



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 28, 2024 – 12:31 pm GMT

PDB ID : 6ZTH
Title : Phospholipase PlaB from Legionella pneumophila
Authors : Diwo, M.G.; Flieger, A.; Blankenfeldt, W.
Deposited on : 2020-07-20
Resolution : 2.30 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

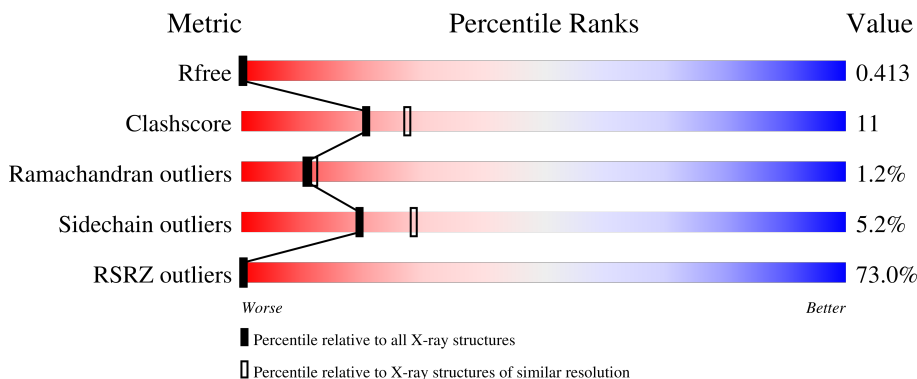
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
R_{free}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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	489	<div> <div>66%</div> <div> <div>72%</div> <div>23%</div> <div>• •</div> </div> </div>
1	B	489	<div> <div>67%</div> <div> <div>72%</div> <div>22%</div> <div>• •</div> </div> </div>
1	C	489	<div> <div>69%</div> <div> <div>73%</div> <div>20%</div> <div>• •</div> </div> </div>
1	D	489	<div> <div>72%</div> <div> <div>71%</div> <div>23%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30812 atoms, of which 14970 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 PlaB phospholipase.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
1	A	470	Total	C	H	N	O	S	Se		0	7	0
			7444	2372	3694	661	699	5	13				
1	B	470	Total	C	H	N	O	S	Se		0	1	0
			7417	2360	3683	661	695	5	13				
1	C	467	Total	C	H	N	O	S	Se		0	2	0
			7417	2358	3697	657	687	5	13				
1	D	474	Total	C	H	N	O	S	Se		1	0	0
			7431	2369	3688	658	698	5	13				

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MSE	-	initiating methionine	UNP A0A378K488
A	-13	ALA	-	expression tag	UNP A0A378K488
A	-12	SER	-	expression tag	UNP A0A378K488
A	-11	TRP	-	expression tag	UNP A0A378K488
A	-10	SER	-	expression tag	UNP A0A378K488
A	-9	HIS	-	expression tag	UNP A0A378K488
A	-8	PRO	-	expression tag	UNP A0A378K488
A	-7	GLN	-	expression tag	UNP A0A378K488
A	-6	PHE	-	expression tag	UNP A0A378K488
A	-5	GLU	-	expression tag	UNP A0A378K488
A	-4	LYS	-	expression tag	UNP A0A378K488
A	-3	GLY	-	expression tag	UNP A0A378K488
A	-2	ALA	-	expression tag	UNP A0A378K488
A	-1	GLY	-	expression tag	UNP A0A378K488
A	0	THR	-	expression tag	UNP A0A378K488
A	203	ASN	ASP	conflict	UNP A0A378K488
B	-14	MSE	-	initiating methionine	UNP A0A378K488
B	-13	ALA	-	expression tag	UNP A0A378K488
B	-12	SER	-	expression tag	UNP A0A378K488
B	-11	TRP	-	expression tag	UNP A0A378K488
B	-10	SER	-	expression tag	UNP A0A378K488

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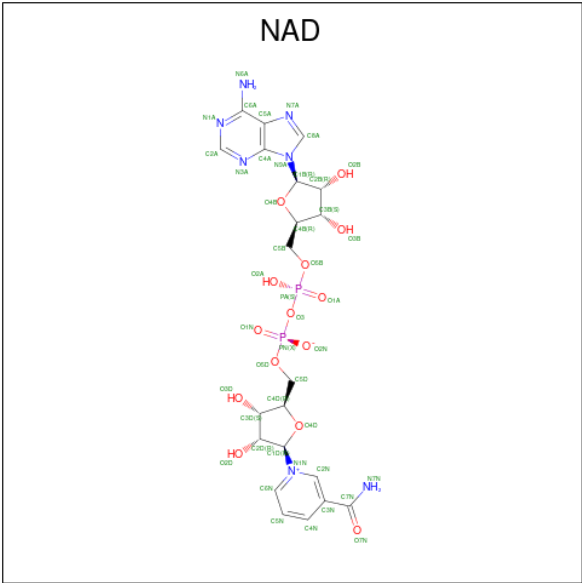
Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	HIS	-	expression tag	UNP A0A378K488
B	-8	PRO	-	expression tag	UNP A0A378K488
B	-7	GLN	-	expression tag	UNP A0A378K488
B	-6	PHE	-	expression tag	UNP A0A378K488
B	-5	GLU	-	expression tag	UNP A0A378K488
B	-4	LYS	-	expression tag	UNP A0A378K488
B	-3	GLY	-	expression tag	UNP A0A378K488
B	-2	ALA	-	expression tag	UNP A0A378K488
B	-1	GLY	-	expression tag	UNP A0A378K488
B	0	THR	-	expression tag	UNP A0A378K488
B	203	ASN	ASP	conflict	UNP A0A378K488
C	-14	MSE	-	initiating methionine	UNP A0A378K488
C	-13	ALA	-	expression tag	UNP A0A378K488
C	-12	SER	-	expression tag	UNP A0A378K488
C	-11	TRP	-	expression tag	UNP A0A378K488
C	-10	SER	-	expression tag	UNP A0A378K488
C	-9	HIS	-	expression tag	UNP A0A378K488
C	-8	PRO	-	expression tag	UNP A0A378K488
C	-7	GLN	-	expression tag	UNP A0A378K488
C	-6	PHE	-	expression tag	UNP A0A378K488
C	-5	GLU	-	expression tag	UNP A0A378K488
C	-4	LYS	-	expression tag	UNP A0A378K488
C	-3	GLY	-	expression tag	UNP A0A378K488
C	-2	ALA	-	expression tag	UNP A0A378K488
C	-1	GLY	-	expression tag	UNP A0A378K488
C	0	THR	-	expression tag	UNP A0A378K488
C	203	ASN	ASP	conflict	UNP A0A378K488
D	-14	MSE	-	initiating methionine	UNP A0A378K488
D	-13	ALA	-	expression tag	UNP A0A378K488
D	-12	SER	-	expression tag	UNP A0A378K488
D	-11	TRP	-	expression tag	UNP A0A378K488
D	-10	SER	-	expression tag	UNP A0A378K488
D	-9	HIS	-	expression tag	UNP A0A378K488
D	-8	PRO	-	expression tag	UNP A0A378K488
D	-7	GLN	-	expression tag	UNP A0A378K488
D	-6	PHE	-	expression tag	UNP A0A378K488
D	-5	GLU	-	expression tag	UNP A0A378K488
D	-4	LYS	-	expression tag	UNP A0A378K488
D	-3	GLY	-	expression tag	UNP A0A378K488
D	-2	ALA	-	expression tag	UNP A0A378K488
D	-1	GLY	-	expression tag	UNP A0A378K488
D	0	THR	-	expression tag	UNP A0A378K488

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Chain	Residue	Modelled	Actual	Comment	Reference
D	203	ASN	ASP	conflict	UNP A0A378K488

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	A	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	B	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	B	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	C	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	C	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	D	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	D	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	131	Total 131	O 131	0	0
3	B	125	Total 125	O 125	0	0
3	C	148	Total 148	O 148	0	0
3	D	139	Total 139	O 139	0	0

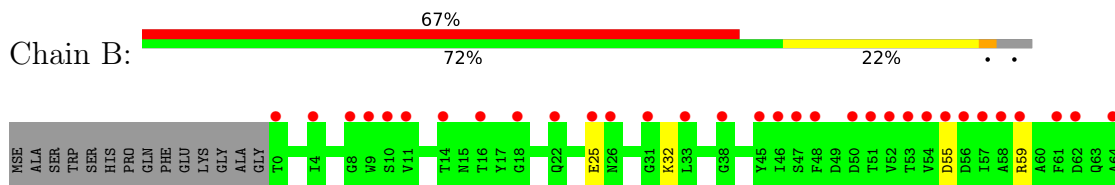
3 Residue-property plots

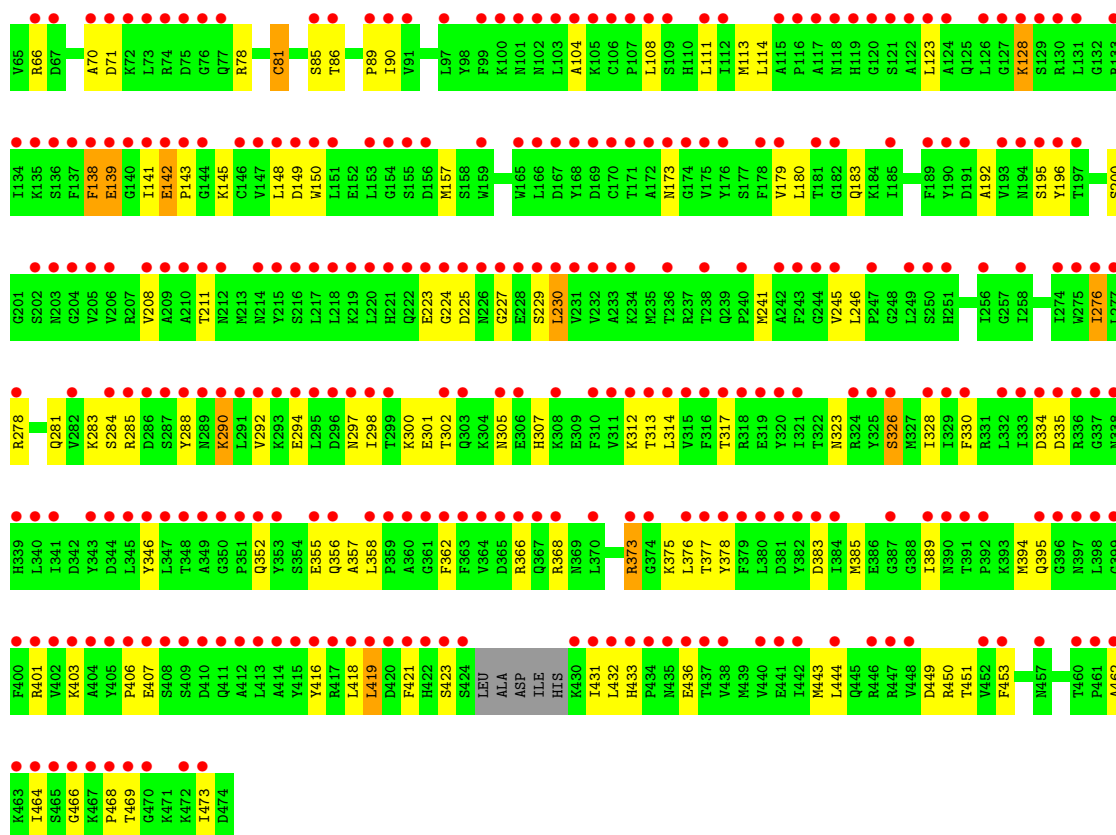
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

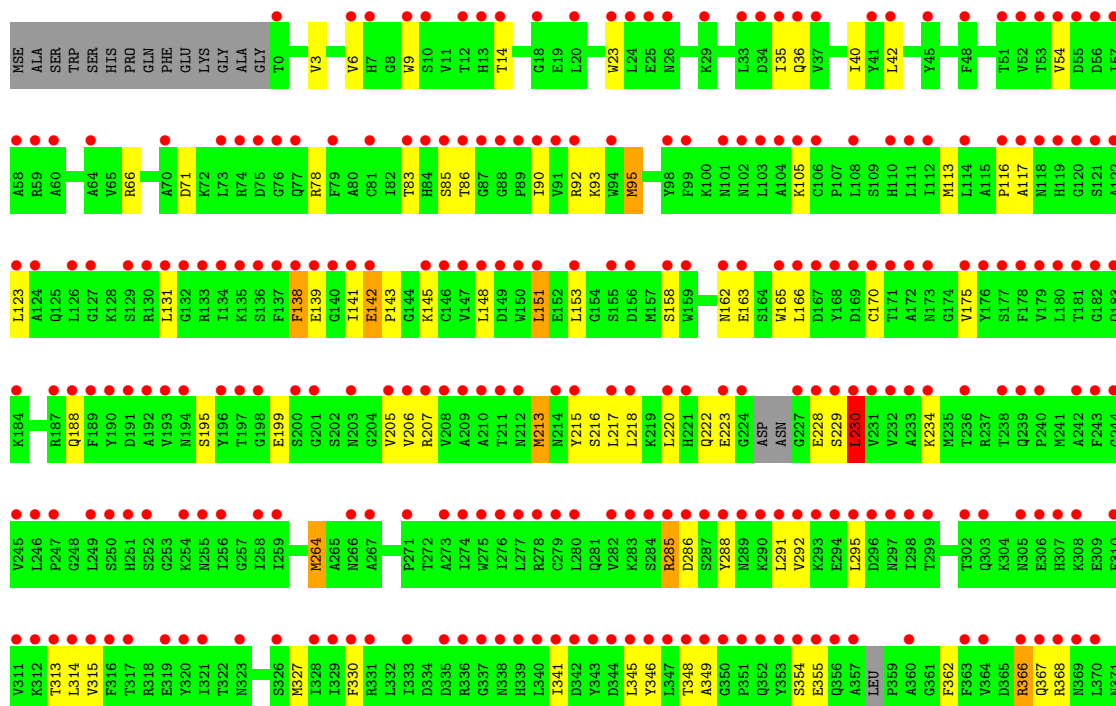
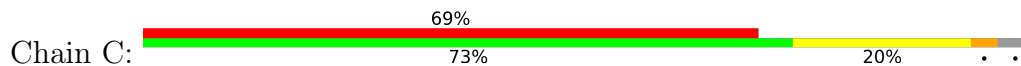


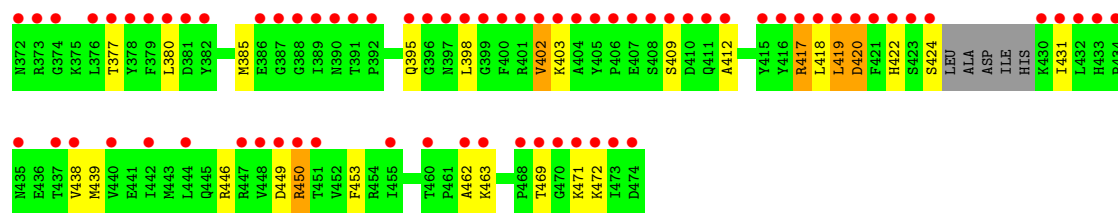
• Molecule 1: PlaB phospholipase



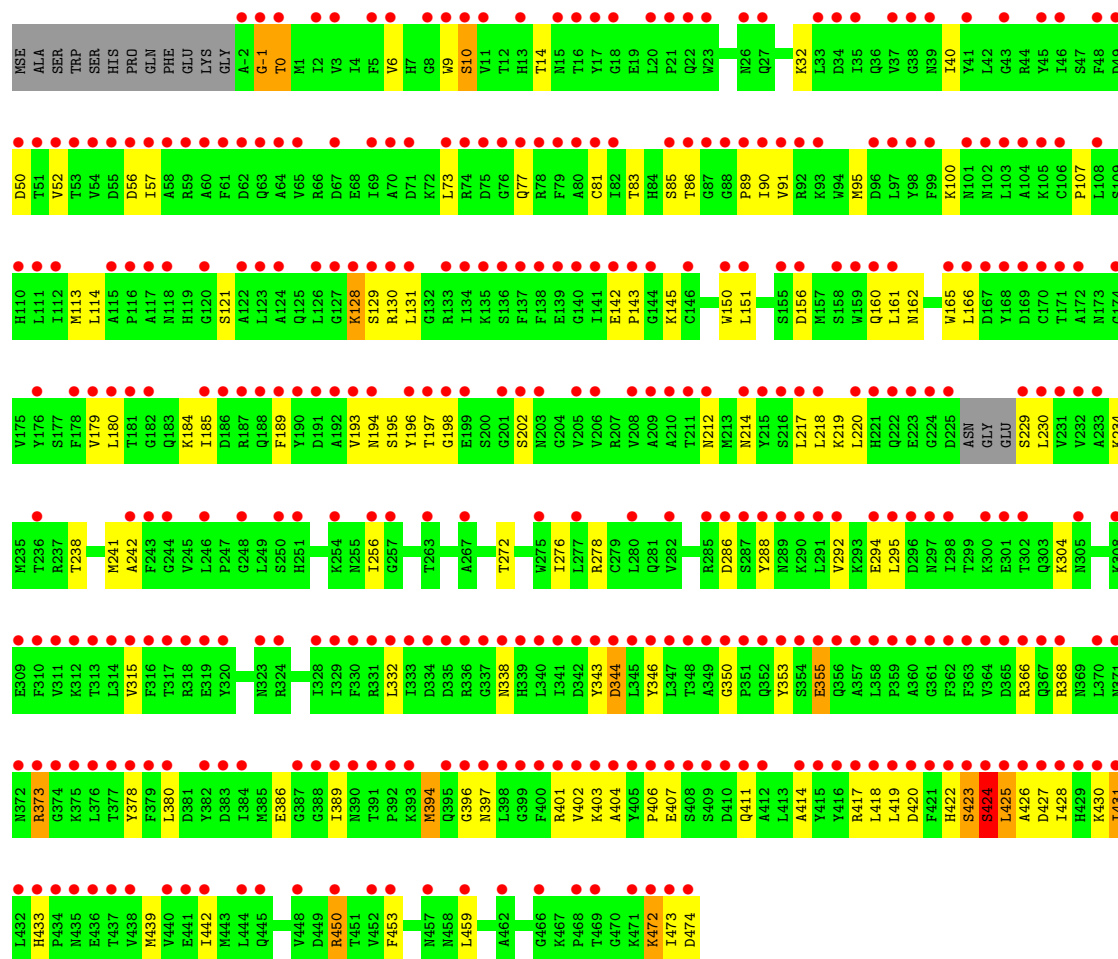
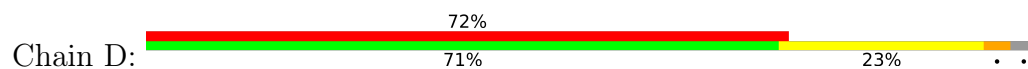


• Molecule 1: PlaB phospholipase





● Molecule 1: PlaB phospholipase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.81Å 170.58Å 93.48Å 90.00° 92.86° 90.00°	Depositor
Resolution (Å)	49.24 – 2.30 49.24 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.24-2.30) 99.7 (49.24-2.30)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.29Å)	Xtriage
Refinement program	PHENIX dev_3922	Depositor
R, R_{free}	0.364 , 0.413 0.363 , 0.413	Depositor DCC
R_{free} test set	5259 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	30812	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7605e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.27	0/3858	0.47	0/5192
1	B	0.25	0/3800	0.47	0/5115
1	C	0.26	0/3788	0.45	0/5094
1	D	0.49	2/3807 (0.1%)	0.47	1/5130 (0.0%)
All	All	0.33	2/15253 (0.0%)	0.47	1/20531 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	424	SER	CB-OG	-23.99	1.11	1.42
1	D	431	ILE	CG1-CD1	-8.62	0.91	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	431	ILE	CB-CG1-CD1	6.52	132.16	113.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	423	SER	Peptide
1	C	230	LEU	Peptide
1	D	424	SER	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3750	3694	3662	79	0
1	B	3734	3683	3700	77	0
1	C	3720	3697	3701	75	0
1	D	3743	3688	3689	106	0
2	A	88	52	51	6	0
2	B	88	52	49	1	0
2	C	88	52	50	4	0
2	D	88	52	52	12	0
3	A	131	0	0	15	0
3	B	125	0	0	11	1
3	C	148	0	0	7	0
3	D	139	0	0	11	1
All	All	15842	14970	14954	333	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 11.

