



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:04 PM GMT

PDB ID : 1NDA
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

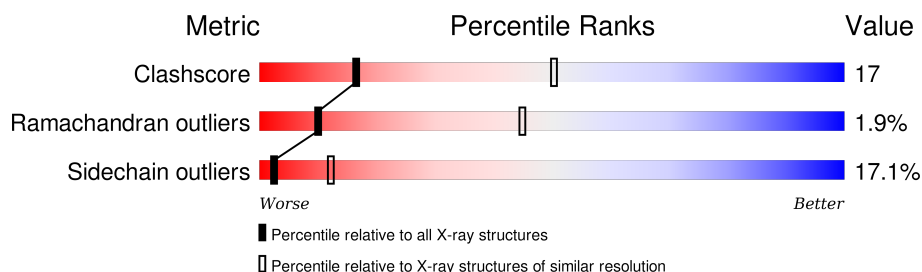
1 Overall quality at a glance

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	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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 [i](#)

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 TRYPTANOTHIONE 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 (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

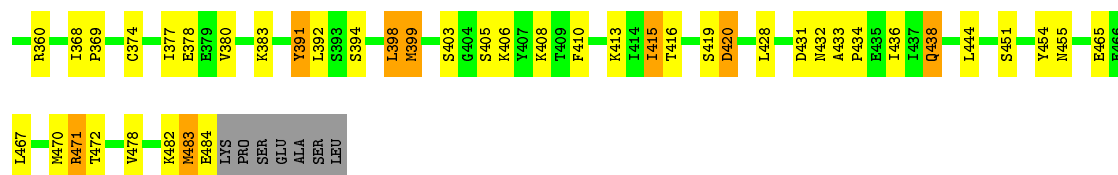


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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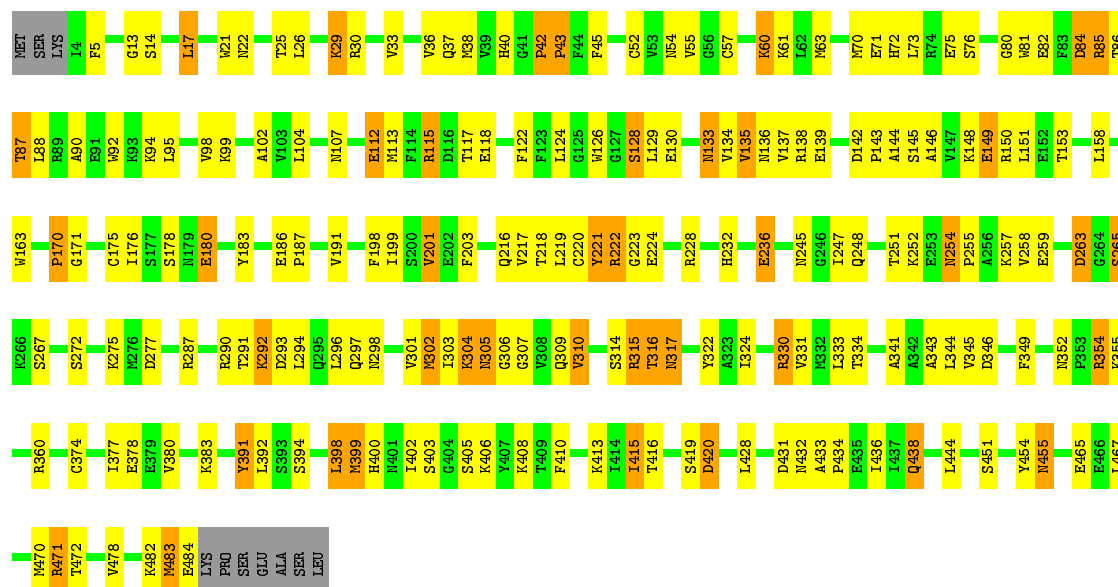
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		



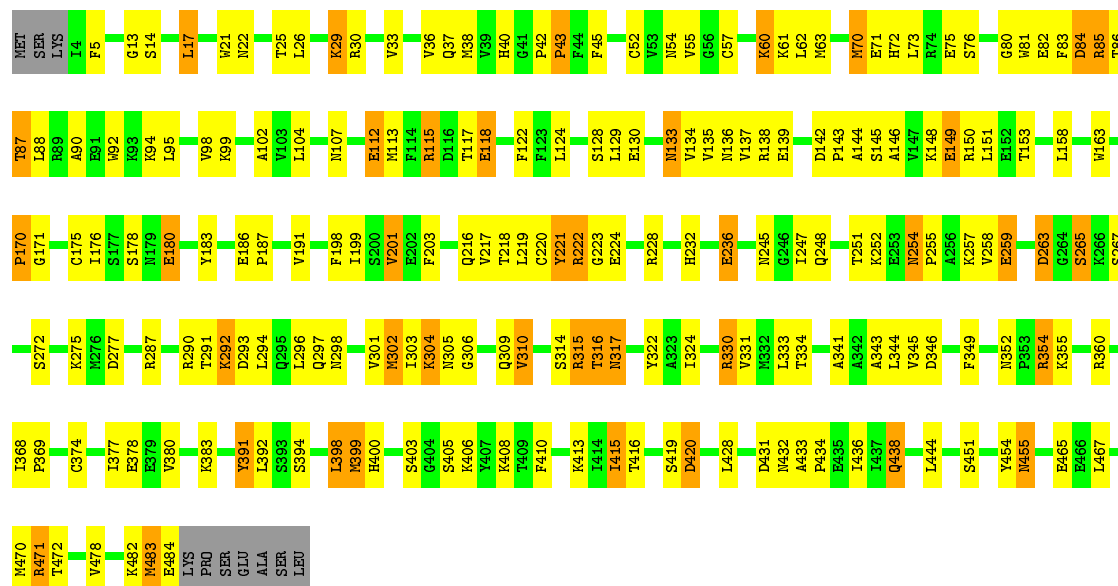
• Molecule 1: TRYPANOTHIONE OXIDOREDUCTASE

