3	1.92	0.50
1:A:88:LEU:O	1:A:88:LEU:HG	2.10	0.50
1:A:102:ALA:HB1	1:B:398:LEU:HD11	1.92	0.50
1:D:133:ASN:N	1:D:133:ASN:ND2	2.58	0.50
1:D:303:ILE:N	1:D:303:ILE:HD12	2.27	0.50
1:C:13:GLY:O	1:C:17:LEU:HB2	2.12	0.50
1:C:29:LYS:HG2	1:C:349:PHE:CE1	2.47	0.50
1:D:224:GLU:HG2	1:D:252:LYS:HE3	1.92	0.50
1:D:13:GLY:O	1:D:17:LEU:HB2	2.12	0.50
1:A:75:GLU:HB2	1:A:403:SER:HB2	1.93	0.50
1:A:221:TYR:CE2	1:A:223:GLY:HA3	2.47	0.50
1:B:221:TYR:CE2	1:B:223:GLY:HA3	2.47	0.49
1:B:13:GLY:O	1:B:17:LEU:HB2	2.12	0.49
1:C:104:LEU:O	1:C:107:ASN:HB2	2.12	0.49
1:A:13:GLY:O	1:A:17:LEU:HB2	2.12	0.49
1:A:104:LEU:O	1:A:107:ASN:HB2	2.12	0.49
1:C:303:ILE:HD12	1:C:303:ILE:N	2.27	0.49
1:C:438:GLN:HE21	1:C:438:GLN:CA	2.25	0.49
1:A:29:LYS:HG2	1:A:349:PHE:CE1	2.47	0.49
1:C:221:TYR:CE2	1:C:223:GLY:HA3	2.47	0.49
1:B:29:LYS:HG2	1:B:349:PHE:CE1	2.47	0.49
1:B:104:LEU:O	1:B:107:ASN:HB2	2.12	0.49
1:D:104:LEU:O	1:D:107:ASN:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:TYR:CE2	1:D:223:GLY:HA3	2.47	0.49
1:B:380:VAL:HA	1:B:383:LYS:HE2	1.95	0.49
1:D:29:LYS:HG2	1:D:349:PHE:CE1	2.47	0.49
1:A:303:ILE:HD12	1:A:303:ILE:N	2.27	0.49
1:B:303:ILE:N	1:B:303:ILE:HD12	2.27	0.49
1:B:438:GLN:HE21	1:B:438:GLN:CA	2.25	0.48
1:C:380:VAL:HA	1:C:383:LYS:HE2	1.95	0.48
1:D:438:GLN:HE21	1:D:438:GLN:CA	2.25	0.48
1:A:380:VAL:HA	1:A:383:LYS:HE2	1.95	0.48
1:B:467:LEU:HA	1:B:470:MET:CE	2.43	0.48
1:C:467:LEU:HA	1:C:470:MET:CE	2.43	0.48
1:D:139:GLU:HG2	1:D:146:ALA:N	2.28	0.48
1:A:377:ILE:HG13	1:A:380:VAL:HG23	1.96	0.48
1:B:467:LEU:HA	1:B:470:MET:HE3	1.96	0.48
1:D:467:LEU:HA	1:D:470:MET:CE	2.43	0.48
1:A:139:GLU:HG2	1:A:146:ALA:N	2.28	0.48
1:C:467:LEU:HA	1:C:470:MET:HE3	1.96	0.48
1:A:399:MET:O	1:A:403:SER:HB3	2.14	0.48
1:B:377:ILE:HG13	1:B:380:VAL:HG23	1.96	0.48
1:C:90:ALA:HB2	1:D:81:TRP:CH2	2.49	0.48
1:C:139:GLU:HG2	1:C:146:ALA:N	2.28	0.48
1:C:399:MET:O	1:C:403:SER:HB3	2.14	0.48
1:D:467:LEU:HA	1:D:470:MET:HE3	1.96	0.48
1:A:467:LEU:HA	1:A:470:MET:CE	2.43	0.48
1:C:133:ASN:N	1:C:133:ASN:ND2	2.58	0.48
1:D:380:VAL:HA	1:D:383:LYS:HE2	1.95	0.48
1:A:133:ASN:N	1:A:133:ASN:ND2	2.58	0.48
1:B:139:GLU:HG2	1:B:146:ALA:N	2.28	0.48
1:C:377:ILE:HG13	1:C:380:VAL:HG23	1.96	0.48
1:B:399:MET:O	1:B:403:SER:HB3	2.14	0.48
1:A:90:ALA:HB2	1:B:81:TRP:CH2	2.49	0.47
1:D:304:LYS:HB2	1:D:309:GLN:HB3	1.96	0.47
1:C:84:ASP:H	1:D:87:THR:HG23	1.80	0.47
1:D:317:ASN:H	1:D:317:ASN:HD22	1.57	0.47
1:A:304:LYS:HB2	1:A:309:GLN:HB3	1.95	0.47
1:C:142:ASP:OD2	1:C:144:ALA:HB3	2.14	0.47
1:D:399:MET:O	1:D:403:SER:HB3	2.14	0.47
1:B:296:LEU:HB3	1:B:301:VAL:HB	1.96	0.47
1:A:296:LEU:HB3	1:A:301:VAL:HB	1.96	0.47
1:C:304:LYS:HB2	1:C:309:GLN:HB3	1.95	0.47
1:D:142:ASP:OD2	1:D:144:ALA:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:405:SER:HB3	1:D:408:LYS:HG3	1.96	0.47
1:B:304:LYS:HB2	1:B:309:GLN:HB3	1.96	0.47
1:C:81:TRP:CH2	1:D:70:MET:HB2	2.50	0.47
1:D:296:LEU:HB3	1:D:301:VAL:HB	1.96	0.47
1:A:405:SER:HB3	1:A:408:LYS:HG3	1.97	0.47
1:B:63:MET:HE2	1:B:206:ILE:HG21	1.97	0.46
1:B:405:SER:HB3	1:B:408:LYS:HG3	1.96	0.46
1:A:142:ASP:OD2	1:A:144:ALA:HB3	2.14	0.46
1:A:467:LEU:HA	1:A:470:MET:HE3	1.96	0.46
1:A:63:MET:HE2	1:A:206:ILE:HG21	1.97	0.46
1:B:36:VAL:HG12	1:B:37:GLN:HG2	1.98	0.46
1:C:63:MET:HE2	1:C:206:ILE:HG21	1.97	0.46
1:C:398:LEU:HD11	1:D:102:ALA:HB1	1.98	0.46
1:C:405:SER:HB3	1:C:408:LYS:HG3	1.96	0.46
1:D:63:MET:HE2	1:D:206:ILE:HG21	1.97	0.46
1:A:84:ASP:H	1:B:87:THR:HG23	1.79	0.46
1:B:431:ASP:O	1:B:432:ASN:HB2	2.15	0.46
1:C:296:LEU:HB3	1:C:301:VAL:HB	1.96	0.46
1:A:81:TRP:CH2	1:B:70:MET:HB2	2.50	0.46
1:A:431:ASP:O	1:A:432:ASN:HB2	2.15	0.46
1:C:354:ARG:HG3	1:C:354:ARG:HH11	1.81	0.46
1:D:377:ILE:HG13	1:D:380:VAL:HG23	1.96	0.46
1:B:354:ARG:HG3	1:B:354:ARG:HH11	1.81	0.46
1:C:433:ALA:HB3	1:C:434:PRO:HD3	1.98	0.46
1:D:36:VAL:HG12	1:D:37:GLN:HG2	1.98	0.46
1:B:142:ASP:OD2	1:B:144:ALA:HB3	2.15	0.46
1:B:433:ALA:HB3	1:B:434:PRO:HD3	1.98	0.46
1:A:433:ALA:HB3	1:A:434:PRO:HD3	1.98	0.46
1:D:354:ARG:HG3	1:D:354:ARG:HH11	1.81	0.46
1:D:431:ASP:O	1:D:432:ASN:HB2	2.15	0.46
1:D:218:THR:HG23	1:D:248:GLN:HB3	1.98	0.46
1:D:433:ALA:HB3	1:D:434:PRO:HD3	1.98	0.46
1:A:354:ARG:HH11	1:A:354:ARG:HG3	1.81	0.45
1:A:36:VAL:HG12	1:A:37:GLN:HG2	1.98	0.45
1:A:290:ARG:HG2	1:A:292:LYS:HD3	1.99	0.45
1:C:218:THR:HG23	1:C:248:GLN:HB3	1.99	0.45
1:D:330:ARG:HB3	1:D:331:VAL:H	1.53	0.45
1:A:198:PHE:CD2	1:A:199:ILE:HG13	2.52	0.45
1:A:374:CYS:SG	1:A:444:LEU:HD22	2.57	0.45
1:A:398:LEU:HD11	1:B:102:ALA:HB1	1.98	0.45
1:B:129:LEU:HD12	1:B:129:LEU:HA	1.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:PHE:CD2	1:B:199:ILE:HG13	2.52	0.45