All (333) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:431:ILE:CD1	1:D:431:ILE:CB	2.24	1.14
1:D:431:ILE:CG1	1:D:431:ILE:HD11	1.53	1.05
1:D:431:ILE:CG1	1:D:431:ILE:HD12	1.53	1.02
1:D:431:ILE:CG1	1:D:431:ILE:HD13	1.53	1.02
1:D:431:ILE:CD1	1:D:431:ILE:HG13	1.48	0.99
1:D:431:ILE:CD1	1:D:431:ILE:HG12	1.48	0.98
1:B:352:GLN:NE2	3:B:702:HOH:O	1.98	0.94
1:D:431:ILE:CD1	1:D:431:ILE:CG1	0.91	0.90
1:B:297:ASN:OD1	1:B:300:LYS:NZ	2.03	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:GLN:O	1:B:283:LYS:NZ	2.06	0.88
1:A:142:GLU:OE2	3:A:601:HOH:O	1.94	0.85
1:A:62:ASP:OD2	1:A:66:ARG:NH1	2.11	0.84
1:B:183:GLN:OE1	3:B:701:HOH:O	1.96	0.82
1:D:286:ASP:OD2	3:D:601:HOH:O	1.99	0.81
1:D:472:LYS:NZ	3:D:602:HOH:O	2.16	0.79
1:B:375:LYS:NZ	3:B:706:HOH:O	2.16	0.78
1:A:272:THR:HG22	1:A:276:ILE:HD12	1.65	0.78
1:C:188:GLN:O	3:C:601:HOH:O	2.01	0.78
1:B:421:PHE:HE1	1:B:431:ILE:HD11	1.48	0.77
1:B:449:ASP:OD1	1:B:450:ARG:N	2.17	0.77
1:D:474:ASP:OD1	3:D:602:HOH:O	2.04	0.76
1:B:431:ILE:O	3:B:703:HOH:O	2.05	0.75
1:C:153:LEU:HD22	1:C:327:MSE:HE1	1.66	0.75
1:D:197:THR:O	3:D:603:HOH:O	2.04	0.75
1:A:451:THR:HG23	1:A:469:THR:HG23	1.68	0.75
1:C:35:ILE:HG21	1:C:40:ILE:HD11	1.69	0.74
1:D:417:ARG:NH2	3:D:611:HOH:O	2.21	0.74
1:B:401:ARG:NH1	3:B:708:HOH:O	2.19	0.74
1:C:431:ILE:O	1:C:438:VAL:HG11	1.88	0.74
1:A:348:THR:O	1:A:398:LEU:HD12	1.88	0.73
1:B:383:ASP:OD2	3:B:705:HOH:O	2.06	0.73
1:C:117:ALA:HB3	1:C:151:LEU:HD21	1.69	0.73
1:B:196:TYR:O	3:B:704:HOH:O	2.05	0.73
1:D:424:SER:O	1:D:426:ALA:N	2.22	0.72
1:C:14:THR:HG21	1:C:42:LEU:HD13	1.71	0.72
1:A:59:ARG:NH1	3:A:608:HOH:O	2.22	0.71
1:B:368:ARG:NH2	1:B:373:ARG:O	2.23	0.71
1:C:420:ASP:N	3:C:606:HOH:O	2.23	0.71
1:D:368:ARG:NH1	1:D:373:ARG:O	2.24	0.71
1:D:100:LYS:O	3:D:605:HOH:O	2.09	0.70
1:B:104:ALA:HB2	1:B:173:ASN:OD1	1.90	0.70
1:D:424:SER:OG	1:D:431:ILE:HD13	1.91	0.69
1:B:301:GLU:OE1	1:B:305:ASN:ND2	2.26	0.68
1:A:437:THR:O	3:A:602:HOH:O	2.11	0.68
1:A:408:SER:OG	1:A:417:ARG:NH1	2.27	0.67
1:D:129:SER:OG	3:D:606:HOH:O	2.12	0.67
1:A:128:LYS:HZ2	1:A:142:GLU:HB2	1.59	0.67
1:C:23:TRP:HA	1:C:264:MSE:HE1	1.77	0.67
1:B:143:PRO:HG2	1:B:148:LEU:HD11	1.77	0.67
1:B:431:ILE:HG22	1:B:432:LEU:HG	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ASN:OD1	3:A:603:HOH:O	2.13	0.66
1:C:6:VAL:HB	1:C:83:THR:HG22	1.78	0.66
1:A:124:ALA:O	3:A:604:HOH:O	2.14	0.65
1:D:52:VAL:HG11	1:D:57:ILE:HD11	1.79	0.65
1:B:355:GLU:OE2	1:B:356:GLN:NE2	2.30	0.65
1:D:420:ASP:O	3:D:609:HOH:O	2.15	0.65
1:A:410:ASP:OD1	3:A:605:HOH:O	2.15	0.65
1:D:423:SER:OG	1:D:424:SER:N	2.30	0.65
1:B:378:TYR:OH	2:D:502:NAD:N6A	2.21	0.65
1:C:395:GLN:O	3:C:602:HOH:O	2.13	0.64
2:D:501:NAD:O1A	2:D:502:NAD:O3D	2.14	0.64
1:B:328:ILE:HG21	1:B:330:PHE:CZ	2.33	0.64
1:D:162:ASN:OD1	3:D:607:HOH:O	2.15	0.64
1:D:52:VAL:CG1	1:D:57:ILE:HD11	2.28	0.64
1:D:344:ASP:OD2	1:D:403:LYS:NZ	2.31	0.64
1:A:327:MSE:HB3	1:A:437:THR:HG22	1.80	0.63
1:A:451:THR:HG21	1:A:467:LYS:O	1.97	0.63
1:B:358:LEU:HD23	1:B:362:PHE:CD2	2.34	0.63
1:A:332:LEU:HG	1:A:340:LEU:HD12	1.81	0.62
1:A:356:GLN:NE2	3:A:614:HOH:O	2.32	0.62
1:D:6:VAL:CG1	1:D:83:THR:HG22	2.30	0.62
1:C:35:ILE:HG21	1:C:40:ILE:CD1	2.30	0.61
1:A:348:THR:HB	1:A:353:TYR:HB3	1.82	0.61
1:D:407:GLU:OE2	3:D:610:HOH:O	2.16	0.61
1:A:451:THR:CG2	1:A:469:THR:HG23	2.31	0.61
1:B:208:VAL:O	1:B:211:THR:OG1	2.14	0.61
1:C:450:ARG:NE	1:C:472:LYS:O	2.34	0.61
1:C:42:LEU:HD11	1:D:459:LEU:HA	1.82	0.60
1:A:411:GLN:OE1	3:A:605:HOH:O	2.15	0.60
1:A:421:PHE:HE2	1:A:431:ILE:HD11	1.67	0.60
1:A:313:THR:HG23	1:A:316:PHE:H	1.67	0.60
1:C:380:LEU:HD13	1:C:385:MSE:HE2	1.82	0.60
1:A:128:LYS:NZ	1:A:142:GLU:HB2	2.15	0.59
1:D:89:PRO:HB3	1:D:150:TRP:CH2	2.36	0.59
1:C:341:ILE:O	1:C:368:ARG:NH1	2.36	0.59
1:A:331:ARG:NH2	3:A:615:HOH:O	2.33	0.59
1:B:223:GLU:N	1:B:230:LEU:O	2.35	0.59
1:D:195:SER:OG	2:D:502:NAD:H4N	2.02	0.59
1:A:250:SER:OG	1:A:251:HIS:N	2.35	0.59
1:A:294:GLU:OE2	3:A:606:HOH:O	2.17	0.59
1:C:71:ASP:N	1:C:71:ASP:OD1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:ILE:O	1:B:302:THR:HG23	2.02	0.58
1:B:451:THR:OG1	1:B:469:THR:HG23	2.03	0.58
1:C:95:MSE:HE3	1:C:165:TRP:CZ2	2.38	0.58
1:D:128:LYS:HD2	1:D:142:GLU:HB3	1.86	0.58
1:C:66:ARG:NH2	3:C:613:HOH:O	2.37	0.57
1:A:209:ALA:O	1:A:437:THR:HG23	2.03	0.57
1:D:450:ARG:NE	1:D:472:LYS:O	2.37	0.57
1:D:6:VAL:HG12	1:D:83:THR:HG22	1.86	0.57
1:C:195:SER:OG	2:C:501:NAD:H4N	2.04	0.57
1:C:207:ARG:NH1	1:C:327:MSE:HE3	2.19	0.57
1:C:207:ARG:HH11	1:C:327:MSE:HE3	1.69	0.56
1:C:213:MSE:O	3:C:604:HOH:O	2.17	0.56
1:C:327:MSE:HE2	1:C:377:THR:CG2	2.35	0.56
1:A:391:THR:HB	1:A:392:PRO:CD	2.35	0.56
1:D:450:ARG:HG3	1:D:473:ILE:HG22	1.87	0.56
1:A:-1:GLY:O	1:A:0:THR:CB	2.54	0.56
1:C:450:ARG:HE	1:C:472:LYS:C	2.09	0.56
1:D:355:GLU:OE2	1:D:401:ARG:NH1	2.39	0.55
1:B:335:ASP:OD1	1:B:335:ASP:N	2.40	0.55
1:A:113:MSE:HB3	1:A:116:PRO:HG3	1.88	0.55
1:A:419:LEU:HD23	1:A:420:ASP:N	2.22	0.55
1:C:123:LEU:HB3	1:C:131:LEU:HD21	1.87	0.55
1:A:184:LYS:HD3	1:A:256:ILE:HD13	1.89	0.55
1:B:114:LEU:HD21	1:B:276:ILE:HD11	1.89	0.55
1:D:332:LEU:HD13	1:D:343:TYR:CZ	2.42	0.55
1:C:85:SER:OG	1:C:86:THR:N	2.40	0.55
1:A:275:TRP:CZ2	1:A:298:ILE:HG13	2.41	0.54
1:A:342:ASP:OD2	1:A:405:TYR:HB2	2.08	0.54
1:D:218:LEU:HD21	1:D:220:LEU:HD21	1.89	0.54
1:D:272:THR:HG22	1:D:276:ILE:HD12	1.89	0.54
1:D:423:SER:O	1:D:424:SER:HB2	2.07	0.54
1:C:222:GLN:HB2	1:C:419:LEU:HD12	1.89	0.54
1:D:402:VAL:HG12	1:D:419:LEU:HB3	1.90	0.53
1:B:436:GLU:OE1	3:B:707:HOH:O	2.18	0.53
1:B:111:LEU:HD21	1:B:113:MSE:HE2	1.91	0.53
1:C:409:SER:OG	1:C:412:ALA:N	2.41	0.53
1:A:450:ARG:NH2	3:A:625:HOH:O	2.39	0.53
1:B:418:LEU:HD21	3:B:722:HOH:O	2.08	0.53
1:C:417:ARG:NH2	1:C:418:LEU:HB3	2.23	0.53
1:B:85:SER:OG	1:B:86:THR:N	2.42	0.53
1:C:95:MSE:HE3	1:C:165:TRP:HZ2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:LYS:HD2	1:A:418:LEU:HD11	1.91	0.52
1:C:213:MSE:HE3	1:C:215:TYR:CE1	2.44	0.52
1:D:420:ASP:OD1	1:D:422:HIS:NE2	2.41	0.52
1:D:353:TYR:CZ	1:D:422:HIS:HB3	2.43	0.52
1:A:421:PHE:CE2	1:A:431:ILE:HD11	2.45	0.52
1:D:278:ARG:NH2	1:D:294:GLU:OE1	2.42	0.52
1:D:-1:GLY:O	1:D:0:THR:CB	2.57	0.52
1:B:326:SER:HB3	1:B:432:LEU:HD22	1.92	0.51
1:C:54:VAL:HG13	1:C:90:ILE:HD13	1.92	0.51
1:D:196:TYR:CE1	2:D:502:NAD:C2N	2.94	0.51
1:A:391:THR:HB	1:A:392:PRO:HD2	1.93	0.51
1:B:394:MSE:HE2	1:D:315:VAL:HG12	1.93	0.51
1:C:313:THR:HG22	1:C:315:VAL:H	1.76	0.51
1:B:385:MSE:O	1:B:389:ILE:HD13	2.11	0.51
1:C:218:LEU:HD21	1:C:220:LEU:HG	1.93	0.51
1:A:195:SER:OG	2:A:501:NAD:H4N	2.11	0.50
1:D:406:PRO:HG2	1:D:414:ALA:O	2.12	0.50
1:A:128:LYS:HZ2	1:A:142:GLU:CB	2.24	0.50
1:C:93:LYS:NZ	3:C:608:HOH:O	2.29	0.50
1:C:217:LEU:HD13	1:C:439:MSE:HB2	1.93	0.50
1:C:349:ALA:O	1:C:354:SER:N	2.44	0.49
1:B:421:PHE:CZ	1:B:423:SER:HB2	2.47	0.49
1:A:24:LEU:HD12	1:A:33:LEU:HD13	1.94	0.49
1:B:195:SER:HB2	2:D:501:NAD:H4N	1.94	0.49
1:C:162:ASN:CB	1:C:439:MSE:HE1	2.43	0.49
1:C:348:THR:O	1:C:398:LEU:HD12	2.12	0.49
1:D:73:LEU:HD23	1:D:77:GLN:O	2.13	0.49
1:C:228:GLU:O	1:C:229:SER:HB3	2.13	0.49
1:A:150:TRP:HA	1:A:157:MSE:HE3	1.95	0.49
1:D:242:ALA:HB1	1:D:295:LEU:HD12	1.94	0.49
1:D:332:LEU:CD2	1:D:402:VAL:HG21	2.43	0.48
1:A:237:ARG:NH2	1:A:436:GLU:OE2	2.46	0.48
1:D:344:ASP:HB2	1:D:403:LYS:NZ	2.27	0.48
1:D:91:VAL:O	1:D:95:MSE:HG3	2.13	0.48
1:A:331:ARG:NH1	3:A:632:HOH:O	2.46	0.48
1:A:403:LYS:NZ	1:A:407:GLU:OE1	2.46	0.48
1:A:345:LEU:HD12	1:A:402:VAL:HG12	1.96	0.48
1:B:358:LEU:HD23	1:B:362:PHE:CE2	2.48	0.48
1:D:189:PHE:CD1	1:D:189:PHE:N	2.81	0.48
1:D:344:ASP:HA	2:D:501:NAD:H2A	1.95	0.48
2:A:502:NAD:O3B	1:C:366:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:386:GLU:HA	1:D:425:LEU:HD23	1.96	0.48
1:D:431:ILE:HD12	1:D:431:ILE:N	2.29	0.48
1:B:278:ARG:HD2	1:B:281:GLN:NE2	2.29	0.48
1:B:335:ASP:HB3	1:B:443:MSE:HE3	1.96	0.48
1:C:446:ARG:NH1	1:D:56:ASP:OD2	2.46	0.48
1:D:229:SER:C	1:D:230:LEU:HD23	2.35	0.48
1:B:149:ASP:HB3	1:B:157:MSE:HE1	1.96	0.47
1:C:450:ARG:HB2	1:C:469:THR:HG21	1.96	0.47
1:A:123:LEU:HD22	1:A:126:LEU:HD12	1.96	0.47
1:B:224:GLY:O	1:B:227:GLY:N	2.46	0.47
1:C:170:CYS:HB3	1:C:175:VAL:HB	1.95	0.47
1:D:344:ASP:HB2	1:D:403:LYS:HZ2	1.78	0.47
1:B:368:ARG:HD3	2:D:502:NAD:O4B	2.14	0.47
1:B:138:PHE:O	1:B:139:GLU:CB	2.62	0.47
1:C:330:PHE:CE1	1:C:345:LEU:HD21	2.49	0.47
1:B:290:LYS:HD3	1:B:294:GLU:OE1	2.15	0.47
1:A:355:GLU:O	2:C:502:NAD:N6A	2.44	0.47
1:C:54:VAL:HG13	1:C:90:ILE:CD1	2.44	0.47
1:C:123:LEU:HD12	1:C:205:VAL:HG13	1.97	0.47
1:D:220:LEU:HD12	1:D:442:ILE:HD13	1.96	0.47
1:D:366:ARG:NH2	2:D:501:NAD:O1N	2.47	0.47
1:A:24:LEU:HD12	1:A:33:LEU:CD1	2.45	0.47
1:D:85:SER:OG	1:D:86:THR:N	2.47	0.47
2:A:501:NAD:O1A	2:C:501:NAD:O3D	2.24	0.47
1:B:401:ARG:NH1	3:B:722:HOH:O	2.48	0.46
1:B:128:LYS:HD2	1:B:141:ILE:HG23	1.96	0.46
1:C:143:PRO:HG2	1:C:148:LEU:HD11	1.97	0.46
1:C:420:ASP:OD1	1:C:422:HIS:CE1	2.68	0.46
1:C:92:ARG:NH2	1:C:162:ASN:OD1	2.48	0.46
1:C:450:ARG:NH2	1:C:472:LYS:O	2.48	0.46
1:C:213:MSE:HE3	1:C:215:TYR:HE1	1.81	0.46
1:C:449:ASP:OD1	1:C:469:THR:HG22	2.15	0.46
1:D:9:TRP:HZ2	1:D:131:LEU:HD11	1.81	0.46
1:D:50:ASP:OD1	1:D:145:LYS:N	2.42	0.46
1:D:212:ASN:HD21	1:D:214:ASN:HB2	1.79	0.46
1:D:389:ILE:HA	1:D:394:MSE:HG2	1.97	0.46
1:C:3:VAL:HB	1:C:40:ILE:HD12	1.97	0.46
1:A:417:ARG:NH2	1:A:418:LEU:HD13	2.31	0.46
1:B:328:ILE:O	1:B:377:THR:HA	2.16	0.46
1:A:358:LEU:HD23	1:A:362:PHE:CD2	2.50	0.46
1:A:402:VAL:HG22	1:A:419:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:VAL:O	3:A:607:HOH:O	2.21	0.46
1:B:288:TYR:O	1:B:292:VAL:HG23	2.15	0.46
1:D:288:TYR:O	1:D:292:VAL:HG13	2.16	0.46
1:C:462:ALA:N	1:D:14:THR:OG1	2.44	0.45
1:D:160:GLN:OE1	1:D:160:GLN:HA	2.16	0.45
1:D:350:GLY:HA3	1:D:394:MSE:HE3	1.97	0.45
2:C:501:NAD:O5D	2:C:501:NAD:H2N	2.17	0.45
1:B:313:THR:HG22	1:B:314:LEU:N	2.32	0.45
1:D:401:ARG:HG3	1:D:418:LEU:HD11	1.98	0.45
1:B:180:LEU:HD22	1:B:246:LEU:HD21	1.97	0.45
1:D:166:LEU:HA	1:D:238:THR:HG22	1.99	0.45
1:B:86:THR:HG22	1:B:90:ILE:HG13	1.98	0.45
1:B:89:PRO:HB3	1:B:150:TRP:CH2	2.52	0.45
1:D:73:LEU:HD22	1:D:107:PRO:HB2	1.99	0.45
1:D:166:LEU:HD21	1:D:217:LEU:HB3	1.98	0.45
1:A:328:ILE:HD11	1:A:380:LEU:HD11	1.99	0.45
2:A:501:NAD:H2N	2:A:501:NAD:O5D	2.16	0.45
1:D:57:ILE:HG21	1:D:90:ILE:HD13	1.99	0.45
1:D:114:LEU:O	1:D:180:LEU:O	2.34	0.44
1:D:131:LEU:HD23	1:D:143:PRO:HG3	1.98	0.44
1:B:334:ASP:OD2	1:B:416:TYR:OH	2.30	0.44
1:D:156:ASP:O	1:D:160:GLN:HG2	2.17	0.44
1:A:85:SER:OG	1:A:86:THR:N	2.50	0.44
1:A:153:LEU:HD13	1:A:377:THR:HG21	2.00	0.44
1:B:355:GLU:O	2:B:602:NAD:N6A	2.47	0.44
1:D:9:TRP:CE3	1:D:143:PRO:HB3	2.52	0.44
1:D:130:ARG:NH2	1:D:194:ASN:OD1	2.46	0.44
1:C:113:MSE:HB3	1:C:116:PRO:HG3	2.00	0.44
1:D:131:LEU:CD2	1:D:143:PRO:HG3	2.47	0.44
1:D:366:ARG:NE	2:D:501:NAD:O2A	2.49	0.44
1:A:23:TRP:HA	1:A:264:MSE:HE1	1.99	0.44
1:A:219:LYS:O	1:A:219:LYS:HG3	2.18	0.44
1:C:288:TYR:O	1:C:292:VAL:HG23	2.17	0.44
1:D:95:MSE:SE	1:D:165:TRP:HH2	2.50	0.44
2:D:502:NAD:O5D	2:D:502:NAD:H2N	2.17	0.44
1:A:334:ASP:OD2	1:A:416:TYR:OH	2.34	0.44
1:B:245:VAL:O	1:B:302:THR:HG21	2.17	0.44
1:C:117:ALA:CB	1:C:151:LEU:HD21	2.43	0.44
1:B:128:LYS:CD	1:B:141:ILE:HG23	2.48	0.44
1:C:142:GLU:HB2	1:C:143:PRO:HD3	1.99	0.44
1:D:217:LEU:C	1:D:217:LEU:HD13	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:MSE:HE3	1:D:179:VAL:HG22	1.99	0.44
1:A:192:ALA:HB3	1:C:346:TYR:HE1	1.82	0.43
1:A:270:HIS:HD2	1:A:272:THR:H	1.64	0.43
1:B:55:ASP:O	1:B:59:ARG:HG3	2.18	0.43
1:B:179:VAL:HG23	1:B:241:MSE:SE	2.68	0.43
1:C:345:LEU:HD12	1:C:402:VAL:HG12	1.99	0.43
1:A:20:LEU:HD21	1:A:276:ILE:HD13	2.00	0.43
1:A:401:ARG:NH1	3:A:634:HOH:O	2.50	0.43
1:B:419:LEU:HD13	1:B:444:LEU:CD2	2.48	0.43
1:B:450:ARG:HG3	1:B:473:ILE:HG22	1.99	0.43
1:C:145:LYS:NZ	3:C:603:HOH:O	2.17	0.43
1:D:9:TRP:CE3	1:D:10:SER:N	2.87	0.43
1:D:424:SER:HB3	1:D:425:LEU:H	1.50	0.43
1:B:81:CYS:HB2	1:B:108:LEU:HD11	2.00	0.43
1:C:380:LEU:HD13	1:C:385:MSE:CE	2.48	0.43
1:A:362:PHE:HD2	1:A:380:LEU:HD22	1.83	0.43
1:B:362:PHE:HB2	1:B:385:MSE:HG3	2.00	0.43
1:C:92:ARG:HA	1:C:95:MSE:HE2	2.01	0.43
1:A:345:LEU:CD1	1:A:402:VAL:HG12	2.48	0.42
1:D:185:ILE:HD12	1:D:198:GLY:HA2	2.01	0.42
1:D:161:LEU:HD11	1:D:165:TRP:HE1	1.84	0.42
1:D:366:ARG:NE	2:D:501:NAD:H8A	2.35	0.42
1:A:419:LEU:HD13	1:A:442:ILE:HG21	2.02	0.42
1:A:246:LEU:HB2	1:A:249:LEU:HD12	2.02	0.42
1:A:313:THR:HG23	1:A:316:PHE:N	2.32	0.42
1:A:362:PHE:CD2	1:A:380:LEU:HD22	2.54	0.42
1:A:400:PHE:CZ	1:A:431:ILE:HD13	2.54	0.42
1:C:162:ASN:HB2	1:C:439:MSE:HE1	2.01	0.42
1:D:353:TYR:CE2	1:D:397:ASN:HB3	2.55	0.42
1:D:426:ALA:HB1	1:D:428:ILE:HD12	2.02	0.42
1:A:14:THR:HG1	1:B:462:ALA:H	1.63	0.42
1:B:326:SER:OG	1:B:433:HIS:O	2.37	0.42
1:A:44:ARG:HB2	1:B:464:ILE:HG23	2.00	0.42
1:B:71:ASP:OD1	1:B:71:ASP:N	2.52	0.42
1:D:128:LYS:CD	1:D:142:GLU:HB3	2.48	0.42
1:A:132:GLY:HA3	1:A:142:GLU:HG2	2.02	0.42
1:B:376:LEU:HD21	2:D:502:NAD:C5A	2.50	0.42
1:D:217:LEU:HD11	1:D:219:LYS:HE2	2.01	0.42
1:D:422:HIS:O	1:D:423:SER:HB2	2.19	0.42
1:D:234:LYS:N	3:D:632:HOH:O	2.52	0.42
1:A:208:VAL:O	1:A:211:THR:OG1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:ALA:HB3	1:D:346:TYR:CE2	2.55	0.42
1:D:332:LEU:HD21	1:D:402:VAL:HG21	2.01	0.42
1:C:163:GLU:HA	1:C:166:LEU:HD12	2.01	0.41
1:A:420:ASP:HB3	1:A:422:HIS:CE1	2.55	0.41
1:C:314:LEU:HD12	1:C:314:LEU:H	1.85	0.41
1:A:54:VAL:HG13	1:A:90:ILE:HD13	2.01	0.41
2:A:502:NAD:N6A	1:C:355:GLU:O	2.54	0.41
1:C:291:LEU:HD13	1:C:295:LEU:HG	2.02	0.41
2:A:502:NAD:H5N	3:A:635:HOH:O	2.21	0.41
1:B:312:LYS:HE2	1:B:317:THR:HG23	2.02	0.41
1:C:199:GLU:OE1	1:C:207:ARG:NE	2.48	0.41
1:D:86:THR:CG2	1:D:151:LEU:HD11	2.50	0.41
1:D:378:TYR:HD2	1:D:380:LEU:HD21	1.85	0.41
1:C:223:GLU:O	1:C:230:LEU:HA	2.21	0.41
1:B:466:GLY:O	1:B:468:PRO:HD3	2.20	0.41
1:C:403:LYS:CB	1:C:418:LEU:HD12	2.51	0.41
1:D:389:ILE:HG22	1:D:396:GLY:HA2	2.03	0.41
1:B:142:GLU:HB2	1:B:143:PRO:HD3	2.02	0.41
1:B:346:TYR:CE1	1:D:193:VAL:HG23	2.56	0.41
1:D:217:LEU:HD11	1:D:219:LYS:HG3	2.03	0.41
1:B:66:ARG:O	1:B:70:ALA:HB2	2.21	0.41
1:B:307:HIS:NE2	1:B:323:ASN:OD1	2.54	0.41
1:D:179:VAL:HG23	1:D:241:MSE:SE	2.71	0.41
1:D:430:LYS:HE2	1:D:433:HIS:ND1	2.35	0.41
1:A:51:THR:HG21	1:B:406:PRO:HG2	2.03	0.40
1:D:184:LYS:HD3	1:D:256:ILE:CD1	2.51	0.40
1:B:357:ALA:HB2	3:B:702:HOH:O	2.22	0.40
1:C:285[A]:ARG:HD3	1:C:285[A]:ARG:H	1.87	0.40
1:D:332:LEU:HD22	1:D:343:TYR:CD2	2.57	0.40
1:D:162:ASN:CB	1:D:439:MSE:HE1	2.51	0.40
1:A:405:TYR:HB3	1:A:406:PRO:HA	2.03	0.40
1:B:403:LYS:NZ	1:B:407:GLU:OE2	2.52	0.40
1:C:291:LEU:O	1:C:295:LEU:HG	2.21	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)
3:B:790:HOH:O	3:D:652:HOH:O[1_655]	2.15	0.05