Chain C: 57% 32% 9%



• Molecule 1: TRYPANOTHIONE OXIDOREDUCTASE

Chain D: 57% 33% 8%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.30 Å 91.10 Å 126.00 Å 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	0.47	0/3776	0.59	0/5116
1	B	0.47	0/3776	0.59	0/5116
1	C	0.47	0/3776	0.59	0/5116
1	D	0.47	0/3776	0.59	0/5116
All	All	0.47	0/15104	0.59	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 [i](#)

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	136	0
1	B	3701	0	3705	131	1
1	C	3701	0	3705	137	1
1	D	3701	0	3705	134	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	493	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 (493) 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:B:391:TYR:HE2	1:B:471:ARG:O	1.72	0.72
1:A:301:VAL:HG13	1:A:316:THR:HG21	1.69	0.72
1:A:317:ASN:H	1:A:317:ASN:ND2	1.87	0.72
1:C:317:ASN:ND2	1:C:317:ASN:H	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:C:391:TYR:HE2	1:C:471:ARG:O	1.72	0.71
1:A:73:LEU:HD12	1:B:73:LEU:HD12	1.72	0.71
1:C:310:VAL:HG13	1:C:314:SER:HA	1.74	0.70
1:D:317:ASN:ND2	1:D:317:ASN:H	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:D:310:VAL:HG13	1:D:314:SER:HA	1.74	0.69
1:A:310:VAL:HG13	1:A: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:HD22	1:C:133:ASN:N	1.92	0.68
1:A:133:ASN:HD22	1:A:133:ASN:N	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:HD22	1:B:133:ASN:N	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: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: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:D:296:LEU:HD12	1:D:303:ILE:HD11	1.84	0.60
1:C:296:LEU:HD12	1:C:303:ILE:HD11	1.84	0.60
1:A:133:ASN:HB2	1:A:153:THR:O	2.02	0.60
1:B:296:LEU:HD12	1:B:303:ILE:HD11	1.84	0.60
1:D:133:ASN:HB2	1:D:153:THR:O	2.02	0.60
1:C:136:ASN:HD22	1:C:150:ARG:HG2	1.66	0.60
1:B:5:PHE:CD1	1:B:30:ARG:HG2	2.37	0.60
1:D:73:LEU:HD23	1:D:88:LEU:HD11	1.84	0.60
1:D:315:ARG:HB3	1:D:322:TYR:CD2	2.37	0.60
1:D:5:PHE:CD1	1:D:30:ARG:HG2	2.37	0.60
1:C:133:ASN:HB2	1:C:153:THR:O	2.02	0.60
1:B:133:ASN:HB2	1:B: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
1:C:73:LEU:HD23	1:C:88:LEU:HD11	1.83	0.59
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:B:315:ARG:HB3	1:B:322:TYR:CD2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:71:GLU:O	1:A: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:B:483:MET:SD	1:B:483:MET:C	2.84	0.56
1:A:87:THR:HG21	1:B:84:ASP:H	1.70	0.56
1:D:392:LEU:HD23	1:D:413:LYS:HG3	1.87	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:A:483:MET:C	1:A:483:MET:SD	2.84	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:C:483:MET:SD	1:C:483:MET:C	2.84	0.56
1:A:402:ILE:HD11	1:B:62:LEU:HG	1.88	0.55
1:D:483:MET:C	1:D:483:MET:SD	2.84	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:C:301:VAL:CG1	1:C:316:THR:HG21	2.37	0.55
1:A:45:PHE:HB3	1:A:55:VAL:HG11	1.89	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:HA	1:A:438:GLN:HE21	1.72	0.54
1:D:45:PHE:HB3	1:D:55:VAL:HG11	1.89	0.54
1:C:73:LEU:HD12	1:D:73:LEU:CD1	2.36	0.54
1:D:302:MET:HB2	1:D:317:ASN:HD21	1.73	0.54
1:C:80:GLY:HA2	1:D:94:LYS:HE3	1.88	0.54
1:C:438:GLN:HA	1:C:438:GLN:HE21	1.72	0.54
1:A:90:ALA:HB2	1:B:81:TRP:CZ3	2.43	0.54
1:C:90:ALA:HB2	1:D:81:TRP:CZ3	2.43	0.54
1:A:302:MET:HB2	1:A:317:ASN:HD21	1.72	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:D:343:ALA:HB1	1:D:354:ARG:HB3	1.90	0.53
1:C:343:ALA:HB1	1:C:354:ARG:HB3	1.90	0.53
1:B:84:ASP:O	1:B:87:THR:HG22	2.08	0.53
1:C:84:ASP:O	1:C:87:THR:HG22	2.08	0.53
1:C:45:PHE:HB3	1:C:55:VAL:HG11	1.89	0.53
1:C:302:MET:HB2	1:C:317:ASN:HD21	1.73	0.53
1:A:84:ASP:O	1:A:87:THR:HG22	2.08	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:232:HIS:O	1:A: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:B:317:ASN:H	1:B:317:ASN:HD22	1.57	0.52
1:A:343:ALA:HB1	1:A:354:ARG:HB3	1.90	0.52
1:C:88:LEU:O	1:C:88:LEU:HG	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:224:GLU:HG2	1:A:252:LYS:HE3	1.92	0.52