1:D:455:ASN:HD22	1:D:455:ASN:HA	1.57	0.45
1:C:129:LEU:HD12	1:C:129:LEU:HA	1.74	0.45
1:D:75:GLU:HG2	1:D:75:GLU:H	1.59	0.45
1:B:218:THR:HG23	1:B:248:GLN:HB3	1.99	0.45
1:C:431:ASP:O	1:C:432:ASN:HB2	2.15	0.45
1:D:186:GLU:HB2	1:D:187:PRO:HD2	1.99	0.45
1:D:290:ARG:HG2	1:D:292:LYS:HD3	1.99	0.45
1:A:180:GLU:H	1:A:180:GLU:HG2	1.55	0.45
1:C:198:PHE:CD2	1:C:199:ILE:HG13	2.52	0.45
1:A:216:GLN:NE2	1:A:248:GLN:HG3	2.32	0.45
1:B:216:GLN:NE2	1:B:248:GLN:HG3	2.32	0.45
1:B:374:CYS:SG	1:B:444:LEU:HD22	2.57	0.45
1:C:216:GLN:NE2	1:C:248:GLN:HG3	2.32	0.45
1:B:254:ASN:HD22	1:B:255:PRO:HD2	1.82	0.44
1:C:374:CYS:SG	1:C:444:LEU:HD22	2.57	0.44
1:D:198:PHE:CD2	1:D:199:ILE:HG13	2.52	0.44
1:A:218:THR:HG23	1:A:248:GLN:HB3	1.99	0.44
1:D:374:CYS:SG	1:D:444:LEU:HD22	2.57	0.44
1:B:415:ILE:O	1:B:415:ILE:HG13	2.18	0.44
1:C:36:VAL:HG12	1:C:37:GLN:HG2	1.98	0.44
1:C:95:LEU:O	1:C:98:VAL:HG22	2.17	0.44
1:A:95:LEU:O	1:A:98:VAL:HG22	2.17	0.44
1:A:415:ILE:O	1:A:415:ILE:HG13	2.17	0.44
1:B:186:GLU:HB2	1:B:187:PRO:HD2	1.99	0.44
1:C:148:LYS:O	1:C:149:GLU:HB2	2.18	0.44
1:C:254:ASN:HD22	1:C:255:PRO:HD2	1.83	0.44
1:C:466:GLU:O	1:C:470:MET:HE2	2.18	0.44
1:D:216:GLN:NE2	1:D:248:GLN:HG3	2.32	0.44
1:C:186:GLU:HB2	1:C:187:PRO:HD2	1.99	0.44
1:A:254:ASN:HD22	1:A:255:PRO:HD2	1.82	0.44
1:B:95:LEU:O	1:B:98:VAL:HG22	2.17	0.44
1:B:290:ARG:HG2	1:B:292:LYS:HD3	1.98	0.44
1:C:330:ARG:HB3	1:C:331:VAL:H	1.53	0.44
1:D:324:ILE:HD12	1:D:341:ALA:HB2	1.99	0.44
1:A:391:TYR:CE2	1:A:471:ARG:O	2.61	0.44
1:C:415:ILE:O	1:C:415:ILE:HG13	2.17	0.44
1:D:95:LEU:O	1:D:98:VAL:HG22	2.17	0.44
1:A:466:GLU:O	1:A:470:MET:HE2	2.18	0.44
1:B:466:GLU:O	1:B:470:MET:HE2	2.18	0.44
1:C:290:ARG:HG2	1:C:292:LYS:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ASN:HD22	1:A:133:ASN:H	1.64	0.44
1:B:330:ARG:HB3	1:B:331:VAL:H	1.53	0.44
1:D:263:ASP:OD1	1:D:265:SER:HB2	2.18	0.44
1:D:368:ILE:HA	1:D:369:PRO:HA	1.77	0.44
1:D:466:GLU:O	1:D:470:MET:HE2	2.18	0.44
1:B:138:ARG:CD	1:B:143:PRO:HA	2.48	0.43
1:D:254:ASN:HD22	1:D:255:PRO:HD2	1.82	0.43
1:A:262:ALA:C	1:A:264:GLY:H	2.26	0.43
1:A:324:ILE:HD12	1:A:341:ALA:HB2	2.00	0.43
1:A:394:SER:HA	1:A:410:PHE:O	2.19	0.43
1:B:73:LEU:HD23	1:B:88:LEU:CD1	2.48	0.43
1:B:262:ALA:C	1:B:264:GLY:H	2.26	0.43
1:D:262:ALA:C	1:D:264:GLY:H	2.26	0.43
1:A:148:LYS:O	1:A:149:GLU:HB2	2.18	0.43
1:A:263:ASP:OD1	1:A:265:SER:HB2	2.18	0.43
1:B:324:ILE:HD12	1:B:341:ALA:HB2	1.99	0.43
1:C:391:TYR:CE2	1:C:471:ARG:O	2.61	0.43
1:D:415:ILE:O	1:D:415:ILE:HG13	2.18	0.43
1:A:186:GLU:HB2	1:A:187:PRO:HD2	1.99	0.43
1:B:138:ARG:HG2	1:B:139:GLU:H	1.83	0.43
1:C:138:ARG:CD	1:C:143:PRO:HA	2.48	0.43
1:D:394:SER:HA	1:D:410:PHE:O	2.19	0.43
1:A:63:MET:HG2	1:A:95:LEU:HD21	2.01	0.43
1:A:138:ARG:CD	1:A:143:PRO:HA	2.48	0.43
1:B:63:MET:HG2	1:B:95:LEU:HD21	2.01	0.43
1:C:133:ASN:HD22	1:C:133:ASN:H	1.64	0.43
1:C:451:SER:HA	1:C:454:TYR:CZ	2.54	0.43
1:D:138:ARG:CD	1:D:143:PRO:HA	2.48	0.43
1:D:139:GLU:HG3	1:D:145:SER:HB2	2.00	0.43
1:D:148:LYS:O	1:D:149:GLU:HB2	2.18	0.43
1:A:82:GLU:HA	1:A:85:ARG:NH2	2.34	0.43
1:A:170:PRO:HB2	1:A:257:LYS:HG3	2.01	0.43
1:C:137:VAL:HB	1:C:149:GLU:HB3	2.01	0.43
1:C:170:PRO:HB2	1:C:257:LYS:HG3	2.01	0.43
1:C:262:ALA:C	1:C:264:GLY:H	2.26	0.43
1:D:82:GLU:HA	1:D:85:ARG:NH2	2.34	0.43
1:D:451:SER:HA	1:D:454:TYR:CZ	2.54	0.43
1:B:52:CYS:SG	1:B:57:CYS:CB	3.06	0.43
1:B:148:LYS:O	1:B:149:GLU:HB2	2.18	0.43
1:C:324:ILE:HD12	1:C:341:ALA:HB2	2.00	0.43
1:D:73:LEU:HD23	1:D:88:LEU:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:CYS:SG	1:A:57:CYS:CB	3.06	0.43
1:B:394:SER:HA	1:B:410:PHE:O	2.19	0.43
1:C:138:ARG:HG2	1:C:139:GLU:H	1.83	0.43
1:A:138:ARG:HG2	1:A:139:GLU:H	1.83	0.43
1:A:139:GLU:HG3	1:A:145:SER:HB2	2.00	0.43
1:B:137:VAL:HB	1:B:149:GLU:HB3	2.01	0.43
1:B:451:SER:HA	1:B:454:TYR:CZ	2.54	0.43
1:C:82:GLU:HA	1:C:85:ARG:NH2	2.34	0.43
1:D:129:LEU:HD12	1:D:129:LEU:HA	1.74	0.43
1:A:112:GLU:HG3	1:A:115:ARG:NH1	2.34	0.43
1:A:482:LYS:HE3	1:A:482:LYS:HB3	1.72	0.43
1:C:455:ASN:HD22	1:C:455:ASN:HA	1.57	0.43
1:D:40:HIS:HB3	1:D:54:ASN:OD1	2.19	0.43
1:D:112:GLU:HG3	1:D:115:ARG:NH1	2.34	0.43
1:A:129:LEU:HA	1:A:129:LEU:HD12	1.74	0.42
1:B:170:PRO:HB2	1:B:257:LYS:HG3	2.01	0.42
1:B:263:ASP:OD1	1:B:265:SER:HB2	2.18	0.42
1:D:289:PRO:C	1:D:291:THR:H	2.27	0.42
1:D:137:VAL:HB	1:D:149:GLU:HB3	2.01	0.42
1:A:137:VAL:HB	1:A:149:GLU:HB3	2.01	0.42
1:C:52:CYS:SG	1:C:57:CYS:CB	3.06	0.42
1:D:432:ASN:O	1:D:436:ILE:HG13	2.19	0.42
1:C:40:HIS:HB3	1:C:54:ASN:OD1	2.19	0.42
1:C:63:MET:HG2	1:C:95:LEU:HD21	2.01	0.42
1:C:394:SER:HA	1:C:410:PHE:O	2.19	0.42