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	471/489 (96%)	445 (94%)	22 (5%)	4 (1%)	16	20
1	B	467/489 (96%)	434 (93%)	27 (6%)	6 (1%)	10	11
1	C	461/489 (94%)	437 (95%)	18 (4%)	6 (1%)	10	11
1	D	470/489 (96%)	439 (93%)	25 (5%)	6 (1%)	10	11
All	All	1869/1956 (96%)	1755 (94%)	92 (5%)	22 (1%)	11	12

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	0	THR
1	A	412	ALA
1	B	139	GLU
1	B	229	SER
1	C	138	PHE
1	D	424	SER
1	D	425	LEU
1	B	142	GLU
1	D	0	THR
1	A	424	SER
1	B	138	PHE
1	B	230	LEU
1	C	78	ARG
1	C	139	GLU
1	C	142	GLU
1	C	230	LEU
1	D	-1	GLY
1	D	404	ALA
1	D	423	SER
1	A	351	PRO
1	B	78	ARG
1	C	141	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	407/408 (100%)	385 (95%)	22 (5%)	18	27
1	B	403/408 (99%)	385 (96%)	18 (4%)	23	34
1	C	402/408 (98%)	374 (93%)	28 (7%)	12	17
1	D	401/408 (98%)	382 (95%)	19 (5%)	22	32
All	All	1613/1632 (99%)	1526 (95%)	87 (5%)	19	27

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	TRP
1	A	106	CYS
1	A	129	SER
1	A	130	ARG
1	A	216	SER
1	A	293	LYS
1	A	296	ASP
1	A	304	LYS
1	A	305	ASN
1	A	308	LYS
1	A	310	PHE
1	A	313	THR
1	A	336	ARG
1	A	353	TYR
1	A	383	ASP
1	A	417	ARG
1	A	424	SER
1	A	438	VAL
1	A	441	GLU
1	A	453	PHE
1	A	471	LYS
1	A	472	LYS
1	B	25	GLU
1	B	32	LYS

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Mol	Chain	Res	Type
1	B	81	CYS
1	B	123	LEU
1	B	128	LYS
1	B	145	LYS
1	B	200	SER
1	B	225	ASP
1	B	276	ILE
1	B	285[A]	ARG
1	B	285[B]	ARG
1	B	290	LYS
1	B	326	SER
1	B	366	ARG
1	B	373	ARG
1	B	395	GLN
1	B	419	LEU
1	B	453	PHE
1	C	9	TRP
1	C	36	GLN
1	C	95	MSE
1	C	105	LYS
1	C	138	PHE
1	C	151	LEU
1	C	158	SER
1	C	206	VAL
1	C	213	MSE
1	C	216	SER
1	C	234	LYS
1	C	264	MSE
1	C	285[A]	ARG
1	C	285[B]	ARG
1	C	286	ASP
1	C	362	PHE
1	C	366	ARG
1	C	367	GLN
1	C	402	VAL
1	C	417	ARG
1	C	419	LEU
1	C	420	ASP
1	C	424	SER
1	C	450	ARG
1	C	453	PHE
1	C	463[A]	LYS

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Mol	Chain	Res	Type
1	C	463[B]	LYS
1	C	471	LYS
1	D	10	SER
1	D	32	LYS
1	D	40	ILE
1	D	81	CYS
1	D	121	SER
1	D	128	LYS
1	D	202	SER
1	D	304	LYS
1	D	338	ASN
1	D	344	ASP
1	D	355	GLU
1	D	373	ARG
1	D	394	MSE
1	D	411	GLN
1	D	424	SER
1	D	427	ASP
1	D	450	ARG
1	D	453	PHE
1	D	472	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	270	HIS
1	A	356	GLN
1	B	281	GLN
1	C	305	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	NAD	C	501	-	42,48,48	4.73	19 (45%)	50,73,73	1.77	6 (12%)
2	NAD	A	501	-	42,48,48	4.72	19 (45%)	50,73,73	1.81	10 (20%)
2	NAD	D	501	-	42,48,48	4.70	19 (45%)	50,73,73	1.76	7 (14%)
2	NAD	B	601	-	42,48,48	4.85	19 (45%)	50,73,73	1.76	10 (20%)
2	NAD	C	502	-	42,48,48	5.04	19 (45%)	50,73,73	1.82	9 (18%)
2	NAD	D	502	-	42,48,48	4.71	19 (45%)	50,73,73	1.82	11 (22%)
2	NAD	A	502	-	42,48,48	5.05	19 (45%)	50,73,73	1.80	10 (20%)
2	NAD	B	602	-	42,48,48	4.83	19 (45%)	50,73,73	1.75	9 (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	NAD	C	501	-	-	3/26/62/62	0/5/5/5
2	NAD	A	501	-	-	5/26/62/62	0/5/5/5
2	NAD	D	501	-	-	2/26/62/62	0/5/5/5
2	NAD	B	601	-	-	4/26/62/62	0/5/5/5
2	NAD	C	502	-	-	6/26/62/62	0/5/5/5
2	NAD	D	502	-	-	3/26/62/62	0/5/5/5
2	NAD	A	502	-	-	4/26/62/62	0/5/5/5
2	NAD	B	602	-	-	2/26/62/62	0/5/5/5

All (152) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	502	NAD	C2B-C1B	-18.51	1.25	1.53
2	A	502	NAD	C2B-C1B	-18.32	1.26	1.53
2	B	601	NAD	C2B-C1B	-17.30	1.27	1.53
2	B	602	NAD	C2B-C1B	-17.15	1.27	1.53
2	C	501	NAD	C2B-C1B	-16.37	1.28	1.53
2	A	501	NAD	C2B-C1B	-16.23	1.29	1.53
2	D	501	NAD	C2B-C1B	-16.18	1.29	1.53
2	D	502	NAD	C2B-C1B	-16.15	1.29	1.53
2	A	502	NAD	O4B-C1B	12.52	1.58	1.41
2	C	502	NAD	O4B-C1B	12.32	1.58	1.41
2	C	502	NAD	C2D-C3D	-10.63	1.24	1.53
2	C	501	NAD	C2D-C3D	-10.60	1.24	1.53
2	D	502	NAD	C2D-C3D	-10.58	1.24	1.53
2	B	602	NAD	C2D-C3D	-10.56	1.24	1.53
2	D	501	NAD	C2D-C3D	-10.55	1.24	1.53
2	B	601	NAD	O4B-C1B	10.55	1.55	1.41
2	A	501	NAD	C2D-C3D	-10.54	1.24	1.53
2	B	601	NAD	C2D-C3D	-10.47	1.24	1.53
2	B	602	NAD	O4B-C1B	10.46	1.55	1.41
2	A	502	NAD	C2D-C3D	-10.46	1.24	1.53
2	D	502	NAD	C3B-C4B	-10.27	1.26	1.53
2	B	602	NAD	C3B-C4B	-10.25	1.26	1.53
2	C	502	NAD	C3B-C4B	-10.22	1.26	1.53
2	A	502	NAD	C3B-C4B	-10.20	1.26	1.53
2	C	501	NAD	C3B-C4B	-10.19	1.27	1.53
2	D	501	NAD	C3B-C4B	-10.16	1.27	1.53
2	B	601	NAD	C3B-C4B	-10.15	1.27	1.53
2	A	501	NAD	C3B-C4B	-10.13	1.27	1.53
2	C	501	NAD	O4B-C1B	9.98	1.55	1.41
2	A	501	NAD	O4B-C1B	9.96	1.55	1.41
2	D	501	NAD	O4B-C1B	9.68	1.54	1.41
2	D	502	NAD	O4B-C1B	9.60	1.54	1.41
2	C	502	NAD	C7N-N7N	7.96	1.48	1.33
2	A	502	NAD	C7N-N7N	7.91	1.48	1.33
2	D	502	NAD	O4D-C1D	7.90	1.52	1.41
2	B	601	NAD	C7N-N7N	7.89	1.48	1.33
2	B	602	NAD	C7N-N7N	7.85	1.48	1.33
2	D	502	NAD	C7N-N7N	7.84	1.47	1.33
2	C	501	NAD	C7N-N7N	7.84	1.47	1.33
2	A	501	NAD	C7N-N7N	7.84	1.47	1.33
2	D	501	NAD	C7N-N7N	7.81	1.47	1.33
2	A	502	NAD	O4D-C1D	7.54	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	NAD	O4D-C1D	7.52	1.51	1.41
2	B	601	NAD	O4D-C1D	7.40	1.51	1.41
2	C	501	NAD	O4D-C1D	7.40	1.51	1.41
2	A	501	NAD	O4D-C1D	7.36	1.51	1.41
2	B	602	NAD	O4D-C1D	7.32	1.51	1.41
2	C	502	NAD	O4D-C1D	7.21	1.51	1.41
2	A	502	NAD	O4D-C4D	-6.50	1.30	1.45
2	B	602	NAD	O4D-C4D	-6.50	1.30	1.45
2	B	601	NAD	O4D-C4D	-6.45	1.30	1.45
2	C	502	NAD	O4D-C4D	-6.45	1.30	1.45
2	C	501	NAD	O4D-C4D	-6.38	1.30	1.45
2	D	502	NAD	O4D-C4D	-6.33	1.30	1.45
2	A	501	NAD	O4D-C4D	-6.32	1.30	1.45
2	D	501	NAD	O4D-C4D	-6.26	1.31	1.45
2	A	501	NAD	C3D-C4D	5.21	1.66	1.53
2	D	501	NAD	C3D-C4D	5.19	1.66	1.53
2	A	502	NAD	O4B-C4B	5.16	1.56	1.45
2	C	502	NAD	C3D-C4D	5.14	1.66	1.53
2	A	501	NAD	O4B-C4B	5.12	1.56	1.45
2	D	501	NAD	O4B-C4B	5.12	1.56	1.45
2	D	502	NAD	C3D-C4D	5.12	1.66	1.53
2	B	601	NAD	C3D-C4D	5.11	1.66	1.53
2	B	601	NAD	O4B-C4B	5.10	1.56	1.45
2	C	501	NAD	C3D-C4D	5.10	1.66	1.53
2	B	601	NAD	C2B-C3B	5.09	1.67	1.53
2	D	502	NAD	O4B-C4B	5.09	1.56	1.45
2	A	502	NAD	C3D-C4D	5.09	1.66	1.53
2	B	602	NAD	O4B-C4B	5.08	1.56	1.45
2	B	602	NAD	C3D-C4D	5.07	1.65	1.53
2	C	501	NAD	O4B-C4B	5.04	1.56	1.45
2	C	501	NAD	C2B-C3B	5.03	1.67	1.53
2	C	502	NAD	O4B-C4B	5.03	1.56	1.45
2	B	602	NAD	C2B-C3B	5.03	1.67	1.53
2	A	502	NAD	C2B-C3B	5.01	1.67	1.53
2	C	502	NAD	C2B-C3B	5.00	1.67	1.53
2	A	501	NAD	C2B-C3B	4.98	1.67	1.53
2	D	501	NAD	C2B-C3B	4.96	1.66	1.53
2	D	502	NAD	C2B-C3B	4.84	1.66	1.53
2	A	501	NAD	C3N-C7N	4.18	1.56	1.50
2	D	502	NAD	C3N-C7N	4.12	1.56	1.50
2	C	501	NAD	C3N-C7N	4.08	1.56	1.50
2	D	501	NAD	C3N-C7N	4.06	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	NAD	C3N-C7N	4.05	1.56	1.50
2	D	501	NAD	C2D-C1D	4.01	1.59	1.53
2	C	502	NAD	O2D-C2D	4.00	1.52	1.43
2	B	601	NAD	C2D-C1D	4.00	1.59	1.53
2	B	601	NAD	O2D-C2D	4.00	1.52	1.43
2	B	602	NAD	C2D-C1D	3.99	1.59	1.53
2	A	501	NAD	C2D-C1D	3.99	1.59	1.53
2	A	502	NAD	C2D-C1D	3.97	1.59	1.53
2	A	502	NAD	O2D-C2D	3.97	1.52	1.43
2	C	502	NAD	C2D-C1D	3.95	1.59	1.53
2	C	501	NAD	C6A-N6A	3.94	1.48	1.34
2	A	502	NAD	C3N-C7N	3.94	1.56	1.50
2	C	502	NAD	C6A-N6A	3.92	1.48	1.34
2	B	602	NAD	C3N-C7N	3.92	1.56	1.50
2	D	502	NAD	C6A-N6A	3.91	1.48	1.34
2	B	602	NAD	O2D-C2D	3.90	1.52	1.43
2	A	502	NAD	C6A-N6A	3.89	1.48	1.34
2	B	602	NAD	C6A-N6A	3.88	1.48	1.34
2	B	601	NAD	C6A-N6A	3.88	1.48	1.34
2	D	502	NAD	O2D-C2D	3.88	1.52	1.43
2	D	501	NAD	C6A-N6A	3.88	1.48	1.34
2	A	501	NAD	C6A-N6A	3.87	1.48	1.34
2	C	502	NAD	C3N-C7N	3.86	1.56	1.50
2	C	501	NAD	O2D-C2D	3.84	1.52	1.43
2	A	501	NAD	O2D-C2D	3.82	1.52	1.43
2	C	501	NAD	C2D-C1D	3.79	1.59	1.53
2	D	501	NAD	O2D-C2D	3.74	1.51	1.43
2	D	502	NAD	C2D-C1D	3.49	1.59	1.53
2	A	502	NAD	O7N-C7N	-3.21	1.18	1.24
2	C	502	NAD	O7N-C7N	-3.20	1.18	1.24
2	B	601	NAD	O7N-C7N	-3.19	1.18	1.24
2	B	602	NAD	O7N-C7N	-3.13	1.18	1.24
2	C	501	NAD	O7N-C7N	-3.13	1.18	1.24
2	A	501	NAD	O7N-C7N	-3.12	1.18	1.24
2	D	501	NAD	O7N-C7N	-3.10	1.18	1.24
2	D	502	NAD	O7N-C7N	-3.08	1.18	1.24
2	B	601	NAD	C2A-N3A	2.86	1.36	1.32
2	A	502	NAD	C2A-N3A	2.83	1.36	1.32
2	A	502	NAD	O3D-C3D	2.82	1.49	1.43
2	B	601	NAD	O3D-C3D	2.81	1.49	1.43
2	D	502	NAD	O3D-C3D	2.80	1.49	1.43
2	C	501	NAD	C2A-N3A	2.79	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NAD	C2A-N3A	2.78	1.36	1.32
2	B	602	NAD	O3D-C3D	2.77	1.49	1.43
2	B	602	NAD	C2A-N3A	2.76	1.36	1.32
2	C	502	NAD	O3D-C3D	2.75	1.49	1.43
2	C	501	NAD	O3D-C3D	2.72	1.49	1.43
2	D	501	NAD	O3D-C3D	2.71	1.49	1.43
2	D	501	NAD	C2A-N3A	2.69	1.36	1.32
2	D	502	NAD	C2A-N3A	2.68	1.36	1.32
2	A	501	NAD	O3D-C3D	2.68	1.49	1.43
2	C	502	NAD	C2A-N3A	2.61	1.36	1.32
2	B	602	NAD	C5A-C4A	-2.47	1.34	1.40
2	C	501	NAD	C5B-C4B	2.47	1.59	1.51
2	D	502	NAD	C5A-C4A	-2.47	1.34	1.40
2	D	501	NAD	C5B-C4B	2.46	1.59	1.51
2	A	501	NAD	C5B-C4B	2.46	1.59	1.51
2	D	501	NAD	C5A-C4A	-2.45	1.34	1.40
2	A	501	NAD	C5A-C4A	-2.43	1.34	1.40
2	C	502	NAD	C5A-C4A	-2.43	1.34	1.40
2	B	601	NAD	C5A-C4A	-2.42	1.34	1.40
2	A	502	NAD	C5A-C4A	-2.42	1.34	1.40
2	D	502	NAD	C5B-C4B	2.40	1.59	1.51
2	B	602	NAD	C5B-C4B	2.36	1.59	1.51
2	C	501	NAD	C5A-C4A	-2.35	1.34	1.40
2	A	502	NAD	C5B-C4B	2.35	1.58	1.51
2	C	502	NAD	C5B-C4B	2.34	1.58	1.51
2	B	601	NAD	C5B-C4B	2.34	1.58	1.51