1:A:38:MET:SD	1:A:124:LEU:HD13	2.50	0.52
1:C:482:LYS:HE3	1:C:484:GLU:HB2	1.91	0.52
1:B:88:LEU:O	1:B:88:LEU:HG	2.10	0.51
1:B:38:MET:SD	1:B:124:LEU:HD13	2.50	0.51
1:A:471:ARG:NH1	1:A:472:THR:HA	2.25	0.51
1:B:471:ARG:NH1	1:B:472:THR:HA	2.26	0.51
1:C:224:GLU:HG2	1:C:252:LYS:HE3	1.92	0.51
1:B:482:LYS:HE3	1:B:484:GLU:HB2	1.91	0.51
1:D:391:TYR:CE2	1:D:471:ARG:O	2.61	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:317:ASN:HD22	1:C:317:ASN:H	1.57	0.51
1:C:471:ARG:NH1	1:C:472:THR:HA	2.25	0.51
1:C:75:GLU:HB2	1:C:403:SER:HB2	1.93	0.51
1:C:38:MET:SD	1:C:124:LEU:HD13	2.50	0.51
1:A:317:ASN:H	1:A:317:ASN:HD22	1.57	0.51
1:D:88:LEU:HG	1:D:88:LEU:O	2.10	0.51
1:B:302:MET:HB2	1:B:317:ASN:HD21	1.73	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:D:471:ARG:NH1	1:D:472:THR:HA	2.25	0.50
1:A:438:GLN:HE21	1:A:438:GLN:CA	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:C:303:ILE:N	1:C:303:ILE:HD12	2.27	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:438:GLN:CA	1:C:438:GLN:HE21	2.25	0.49
1:B:133:ASN:N	1:B:133:ASN:ND2	2.58	0.49
1:C:29:LYS:HZ3	1:C:349:PHE:HD1	1.59	0.49
1:C:221:TYR:CE2	1:C:223:GLY:HA3	2.47	0.49
1:A:29:LYS:HG2	1:A:349:PHE:CE1	2.47	0.49
1:B:104:LEU:O	1:B:107:ASN:HB2	2.12	0.49
1:B:29:LYS:HG2	1:B:349:PHE:CE1	2.47	0.49
1:D:221:TYR:CE2	1:D:223:GLY:HA3	2.47	0.49
1:D:104:LEU:O	1:D:107:ASN:HB2	2.12	0.49
1:B:380:VAL:HA	1:B:383:LYS:HE2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:LYS:HG2	1:D:349:PHE:CE1	2.47	0.49
1:B:303:ILE:HD12	1:B:303:ILE:N	2.27	0.49
1:A:303:ILE:HD12	1:A:303:ILE:N	2.27	0.49
1:C:60:LYS:HD3	1:C:60:LYS:C	2.33	0.49
1:A:60:LYS:C	1:A:60:LYS:HD3	2.33	0.49
1:D:60:LYS:C	1:D:60:LYS:HD3	2.33	0.49
1:B:438:GLN:CA	1:B:438:GLN:HE21	2.25	0.48
1:C:380:VAL:HA	1:C:383:LYS:HE2	1.95	0.48
1:D:438:GLN:CA	1:D:438:GLN:HE21	2.25	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: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:A:377:ILE:HG13	1:A:380:VAL:HG23	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:399:MET:O	1:C:403:SER:HB3	2.14	0.48
1:A:399:MET:O	1:A:403:SER:HB3	2.14	0.48
1:C:90:ALA:HB2	1:D:81:TRP:CH2	2.49	0.48
1:B:377:ILE:HG13	1:B:380:VAL:HG23	1.96	0.48
1:C:139:GLU:HG2	1:C:146:ALA:N	2.28	0.48
1:B:60:LYS:C	1:B:60:LYS:HD3	2.33	0.48
1:C:133:ASN:N	1:C:133:ASN:ND2	2.58	0.48
1:A:467:LEU:HA	1:A:470:MET:CE	2.43	0.48
1:D:380:VAL:HA	1:D:383:LYS:HE2	1.95	0.48
1:A:133:ASN:ND2	1:A:133:ASN:N	2.58	0.48
1:C:377:ILE:HG13	1:C:380:VAL:HG23	1.96	0.48
1:B:139:GLU:HG2	1:B:146:ALA:N	2.28	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:D:317:ASN:HD22	1:D:317:ASN:H	1.57	0.47
1:C:84:ASP:H	1:D:87:THR:HG23	1.80	0.47
1:D:399:MET:O	1:D:403:SER:HB3	2.14	0.47
1:C:142:ASP:OD2	1:C:144:ALA:HB3	2.14	0.47
1:A:304:LYS:HB2	1:A:309:GLN:HB3	1.95	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:B:29:LYS:HZ3	1:B:349:PHE:HD1	1.63	0.47
1:D:142:ASP:OD2	1:D:144:ALA:HB3	2.14	0.47
1:C:304:LYS:HB2	1:C:309:GLN:HB3	1.95	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:A:29:LYS:HZ3	1:A:349:PHE:HD1	1.63	0.47
1:B:304:LYS:HB2	1:B:309:GLN:HB3	1.96	0.47
1:D:296:LEU:HB3	1:D:301:VAL:HB	1.96	0.47
1:C:81:TRP:CH2	1:D:70:MET:HB2	2.50	0.47
1:A:405:SER:HB3	1:A:408:LYS:HG3	1.97	0.47
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:C:405:SER:HB3	1:C:408:LYS:HG3	1.96	0.46
1:B:36:VAL:HG12	1:B:37:GLN:HG2	1.98	0.46
1:C:398:LEU:HD11	1:D:102:ALA:HB1	1.98	0.46
1:C:296:LEU:HB3	1:C:301:VAL:HB	1.96	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:354:ARG:HH11	1:C:354:ARG:HG3	1.81	0.46
1:D:377:ILE:HG13	1:D:380:VAL:HG23	1.96	0.46
1:A:431:ASP:O	1:A:432:ASN:HB2	2.15	0.46
1:A:81:TRP:CH2	1:B:70:MET:HB2	2.50	0.46
1:B:354:ARG:HH11	1:B:354:ARG:HG3	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:D:354:ARG:HG3	1:D:354:ARG:HH11	1.81	0.46
1:A:433:ALA:HB3	1:A:434:PRO:HD3	1.98	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:HG3	1:A:354:ARG:HH11	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:D:330:ARG:HB3	1:D:331:VAL:H	1.53	0.45