1:D:133:ASN:HD22	1:D:133:ASN:H	1.64	0.42
1:A:14:SER:HB3	1:A:334:THR:HG23	2.02	0.42
1:B:92:TRP:CG	1:B:187:PRO:HD3	2.55	0.42
1:C:112:GLU:HG3	1:C:115:ARG:NH1	2.34	0.42
1:C:139:GLU:HG3	1:C:145:SER:HB2	2.00	0.42
1:C:263:ASP:OD1	1:C:265:SER:HB2	2.18	0.42
1:C:289:PRO:C	1:C:291:THR:H	2.27	0.42
1:D:391:TYR:O	1:D:413:LYS:HA	2.20	0.42
1:A:289:PRO:C	1:A:291:THR:H	2.27	0.42
1:A:317:ASN:ND2	1:A:317:ASN:N	2.64	0.42
1:A:391:TYR:O	1:A:413:LYS:HA	2.20	0.42
1:A:451:SER:HA	1:A:454:TYR:CZ	2.54	0.42
1:B:112:GLU:HG3	1:B:115:ARG:NH1	2.34	0.42
1:C:201:VAL:HG12	1:C:219:LEU:HD11	2.02	0.42
1:B:14:SER:HB3	1:B:334:THR:HG23	2.02	0.42
1:B:40:HIS:HB3	1:B:54:ASN:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:GLN:OE1	1:D:43:PRO:HD2	2.20	0.42
1:D:92:TRP:CG	1:D:187:PRO:HD3	2.55	0.42
1:C:14:SER:HB3	1:C:334:THR:HG23	2.02	0.42
1:D:52:CYS:SG	1:D:57:CYS:CB	3.06	0.42
1:B:82:GLU:HA	1:B:85:ARG:NH2	2.34	0.42
1:B:139:GLU:HG3	1:B:145:SER:HB2	2.00	0.42
1:C:92:TRP:CG	1:C:187:PRO:HD3	2.55	0.42
1:C:391:TYR:O	1:C:413:LYS:HA	2.20	0.42
1:D:138:ARG:HG2	1:D:139:GLU:H	1.83	0.42
1:D:170:PRO:HB2	1:D:257:LYS:HG3	2.01	0.42
1:A:218:THR:HA	1:A:248:GLN:HB2	2.02	0.42
1:B:21:TRP:O	1:B:25:THR:HB	2.20	0.42
1:B:218:THR:HA	1:B:248:GLN:HB2	2.02	0.42
1:A:40:HIS:HB3	1:A:54:ASN:OD1	2.19	0.41
1:A:432:ASN:O	1:A:436:ILE:HG13	2.19	0.41
1:B:259:GLU:HG2	1:B:267:SER:HB2	2.02	0.41
1:B:432:ASN:O	1:B:436:ILE:HG13	2.19	0.41
1:C:297:GLN:HG2	1:C:298:ASN:N	2.35	0.41
1:A:297:GLN:HG2	1:A:298:ASN:N	2.35	0.41
1:B:37:GLN:OE1	1:B:43:PRO:HD2	2.20	0.41
1:B:222:ARG:HB3	1:B:254:ASN:HB2	2.02	0.41
1:B:391:TYR:O	1:B:413:LYS:HA	2.20	0.41
1:A:201:VAL:HG12	1:A:219:LEU:HD11	2.02	0.41
1:A:455:ASN:HD22	1:A:455:ASN:HA	1.57	0.41
1:C:37:GLN:OE1	1:C:43:PRO:HD2	2.20	0.41
1:D:14:SER:HB3	1:D:334:THR:HG23	2.02	0.41
1:A:222:ARG:HB3	1:A:254:ASN:HB2	2.02	0.41
1:C:21:TRP:O	1:C:25:THR:HB	2.20	0.41
1:C:218:THR:HA	1:C:248:GLN:HB2	2.02	0.41
1:D:63:MET:HG2	1:D:95:LEU:HD21	2.01	0.41
1:D:259:GLU:HG2	1:D:267:SER:HB2	2.02	0.41
1:D:297:GLN:HG2	1:D:298:ASN:N	2.35	0.41
1:A:21:TRP:O	1:A:25:THR:HB	2.20	0.41
1:A:33:VAL:O	1:A:122:PHE:HA	2.21	0.41
1:C:33:VAL:O	1:C:122:PHE:HA	2.21	0.41
1:D:21:TRP:O	1:D:25:THR:HB	2.20	0.41
1:A:92:TRP:CG	1:A:187:PRO:HD3	2.55	0.41
1:A:471:ARG:O	1:A:471:ARG:CZ	2.68	0.41
1:B:133:ASN:HD22	1:B:133:ASN:H	1.64	0.41
1:B:133:ASN:HA	1:B:156:ILE:HD11	2.03	0.41
1:C:73:LEU:HD23	1:C:88:LEU:CD1	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:ASN:HA	1:C:255:PRO:HD2	1.94	0.41
1:C:432:ASN:O	1:C:436:ILE:HG13	2.19	0.41
1:D:222:ARG:HB3	1:D:254:ASN:HB2	2.02	0.41
1:A:259:GLU:HG2	1:A:267:SER:HB2	2.02	0.41
1:B:33:VAL:O	1:B:122:PHE:HA	2.21	0.41
1:B:133:ASN:N	1:B:133:ASN:ND2	2.58	0.41
1:D:117:THR:HG22	1:D:118:GLU:O	2.21	0.41
1:A:263:ASP:OD1	1:A:263:ASP:N	2.54	0.41
1:A:479:LYS:HE2	1:C:42:PRO:O	2.20	0.41
1:B:289:PRO:C	1:B:291:THR:H	2.27	0.41
1:B:391:TYR:N	1:B:391:TYR:CD1	2.89	0.41
1:C:222:ARG:HB3	1:C:254:ASN:HB2	2.02	0.41
1:C:391:TYR:CD1	1:C:391:TYR:N	2.89	0.41
1:D:33:VAL:O	1:D:122:PHE:HA	2.21	0.41
1:D:175:CYS:SG	1:D:258:VAL:HG21	2.61	0.41
1:D:201:VAL:HG12	1:D:219:LEU:HD11	2.02	0.41
1:D:218:THR:HA	1:D:248:GLN:HB2	2.02	0.41
1:D:263:ASP:OD1	1:D:263:ASP:N	2.54	0.41
1:D:471:ARG:O	1:D:471:ARG:CZ	2.68	0.41
1:A:105:ASN:N	1:A:105:ASN:ND2	2.69	0.41
1:B:117:THR:HG22	1:B:118:GLU:O	2.21	0.41
1:B:314:SER:O	1:B:322:TYR:HB3	2.21	0.41
1:B:368:ILE:HA	1:B:369:PRO:HA	1.77	0.41
1:A:37:GLN:OE1	1:A:43:PRO:HD2	2.20	0.40
1:B:36:VAL:HG22	1:B:126:TRP:CD2	2.57	0.40
1:B:263:ASP:OD1	1:B:263:ASP:N	2.54	0.40
1:C:117:THR:HG22	1:C:118:GLU:O	2.21	0.40
1:C:175:CYS:SG	1:C:258:VAL:HG21	2.61	0.40
1:D:400:HIS:HA	1:D:403:SER:OG	2.22	0.40
1:A:400:HIS:HA	1:A:403:SER:OG	2.22	0.40
1:B:297:GLN:HG2	1:B:298:ASN:N	2.35	0.40
1:C:400:HIS:HA	1:C:403:SER:OG	2.21	0.40
1:C:471:ARG:O	1:C:471:ARG:CZ	2.68	0.40
1:D:99:LYS:HD2	1:D:99:LYS:C	2.46	0.40
1:B:201:VAL:HG12	1:B:219:LEU:HD11	2.02	0.40
1:C:81:TRP:CZ3	1:D:90:ALA:HB2	2.56	0.40
1:D:482:LYS:HE3	1:D:482:LYS:HB3	1.72	0.40
1:A:73:LEU:HD23	1:A:88:LEU:CD1	2.48	0.40
1:A:117:THR:HG22	1:A:118:GLU:O	2.21	0.40
1:B:471:ARG:O	1:B:471:ARG:CZ	2.68	0.40
1:C:128:SER:O	1:C:135:VAL:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:SER:O	1:D:322:TYR:HB3	2.21	0.40
1:A:391:TYR:CD1	1:A:391:TYR:N	2.89	0.40
1:A:438:GLN:OE1	1:B:465:GLU:HA	2.21	0.40
1:C:36:VAL:HG22	1:C:126:TRP:CD2	2.57	0.40
1:C:305:ASN:O	1:C:307:GLY:N	2.55	0.40
1:C:438:GLN:OE1	1:D:465:GLU:HA	2.21	0.40
1:D:391:TYR:CD1	1:D:391:TYR:N	2.89	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:173:GLU:CG	1:C:118:GLU:OE2[2_655]	1.93	0.27