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	502	NAD	C5A-C6A-N6A	7.17	131.25	120.35
2	C	502	NAD	C5A-C6A-N6A	7.16	131.23	120.35
2	D	501	NAD	C5A-C6A-N6A	7.13	131.19	120.35
2	C	501	NAD	C5A-C6A-N6A	7.05	131.07	120.35
2	A	501	NAD	C5A-C6A-N6A	6.78	130.66	120.35
2	B	602	NAD	C5A-C6A-N6A	6.78	130.65	120.35
2	A	502	NAD	C5A-C6A-N6A	6.75	130.61	120.35
2	B	601	NAD	C5A-C6A-N6A	6.68	130.50	120.35
2	B	601	NAD	N3A-C2A-N1A	-5.41	120.22	128.68
2	A	501	NAD	N3A-C2A-N1A	-5.39	120.26	128.68
2	C	502	NAD	N3A-C2A-N1A	-5.36	120.30	128.68
2	B	602	NAD	N3A-C2A-N1A	-5.35	120.32	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	NAD	N3A-C2A-N1A	-5.33	120.35	128.68
2	D	502	NAD	N3A-C2A-N1A	-5.28	120.43	128.68
2	D	501	NAD	N3A-C2A-N1A	-5.27	120.45	128.68
2	C	501	NAD	N3A-C2A-N1A	-5.26	120.46	128.68
2	D	501	NAD	N6A-C6A-N1A	-4.51	109.22	118.57
2	C	502	NAD	N6A-C6A-N1A	-4.47	109.29	118.57
2	A	501	NAD	N6A-C6A-N1A	-4.45	109.33	118.57
2	C	501	NAD	N6A-C6A-N1A	-4.44	109.36	118.57
2	D	502	NAD	N6A-C6A-N1A	-4.41	109.43	118.57
2	B	602	NAD	N6A-C6A-N1A	-4.40	109.45	118.57
2	A	502	NAD	N6A-C6A-N1A	-4.36	109.52	118.57
2	B	601	NAD	N6A-C6A-N1A	-4.34	109.56	118.57
2	A	501	NAD	C1B-N9A-C4A	3.26	132.36	126.64
2	C	502	NAD	C3B-C2B-C1B	3.21	105.81	100.98
2	C	501	NAD	C1B-N9A-C4A	3.08	132.04	126.64
2	A	502	NAD	C3B-C2B-C1B	3.07	105.59	100.98
2	A	501	NAD	PN-O3-PA	-2.88	122.94	132.83
2	D	502	NAD	C1B-N9A-C4A	2.85	131.64	126.64
2	C	501	NAD	PN-O3-PA	-2.70	123.57	132.83
2	B	602	NAD	C1B-N9A-C4A	2.63	131.26	126.64
2	A	502	NAD	C1B-N9A-C4A	2.59	131.19	126.64
2	D	501	NAD	PN-O3-PA	-2.59	123.94	132.83
2	D	502	NAD	O4B-C1B-C2B	-2.55	103.20	106.93
2	B	601	NAD	PN-O3-PA	-2.54	124.11	132.83
2	B	601	NAD	C1B-N9A-C4A	2.53	131.08	126.64
2	C	502	NAD	C3D-C2D-C1D	2.52	104.77	100.98
2	B	602	NAD	PN-O3-PA	-2.51	124.21	132.83
2	A	502	NAD	C6N-N1N-C2N	-2.51	119.69	121.97
2	D	502	NAD	C3N-C7N-N7N	2.51	120.76	117.75
2	C	502	NAD	C1B-N9A-C4A	2.48	131.00	126.64
2	B	601	NAD	C6N-N1N-C2N	-2.44	119.75	121.97
2	B	602	NAD	C6N-N1N-C2N	-2.36	119.82	121.97
2	D	502	NAD	PN-O3-PA	-2.34	124.79	132.83
2	A	502	NAD	PN-O3-PA	-2.32	124.86	132.83
2	C	502	NAD	C6N-N1N-C2N	-2.29	119.88	121.97
2	D	501	NAD	C1B-N9A-C4A	2.26	130.62	126.64
2	B	602	NAD	C3D-C2D-C1D	2.26	104.38	100.98
2	A	501	NAD	C3N-C7N-N7N	2.26	120.46	117.75
2	B	601	NAD	O4D-C1D-C2D	-2.20	103.71	106.93
2	B	602	NAD	O4D-C1D-C2D	-2.20	103.71	106.93
2	A	502	NAD	O4D-C1D-C2D	-2.18	103.74	106.93
2	C	501	NAD	C3B-C2B-C1B	2.16	104.23	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	NAD	C3D-C2D-C1D	2.14	104.21	100.98
2	A	501	NAD	C3B-C2B-C1B	2.14	104.19	100.98
2	D	501	NAD	O4D-C1D-C2D	-2.14	103.80	106.93
2	D	502	NAD	C2B-C3B-C4B	2.12	106.77	102.64
2	A	501	NAD	C2B-C3B-C4B	2.11	106.75	102.64
2	D	501	NAD	C3N-C7N-N7N	2.11	120.29	117.75
2	A	502	NAD	C2D-C3D-C4D	2.11	106.73	102.64
2	B	602	NAD	C2D-C3D-C4D	2.10	106.73	102.64
2	B	601	NAD	C3D-C2D-C1D	2.10	104.14	100.98
2	B	601	NAD	C3B-C2B-C1B	2.09	104.13	100.98
2	D	502	NAD	C2D-C3D-C4D	2.08	106.69	102.64
2	A	501	NAD	O4B-C1B-C2B	-2.08	103.89	106.93
2	A	501	NAD	O4D-C1D-C2D	-2.07	103.91	106.93
2	C	502	NAD	C2D-C3D-C4D	2.06	106.65	102.64
2	C	502	NAD	PN-O3-PA	-2.05	125.80	132.83
2	D	502	NAD	O4D-C1D-C2D	-2.04	103.95	106.93
2	D	502	NAD	O7N-C7N-N7N	-2.03	119.70	122.58
2	B	601	NAD	C2D-C3D-C4D	2.01	106.54	102.64

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAD	PN-O3-PA-O5B
2	A	502	NAD	C5D-O5D-PN-O1N
2	A	502	NAD	O4D-C1D-N1N-C6N
2	B	601	NAD	C5D-O5D-PN-O3
2	B	601	NAD	C5D-O5D-PN-O1N
2	B	601	NAD	O4D-C1D-N1N-C6N
2	B	602	NAD	C5D-O5D-PN-O1N
2	C	501	NAD	PN-O3-PA-O5B
2	C	502	NAD	PA-O3-PN-O5D
2	C	502	NAD	C5D-O5D-PN-O1N
2	C	502	NAD	O4D-C1D-N1N-C6N
2	D	502	NAD	O4D-C4D-C5D-O5D
2	D	502	NAD	C3D-C4D-C5D-O5D
2	A	502	NAD	PA-O3-PN-O5D
2	B	601	NAD	PA-O3-PN-O5D
2	D	502	NAD	PN-O3-PA-O5B
2	A	501	NAD	O4D-C4D-C5D-O5D
2	A	501	NAD	C4N-C3N-C7N-N7N
2	A	501	NAD	C4N-C3N-C7N-O7N

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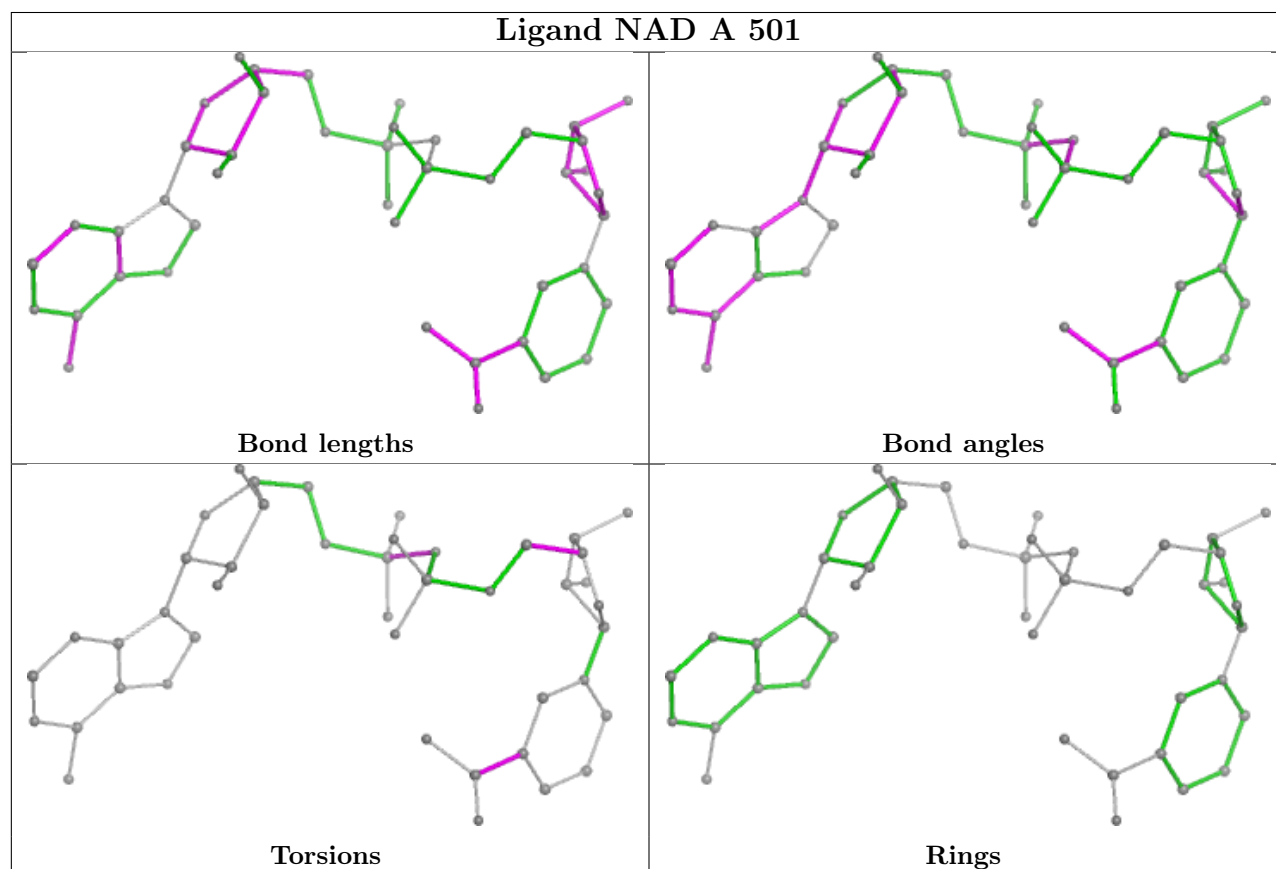
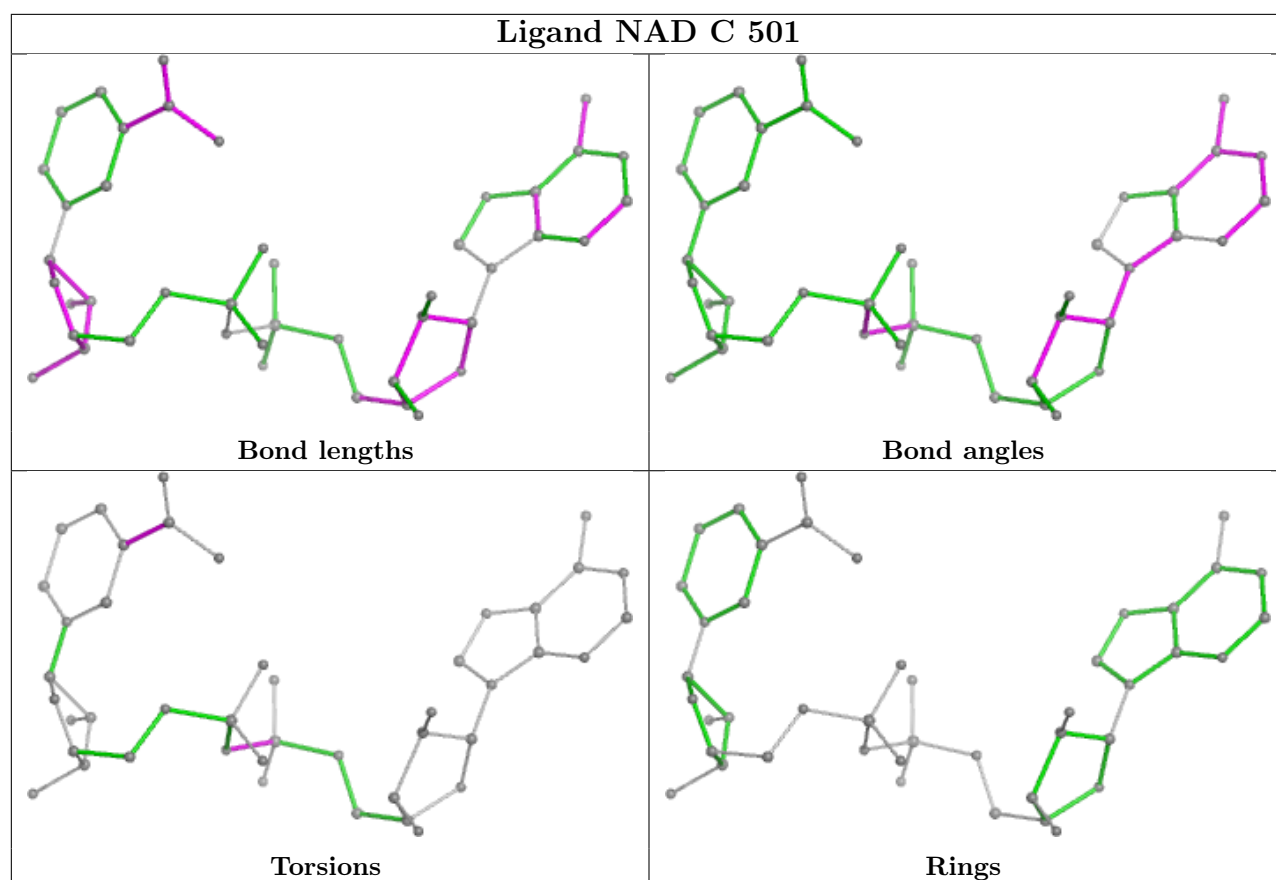
Mol	Chain	Res	Type	Atoms
2	C	501	NAD	C4N-C3N-C7N-N7N
2	C	501	NAD	C4N-C3N-C7N-O7N
2	A	502	NAD	C5D-O5D-PN-O3
2	B	602	NAD	C5D-O5D-PN-O3
2	C	502	NAD	C5D-O5D-PN-O3
2	D	501	NAD	C4N-C3N-C7N-O7N
2	D	501	NAD	C4N-C3N-C7N-N7N
2	C	502	NAD	PN-O3-PA-O1A
2	C	502	NAD	PN-O3-PA-O2A
2	A	501	NAD	C3D-C4D-C5D-O5D

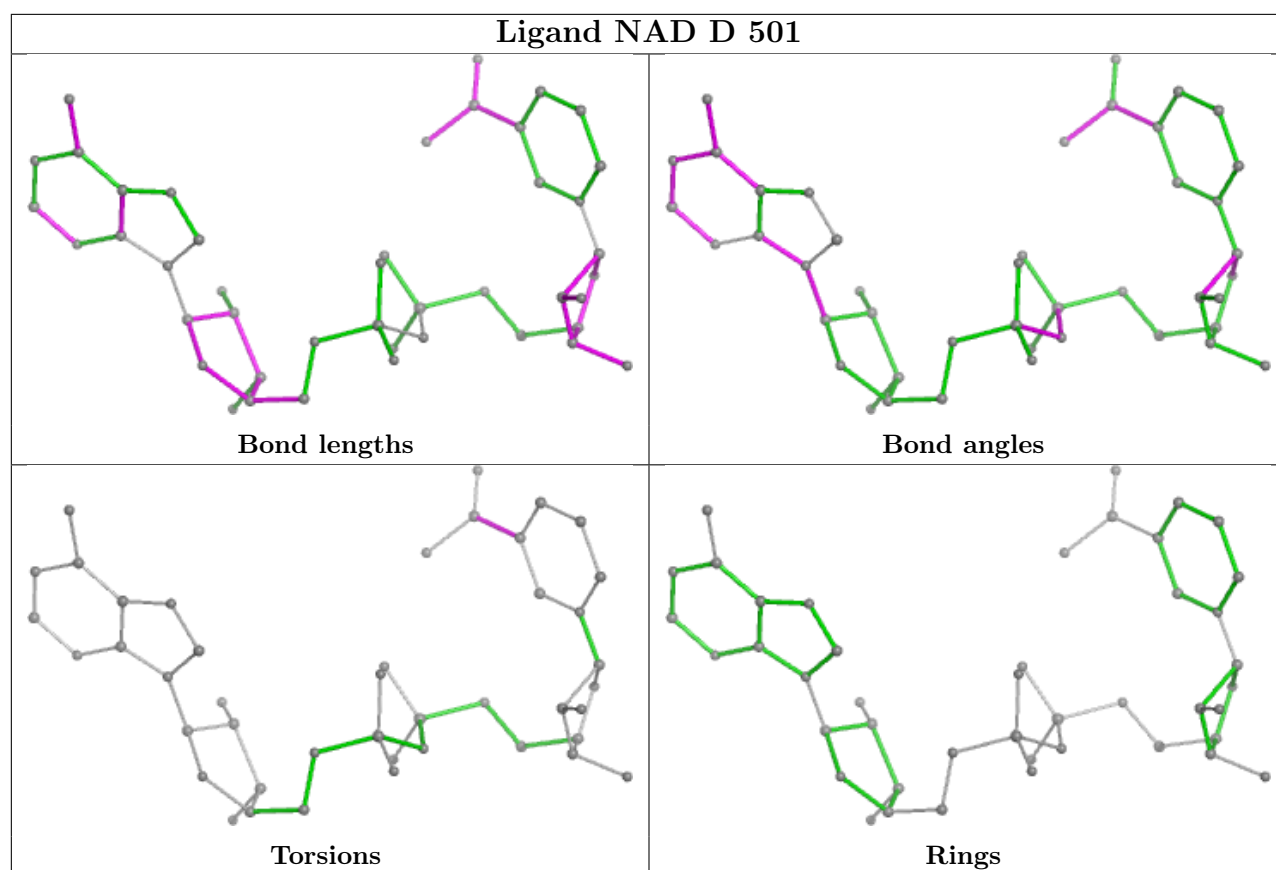
There are no ring outliers.