1:C:218:THR:HG23	1:C:248:GLN:HB3	1.99	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:B:129:LEU:HD12	1:B:129:LEU:HA	1.74	0.45
1:A:398:LEU:HD11	1:B:102:ALA:HB1	1.98	0.45
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:D:75:GLU:HG2	1:D:75:GLU:H	1.59	0.45
1:C:129:LEU:HA	1:C:129:LEU:HD12	1.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:218:THR:HG23	1:B:248:GLN:HB3	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:B:216:GLN:NE2	1:B:248:GLN:HG3	2.32	0.45
1:A:216:GLN:NE2	1:A: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:C:374:CYS:SG	1:C:444:LEU:HD22	2.57	0.44
1:B:254:ASN:HD22	1:B:255:PRO:HD2	1.82	0.44
1:D:198:PHE:CD2	1:D:199:ILE:HG13	2.52	0.44
1:B:467:LEU:HA	1:B:470:MET:HE3	1.99	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:C:36:VAL:HG12	1:C:37:GLN:HG2	1.98	0.44
1:B:415:ILE:HG13	1:B:415:ILE:O	2.18	0.44
1:C:95:LEU:O	1:C:98:VAL:HG22	2.17	0.44
1:C:467:LEU:HA	1:C:470:MET:HE3	1.99	0.44
1:D:216:GLN:NE2	1:D:248:GLN:HG3	2.32	0.44
1:C:254:ASN:HD22	1:C:255:PRO:HD2	1.83	0.44
1:C:148:LYS:O	1:C:149:GLU:HB2	2.18	0.44
1:B:186:GLU:HB2	1:B:187:PRO:HD2	1.99	0.44
1:A:415:ILE:HG13	1:A:415:ILE:O	2.17	0.44
1:A:95:LEU:O	1:A:98:VAL:HG22	2.17	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: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:B:290:ARG:HG2	1:B:292:LYS:HD3	1.98	0.44
1:B:95:LEU:O	1:B:98:VAL:HG22	2.17	0.44
1:A:391:TYR:CE2	1:A:471:ARG:O	2.61	0.44
1:D:95:LEU:O	1:D:98:VAL:HG22	2.17	0.44
1:C:415:ILE:O	1:C:415:ILE:HG13	2.17	0.44
1:C:290:ARG:HG2	1:C:292:LYS:HD3	1.99	0.44
1:A:133:ASN:H	1:A:133:ASN:HD22	1.64	0.44
1:B:330:ARG:HB3	1:B:331:VAL:H	1.53	0.44
1:D:368:ILE:HA	1:D:369:PRO:HA	1.77	0.44
1:D:263:ASP:OD1	1:D:265:SER:HB2	2.18	0.44
1:B:138:ARG:CD	1:B:143:PRO:HA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:ASN:HD22	1:D:255:PRO:HD2	1.82	0.43
1:B:73:LEU:HD23	1:B:88:LEU:CD1	2.48	0.43
1:A:394:SER:HA	1:A:410:PHE:O	2.19	0.43
1:A:324:ILE:HD12	1:A:341:ALA:HB2	2.00	0.43
1:C:391:TYR:CE2	1:C:471:ARG:O	2.61	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:D:415:ILE:HG13	1:D:415:ILE:O	2.18	0.43
1:A:148:LYS:O	1:A:149:GLU:HB2	2.18	0.43
1:C:138:ARG:CD	1:C:143:PRO:HA	2.48	0.43
1:B:138:ARG:HG2	1:B:139:GLU:H	1.83	0.43
1:B:148:LYS:O	1:B:149:GLU:HB2	2.18	0.43
1:A:186:GLU:HB2	1:A:187:PRO:HD2	1.99	0.43
1:D:394:SER:HA	1:D:410:PHE:O	2.19	0.43
1:D:148:LYS:O	1:D:149:GLU:HB2	2.18	0.43
1:C:133:ASN:HD22	1:C:133:ASN:H	1.64	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:A:138:ARG:CD	1:A:143:PRO:HA	2.48	0.43
1:A:63:MET:HG2	1:A:95:LEU:HD21	2.01	0.43
1:B:63:MET:HG2	1:B:95:LEU:HD21	2.01	0.43
1:C:451:SER:HA	1:C:454:TYR:CZ	2.54	0.43
1:C:137:VAL:HB	1:C:149:GLU:HB3	2.01	0.43
1:A:170:PRO:HB2	1:A:257:LYS:HG3	2.01	0.43
1:D:82:GLU:HA	1:D:85:ARG:NH2	2.34	0.43
1:C:170:PRO:HB2	1:C:257:LYS:HG3	2.01	0.43
1:D:451:SER:HA	1:D:454:TYR:CZ	2.54	0.43
1:A:82:GLU:HA	1:A:85:ARG:NH2	2.34	0.43
1:B:52:CYS:SG	1:B:57:CYS:CB	3.06	0.43
1:D:73:LEU:HD23	1:D:88:LEU:CD1	2.48	0.43
1:C:324:ILE:HD12	1:C:341:ALA:HB2	2.00	0.43
1:A:52:CYS:SG	1:A:57:CYS:CB	3.06	0.43
1:C:138:ARG:HG2	1:C:139:GLU:H	1.83	0.43
1:A:467:LEU:HA	1:A:470:MET:HE3	2.00	0.43
1:B:394:SER:HA	1:B:410:PHE:O	2.19	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:C:82:GLU:HA	1:C:85:ARG:NH2	2.34	0.43
1:B:451:SER:HA	1:B:454:TYR:CZ	2.54	0.43
1:D:129:LEU:HD12	1:D:129:LEU:HA	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:LYS:HE3	1:A:482:LYS:HB3	1.72	0.43
1:D:112:GLU:HG3	1:D:115:ARG:NH1	2.34	0.43
1:A:112:GLU:HG3	1:A:115:ARG:NH1	2.34	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: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:A:129:LEU:HA	1:A:129:LEU:HD12	1.74	0.42
1:D:137:VAL:HB	1:D: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:A:137:VAL:HB	1:A:149:GLU:HB3	2.01	0.42
1:D:133:ASN:H	1:D:133:ASN:HD22	1.64	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:C:40:HIS:HB3	1:C:54:ASN:OD1	2.19	0.42