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	415/491 (84%)	376 (91%)	32 (8%)	7 (2%)	7	30
1	B	479/491 (98%)	432 (90%)	38 (8%)	9 (2%)	6	28
1	C	479/491 (98%)	432 (90%)	38 (8%)	9 (2%)	6	28
1	D	479/491 (98%)	432 (90%)	38 (8%)	9 (2%)	6	28
All	All	1852/1964 (94%)	1672 (90%)	146 (8%)	34 (2%)	6	29

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	84	ASP
1	C	84	ASP
1	D	84	ASP

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Mol	Chain	Res	Type
1	A	263	ASP
1	A	292	LYS
1	B	263	ASP
1	B	292	LYS
1	C	263	ASP
1	C	292	LYS
1	D	263	ASP
1	D	292	LYS
1	A	149	GLU
1	B	149	GLU
1	C	149	GLU
1	D	149	GLU
1	A	170	PRO
1	A	306	GLY
1	A	420	ASP
1	B	170	PRO
1	B	306	GLY
1	B	420	ASP
1	C	170	PRO
1	C	306	GLY
1	C	420	ASP
1	D	170	PRO
1	D	306	GLY
1	D	420	ASP
1	A	378	GLU
1	B	378	GLU
1	C	378	GLU
1	D	378	GLU
1	B	43	PRO
1	C	43	PRO
1	D	43	PRO

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	402/411 (98%)	325 (81%)	77 (19%)	1	7
1	B	402/411 (98%)	325 (81%)	77 (19%)	1	7
1	C	402/411 (98%)	325 (81%)	77 (19%)	1	7
1	D	402/411 (98%)	325 (81%)	77 (19%)	1	7
All	All	1608/1644 (98%)	1300 (81%)	308 (19%)	1	7

All (308) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	25	THR
1	A	28	LYS
1	A	60	LYS
1	A	61	LYS
1	A	62	LEU
1	A	70	MET
1	A	73	LEU
1	A	75	GLU
1	A	85	ARG
1	A	86	THR
1	A	87	THR
1	A	112	GLU
1	A	113	MET
1	A	120	LEU
1	A	128	SER
1	A	129	LEU
1	A	133	ASN
1	A	135	VAL
1	A	151	LEU
1	A	158	LEU
1	A	163	TRP
1	A	168	ASN
1	A	169	ILE
1	A	178	SER
1	A	180	GLU
1	A	191	VAL
1	A	201	VAL
1	A	213	LYS
1	A	217	VAL

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Mol	Chain	Res	Type
1	A	220	CYS
1	A	222	ARG
1	A	228	ARG
1	A	236	GLU
1	A	245	ASN
1	A	247	ILE
1	A	251	THR
1	A	259	GLU
1	A	265	SER
1	A	272	SER
1	A	277	ASP
1	A	291	THR
1	A	293	ASP
1	A	294	LEU
1	A	302	MET
1	A	304	LYS
1	A	305	ASN
1	A	310	VAL
1	A	315	ARG
1	A	316	THR
1	A	317	ASN
1	A	330	ARG
1	A	333	LEU
1	A	344	LEU
1	A	348	VAL
1	A	351	THR
1	A	354	ARG
1	A	355	LYS
1	A	384	ARG
1	A	391	TYR
1	A	392	LEU
1	A	398	LEU
1	A	399	MET
1	A	406	LYS
1	A	415	ILE
1	A	416	THR
1	A	419	SER
1	A	420	ASP
1	A	428	LEU
1	A	429	LEU
1	A	438	GLN
1	A	445	LYS

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Mol	Chain	Res	Type
1	A	455	ASN
1	A	471	ARG
1	A	478	VAL
1	A	483	MET
1	A	484	GLU
1	B	17	LEU
1	B	25	THR
1	B	28	LYS
1	B	60	LYS
1	B	61	LYS
1	B	62	LEU
1	B	70	MET
1	B	73	LEU
1	B	75	GLU
1	B	85	ARG
1	B	86	THR
1	B	87	THR
1	B	112	GLU
1	B	113	MET
1	B	120	LEU
1	B	128	SER
1	B	129	LEU
1	B	133	ASN
1	B	135	VAL
1	B	151	LEU
1	B	158	LEU
1	B	163	TRP
1	B	168	ASN
1	B	169	ILE
1	B	178	SER
1	B	180	GLU
1	B	191	VAL
1	B	201	VAL
1	B	213	LYS
1	B	217	VAL
1	B	220	CYS
1	B	222	ARG
1	B	228	ARG
1	B	236	GLU
1	B	245	ASN
1	B	247	ILE
1	B	251	THR