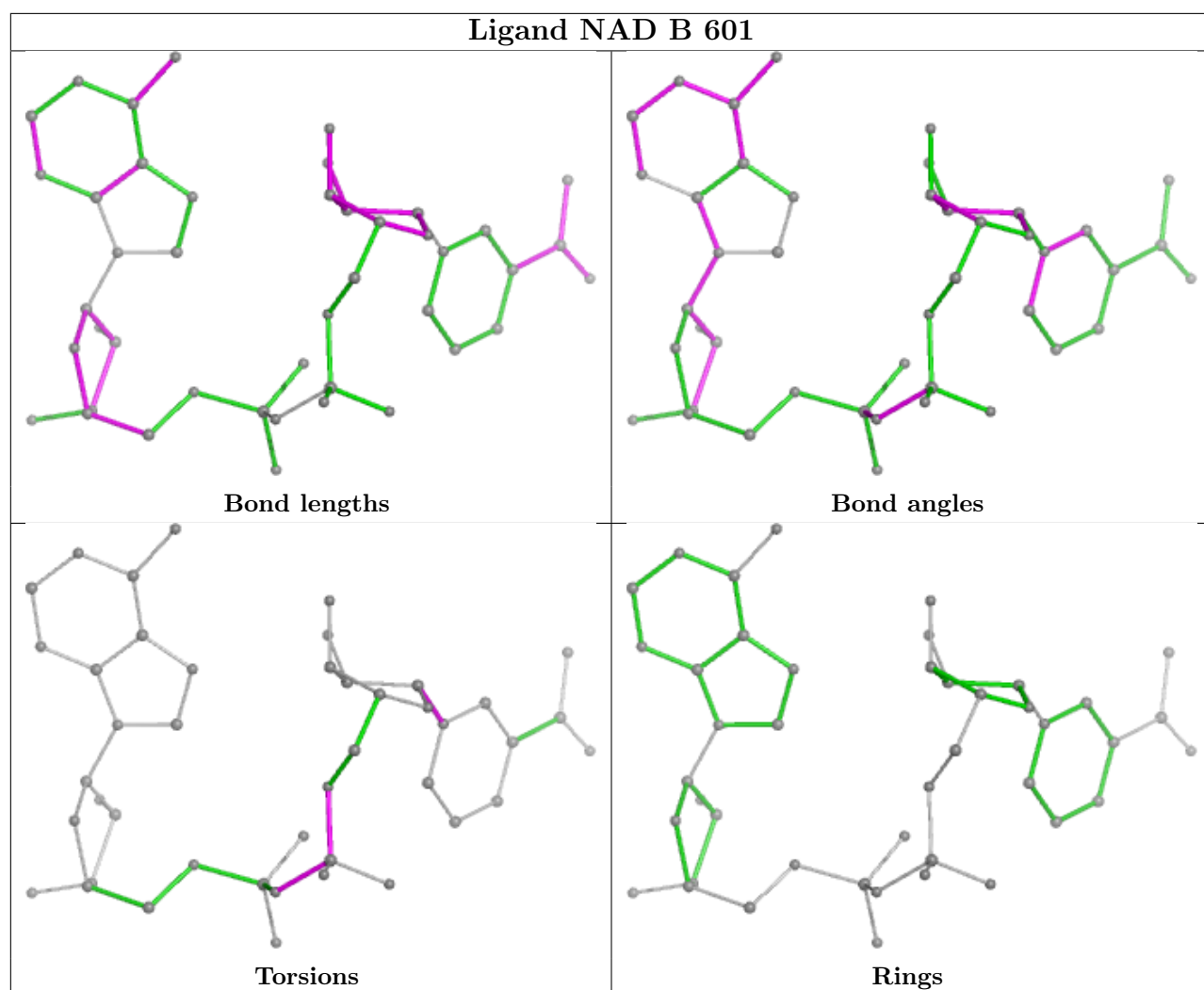
7 monomers are involved in 22 short contacts:

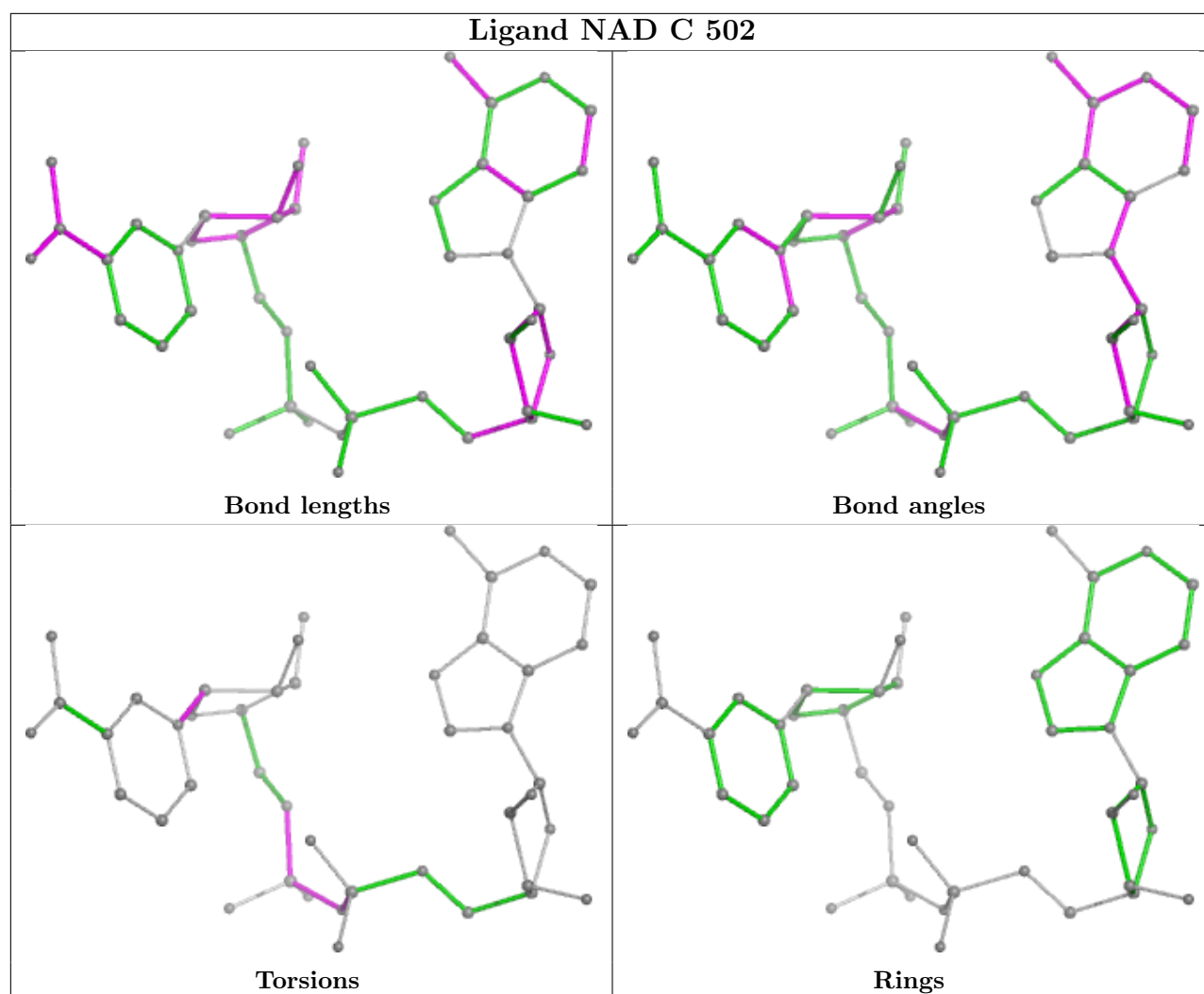
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	NAD	3	0
2	A	501	NAD	3	0
2	D	501	NAD	6	0
2	C	502	NAD	1	0
2	D	502	NAD	7	0
2	A	502	NAD	3	0
2	B	602	NAD	1	0

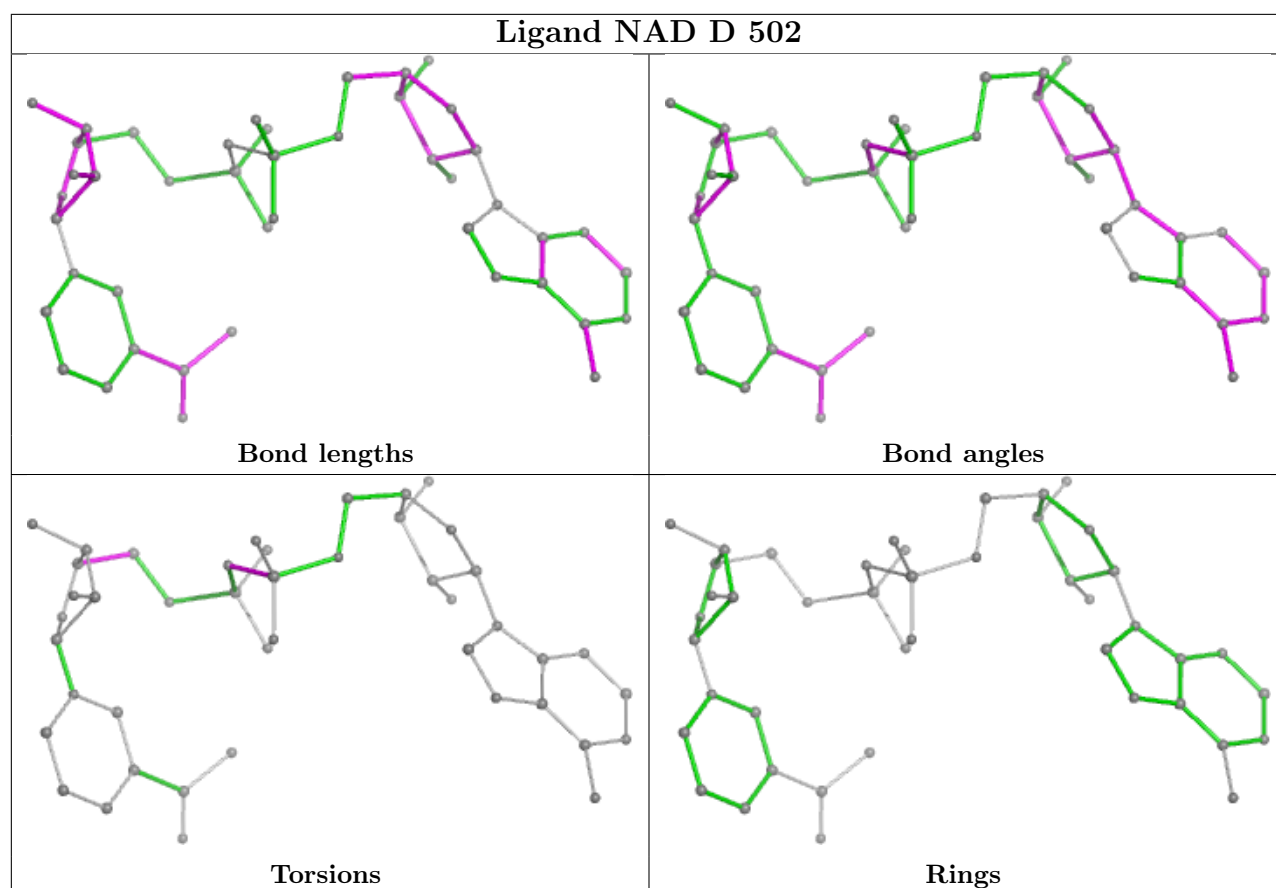
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

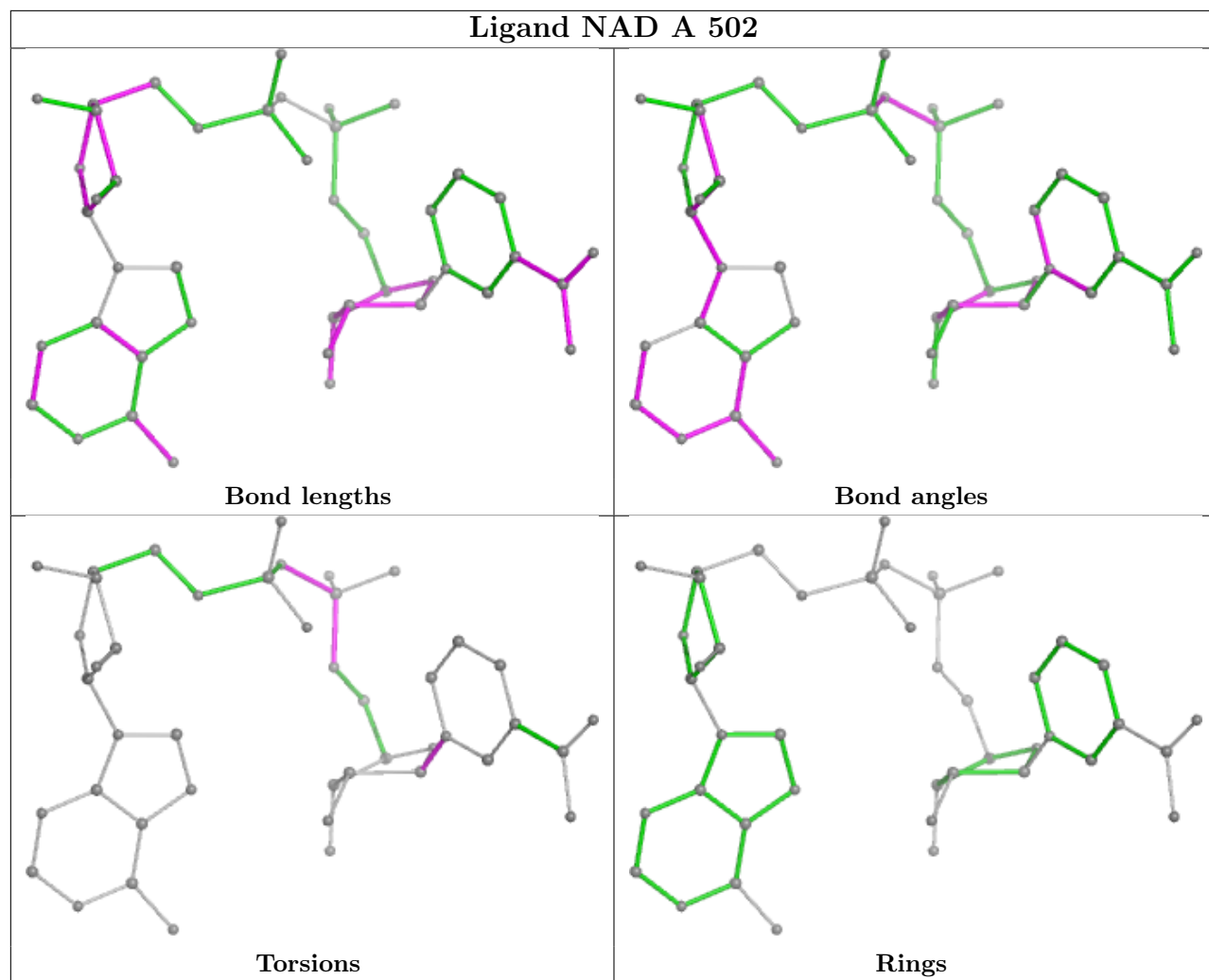


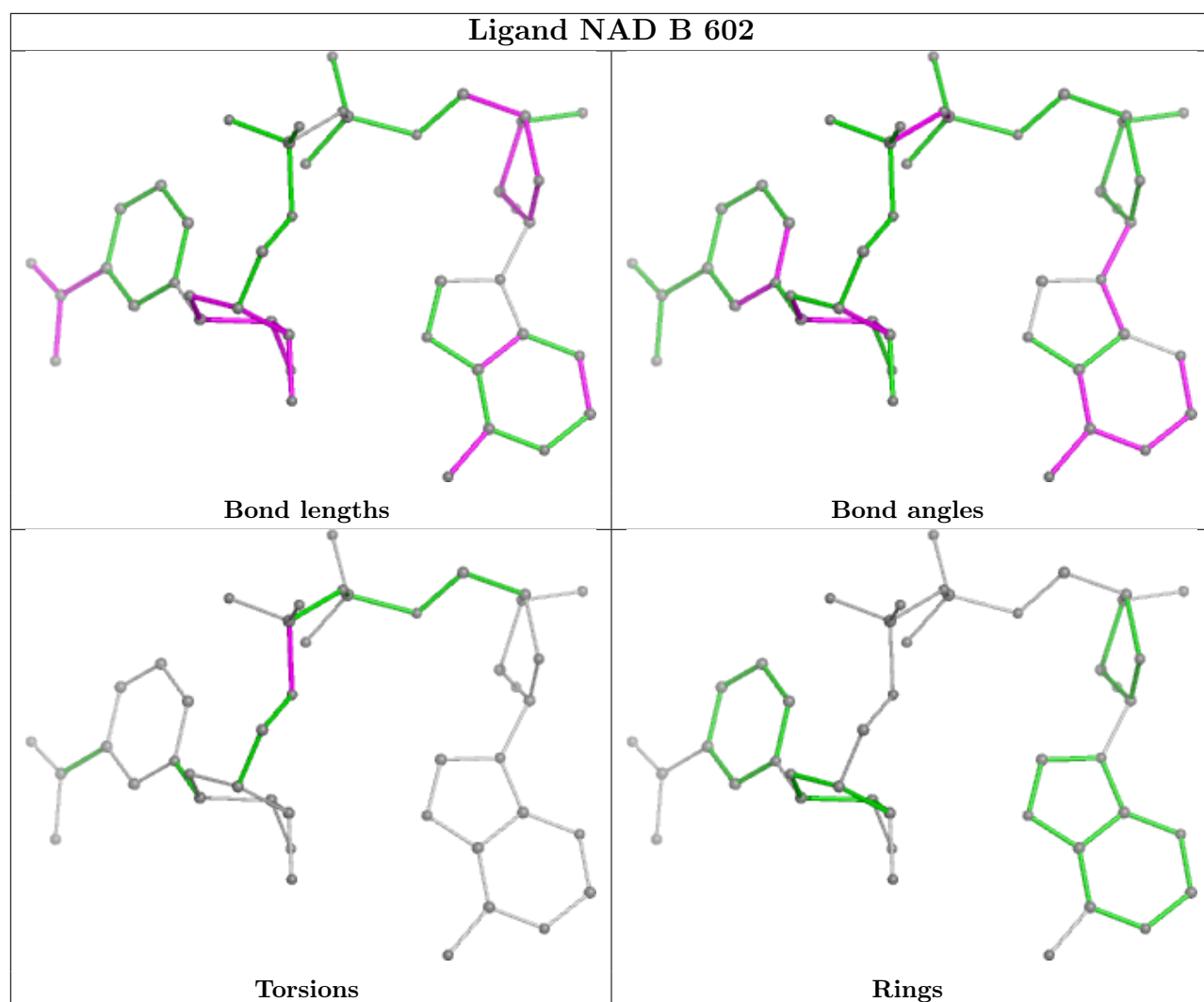












5.7 Other polymers [i](#)

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	457/489 (93%)	2.76	321 (70%) 0 0	19, 35, 56, 82	3 (0%)
1	B	457/489 (93%)	2.89	327 (71%) 0 0	17, 39, 65, 91	1 (0%)
1	C	454/489 (92%)	2.94	338 (74%) 0 0	22, 37, 61, 98	2 (0%)
1	D	461/489 (94%)	3.09	350 (75%) 0 0	25, 41, 65, 97	0
All	All	1829/1956 (93%)	2.92	1336 (73%) 0 0	17, 38, 62, 98	6 (0%)

All (1336) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	127	GLY	11.7
1	B	138	PHE	11.5
1	C	424	SER	11.1
1	D	427	ASP	10.8
1	D	399	GLY	9.5
1	A	136	SER	9.4
1	B	136	SER	9.3
1	D	136	SER	9.3
1	D	424	SER	9.2
1	D	412	ALA	8.8
1	C	10	SER	8.6
1	D	137	PHE	8.4
1	D	425	LEU	8.1
1	B	137	PHE	8.0
1	D	140	GLY	7.9
1	D	343	TYR	7.9
1	D	396	GLY	7.8
1	B	141	ILE	7.7
1	D	428	ILE	7.6
1	C	229	SER	7.5
1	C	104	ALA	7.4

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Mol	Chain	Res	Type	RSRZ
1	C	402	VAL	7.4
1	C	419	LEU	7.3
1	A	189	PHE	7.3
1	D	104	ALA	7.3
1	C	221	HIS	7.2
1	D	138	PHE	7.1
1	D	400	PHE	7.1
1	D	229	SER	7.1
1	C	378	TYR	7.1
1	B	174	GLY	7.0
1	A	-1	GLY	6.9
1	B	379	PHE	6.9
1	A	425	LEU	6.9
1	C	412	ALA	6.8
1	A	229	SER	6.8
1	A	408	SER	6.8
1	D	317	THR	6.8
1	D	350	GLY	6.8
1	D	429	HIS	6.7
1	A	415	TYR	6.7
1	D	134	ILE	6.6
1	B	424	SER	6.6
1	C	231	VAL	6.5
1	A	104	ALA	6.5
1	B	423	SER	6.5
1	D	10	SER	6.5
1	B	352	GLN	6.4
1	A	378	TYR	6.4
1	B	57	ILE	6.4
1	D	402	VAL	6.3
1	D	438	VAL	6.3
1	C	140	GLY	6.3
1	A	127	GLY	6.3
1	D	344	ASP	6.3
1	A	87	GLY	6.2
1	C	230	LEU	6.2
1	C	139	GLU	6.2
1	A	192	ALA	6.1
1	B	348	THR	6.1
1	D	426	ALA	6.0
1	A	424	SER	6.0
1	A	118	ASN	6.0