1:D:391:TYR:O	1:D:413:LYS:HA	2.20	0.42
1:C:139:GLU:HG3	1:C:145:SER:HB2	2.00	0.42
1:B:92:TRP:CG	1:B:187:PRO:HD3	2.55	0.42
1:A:14:SER:HB3	1:A:334:THR:HG23	2.02	0.42
1:C:263:ASP:OD1	1:C:265:SER:HB2	2.18	0.42
1:C:112:GLU:HG3	1:C:115:ARG:NH1	2.34	0.42
1:A:391:TYR:O	1:A:413:LYS:HA	2.20	0.42
1:A:317:ASN:N	1:A:317:ASN:ND2	2.64	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:D:29:LYS:HZ3	1:D:349:PHE:HD1	1.66	0.42
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: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
1:D:52:CYS:SG	1:D:57:CYS:CB	3.06	0.42
1:C:14:SER:HB3	1:C:334:THR:HG23	2.02	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: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:D:170:PRO:HB2	1:D:257:LYS:HG3	2.01	0.42
1:B:82:GLU:HA	1:B:85:ARG:NH2	2.34	0.42
1:B:218:THR:HA	1:B:248:GLN:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:259:GLU:HG2	1:B:267:SER:HB2	2.02	0.41
1:D:467:LEU:HA	1:D:470:MET:HE3	2.00	0.41
1:B:432:ASN:O	1:B:436:ILE:HG13	2.19	0.41
1:A:432:ASN:O	1:A:436:ILE:HG13	2.19	0.41
1:A:40:HIS:HB3	1:A:54:ASN:OD1	2.19	0.41
1:C:297:GLN:HG2	1:C: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:A:297:GLN:HG2	1:A:298:ASN:N	2.35	0.41
1:B:391:TYR:O	1:B:413:LYS:HA	2.20	0.41
1:C:37:GLN:OE1	1:C:43:PRO:HD2	2.20	0.41
1:A:201:VAL:HG12	1:A:219:LEU:HD11	2.02	0.41
1:D:14:SER:HB3	1:D:334:THR:HG23	2.02	0.41
1:A:455:ASN:HA	1:A:455:ASN:HD22	1.57	0.41
1:D:259:GLU:HG2	1:D:267:SER:HB2	2.02	0.41
1:C:218:THR:HA	1:C:248:GLN:HB2	2.02	0.41
1:A:222:ARG:HB3	1:A:254:ASN:HB2	2.02	0.41
1:D:63:MET:HG2	1:D:95:LEU:HD21	2.01	0.41
1:C:21:TRP:O	1:C:25:THR:HB	2.20	0.41
1:D:297:GLN:HG2	1:D:298:ASN:N	2.35	0.41
1:D:21:TRP:O	1:D:25:THR:HB	2.20	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:A:471:ARG:CZ	1:A:471:ARG:O	2.68	0.41
1:C:73:LEU:HD23	1:C:88:LEU:CD1	2.48	0.41
1:B:133:ASN:HA	1:B:156:ILE:HD11	2.03	0.41
1:B:133:ASN:HD22	1:B:133:ASN:H	1.64	0.41
1:C:432:ASN:O	1:C:436:ILE:HG13	2.19	0.41
1:C:254:ASN:HA	1:C:255:PRO:HD2	1.94	0.41
1:D:222:ARG:HB3	1:D:254:ASN:HB2	2.02	0.41
1:A:92:TRP:CG	1:A:187:PRO:HD3	2.55	0.41
1:C:263:ASP:OD1	1:C:263:ASP:N	2.54	0.41
1:B:297:GLN:HG2	1:B:298:ASN:N	2.35	0.41
1:A:259:GLU:HG2	1:A:267:SER:HB2	2.02	0.41
1:D:117:THR:HG22	1:D:118:GLU:O	2.21	0.41
1:B:33:VAL:O	1:B:122:PHE:HA	2.21	0.41
1:A:479:LYS:HE2	1:C:42:PRO:O	2.20	0.41
1:B:391:TYR:N	1:B:391:TYR:CD1	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:471:ARG:O	1:D:471:ARG:CZ	2.68	0.41
1:C:391:TYR:N	1:C:391:TYR:CD1	2.89	0.41
1:D:175:CYS:SG	1:D:258:VAL:HG21	2.61	0.41
1:D:218:THR:HA	1:D:248:GLN:HB2	2.02	0.41
1:C:222:ARG:HB3	1:C:254:ASN:HB2	2.02	0.41
1:D:263:ASP:N	1:D:263:ASP:OD1	2.54	0.41
1:A:263:ASP:N	1:A:263:ASP:OD1	2.54	0.41
1:D:33:VAL:O	1:D:122:PHE:HA	2.21	0.41
1:D:201:VAL:HG12	1:D:219:LEU:HD11	2.02	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:105:ASN:ND2	1:A:105:ASN:N	2.69	0.41
1:B:117:THR:HG22	1:B:118:GLU:O	2.21	0.41
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:B:36:VAL:HG22	1:B:126:TRP:CD2	2.57	0.40
1:A:37:GLN:OE1	1:A:43:PRO:HD2	2.20	0.40
1:B:263:ASP:N	1:B:263:ASP:OD1	2.54	0.40
1:C:117:THR:HG22	1:C:118:GLU:O	2.21	0.40
1:C:471:ARG:O	1:C:471:ARG:CZ	2.68	0.40
1:C:400:HIS:HA	1:C:403:SER:OG	2.21	0.40
1:A:400:HIS:HA	1:A:403:SER:OG	2.22	0.40
1:A:198:PHE:CG	1:A:199:ILE:N	2.90	0.40
1:D:482:LYS:HB3	1:D:482:LYS:HE3	1.72	0.40
1:C:81:TRP:CZ3	1:D:90:ALA:HB2	2.56	0.40
1:B:198:PHE:CG	1:B:199:ILE:N	2.90	0.40
1:B:201:VAL:HG12	1:B:219:LEU:HD11	2.02	0.40
1:B:471:ARG:CZ	1:B:471:ARG:O	2.68	0.40
1:A:73:LEU:HD23	1:A:88:LEU:CD1	2.48	0.40
1:D:314:SER:O	1:D:322:TYR:HB3	2.21	0.40
1:C:128:SER:O	1:C:135:VAL:HG23	2.22	0.40
1:A:117:THR:HG22	1:A:118:GLU:O	2.21	0.40
1:A:391:TYR:CD1	1:A:391:TYR:N	2.89	0.40
1:D:391:TYR:N	1:D:391:TYR:CD1	2.89	0.40
1:A:438:GLN:OE1	1:B:465:GLU:HA	2.21	0.40
1:C:438:GLN:OE1	1:D: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