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Mol	Chain	Res	Type
1	B	259	GLU
1	B	265	SER
1	B	272	SER
1	B	277	ASP
1	B	291	THR
1	B	293	ASP
1	B	294	LEU
1	B	302	MET
1	B	304	LYS
1	B	305	ASN
1	B	310	VAL
1	B	315	ARG
1	B	316	THR
1	B	317	ASN
1	B	330	ARG
1	B	333	LEU
1	B	344	LEU
1	B	348	VAL
1	B	351	THR
1	B	354	ARG
1	B	355	LYS
1	B	384	ARG
1	B	391	TYR
1	B	392	LEU
1	B	398	LEU
1	B	399	MET
1	B	406	LYS
1	B	415	ILE
1	B	416	THR
1	B	419	SER
1	B	420	ASP
1	B	428	LEU
1	B	429	LEU
1	B	438	GLN
1	B	445	LYS
1	B	455	ASN
1	B	471	ARG
1	B	478	VAL
1	B	483	MET
1	B	484	GLU
1	C	17	LEU
1	C	25	THR

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Mol	Chain	Res	Type
1	C	28	LYS
1	C	60	LYS
1	C	61	LYS
1	C	62	LEU
1	C	70	MET
1	C	73	LEU
1	C	75	GLU
1	C	85	ARG
1	C	86	THR
1	C	87	THR
1	C	112	GLU
1	C	113	MET
1	C	120	LEU
1	C	128	SER
1	C	129	LEU
1	C	133	ASN
1	C	135	VAL
1	C	151	LEU
1	C	158	LEU
1	C	163	TRP
1	C	168	ASN
1	C	169	ILE
1	C	178	SER
1	C	180	GLU
1	C	191	VAL
1	C	201	VAL
1	C	213	LYS
1	C	217	VAL
1	C	220	CYS
1	C	222	ARG
1	C	228	ARG
1	C	236	GLU
1	C	245	ASN
1	C	247	ILE
1	C	251	THR
1	C	259	GLU
1	C	265	SER
1	C	272	SER
1	C	277	ASP
1	C	291	THR
1	C	293	ASP
1	C	294	LEU

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Mol	Chain	Res	Type
1	C	302	MET
1	C	304	LYS
1	C	305	ASN
1	C	310	VAL
1	C	315	ARG
1	C	316	THR
1	C	317	ASN
1	C	330	ARG
1	C	333	LEU
1	C	344	LEU
1	C	348	VAL
1	C	351	THR
1	C	354	ARG
1	C	355	LYS
1	C	384	ARG
1	C	391	TYR
1	C	392	LEU
1	C	398	LEU
1	C	399	MET
1	C	406	LYS
1	C	415	ILE
1	C	416	THR
1	C	419	SER
1	C	420	ASP
1	C	428	LEU
1	C	429	LEU
1	C	438	GLN
1	C	445	LYS
1	C	455	ASN
1	C	471	ARG
1	C	478	VAL
1	C	483	MET
1	C	484	GLU
1	D	17	LEU
1	D	25	THR
1	D	28	LYS
1	D	60	LYS
1	D	61	LYS
1	D	62	LEU
1	D	70	MET
1	D	73	LEU
1	D	75	GLU

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Mol	Chain	Res	Type
1	D	85	ARG
1	D	86	THR
1	D	87	THR
1	D	112	GLU
1	D	113	MET
1	D	120	LEU
1	D	128	SER
1	D	129	LEU
1	D	133	ASN
1	D	135	VAL
1	D	151	LEU
1	D	158	LEU
1	D	163	TRP
1	D	168	ASN
1	D	169	ILE
1	D	178	SER
1	D	180	GLU
1	D	191	VAL
1	D	201	VAL
1	D	213	LYS
1	D	217	VAL
1	D	220	CYS
1	D	222	ARG
1	D	228	ARG
1	D	236	GLU
1	D	245	ASN
1	D	247	ILE
1	D	251	THR
1	D	259	GLU
1	D	265	SER
1	D	272	SER
1	D	277	ASP
1	D	291	THR
1	D	293	ASP
1	D	294	LEU
1	D	302	MET
1	D	304	LYS
1	D	305	ASN
1	D	310	VAL
1	D	315	ARG
1	D	316	THR
1	D	317	ASN

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Mol	Chain	Res	Type
1	D	330	ARG
1	D	333	LEU
1	D	344	LEU
1	D	348	VAL
1	D	351	THR
1	D	354	ARG
1	D	355	LYS
1	D	384	ARG
1	D	391	TYR
1	D	392	LEU
1	D	398	LEU
1	D	399	MET
1	D	406	LYS
1	D	415	ILE
1	D	416	THR
1	D	419	SER
1	D	420	ASP
1	D	428	LEU
1	D	429	LEU
1	D	438	GLN
1	D	445	LYS
1	D	455	ASN
1	D	471	ARG
1	D	478	VAL
1	D	483	MET
1	D	484	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	107	ASN
1	A	133	ASN
1	A	136	ASN
1	A	168	ASN
1	A	241	GLN
1	A	245	ASN
1	A	254	ASN
1	A	305	ASN
1	A	309	GLN
1	A	317	ASN
1	A	417	ASN

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Mol	Chain	Res	Type
1	A	418	HIS
1	A	455	ASN
1	B	68	GLN
1	B	107	ASN
1	B	133	ASN
1	B	136	ASN
1	B	168	ASN
1	B	216	GLN
1	B	241	GLN
1	B	245	ASN
1	B	254	ASN
1	B	305	ASN
1	B	309	GLN
1	B	317	ASN
1	B	417	ASN
1	B	455	ASN
1	C	68	GLN
1	C	72	HIS
1	C	107	ASN
1	C	133	ASN
1	C	136	ASN
1	C	168	ASN
1	C	216	GLN
1	C	241	GLN
1	C	245	ASN
1	C	254	ASN
1	C	305	ASN
1	C	309	GLN
1	C	317	ASN
1	C	417	ASN
1	C	455	ASN
1	D	68	GLN
1	D	72	HIS
1	D	107	ASN
1	D	133	ASN
1	D	136	ASN
1	D	168	ASN
1	D	216	GLN
1	D	241	GLN
1	D	245	ASN
1	D	254	ASN
1	D	305	ASN

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Mol	Chain	Res	Type
1	D	309	GLN
1	D	317	ASN
1	D	417	ASN
1	D	455	ASN

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	C	500	-	58,58,58	5.50	7 (12%)	85,89,89	1.52	16 (18%)
2	FAD	A	500	-	58,58,58	5.50	7 (12%)	85,89,89	1.52	16 (18%)
2	FAD	D	500	-	58,58,58	5.49	7 (12%)	85,89,89	1.52	16 (18%)
2	FAD	B	500	-	58,58,58	5.50	7 (12%)	85,89,89	1.52	16 (18%)

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	C	500	-	-	6/34/50/50	0/6/6/6
2	FAD	A	500	-	-	6/34/50/50	0/6/6/6
2	FAD	D	500	-	-	6/34/50/50	0/6/6/6
2	FAD	B	500	-	-	6/34/50/50	0/6/6/6