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Mol	Chain	Res	Type	RSRZ
1	D	9	TRP	6.0
1	A	142	GLU	6.0
1	A	414	ALA	5.9
1	C	134	ILE	5.9
1	B	316	PHE	5.9
1	C	438	VAL	5.9
1	D	198	GLY	5.9
1	D	143	PRO	5.9
1	D	423	SER	5.9
1	C	282	VAL	5.8
1	D	440	VAL	5.8
1	C	218	LEU	5.8
1	A	-2	ALA	5.8
1	A	174	GLY	5.8
1	B	229	SER	5.8
1	D	409	SER	5.8
1	C	431	ILE	5.8
1	A	342	ASP	5.7
1	B	206	VAL	5.7
1	D	193	VAL	5.7
1	D	422	HIS	5.7
1	A	409	SER	5.7
1	B	140	GLY	5.7
1	B	311	VAL	5.7
1	D	98	TYR	5.6
1	C	141	ILE	5.6
1	C	0	THR	5.6
1	D	189	PHE	5.6
1	A	396	GLY	5.6
1	B	135	LYS	5.6
1	C	137	PHE	5.6
1	D	430	LYS	5.6
1	C	404	ALA	5.5
1	D	139	GLU	5.5
1	B	363	PHE	5.5
1	C	314	LEU	5.5
1	A	295	LEU	5.5
1	D	414	ALA	5.5
1	C	9	TRP	5.4
1	A	298	ILE	5.4
1	B	438	VAL	5.4
1	C	285[A]	ARG	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	396	GLY	5.4
1	D	165	TRP	5.4
1	C	74	ARG	5.3
1	C	170	CYS	5.3
1	C	348	THR	5.3
1	B	189	PHE	5.3
1	D	230	LEU	5.3
1	D	159	TRP	5.3
1	C	151	LEU	5.3
1	D	340	LEU	5.3
1	C	390	ASN	5.3
1	C	86	THR	5.3
1	D	349	ALA	5.3
1	B	350	GLY	5.3
1	C	146	CYS	5.3
1	C	444	LEU	5.3
1	C	305	ASN	5.2
1	A	8	GLY	5.2
1	B	230	LEU	5.2
1	D	332	LEU	5.2
1	A	397	ASN	5.2
1	B	233	ALA	5.2
1	D	421	PHE	5.1
1	B	91	VAL	5.1
1	C	354	SER	5.1
1	D	310	PHE	5.1
1	B	102	ASN	5.1
1	B	0	THR	5.1
1	C	227	GLY	5.1
1	D	-2	ALA	5.1
1	B	378	TYR	5.1
1	C	410	ASP	5.1
1	A	447	ARG	5.1
1	C	409	SER	5.1
1	D	387	GLY	5.1
1	C	343	TYR	5.1
1	C	344	ASP	5.1
1	A	70	ALA	5.0
1	C	474	ASP	5.0
1	D	432	LEU	5.0
1	A	423	SER	5.0
1	D	339	HIS	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	9	TRP	5.0
1	A	86	THR	5.0
1	D	161	LEU	5.0
1	B	431	ILE	5.0
1	C	411	GLN	5.0
1	B	227	GLY	5.0
1	C	75	ASP	5.0
1	A	141	ILE	5.0
1	B	120	GLY	4.9
1	B	165	TRP	4.9
1	C	396	GLY	4.9
1	D	248	GLY	4.9
1	B	208	VAL	4.9
1	B	345	LEU	4.9
1	C	232	VAL	4.9
1	C	341	ILE	4.9
1	B	130	ARG	4.9
1	B	359	PRO	4.9
1	A	211	THR	4.9
1	C	228	GLU	4.9
1	D	410	ASP	4.9
1	C	430	LYS	4.9
1	B	76	GLY	4.9
1	B	317	THR	4.9
1	C	320	TYR	4.8
1	D	244	GLY	4.8
1	B	55	ASP	4.8
1	D	102	ASN	4.8
1	B	387	GLY	4.8
1	B	405	TYR	4.8
1	A	75	ASP	4.8
1	B	315	VAL	4.8
1	C	339	HIS	4.8
1	A	244	GLY	4.8
1	D	330	PHE	4.8
1	B	310	PHE	4.8
1	D	218	LEU	4.8
1	A	242	ALA	4.7
1	A	88	GLY	4.7
1	B	51	THR	4.7
1	D	126	LEU	4.7
1	D	378	TYR	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	422	HIS	4.7
1	B	154	GLY	4.7
1	D	363	PHE	4.7
1	B	228	GLU	4.7
1	B	380	LEU	4.7
1	A	410	ASP	4.7
1	B	353	TYR	4.7
1	D	215	TYR	4.7
1	D	296	ASP	4.7
1	D	368	ARG	4.7
1	A	33	LEU	4.7
1	A	117	ALA	4.6
1	D	357	ALA	4.6
1	C	102	ASN	4.6
1	C	179	VAL	4.6
1	D	448	VAL	4.6
1	D	341	ILE	4.6
1	A	108	LEU	4.6
1	B	340	LEU	4.6
1	C	295	LEU	4.6
1	C	437	THR	4.6
1	D	191	ASP	4.6
1	C	172	ALA	4.6
1	C	54	VAL	4.6
1	D	135	LYS	4.6
1	A	143	PRO	4.6
1	A	152	GLU	4.6
1	D	142	GLU	4.6
1	D	418	LEU	4.6
1	C	92	ARG	4.6
1	A	288	TYR	4.6
1	B	126	LEU	4.6
1	C	313	THR	4.6
1	D	0	THR	4.6
1	D	86	THR	4.6
1	B	129	SER	4.6
1	C	135	LYS	4.6
1	C	136	SER	4.6
1	D	354	SER	4.6
1	B	341	ILE	4.6
1	C	350	GLY	4.5
1	A	135	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	131	LEU	4.5
1	B	368	ARG	4.5
1	A	129	SER	4.5
1	D	115	ALA	4.5
1	B	289	ASN	4.5
1	A	228	GLU	4.5
1	C	76	GLY	4.5
1	C	103	LEU	4.5
1	C	423	SER	4.5
1	A	240	PRO	4.5
1	A	140	GLY	4.5
1	B	75	ASP	4.5
1	D	158	SER	4.5
1	D	337	GLY	4.4
1	A	444	LEU	4.4
1	B	123	LEU	4.4
1	B	178	PHE	4.4
1	C	403	LYS	4.4
1	D	120	GLY	4.4
1	D	374	GLY	4.4
1	B	437	THR	4.4
1	D	150	TRP	4.4
1	B	103	LEU	4.4
1	D	366	ARG	4.4
1	A	11	VAL	4.4
1	A	208	VAL	4.4
1	A	413	LEU	4.4
1	B	211	THR	4.3
1	B	121	SER	4.3
1	D	285	ARG	4.3
1	C	421	PHE	4.3
1	C	258	ILE	4.3
1	D	185	ILE	4.3
1	A	51	THR	4.3
1	C	34	ASP	4.3
1	C	51	THR	4.3
1	C	366	ARG	4.3
1	B	172	ALA	4.3
1	B	182	GLY	4.3
1	B	147	VAL	4.3
1	B	440	VAL	4.3
1	C	448	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	169	ASP	4.3
1	B	346	TYR	4.3
1	C	374	GLY	4.3
1	D	331	ARG	4.3
1	B	415	TYR	4.3
1	B	287	SER	4.3
1	A	330	PHE	4.3
1	C	87	GLY	4.3
1	D	404	ALA	4.3
1	A	231	VAL	4.3
1	B	179	VAL	4.3
1	D	52	VAL	4.3
1	B	397	ASN	4.2
1	D	411	GLN	4.2
1	C	389	ILE	4.2
1	A	230	LEU	4.2
1	A	411	GLN	4.2
1	C	238	THR	4.2
1	D	391	THR	4.2
1	A	10	SER	4.2
1	B	442	ILE	4.2
1	D	112	ILE	4.2
1	A	305	ASN	4.2
1	D	469	THR	4.2
1	B	240	PRO	4.2
1	D	85	SER	4.2
1	D	23	TRP	4.2
1	D	431	ILE	4.2
1	B	422	HIS	4.2
1	B	9	TRP	4.1
1	D	91	VAL	4.1
1	D	232	VAL	4.1
1	A	103	LEU	4.1
1	D	334	ASP	4.1
1	C	351	PRO	4.1
1	D	351	PRO	4.1
1	A	361	GLY	4.1
1	A	81	CYS	4.1
1	C	189	PHE	4.1
1	A	147	VAL	4.1
1	C	33	LEU	4.1
1	A	102	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	138	PHE	4.1
1	C	329	ILE	4.1
1	B	448	VAL	4.1
1	A	167	ASP	4.1
1	B	297	ASN	4.1
1	C	171	THR	4.1
1	C	355	GLU	4.1
1	C	85	SER	4.1
1	B	433	HIS	4.1
1	B	313	THR	4.1
1	D	-1	GLY	4.0
1	D	408	SER	4.0
1	B	170	CYS	4.0
1	C	131	LEU	4.0
1	C	291	LEU	4.0
1	C	193	VAL	4.0
1	C	364	VAL	4.0
1	D	205	VAL	4.0
1	A	120	GLY	4.0
1	D	243	PHE	4.0
1	B	373	ARG	4.0
1	C	417	ARG	4.0
1	A	422	HIS	4.0
1	C	98	TYR	4.0
1	C	415	TYR	4.0
1	D	168	TYR	4.0
1	B	351	PRO	4.0
1	D	225	ASP	4.0
1	C	469	THR	4.0
1	D	437	THR	4.0
1	A	76	GLY	4.0
1	A	250	SER	4.0
1	A	284	SER	4.0
1	B	104	ALA	4.0
1	B	324	ARG	4.0
1	A	246	LEU	4.0
1	A	419	LEU	4.0
1	D	57	ILE	4.0
1	B	176	TYR	4.0
1	B	193	VAL	4.0
1	A	224	GLY	4.0
1	B	284	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	398	LEU	4.0
1	A	442	ILE	4.0
1	D	389	ILE	4.0
1	A	179	VAL	3.9
1	C	118	ASN	3.9
1	C	299	THR	3.9
1	C	284	SER	3.9
1	D	324	ARG	3.9
1	D	58	ALA	3.9
1	A	137	PHE	3.9
1	C	363	PHE	3.9
1	D	131	LEU	3.9
1	A	351	PRO	3.9
1	B	54	VAL	3.9
1	D	348	THR	3.9
1	B	275	TRP	3.9
1	D	221	HIS	3.9
1	D	471	LYS	3.9
1	C	333	ILE	3.9
1	C	342	ASP	3.9
1	A	401	ARG	3.9
1	B	285[A]	ARG	3.9
1	A	465	SER	3.9
1	C	312	LYS	3.9
1	B	298	ILE	3.9
1	B	435	ASN	3.9
1	D	130	ARG	3.9
1	D	315	VAL	3.9
1	D	342	ASP	3.9
1	B	360	ALA	3.9
1	C	298	ILE	3.8
1	C	401	ARG	3.8
1	D	92	ARG	3.8
1	B	391	THR	3.8
1	B	325	TYR	3.8
1	D	433	HIS	3.8
1	B	117	ALA	3.8
1	A	218	LEU	3.8
1	D	217	LEU	3.8
1	C	243	PHE	3.8
1	B	118	ASN	3.8
1	C	435	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	101	ASN	3.8
1	D	328	ILE	3.8
1	A	169	ASP	3.8
1	B	53	THR	3.8
1	B	197	THR	3.8
1	B	150	TRP	3.8
1	D	347	LEU	3.8
1	A	247	PRO	3.8
1	D	316	PHE	3.8
1	B	101	ASN	3.8
1	B	194	ASN	3.8
1	D	435	ASN	3.8
1	A	403	LYS	3.8
1	C	399	GLY	3.8
1	C	223	GLU	3.8
1	C	408	SER	3.8
1	C	416	TYR	3.8
1	B	462	ALA	3.8
1	D	172	ALA	3.8
1	A	123	LEU	3.8
1	B	398	LEU	3.8
1	B	419	LEU	3.8
1	D	444	LEU	3.8
1	D	338	ASN	3.8
1	A	184	LYS	3.8
1	D	141	ILE	3.8
1	C	405	TYR	3.7
1	B	414	ALA	3.7
1	A	390	ASN	3.7
1	B	338	ASN	3.7
1	B	390	ASN	3.7
1	D	329	ILE	3.7
1	A	204	GLY	3.7
1	D	59	ARG	3.7
1	B	196	TYR	3.7
1	B	343	TYR	3.7
1	C	346	TYR	3.7
1	A	249	LEU	3.7
1	D	295	LEU	3.7
1	D	314	LEU	3.7
1	B	204	GLY	3.7
1	C	23	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	337	GLY	3.7
1	A	451	THR	3.7
1	B	409	SER	3.7
1	A	114	LEU	3.7
1	B	358	LEU	3.7
1	C	89	PRO	3.7
1	C	214	ASN	3.7
1	A	154	GLY	3.7
1	A	421	PHE	3.7
1	C	373	ARG	3.7
1	B	86	THR	3.7
1	C	377	THR	3.7
1	D	54	VAL	3.7
1	D	206	VAL	3.7
1	D	236	THR	3.7
1	D	415	TYR	3.7
1	A	151[A]	LEU	3.7
1	A	432	LEU	3.7
1	B	370	LEU	3.7
1	D	406	PRO	3.7
1	D	420	ASP	3.7
1	A	329	ILE	3.7
1	A	100	LYS	3.6
1	B	432	LEU	3.6
1	D	8	GLY	3.6
1	B	421	PHE	3.6
1	C	90	ILE	3.6
1	A	348	THR	3.6
1	C	150	TRP	3.6
1	B	58	ALA	3.6
1	B	332	LEU	3.6
1	C	392	PRO	3.6
1	D	345	LEU	3.6
1	A	243	PHE	3.6
1	A	363	PHE	3.6
1	D	90	ILE	3.6
1	B	216	SER	3.6
1	B	392	PRO	3.6
1	D	434	PRO	3.6
1	A	73	LEU	3.6
1	A	196	TYR	3.6
1	D	106	CYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	410	ASP	3.6
1	A	302	THR	3.6
1	D	51	THR	3.6
1	B	339	HIS	3.6
1	B	364	VAL	3.6
1	B	139	GLU	3.6
1	B	10	SER	3.6
1	C	130	ARG	3.6
1	D	15	ASN	3.5
1	D	257	GLY	3.5
1	B	330	PHE	3.5
1	A	171	THR	3.5
1	B	452	VAL	3.5
1	D	373	ARG	3.5
1	C	126	LEU	3.5
1	C	117	ALA	3.5
1	C	182	GLY	3.5
1	A	186	ASP	3.5
1	A	191	ASP	3.5
1	B	146	CYS	3.5
1	B	464	ILE	3.5
1	D	442	ILE	3.5
1	A	301	GLU	3.5
1	C	311	VAL	3.5
1	A	275	TRP	3.5
1	C	217	LEU	3.5
1	B	356	GLN	3.5
1	D	176	TYR	3.5
1	B	407	GLU	3.5
1	C	138	PHE	3.5
1	B	205	VAL	3.5
1	A	392	PRO	3.5
1	A	173	ASN	3.5
1	B	159	TRP	3.5
1	C	349	ALA	3.5
1	D	194	ASN	3.5
1	D	242	ALA	3.5
1	B	420	ASP	3.5
1	A	134	ILE	3.5
1	D	133	ARG	3.5
1	A	316	PHE	3.5
1	C	316	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	466	GLY	3.4
1	C	127	GLY	3.4
1	D	233	ALA	3.4
1	B	286	ASP	3.4
1	B	142	GLU	3.4
1	D	309	GLU	3.4
1	C	181	THR	3.4
1	D	16	THR	3.4
1	D	48	PHE	3.4
1	D	128	LYS	3.4
1	D	377	THR	3.4
1	A	216	SER	3.4
1	C	108	LEU	3.4
1	C	280	LEU	3.4
1	C	101	ASN	3.4
1	C	212	ASN	3.4
1	C	159	TRP	3.4
1	C	463[A]	LYS	3.4
1	B	329	ILE	3.4
1	A	0	THR	3.4
1	D	171	THR	3.4
1	A	168	TYR	3.4
1	A	416	TYR	3.4
1	B	288	TYR	3.4
1	B	411	GLN	3.4
1	C	147	VAL	3.4
1	B	314	LEU	3.4
1	C	166	LEU	3.4
1	A	289	ASN	3.4
1	B	366	ARG	3.4
1	D	254	LYS	3.4
1	D	384	ILE	3.4
1	A	400	PHE	3.4
1	B	292	VAL	3.4
1	B	402	VAL	3.4
1	C	315	VAL	3.4
1	D	216	SER	3.4
1	A	291	LEU	3.4
1	B	447	ARG	3.4
1	A	182	GLY	3.4
1	B	399	GLY	3.4
1	A	412	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	349	ALA	3.4
1	C	293	LYS	3.4
1	D	403	LYS	3.4
1	D	335	ASP	3.4
1	D	405	TYR	3.3
1	C	336	ARG	3.3
1	C	114	LEU	3.3
1	D	291	LEU	3.3
1	C	142	GLU	3.3
1	D	223	GLU	3.3
1	C	297	ASN	3.3
1	D	88	GLY	3.3
1	C	357	ALA	3.3
1	C	53	THR	3.3
1	C	77	GLN	3.3
1	D	352	GLN	3.3
1	C	178	PHE	3.3
1	C	406	PRO	3.3
1	A	336	ARG	3.3
1	A	193	VAL	3.3
1	D	6	VAL	3.3
1	A	24	LEU	3.3
1	A	166	LEU	3.3
1	D	372	ASN	3.3
1	A	420	ASP	3.3
1	A	313	THR	3.3
1	B	185	ILE	3.3
1	C	57	ILE	3.3
1	D	302	THR	3.3
1	D	379	PHE	3.3
1	A	311	VAL	3.3
1	A	161	LEU	3.3
1	B	166	LEU	3.3
1	B	347	LEU	3.3
1	D	151	LEU	3.3
1	D	196	TYR	3.3
1	D	118	ASN	3.3
1	D	75	ASP	3.3
1	B	181	THR	3.3
1	B	389	ILE	3.3
1	C	451	THR	3.3
1	C	91	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	166	LEU	3.3
1	D	452	VAL	3.3
1	B	212	ASN	3.3
1	D	76	GLY	3.3
1	A	279[A]	CYS	3.3
1	A	122	ALA	3.3
1	A	349	ALA	3.3
1	C	192	ALA	3.3
1	D	124	ALA	3.3
1	B	167	ASP	3.2
1	D	356	GLN	3.2
1	A	105	LYS	3.2
1	B	100	LYS	3.2
1	C	442	ILE	3.2
1	B	400	PHE	3.2
1	C	330	PHE	3.2
1	C	148	LEU	3.2
1	C	418	LEU	3.2
1	D	73	LEU	3.2
1	A	214	ASN	3.2
1	D	390	ASN	3.2
1	C	288	TYR	3.2
1	D	353	TYR	3.2
1	B	191	ASP	3.2
1	B	334	ASP	3.2
1	D	192	ALA	3.2
1	A	74	ARG	3.2
1	D	336	ARG	3.2
1	B	467	LYS	3.2
1	C	310	PHE	3.2
1	C	400	PHE	3.2
1	B	109	SER	3.2
1	D	129	SER	3.2
1	A	212	ASN	3.2
1	B	226	ASN	3.2
1	B	395	GLN	3.2
1	D	320	TYR	3.2
1	B	344	ASP	3.2
1	C	273	ALA	3.2
1	D	472	LYS	3.2
1	D	436	GLU	3.2
1	A	299	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	171	THR	3.2
1	C	468	PRO	3.2
1	A	347	LEU	3.2
1	A	315	VAL	3.2
1	D	39	ASN	3.2
1	D	371	ASN	3.2
1	A	176	TYR	3.2
1	B	219	LYS	3.2
1	B	251	HIS	3.2
1	C	290	LYS	3.2
1	D	346	TYR	3.2
1	A	464	ILE	3.2
1	A	332	LEU	3.2
1	A	354	SER	3.2
1	B	243	PHE	3.2
1	C	48	PHE	3.2
1	C	153	LEU	3.2
1	D	370	LEU	3.2
1	A	368	ARG	3.1
1	A	448	VAL	3.1
1	A	150	TRP	3.1
1	A	55	ASP	3.1
1	A	58	ALA	3.1
1	C	70	ALA	3.1
1	C	197	THR	3.1
1	B	384	ILE	3.1
1	D	97	LEU	3.1
1	C	191	ASP	3.1
1	C	296	ASP	3.1
1	A	45	TYR	3.1
1	B	416	TYR	3.1
1	C	215	TYR	3.1
1	A	148	LEU	3.1
1	B	277	LEU	3.1
1	C	376	LEU	3.1
1	D	419	LEU	3.1
1	A	47	SER	3.1
1	A	99	PHE	3.1
1	D	388	GLY	3.1
1	A	52	VAL	3.1
1	A	440	VAL	3.1
1	C	52	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	208	VAL	3.1
1	A	286	ASP	3.1
1	B	225	ASP	3.1
1	C	381	ASP	3.1
1	D	55	ASP	3.1
1	B	468	PRO	3.1
1	B	299	THR	3.1
1	D	160	GLN	3.1
1	A	374	GLY	3.1
1	C	88	GLY	3.1
1	D	123	LEU	3.1
1	A	338	ASN	3.1
1	C	369	ASN	3.1
1	C	379	PHE	3.1
1	D	62	ASP	3.1
1	A	343	TYR	3.1
1	B	247	PRO	3.1
1	D	190	TYR	3.1
1	C	450	ARG	3.1
1	D	78	ARG	3.1
1	C	188	GLN	3.0
1	D	395	GLN	3.0
1	A	119	HIS	3.0
1	D	103	LEU	3.0
1	D	323	ASN	3.0
1	A	379	PHE	3.0
1	D	65	VAL	3.0
1	D	311	VAL	3.0
1	A	116	PRO	3.0
1	A	293	LYS	3.0
1	D	290	LYS	3.0
1	B	320	TYR	3.0
1	D	416	TYR	3.0
1	A	222	GLN	3.0
1	C	239	GLN	3.0
1	C	395	GLN	3.0
1	C	35	ILE	3.0
1	A	217	LEU	3.0
1	A	337	GLY	3.0
1	B	8	GLY	3.0
1	A	355	GLU	3.0
1	C	169	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	285	ARG	3.0
1	B	417	ARG	3.0
1	D	117	ALA	3.0
1	A	353	TYR	3.0
1	C	275	TRP	3.0
1	C	353	TYR	3.0
1	A	2	ILE	3.0
1	C	224	GLY	3.0
1	C	370	LEU	3.0
1	C	289	ASN	3.0
1	D	99	PHE	3.0
1	C	175	VAL	3.0
1	D	231	VAL	3.0
1	A	393	LYS	3.0
1	C	59	ARG	3.0
1	C	133	ARG	3.0
1	D	169	ASP	3.0
1	B	124	ALA	3.0
1	C	267	ALA	3.0
1	D	267	ALA	3.0
1	D	392	PRO	3.0
1	D	13	HIS	3.0
1	C	473	ILE	3.0
1	D	333	ILE	3.0
1	B	355	GLU	3.0
1	C	470	GLY	3.0
1	D	376	LEU	3.0
1	B	465	SER	3.0
1	D	318	ARG	3.0
1	B	245	VAL	3.0
1	D	56	ASP	3.0
1	A	267	ALA	3.0
1	B	236	THR	2.9
1	A	112	ILE	2.9
1	A	306	GLU	2.9
1	A	345	LEU	2.9
1	B	31	GLY	2.9
1	B	361	GLY	2.9
1	B	374	GLY	2.9
1	C	112	ILE	2.9
1	D	473	ILE	2.9
1	B	376	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	275	TRP	2.9
1	C	287	SER	2.9
1	A	170	CYS	2.9
1	B	232	VAL	2.9
1	C	440	VAL	2.9
1	A	36	GLN	2.9
1	C	36	GLN	2.9
1	D	367	GLN	2.9
1	A	115	ALA	2.9
1	C	122	ALA	2.9
1	A	53	THR	2.9
1	D	181	THR	2.9
1	B	244	GLY	2.9
1	B	413	LEU	2.9
1	B	444	LEU	2.9
1	A	155	SER	2.9
1	C	121	SER	2.9
1	D	50	ASP	2.9
1	D	208	VAL	2.9
1	D	116	PRO	2.9
1	A	163[A]	GLU	2.9
1	A	322	THR	2.9
1	B	312	LYS	2.9
1	B	90	ILE	2.9
1	B	328	ILE	2.9
1	C	42	LEU	2.9
1	C	328	ILE	2.9
1	C	26	ASN	2.9
1	A	190	TYR	2.9
1	C	190	TYR	2.9
1	C	155	SER	2.9
1	C	79	PHE	2.9
1	A	402	VAL	2.9
1	B	406	PRO	2.9
1	D	312	LYS	2.9
1	C	14	THR	2.9
1	B	111	LEU	2.9
1	C	173	ASN	2.9
1	B	77	GLN	2.9
1	D	445	GLN	2.9
1	A	165	TRP	2.8
1	C	420	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	3	VAL	2.8
1	A	294	GLU	2.8
1	B	436	GLU	2.8
1	B	128	LYS	2.8
1	C	472	LYS	2.8
1	A	236	THR	2.8
1	B	302	THR	2.8
1	C	180	LEU	2.8
1	D	220	LEU	2.8
1	A	101	ASN	2.8
1	A	258	ILE	2.8
1	D	2	ILE	2.8
1	D	256	ILE	2.8
1	D	298	ILE	2.8
1	A	177	SER	2.8
1	D	155	SER	2.8
1	B	190	TYR	2.8
1	B	362	PHE	2.8
1	C	449	ASP	2.8
1	B	441	GLU	2.8
1	C	187	ARG	2.8
1	B	108	LEU	2.8
1	D	398	LEU	2.8
1	A	82	ILE	2.8
1	A	473	ILE	2.8
1	D	156	ASP	2.8
1	B	48	PHE	2.8
1	D	300	LYS	2.8
1	D	453	PHE	2.8
1	C	81	CYS	2.8
1	D	360	ALA	2.8
1	A	238	THR	2.8
1	A	314	LEU	2.8
1	C	73	LEU	2.8
1	B	173	ASN	2.8
1	D	26	ASN	2.8
1	D	214	ASN	2.8
1	B	59	ARG	2.8
1	B	89	PRO	2.8
1	A	159[A]	TRP	2.8
1	B	404	ALA	2.8
1	C	124	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	122	ALA	2.8
1	B	221	HIS	2.8
1	C	340	LEU	2.8
1	D	459	LEU	2.8
1	A	297	ASN	2.8
1	B	26	ASN	2.8
1	A	276	ILE	2.7
1	D	46	ILE	2.7
1	C	184	LYS	2.7
1	C	294	GLU	2.7
1	A	271	PRO	2.7
1	C	271	PRO	2.7
1	A	310	PHE	2.7
1	A	346	TYR	2.7
1	A	282	VAL	2.7
1	A	181	THR	2.7
1	A	126	LEU	2.7
1	D	212	ASN	2.7
1	A	219	LYS	2.7
1	B	333	ILE	2.7
1	B	336	ARG	2.7
1	C	200	SER	2.7
1	C	306	GLU	2.7
1	B	461	PRO	2.7
1	A	320	TYR	2.7
1	C	205	VAL	2.7
1	D	87	GLY	2.7
1	A	106	CYS	2.7
1	A	272	THR	2.7
1	D	313	THR	2.7
1	A	180	LEU	2.7
1	A	370	LEU	2.7
1	B	33	LEU	2.7
1	C	254	LYS	2.7
1	B	214	ASN	2.7
1	B	306	GLU	2.7
1	B	446	ARG	2.7
1	B	155	SER	2.7
1	B	202	SER	2.7
1	B	434	PRO	2.7
1	C	335	ASP	2.7
1	D	67	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	365	ASP	2.7
1	A	91	VAL	2.7
1	A	178	PHE	2.7
1	B	52	VAL	2.7
1	C	176	TYR	2.7
1	B	412	ALA	2.7
1	B	463	LYS	2.7
1	C	308	LYS	2.7
1	D	146	CYS	2.7
1	A	130	ARG	2.7
1	D	187	ARG	2.7
1	A	256	ILE	2.7
1	A	384	ILE	2.7
1	C	177	SER	2.7
1	C	252	SER	2.7
1	B	50	ASP	2.7
1	D	286	ASP	2.7
1	A	232	VAL	2.7
1	C	206	VAL	2.7
1	D	292	VAL	2.7
1	C	64	ALA	2.7
1	C	105	LYS	2.7
1	B	144	GLY	2.6
1	A	318	ARG	2.6
1	B	133	ARG	2.6
1	B	295	LEU	2.6
1	C	163	GLU	2.6
1	D	199	GLU	2.6
1	B	276	ILE	2.6
1	C	129	SER	2.6
1	A	34	ASP	2.6
1	D	71	ASP	2.6
1	D	60	ALA	2.6
1	D	210	ALA	2.6
1	B	382	TYR	2.6
1	A	377	THR	2.6
1	B	218	LEU	2.6
1	C	12	THR	2.6
1	C	236	THR	2.6
1	C	386	GLU	2.6
1	D	20	LEU	2.6
1	A	194	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	431	ILE	2.6
1	D	82	ILE	2.6
1	B	326	SER	2.6
1	D	21	PRO	2.6
1	D	89	PRO	2.6
1	D	49	ASP	2.6
1	A	339	HIS	2.6
1	B	222	GLN	2.6
1	C	119	HIS	2.6
1	D	375	LYS	2.6
1	A	175	VAL	2.6
1	B	74	ARG	2.6
1	C	6	VAL	2.6
1	D	37	VAL	2.6
1	A	399	GLY	2.6
1	C	18	GLY	2.6
1	C	198	GLY	2.6
1	C	319	GLU	2.6
1	B	97	LEU	2.6
1	B	377	THR	2.6
1	C	391	THR	2.6
1	D	53	THR	2.6
1	C	162	ASN	2.6
1	A	94	TRP	2.6
1	B	106	CYS	2.6
1	B	143	PRO	2.6
1	D	287	SER	2.6
1	A	395	GLN	2.6
1	B	22	GLN	2.6
1	A	278[A]	ARG	2.6
1	C	368	ARG	2.6
1	C	447	ARG	2.6
1	A	245	VAL	2.6
1	D	43	GLY	2.6
1	D	61	PHE	2.6
1	B	209	ALA	2.6
1	A	391	THR	2.6
1	B	460	THR	2.6
1	C	211	THR	2.6
1	B	203	ASN	2.6
1	A	434	PRO	2.6
1	B	258	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	383	ASP	2.6
1	A	366	ARG	2.6
1	A	206	VAL	2.5
1	A	273	ALA	2.5
1	D	64	ALA	2.5
1	D	364	VAL	2.5
1	A	153	LEU	2.5
1	C	220	LEU	2.5
1	C	432	LEU	2.5
1	D	380	LEU	2.5
1	C	323	ASN	2.5
1	B	168	TYR	2.5
1	B	472	LYS	2.5
1	A	326	SER	2.5
1	A	344	ASP	2.5
1	B	56	ASP	2.5
1	B	67	ASP	2.5
1	C	286	ASP	2.5
1	D	167	ASP	2.5
1	A	6	VAL	2.5
1	A	124	ALA	2.5
1	B	282	VAL	2.5
1	C	245	VAL	2.5
1	A	340	LEU	2.5
1	C	123	LEU	2.5
1	D	111	LEU	2.5
1	A	435	ASN	2.5
1	B	290	LYS	2.5
1	D	69	ILE	2.5
1	D	74	ARG	2.5
1	B	85	SER	2.5
1	D	202	SER	2.5
1	A	71[A]	ASP	2.5
1	A	296	ASP	2.5
1	B	296	ASP	2.5
1	B	381	ASP	2.5
1	C	149	ASP	2.5
1	B	294	GLU	2.5
1	B	224	GLY	2.5
1	D	361	GLY	2.5
1	C	99	PHE	2.5
1	A	32	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	358	LEU	2.5
1	A	467	LYS	2.5
1	B	72	LYS	2.5
1	B	293	LYS	2.5
1	B	430	LYS	2.5
1	C	234	LYS	2.5
1	D	180	LEU	2.5
1	D	246	LEU	2.5
1	D	308	LYS	2.5
1	C	302	THR	2.5
1	D	397	ASN	2.5
1	A	450	ARG	2.5
1	C	196	TYR	2.5
1	C	276	ILE	2.5
1	A	85	SER	2.5
1	A	195	SER	2.5
1	A	252	SER	2.5
1	A	287	SER	2.5
1	C	25	GLU	2.5
1	D	144	GLY	2.5
1	D	466	GLY	2.5
1	C	471	LYS	2.5
1	A	209	ALA	2.5
1	C	462	ALA	2.5
1	A	133	ARG	2.5
1	A	281	GLN	2.5
1	D	45	TYR	2.4
1	A	56	ASP	2.4
1	B	71	ASP	2.4
1	D	182	GLY	2.4
1	B	210	ALA	2.4
1	B	99	PHE	2.4
1	B	151	LEU	2.4
1	B	453	PHE	2.4
1	C	24	LEU	2.4
1	D	108	LEU	2.4
1	A	89	PRO	2.4
1	B	107	PRO	2.4
1	C	434	PRO	2.4
1	D	17	TYR	2.4
1	A	449	ASP	2.4
1	B	365	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	132	GLY	2.4
1	D	174	GLY	2.4
1	C	84	HIS	2.4
1	A	59	ARG	2.4
1	C	94	TRP	2.4
1	C	165	TRP	2.4
1	C	277	LEU	2.4
1	C	303	GLN	2.4
1	C	380	LEU	2.4
1	A	255	ASN	2.4
1	C	397	ASN	2.4
1	A	269	THR	2.4
1	D	197	THR	2.4
1	A	461	PRO	2.4
1	C	116	PRO	2.4
1	B	319	GLU	2.4
1	B	321	ILE	2.4
1	C	259	ILE	2.4
1	A	382	TYR	2.4
1	C	45	TYR	2.4
1	C	283	LYS	2.4
1	D	38	GLY	2.4
1	A	207	ARG	2.4
1	C	331	ARG	2.4
1	A	20	LEU	2.4
1	A	280	LEU	2.4
1	A	398	LEU	2.4
1	B	64	ALA	2.4
1	B	115	ALA	2.4
1	B	220	LEU	2.4
1	B	291	LEU	2.4
1	C	233	ALA	2.4
1	C	345	LEU	2.4
1	C	347	LEU	2.4
1	D	209	ALA	2.4
1	A	438	VAL	2.4
1	B	175	VAL	2.4
1	C	194	ASN	2.4
1	D	179	VAL	2.4
1	D	297	ASN	2.4
1	D	362	PHE	2.4
1	B	223	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	274	ILE	2.4
1	C	158	SER	2.4
1	A	335	ASP	2.4
1	C	41	TYR	2.4
1	A	22	GLN	2.4
1	B	303	GLN	2.4
1	A	146	CYS	2.4
1	B	148	LEU	2.4
1	B	305	ASN	2.4
1	C	203	ASN	2.4
1	C	266	ASN	2.4
1	C	360	ALA	2.4
1	D	81	CYS	2.4
1	D	203	ASN	2.4
1	D	289	ASN	2.4
1	A	54	VAL	2.3
1	A	364	VAL	2.3
1	D	319	GLU	2.3
1	D	359	PRO	2.3
1	B	112	ILE	2.3
1	B	149	ASP	2.3
1	D	186	ASP	2.3
1	A	325	TYR	2.3
1	D	382	TYR	2.3
1	A	201	GLY	2.3
1	B	38	GLY	2.3
1	C	201	GLY	2.3
1	D	18	GLY	2.3
1	D	63	GLN	2.3
1	A	131	LEU	2.3
1	A	277	LEU	2.3
1	A	376	LEU	2.3
1	C	460	THR	2.3
1	D	79	PHE	2.3
1	A	90	ILE	2.3
1	A	446	ARG	2.3
1	B	335	ASP	2.3
1	C	156	ASP	2.3
1	C	167	ASP	2.3
1	B	337	GLY	2.3
1	C	356	GLN	2.3
1	D	41	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	359	PRO	2.3
1	B	11	VAL	2.3
1	C	37	VAL	2.3
1	B	61	PHE	2.3
1	B	238	THR	2.3
1	C	106	CYS	2.3
1	C	207	ARG	2.3
1	A	259	ILE	2.3
1	B	250	SER	2.3
1	B	473	ILE	2.3
1	A	303	GLN	2.3
1	C	387	GLY	2.3
1	A	471	LYS	2.3
1	B	249	LEU	2.3
1	C	372	ASN	2.3
1	D	305	ASN	2.3
1	C	60	ALA	2.3
1	C	209	ALA	2.3
1	D	11	VAL	2.3
1	D	282	VAL	2.3
1	B	318	ARG	2.3
1	A	188	GLN	2.3
1	C	367	GLN	2.3
1	D	188	GLN	2.3
1	D	224	GLY	2.3
1	C	168	TYR	2.2
1	C	111	LEU	2.2
1	A	437	THR	2.2
1	D	468	PRO	2.2
1	B	231	VAL	2.2
1	B	401	ARG	2.2
1	C	292	VAL	2.2
1	D	401	ARG	2.2
1	B	367	GLN	2.2
1	A	62	ASP	2.2
1	D	34	ASP	2.2
1	A	328	ILE	2.2
1	C	274	ILE	2.2
1	D	407	GLU	2.2
1	A	371	ASN	2.2
1	B	73	LEU	2.2
1	C	249	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	60	ALA	2.2
1	A	404	ALA	2.2
1	B	116	PRO	2.2
1	B	278	ARG	2.2
1	C	242	ALA	2.2
1	D	80	ALA	2.2
1	D	450	ARG	2.2
1	B	16	THR	2.2
1	C	251	HIS	2.2
1	D	27	GLN	2.2
1	D	77	GLN	2.2
1	A	202	SER	2.2
1	A	472	LYS	2.2
1	C	55	ASP	2.2
1	B	18	GLY	2.2
1	C	120	GLY	2.2
1	C	244	GLY	2.2
1	B	25	GLU	2.2
1	D	294	GLU	2.2
1	D	355	GLU	2.2
1	A	418	LEU	2.2
1	D	462	ALA	2.2
1	C	317	THR	2.2
1	A	48	PHE	2.2
1	C	183	GLN	2.2
1	B	105	LYS	2.2
1	B	47	SER	2.2
1	D	474	ASP	2.2
1	B	256	ILE	2.2
1	C	256	ILE	2.2
1	C	321	ILE	2.2
1	D	301	GLU	2.2
1	A	417	ARG	2.2
1	D	280	LEU	2.2
1	A	215	TYR	2.2
1	A	270	HIS	2.2
1	B	45	TYR	2.2
1	C	7	HIS	2.2
1	B	242	ALA	2.2
1	B	469	THR	2.2
1	D	211	THR	2.2
1	A	254	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	105	LYS	2.2
1	A	474	ASP	2.2
1	B	62	ASP	2.2
1	B	383	ASP	2.2
1	B	195	SER	2.1
1	A	4	ILE	2.1
1	A	198	GLY	2.1
1	C	407	GLU	2.1
1	D	170	CYS	2.1
1	A	373	ARG	2.1
1	A	42	LEU	2.1
1	C	110	HIS	2.1
1	D	251	HIS	2.1
1	A	80	ALA	2.1
1	A	12	THR	2.1
1	A	469	THR	2.1
1	C	83	THR	2.1
1	A	79	PHE	2.1
1	D	441	GLU	2.1
1	B	4	ILE	2.1
1	B	66	ARG	2.1
1	C	278	ARG	2.1
1	C	307	HIS	2.1
1	A	39	ASN	2.1
1	D	358	LEU	2.1
1	C	247	PRO	2.1
1	A	125	GLN	2.1
1	C	145	LYS	2.1
1	D	22	GLN	2.1
1	D	222	GLN	2.1
1	B	70	ALA	2.1
1	A	453	PHE	2.1
1	A	237	ARG	2.1
1	C	56	ASP	2.1
1	D	96	ASP	2.1
1	C	250	SER	2.1
1	C	388	GLY	2.1
1	D	250	SER	2.1
1	D	417	ARG	2.1
1	A	321	ILE	2.1
1	A	389	ILE	2.1
1	B	46	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	455	ILE	2.1
1	D	35	ILE	2.1
1	B	119	HIS	2.1
1	B	403	LYS	2.1
1	B	418	LEU	2.1
1	B	457	ASN	2.1
1	D	393	LYS	2.1
1	D	457	ASN	2.1
1	A	468	PRO	2.1
1	C	240	PRO	2.1
1	C	210	ALA	2.1
1	D	70	ALA	2.1
1	A	98	TYR	2.1
1	D	288	TYR	2.1
1	D	5	PHE	2.1
1	B	470	GLY	2.1
1	D	201	GLY	2.1
1	A	274	ILE	2.1
1	A	234	LYS	2.1
1	B	308	LYS	2.1
1	C	29	LYS	2.1
1	D	93	LYS	2.1
1	A	107	PRO	2.1
1	A	220	LEU	2.1
1	B	217	LEU	2.1
1	C	246	LEU	2.1
1	D	33	LEU	2.1
1	A	360	ALA	2.1
1	B	14	THR	2.1
1	B	122	ALA	2.1
1	C	58	ALA	2.1
1	D	263	THR	2.1
1	A	405	TYR	2.0
1	A	452	VAL	2.0
1	C	382	TYR	2.0
1	D	127	GLY	2.0
1	C	13	HIS	2.0
1	C	433	HIS	2.0
1	D	110	HIS	2.0
1	A	283	LYS	2.0
1	B	134	ILE	2.0
1	C	352	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	153	LEU	2.0
1	D	277	LEU	2.0
1	B	215	TYR	2.0
1	A	248	GLY	2.0
1	B	156	ASP	2.0
1	D	178	PHE	2.0
1	B	234	LYS	2.0
1	B	408	SER	2.0
1	C	326	SER	2.0
1	C	20	LEU	2.0
1	C	255	ASN	2.0
1	C	338	ASN	2.0
1	C	279	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.