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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	479/491 (98%)	432 (90%)	38 (8%)	9 (2%)	10	45
1	B	479/491 (98%)	432 (90%)	38 (8%)	9 (2%)	10	45
1	C	479/491 (98%)	432 (90%)	38 (8%)	9 (2%)	10	45
1	D	479/491 (98%)	432 (90%)	38 (8%)	9 (2%)	10	45
All	All	1916/1964 (98%)	1728 (90%)	152 (8%)	36 (2%)	10	45

All (36) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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	A	43	PRO
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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	402/411 (98%)	333 (83%)	69 (17%)	2	12
1	B	402/411 (98%)	333 (83%)	69 (17%)	2	12
1	C	402/411 (98%)	334 (83%)	68 (17%)	2	12
1	D	402/411 (98%)	333 (83%)	69 (17%)	2	12
All	All	1608/1644 (98%)	1333 (83%)	275 (17%)	2	12

All (275) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	29	LYS

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Mol	Chain	Res	Type
1	A	60	LYS
1	A	61	LYS
1	A	70	MET
1	A	85	ARG
1	A	86	THR
1	A	87	THR
1	A	99	LYS
1	A	112	GLU
1	A	113	MET
1	A	115	ARG
1	A	118	GLU
1	A	128	SER
1	A	133	ASN
1	A	135	VAL
1	A	151	LEU
1	A	158	LEU
1	A	163	TRP
1	A	178	SER
1	A	180	GLU
1	A	191	VAL
1	A	201	VAL
1	A	203	PHE
1	A	217	VAL
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	254	ASN
1	A	259	GLU
1	A	265	SER
1	A	272	SER
1	A	277	ASP
1	A	287	ARG
1	A	291	THR
1	A	293	ASP
1	A	294	LEU
1	A	302	MET
1	A	304	LYS
1	A	305	ASN

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Mol	Chain	Res	Type
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	346	ASP
1	A	354	ARG
1	A	355	LYS
1	A	360	ARG
1	A	391	TYR
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	438	GLN
1	A	455	ASN
1	A	471	ARG
1	A	478	VAL
1	A	483	MET
1	B	17	LEU
1	B	29	LYS
1	B	60	LYS
1	B	61	LYS
1	B	70	MET
1	B	85	ARG
1	B	86	THR
1	B	87	THR
1	B	99	LYS
1	B	112	GLU
1	B	113	MET
1	B	115	ARG
1	B	118	GLU
1	B	128	SER
1	B	133	ASN
1	B	135	VAL
1	B	151	LEU

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Mol	Chain	Res	Type
1	B	158	LEU
1	B	163	TRP
1	B	178	SER
1	B	180	GLU
1	B	191	VAL
1	B	201	VAL
1	B	203	PHE
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
1	B	254	ASN
1	B	259	GLU
1	B	265	SER
1	B	272	SER
1	B	277	ASP
1	B	287	ARG
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	346	ASP
1	B	354	ARG
1	B	355	LYS
1	B	360	ARG
1	B	391	TYR
1	B	398	LEU
1	B	399	MET
1	B	406	LYS

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Mol	Chain	Res	Type
1	B	415	ILE
1	B	416	THR
1	B	419	SER
1	B	420	ASP
1	B	428	LEU
1	B	438	GLN
1	B	455	ASN
1	B	471	ARG
1	B	478	VAL
1	B	483	MET
1	C	17	LEU
1	C	29	LYS
1	C	60	LYS
1	C	61	LYS
1	C	70	MET
1	C	85	ARG
1	C	86	THR
1	C	87	THR
1	C	99	LYS
1	C	112	GLU
1	C	113	MET
1	C	115	ARG
1	C	128	SER
1	C	133	ASN
1	C	135	VAL
1	C	151	LEU
1	C	158	LEU
1	C	163	TRP
1	C	178	SER
1	C	180	GLU
1	C	191	VAL
1	C	201	VAL
1	C	203	PHE
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	254	ASN