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	FAD	C8M-C8	-29.36	0.96	1.51
2	A	500	FAD	C8M-C8	-29.34	0.96	1.51
2	B	500	FAD	C8M-C8	-29.33	0.96	1.51
2	D	500	FAD	C8M-C8	-29.31	0.96	1.51
2	B	500	FAD	C7M-C7	-27.36	0.99	1.51
2	A	500	FAD	C7M-C7	-27.36	0.99	1.51
2	C	500	FAD	C7M-C7	-27.36	0.99	1.51
2	D	500	FAD	C7M-C7	-27.34	0.99	1.51
2	D	500	FAD	P-O3P	-5.63	1.53	1.59
2	B	500	FAD	P-O3P	-5.63	1.53	1.59
2	A	500	FAD	P-O3P	-5.63	1.53	1.59
2	C	500	FAD	P-O3P	-5.63	1.53	1.59
2	B	500	FAD	PA-O3P	-5.32	1.53	1.59
2	A	500	FAD	PA-O3P	-5.31	1.53	1.59
2	C	500	FAD	PA-O3P	-5.29	1.53	1.59
2	D	500	FAD	PA-O3P	-5.26	1.53	1.59
2	D	500	FAD	C4'-C3'	-3.48	1.47	1.53
2	B	500	FAD	C4'-C3'	-3.46	1.47	1.53
2	C	500	FAD	C4'-C3'	-3.44	1.47	1.53
2	A	500	FAD	C4'-C3'	-3.43	1.47	1.53
2	D	500	FAD	C5X-N5	-3.18	1.33	1.39
2	B	500	FAD	C5X-N5	-3.18	1.33	1.39
2	A	500	FAD	C5X-N5	-3.16	1.33	1.39
2	C	500	FAD	C5X-N5	-3.13	1.33	1.39
2	C	500	FAD	O4'-C4'	-2.16	1.38	1.43
2	A	500	FAD	O4'-C4'	-2.13	1.38	1.43
2	D	500	FAD	O4'-C4'	-2.13	1.38	1.43
2	B	500	FAD	O4'-C4'	-2.11	1.38	1.43

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	FAD	O3'-C3'-C4'	-5.57	96.28	108.93
2	A	500	FAD	O3'-C3'-C4'	-5.57	96.28	108.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	FAD	O3'-C3'-C4'	-5.56	96.30	108.93
2	C	500	FAD	O3'-C3'-C4'	-5.54	96.33	108.93
2	B	500	FAD	C6-C5X-N5	-3.62	112.44	118.44
2	D	500	FAD	C6-C5X-N5	-3.62	112.44	118.44
2	A	500	FAD	C6-C5X-N5	-3.59	112.48	118.44
2	C	500	FAD	C6-C5X-N5	-3.58	112.50	118.44
2	C	500	FAD	C7M-C7-C8	3.13	127.16	120.76
2	B	500	FAD	C7M-C7-C8	3.12	127.13	120.76
2	A	500	FAD	C7M-C7-C8	3.12	127.12	120.76
2	D	500	FAD	C7M-C7-C8	3.11	127.11	120.76
2	C	500	FAD	O4B-C1B-N9A	-2.93	102.46	108.09
2	D	500	FAD	O4B-C1B-N9A	-2.91	102.49	108.09
2	A	500	FAD	O4B-C1B-N9A	-2.91	102.50	108.09
2	B	500	FAD	O4B-C1B-N9A	-2.91	102.51	108.09
2	C	500	FAD	C6-C7-C8	-2.82	115.55	119.69
2	A	500	FAD	C6-C7-C8	-2.79	115.60	119.69
2	B	500	FAD	C6-C7-C8	-2.77	115.62	119.69
2	D	500	FAD	C6-C7-C8	-2.76	115.63	119.69
2	C	500	FAD	C6-C5X-C9A	2.74	122.82	119.05
2	A	500	FAD	C6-C5X-C9A	2.72	122.79	119.05
2	B	500	FAD	C6-C5X-C9A	2.72	122.78	119.05
2	D	500	FAD	C6-C5X-C9A	2.72	122.78	119.05
2	D	500	FAD	C9-C9A-N10	2.70	125.48	121.85
2	B	500	FAD	C9-C9A-N10	2.70	125.48	121.85
2	A	500	FAD	C9-C9A-N10	2.67	125.45	121.85
2	C	500	FAD	C9-C9A-N10	2.67	125.44	121.85
2	B	500	FAD	O3B-C3B-C4B	-2.58	103.66	111.08
2	B	500	FAD	O4B-C1B-C2B	-2.58	101.09	106.62
2	C	500	FAD	O3B-C3B-C4B	-2.57	103.69	111.08
2	D	500	FAD	O3B-C3B-C4B	-2.57	103.69	111.08
2	D	500	FAD	O4B-C1B-C2B	-2.57	101.11	106.62
2	A	500	FAD	O3B-C3B-C4B	-2.57	103.70	111.08
2	A	500	FAD	O4B-C1B-C2B	-2.56	101.13	106.62
2	C	500	FAD	O4B-C1B-C2B	-2.56	101.15	106.62
2	C	500	FAD	N6A-C6A-N1A	2.47	123.87	118.38
2	A	500	FAD	N6A-C6A-N1A	2.45	123.83	118.38
2	D	500	FAD	N6A-C6A-N1A	2.45	123.83	118.38
2	B	500	FAD	N6A-C6A-N1A	2.44	123.81	118.38
2	A	500	FAD	O2B-C2B-C3B	2.41	119.55	111.82
2	B	500	FAD	O2B-C2B-C3B	2.41	119.53	111.82
2	C	500	FAD	O2B-C2B-C3B	2.40	119.52	111.82
2	D	500	FAD	O2B-C2B-C3B	2.40	119.52	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	FAD	C9-C9A-C5X	-2.37	115.84	120.03
2	A	500	FAD	C9-C9A-C5X	-2.34	115.89	120.03
2	D	500	FAD	C9-C9A-C5X	-2.34	115.90	120.03
2	B	500	FAD	C9-C9A-C5X	-2.33	115.91	120.03
2	D	500	FAD	O2'-C2'-C3'	2.32	114.68	109.25
2	B	500	FAD	O2'-C2'-C3'	2.30	114.62	109.25
2	A	500	FAD	O2'-C2'-C3'	2.28	114.58	109.25
2	C	500	FAD	O2'-C2'-C3'	2.27	114.56	109.25
2	D	500	FAD	O4-C4-C4X	-2.24	120.62	126.53
2	D	500	FAD	O4-C4-N3	2.24	124.33	120.11
2	B	500	FAD	O4-C4-C4X	-2.22	120.68	126.53
2	A	500	FAD	O4-C4-C4X	-2.21	120.69	126.53
2	B	500	FAD	O4-C4-N3	2.20	124.26	120.11
2	A	500	FAD	O4-C4-N3	2.20	124.25	120.11
2	C	500	FAD	O4-C4-C4X	-2.20	120.73	126.53
2	C	500	FAD	O4-C4-N3	2.18	124.21	120.11
2	B	500	FAD	O5'-C5'-C4'	2.11	114.99	109.36
2	D	500	FAD	O5'-C5'-C4'	2.11	114.99	109.36
2	A	500	FAD	O5'-C5'-C4'	2.10	114.96	109.36
2	C	500	FAD	O5'-C5'-C4'	2.10	114.96	109.36

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	FAD	PA-O3P-P-O5'
2	B	500	FAD	PA-O3P-P-O5'
2	C	500	FAD	PA-O3P-P-O5'
2	D	500	FAD	PA-O3P-P-O5'
2	A	500	FAD	C2B-C1B-N9A-C8A
2	B	500	FAD	C2B-C1B-N9A-C8A
2	C	500	FAD	C2B-C1B-N9A-C8A
2	D	500	FAD	C2B-C1B-N9A-C8A
2	A	500	FAD	C5B-O5B-PA-O1A
2	B	500	FAD	C5B-O5B-PA-O1A
2	C	500	FAD	C5B-O5B-PA-O1A
2	D	500	FAD	C5B-O5B-PA-O1A
2	A	500	FAD	O4B-C4B-C5B-O5B
2	B	500	FAD	O4B-C4B-C5B-O5B
2	C	500	FAD	O4B-C4B-C5B-O5B
2	D	500	FAD	O4B-C4B-C5B-O5B
2	A	500	FAD	O2'-C2'-C3'-C4'