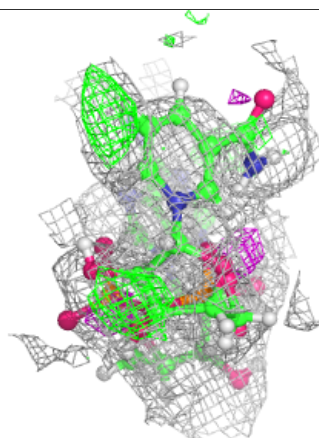
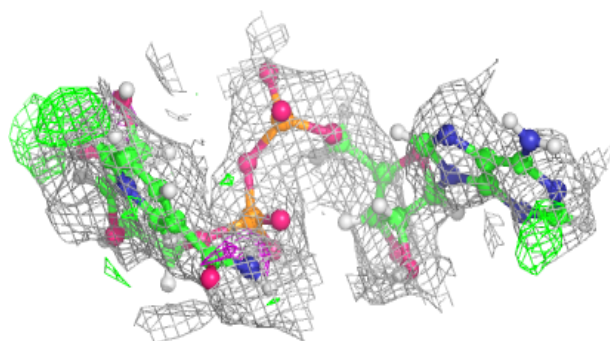
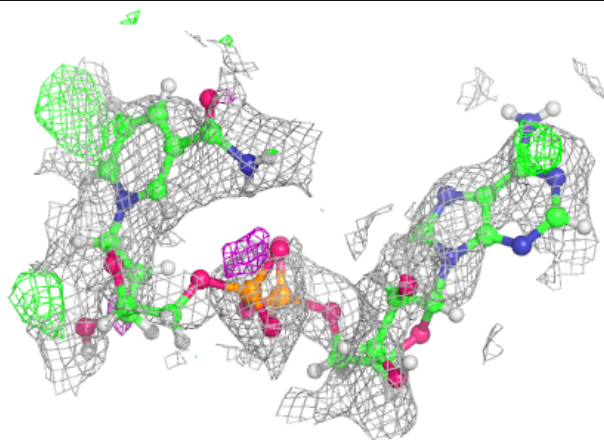
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAD	D	501	44/44	0.57	0.30	23,48,62,69	70
2	NAD	D	502	44/44	0.61	0.33	22,34,44,53	70
2	NAD	A	501	44/44	0.63	0.23	22,38,52,55	0
2	NAD	C	501	44/44	0.69	0.27	15,30,43,49	70
2	NAD	B	601	44/44	0.72	0.23	21,38,51,57	70
2	NAD	B	602	44/44	0.74	0.23	10,28,39,46	0
2	NAD	A	502	44/44	0.76	0.20	18,31,45,55	70
2	NAD	C	502	44/44	0.86	0.16	6,24,34,41	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.