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Mol	Chain	Res	Type
1	C	259	GLU
1	C	265	SER
1	C	272	SER
1	C	277	ASP
1	C	287	ARG
1	C	291	THR
1	C	293	ASP
1	C	294	LEU
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	346	ASP
1	C	354	ARG
1	C	355	LYS
1	C	360	ARG
1	C	391	TYR
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	438	GLN
1	C	455	ASN
1	C	471	ARG
1	C	478	VAL
1	C	483	MET
1	D	17	LEU
1	D	29	LYS
1	D	60	LYS
1	D	61	LYS
1	D	70	MET
1	D	85	ARG

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Mol	Chain	Res	Type
1	D	86	THR
1	D	87	THR
1	D	99	LYS
1	D	112	GLU
1	D	113	MET
1	D	115	ARG
1	D	118	GLU
1	D	128	SER
1	D	133	ASN
1	D	135	VAL
1	D	151	LEU
1	D	158	LEU
1	D	163	TRP
1	D	178	SER
1	D	180	GLU
1	D	191	VAL
1	D	201	VAL
1	D	203	PHE
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	254	ASN
1	D	259	GLU
1	D	265	SER
1	D	272	SER
1	D	277	ASP
1	D	287	ARG
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	346	ASP
1	D	354	ARG
1	D	355	LYS
1	D	360	ARG
1	D	391	TYR
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	438	GLN
1	D	455	ASN
1	D	471	ARG
1	D	478	VAL
1	D	483	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	133	ASN
1	A	136	ASN
1	A	168	ASN
1	A	216	GLN
1	A	245	ASN
1	A	254	ASN
1	A	309	GLN
1	A	317	ASN
1	A	455	ASN
1	B	105	ASN
1	B	133	ASN
1	B	136	ASN
1	B	168	ASN
1	B	216	GLN
1	B	245	ASN
1	B	254	ASN

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Mol	Chain	Res	Type
1	B	309	GLN
1	B	317	ASN
1	B	455	ASN
1	C	105	ASN
1	C	133	ASN
1	C	136	ASN
1	C	168	ASN
1	C	216	GLN
1	C	245	ASN
1	C	254	ASN
1	C	309	GLN
1	C	317	ASN
1	C	455	ASN
1	D	105	ASN
1	D	133	ASN
1	D	136	ASN
1	D	168	ASN
1	D	216	GLN
1	D	245	ASN
1	D	254	ASN
1	D	309	GLN
1	D	317	ASN
1	D	455	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	A	500	-	48,58,58	5.57	10 (20%)	54,89,89	3.10	16 (29%)
2	FAD	B	500	-	48,58,58	5.57	9 (18%)	54,89,89	3.10	16 (29%)
2	FAD	C	500	-	48,58,58	5.58	10 (20%)	54,89,89	3.10	16 (29%)
2	FAD	D	500	-	48,58,58	5.57	9 (18%)	54,89,89	3.11	16 (29%)

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	A	500	-	-	0/30/50/50	0/6/6/6
2	FAD	B	500	-	-	0/30/50/50	0/6/6/6
2	FAD	C	500	-	-	0/30/50/50	0/6/6/6
2	FAD	D	500	-	-	0/30/50/50	0/6/6/6

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	FAD	C8M-C8	-27.20	0.96	1.51
2	A	500	FAD	C8M-C8	-27.18	0.96	1.51
2	B	500	FAD	C8M-C8	-27.17	0.96	1.51
2	D	500	FAD	C8M-C8	-27.15	0.96	1.51
2	B	500	FAD	C7M-C7	-25.34	0.99	1.51
2	A	500	FAD	C7M-C7	-25.34	0.99	1.51
2	C	500	FAD	C7M-C7	-25.34	0.99	1.51
2	D	500	FAD	C7M-C7	-25.32	0.99	1.51
2	C	500	FAD	C4X-N5	-3.01	1.28	1.33
2	D	500	FAD	C4'-C3'	-3.00	1.47	1.53
2	B	500	FAD	C4'-C3'	-2.98	1.47	1.53
2	C	500	FAD	C4'-C3'	-2.97	1.47	1.53
2	D	500	FAD	C4X-N5	-2.96	1.28	1.33
2	A	500	FAD	C4X-N5	-2.96	1.28	1.33
2	A	500	FAD	C4'-C3'	-2.95	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	FAD	C4A-N3A	-2.93	1.31	1.35
2	B	500	FAD	C4X-N5	-2.93	1.28	1.33
2	A	500	FAD	C4A-N3A	-2.88	1.31	1.35
2	B	500	FAD	C4A-N3A	-2.86	1.31	1.35
2	D	500	FAD	C4A-N3A	-2.85	1.31	1.35
2	C	500	FAD	C6-C5X	-2.38	1.38	1.41
2	A	500	FAD	C6-C5X	-2.35	1.38	1.41
2	D	500	FAD	C6-C5X	-2.32	1.38	1.41
2	B	500	FAD	C6-C5X	-2.30	1.38	1.41
2	C	500	FAD	C8A-N7A	-2.27	1.30	1.34
2	A	500	FAD	C8A-N7A	-2.27	1.30	1.34
2	B	500	FAD	C8A-N7A	-2.24	1.30	1.34
2	D	500	FAD	C8A-N7A	-2.23	1.30	1.34
2	C	500	FAD	O4'-C4'	-2.03	1.38	1.43
2	A	500	FAD	O4'-C4'	-2.00	1.38	1.43
2	A	500	FAD	C4X-C10	3.81	1.48	1.41
2	C	500	FAD	C4X-C10	3.82	1.48	1.41
2	D	500	FAD	C4X-C10	3.83	1.48	1.41
2	B	500	FAD	C4X-C10	3.84	1.48	1.41
2	B	500	FAD	C4-C4X	3.93	1.49	1.41
2	A	500	FAD	C4-C4X	3.97	1.49	1.41
2	C	500	FAD	C4-C4X	3.97	1.49	1.41
2	D	500	FAD	C4-C4X	3.98	1.49	1.41