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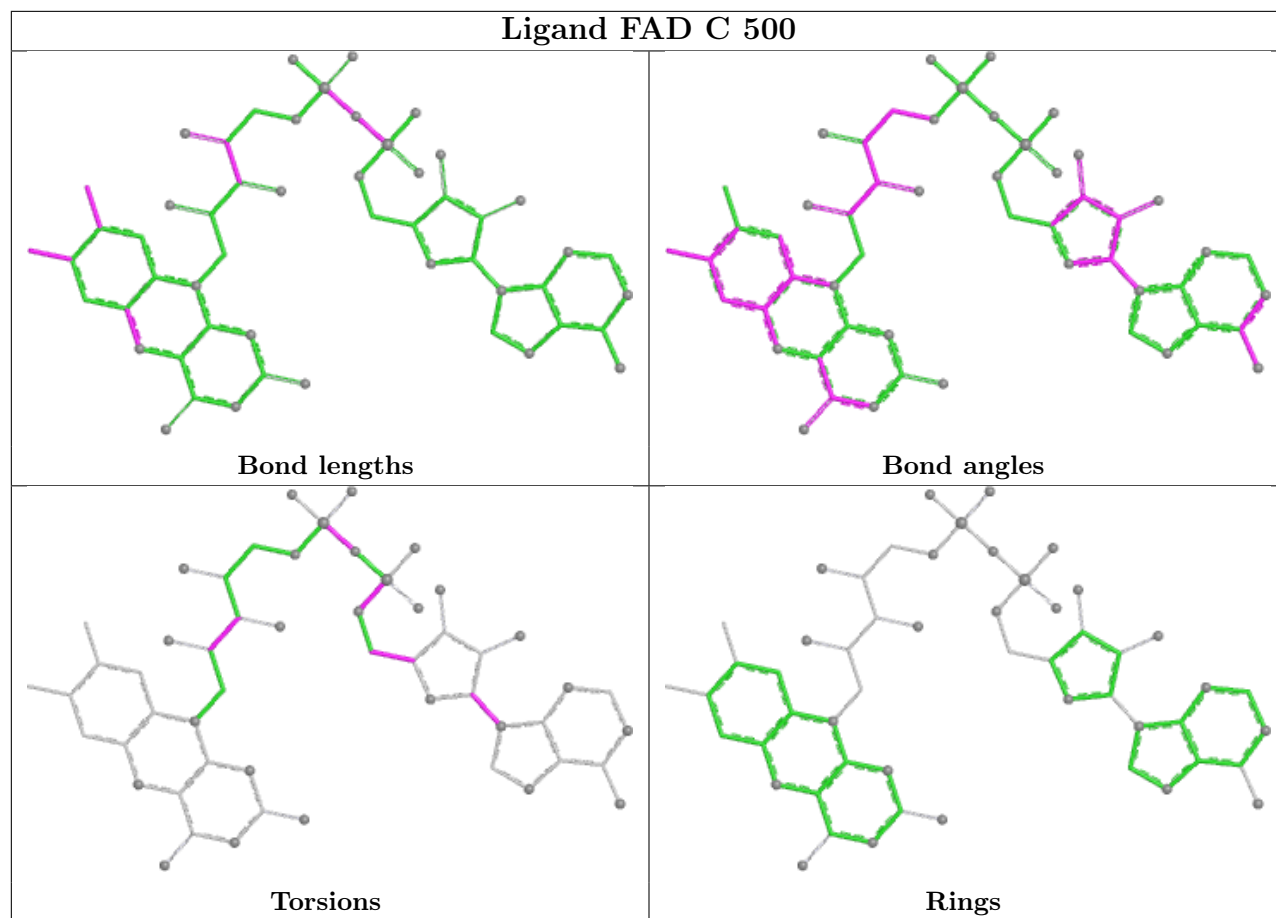
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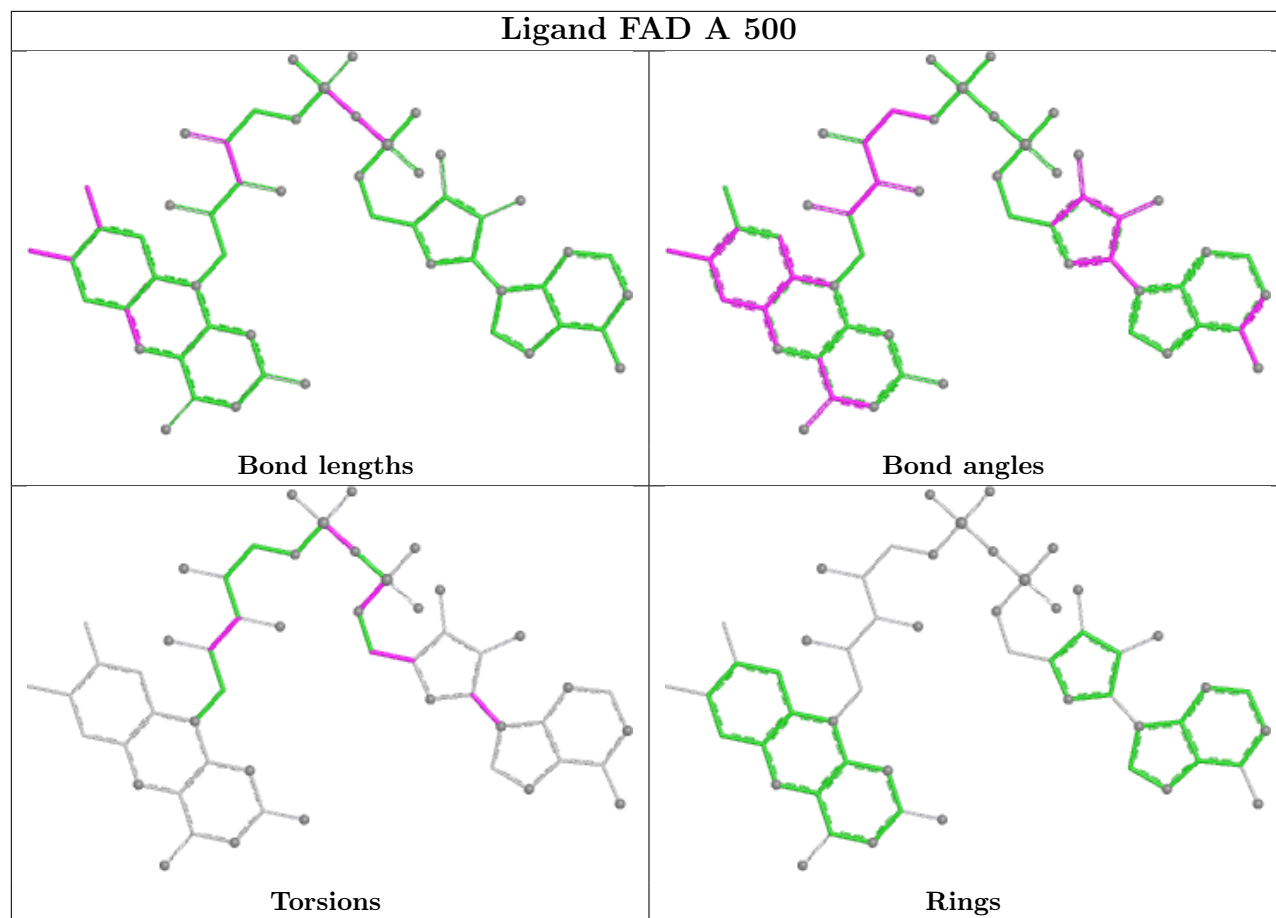
Mol	Chain	Res	Type	Atoms
2	B	500	FAD	O2'-C2'-C3'-C4'
2	C	500	FAD	O2'-C2'-C3'-C4'
2	D	500	FAD	O2'-C2'-C3'-C4'
2	A	500	FAD	PA-O3P-P-O2P
2	B	500	FAD	PA-O3P-P-O2P
2	C	500	FAD	PA-O3P-P-O2P
2	D	500	FAD	PA-O3P-P-O2P