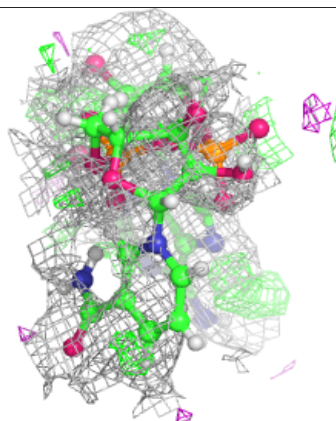
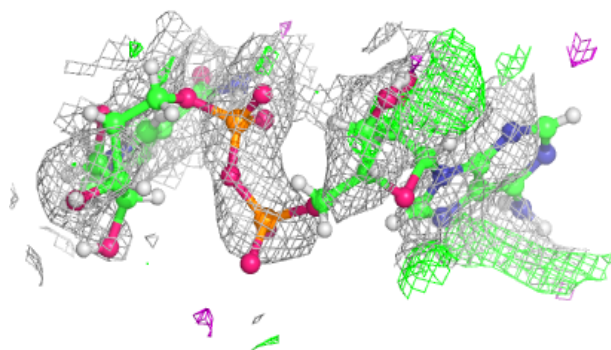
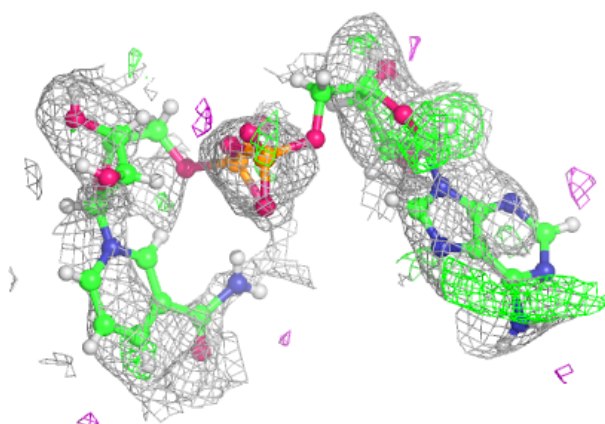
Electron density around NAD D 501:

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

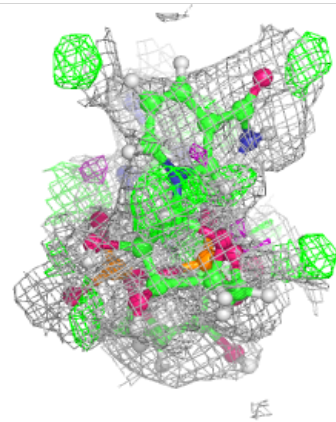
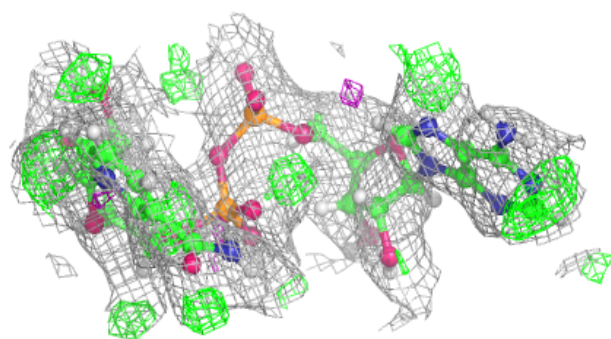
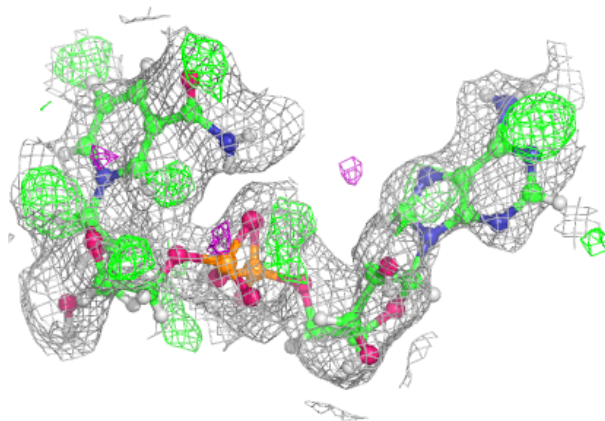


Electron density around NAD D 502:

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

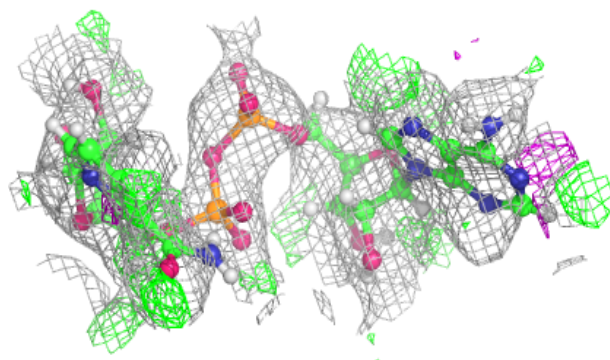
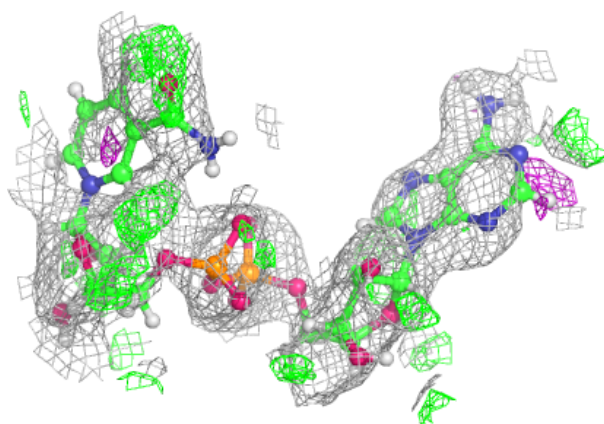
**Electron density around NAD A 501:**

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



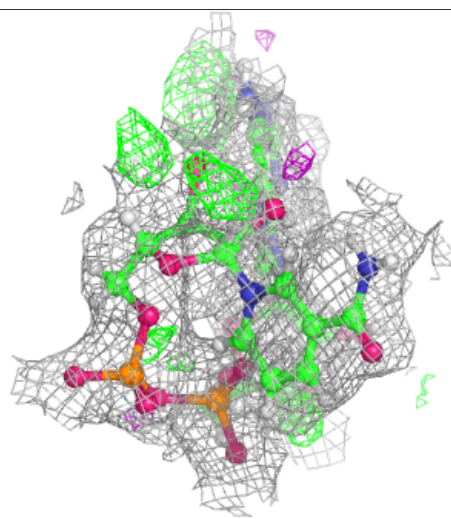
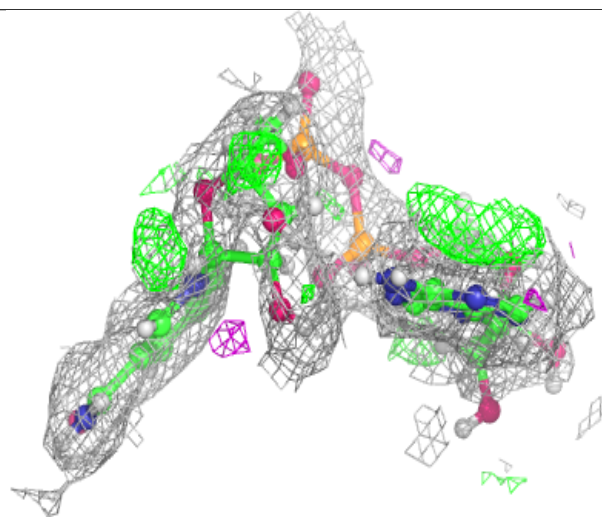
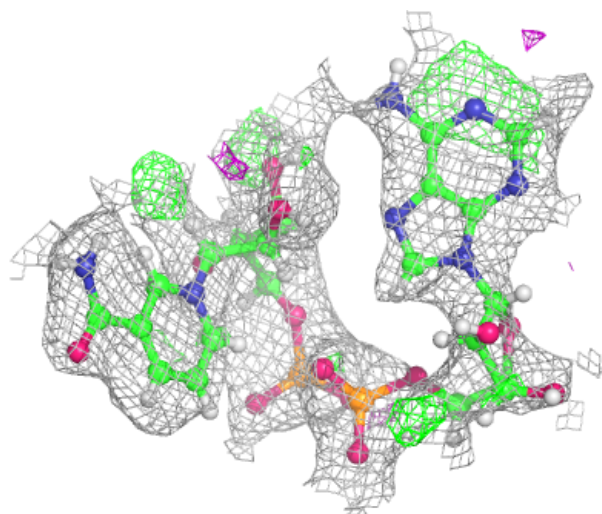
Electron density around NAD C 501:

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



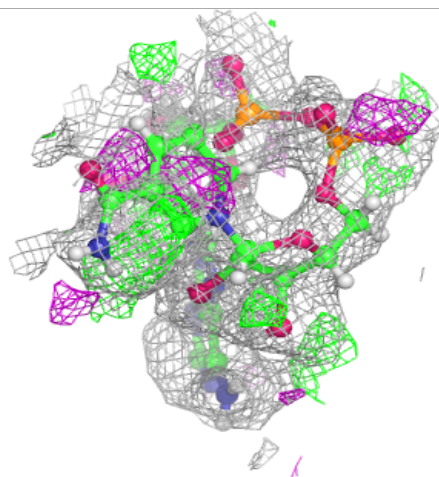
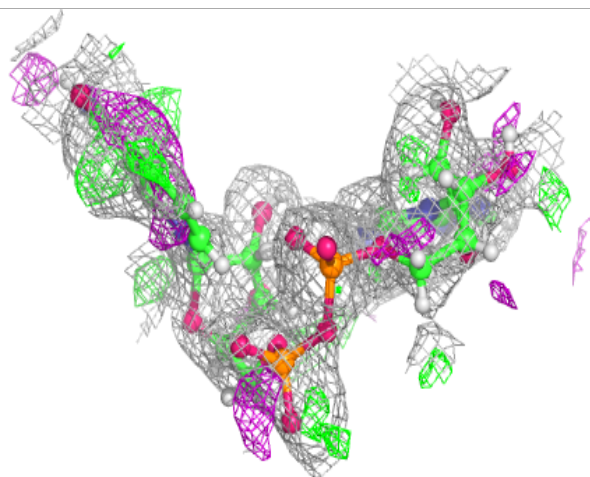
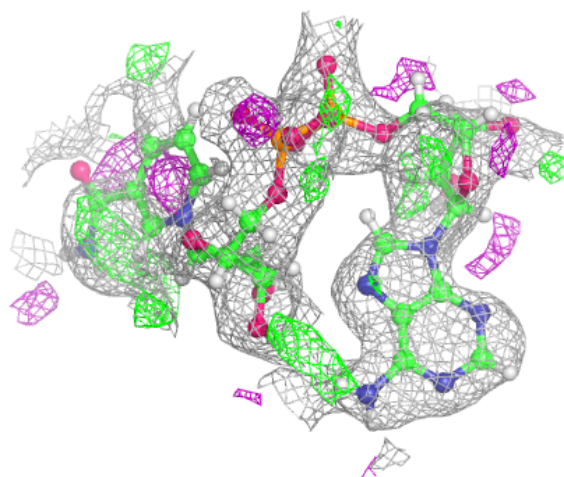
Electron density around NAD B 601:

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



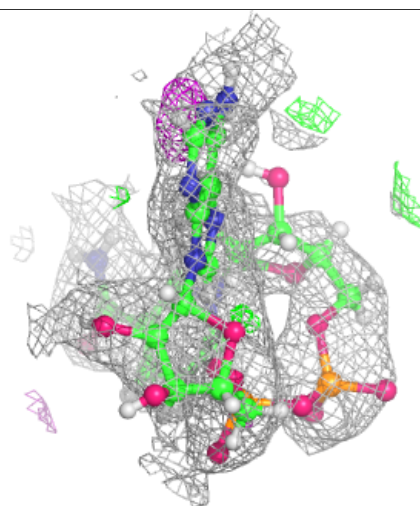
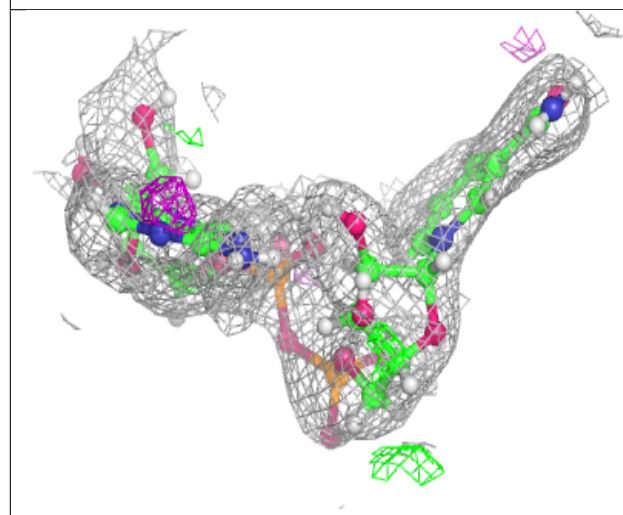
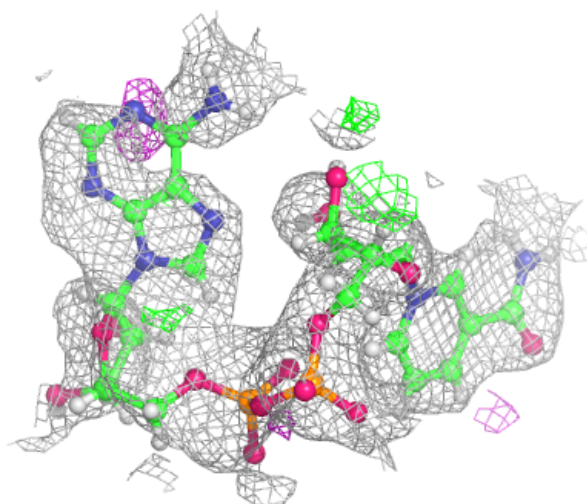
Electron density around NAD B 602:

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



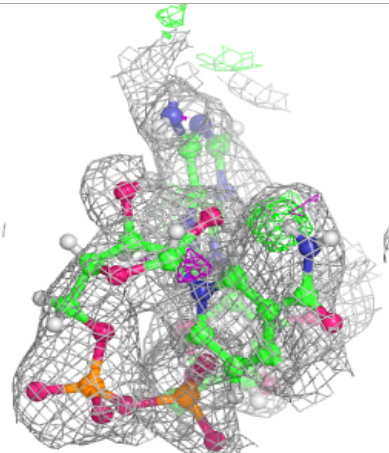
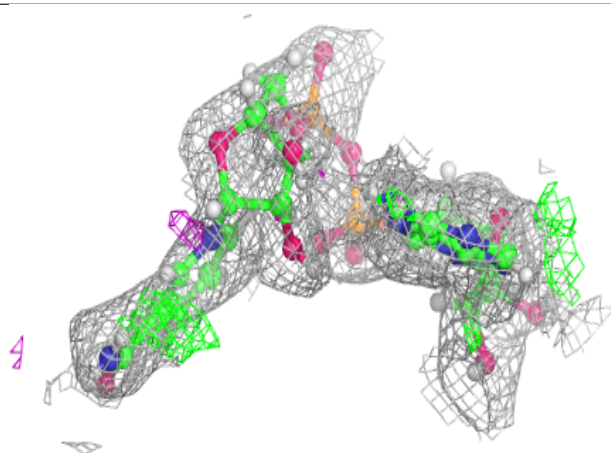
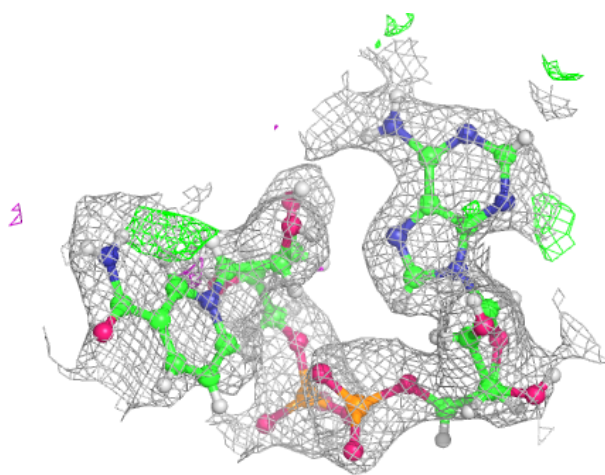
Electron density around NAD A 502:

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



Electron density around NAD C 502:

$2mF_o-DF_c$ (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.