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	FAD	C4X-C10-N10	-10.84	114.13	120.52
2	B	500	FAD	C4X-C10-N10	-10.84	114.13	120.52
2	C	500	FAD	C4X-C10-N10	-10.81	114.15	120.52
2	D	500	FAD	C4X-C10-N10	-10.81	114.15	120.52
2	D	500	FAD	C4-C4X-C10	-6.60	115.72	119.94
2	A	500	FAD	C4-C4X-C10	-6.54	115.76	119.94
2	B	500	FAD	C4-C4X-C10	-6.53	115.77	119.94
2	C	500	FAD	C4-C4X-C10	-6.52	115.77	119.94
2	C	500	FAD	C4X-C4-N3	-6.24	115.05	123.59
2	D	500	FAD	C4X-C4-N3	-6.24	115.05	123.59
2	B	500	FAD	C4X-C4-N3	-6.24	115.06	123.59
2	A	500	FAD	C4X-C4-N3	-6.24	115.06	123.59
2	B	500	FAD	C6-C5X-N5	-5.07	112.44	118.96
2	D	500	FAD	C6-C5X-N5	-5.07	112.44	118.96
2	A	500	FAD	C6-C5X-N5	-5.04	112.48	118.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	FAD	C6-C5X-N5	-5.02	112.50	118.96
2	B	500	FAD	O3'-C3'-C4'	-4.95	96.28	108.75
2	A	500	FAD	O3'-C3'-C4'	-4.95	96.28	108.75
2	D	500	FAD	O3'-C3'-C4'	-4.94	96.30	108.75
2	C	500	FAD	O3'-C3'-C4'	-4.93	96.33	108.75
2	C	500	FAD	O4B-C1B-N9A	-2.69	102.46	108.10
2	D	500	FAD	O4B-C1B-N9A	-2.68	102.49	108.10
2	A	500	FAD	O4B-C1B-N9A	-2.67	102.50	108.10
2	B	500	FAD	O4B-C1B-N9A	-2.67	102.51	108.10
2	B	500	FAD	O3B-C3B-C4B	-2.46	103.66	111.05
2	C	500	FAD	O3B-C3B-C4B	-2.46	103.69	111.05
2	D	500	FAD	O3B-C3B-C4B	-2.45	103.69	111.05
2	A	500	FAD	O3B-C3B-C4B	-2.45	103.70	111.05
2	C	500	FAD	C6-C7-C8	-2.35	115.55	120.04
2	A	500	FAD	C6-C7-C8	-2.33	115.60	120.04
2	B	500	FAD	C6-C7-C8	-2.32	115.62	120.04
2	D	500	FAD	C6-C7-C8	-2.31	115.63	120.04
2	C	500	FAD	C9-C9A-C5X	-2.13	115.84	119.62
2	A	500	FAD	C9-C9A-C5X	-2.10	115.89	119.62
2	D	500	FAD	C9-C9A-C5X	-2.09	115.90	119.62
2	B	500	FAD	C9-C9A-C5X	-2.09	115.91	119.62
2	B	500	FAD	N6A-C6A-N1A	2.15	123.81	119.20
2	D	500	FAD	N6A-C6A-N1A	2.15	123.83	119.20
2	A	500	FAD	N6A-C6A-N1A	2.15	123.83	119.20
2	C	500	FAD	N6A-C6A-N1A	2.17	123.87	119.20
2	C	500	FAD	O2'-C2'-C3'	2.20	114.56	109.02
2	A	500	FAD	O2'-C2'-C3'	2.21	114.58	109.02
2	B	500	FAD	O2'-C2'-C3'	2.23	114.62	109.02
2	D	500	FAD	O2'-C2'-C3'	2.25	114.68	109.02
2	C	500	FAD	O2B-C2B-C3B	2.37	119.52	111.83
2	D	500	FAD	O2B-C2B-C3B	2.37	119.52	111.83
2	B	500	FAD	O2B-C2B-C3B	2.37	119.53	111.83
2	A	500	FAD	O2B-C2B-C3B	2.37	119.55	111.83
2	B	500	FAD	C6-C5X-C9A	2.89	122.78	118.98
2	D	500	FAD	C6-C5X-C9A	2.89	122.78	118.98
2	A	500	FAD	C6-C5X-C9A	2.90	122.79	118.98
2	D	500	FAD	C7M-C7-C8	2.91	127.11	120.73
2	A	500	FAD	C7M-C7-C8	2.91	127.12	120.73
2	B	500	FAD	C7M-C7-C8	2.91	127.13	120.73
2	C	500	FAD	C6-C5X-C9A	2.92	122.82	118.98
2	C	500	FAD	C7M-C7-C8	2.93	127.16	120.73
2	B	500	FAD	C1'-N10-C9A	4.95	124.42	118.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	FAD	C1'-N10-C9A	4.95	124.42	118.86
2	D	500	FAD	C1'-N10-C9A	4.96	124.43	118.86
2	C	500	FAD	C1'-N10-C9A	4.97	124.44	118.86
2	A	500	FAD	C4-N3-C2	12.46	126.02	115.25
2	C	500	FAD	C4-N3-C2	12.47	126.03	115.25
2	B	500	FAD	C4-N3-C2	12.49	126.05	115.25
2	D	500	FAD	C4-N3-C2	12.54	126.09	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.