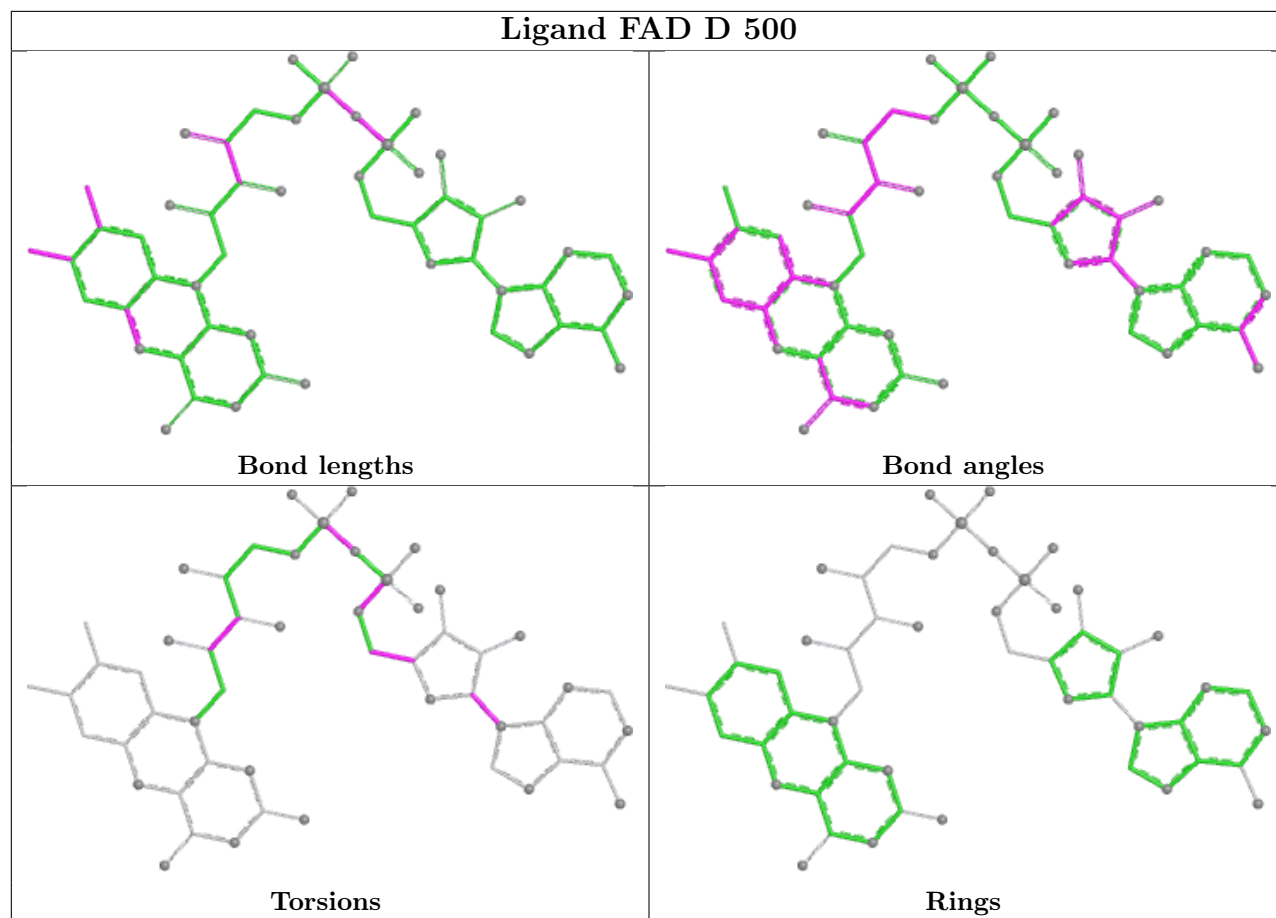
There are no ring outliers.

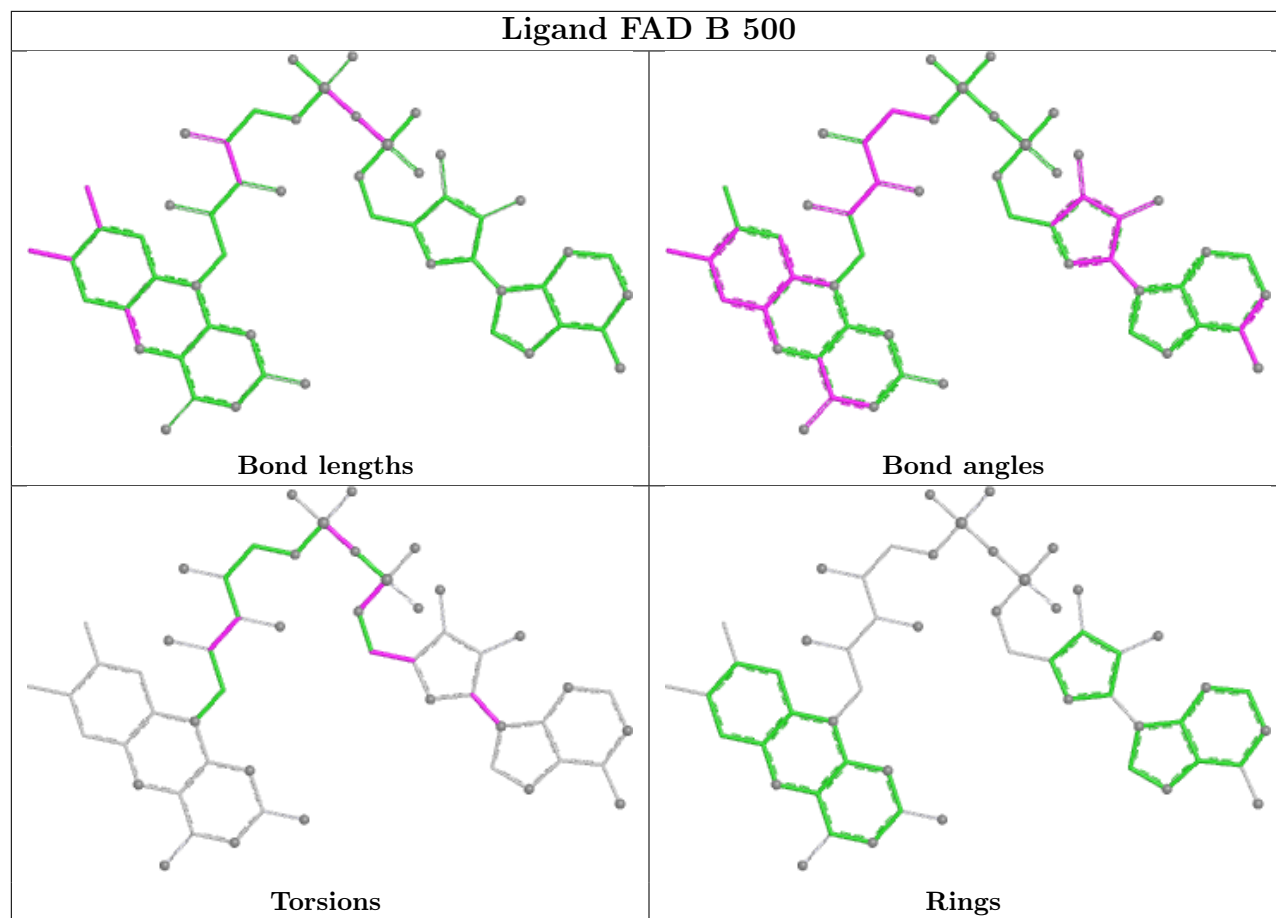
No monomer is involved in short contacts.

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.