



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:12 AM UTC

PDB ID : 3SXP / pdb_00003sxp
Title : Crystal Structure of Helicobacter pylori ADP-L-glycero-D-manno-heptose-6-e pimerase (rfaD, HP0859)
Authors : Shaik, M.M.; Zanotti, G.; Cendron, L.
Deposited on : 2011-07-15
Resolution : 2.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

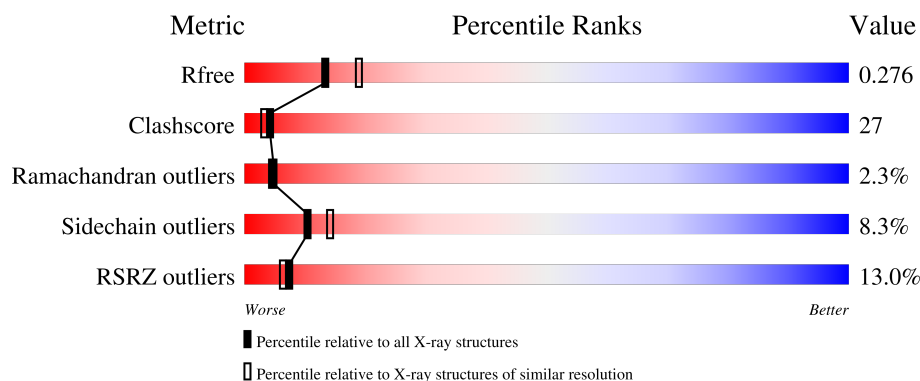
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	362	
1	B	362	
1	C	362	
1	D	362	
1	E	362	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12913 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 ADP-L-glycero-D-mannoheptose-6-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2480	1596	416	460	8			
1	B	311	Total	C	N	O	S	0	0	0
			2489	1601	418	462	8			
1	C	310	Total	C	N	O	S	0	0	0
			2480	1596	416	460	8			
1	D	314	Total	C	N	O	S	0	0	0
			2519	1623	422	466	8			
1	E	310	Total	C	N	O	S	0	0	0
			2480	1596	416	460	8			

There are 165 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	GLU	GLY	engineered mutation	UNP B5Z7L9
A	331	LYS	-	expression tag	UNP B5Z7L9
A	332	GLY	-	expression tag	UNP B5Z7L9
A	333	GLU	-	expression tag	UNP B5Z7L9
A	334	LEU	-	expression tag	UNP B5Z7L9
A	335	ASN	-	expression tag	UNP B5Z7L9
A	336	SER	-	expression tag	UNP B5Z7L9
A	337	LYS	-	expression tag	UNP B5Z7L9
A	338	LEU	-	expression tag	UNP B5Z7L9
A	339	GLU	-	expression tag	UNP B5Z7L9
A	340	GLY	-	expression tag	UNP B5Z7L9
A	341	LYS	-	expression tag	UNP B5Z7L9
A	342	PRO	-	expression tag	UNP B5Z7L9
A	343	ILE	-	expression tag	UNP B5Z7L9
A	344	PRO	-	expression tag	UNP B5Z7L9
A	345	ASN	-	expression tag	UNP B5Z7L9
A	346	LEU	-	expression tag	UNP B5Z7L9
A	347	LEU	-	expression tag	UNP B5Z7L9
A	348	GLY	-	expression tag	UNP B5Z7L9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	349	LEU	-	expression tag	UNP B5Z7L9
A	350	ASP	-	expression tag	UNP B5Z7L9
A	351	SER	-	expression tag	UNP B5Z7L9
A	352	THR	-	expression tag	UNP B5Z7L9
A	353	ARG	-	expression tag	UNP B5Z7L9
A	354	THR	-	expression tag	UNP B5Z7L9
A	355	GLY	-	expression tag	UNP B5Z7L9
A	356	HIS	-	expression tag	UNP B5Z7L9
A	357	HIS	-	expression tag	UNP B5Z7L9
A	358	HIS	-	expression tag	UNP B5Z7L9
A	359	HIS	-	expression tag	UNP B5Z7L9
A	360	HIS	-	expression tag	UNP B5Z7L9
A	361	HIS	-	expression tag	UNP B5Z7L9
A	362	HIS	-	expression tag	UNP B5Z7L9
B	7	GLU	GLY	engineered mutation	UNP B5Z7L9
B	331	LYS	-	expression tag	UNP B5Z7L9
B	332	GLY	-	expression tag	UNP B5Z7L9
B	333	GLU	-	expression tag	UNP B5Z7L9
B	334	LEU	-	expression tag	UNP B5Z7L9
B	335	ASN	-	expression tag	UNP B5Z7L9
B	336	SER	-	expression tag	UNP B5Z7L9
B	337	LYS	-	expression tag	UNP B5Z7L9
B	338	LEU	-	expression tag	UNP B5Z7L9
B	339	GLU	-	expression tag	UNP B5Z7L9
B	340	GLY	-	expression tag	UNP B5Z7L9
B	341	LYS	-	expression tag	UNP B5Z7L9
B	342	PRO	-	expression tag	UNP B5Z7L9
B	343	ILE	-	expression tag	UNP B5Z7L9
B	344	PRO	-	expression tag	UNP B5Z7L9
B	345	ASN	-	expression tag	UNP B5Z7L9
B	346	LEU	-	expression tag	UNP B5Z7L9
B	347	LEU	-	expression tag	UNP B5Z7L9
B	348	GLY	-	expression tag	UNP B5Z7L9
B	349	LEU	-	expression tag	UNP B5Z7L9
B	350	ASP	-	expression tag	UNP B5Z7L9
B	351	SER	-	expression tag	UNP B5Z7L9
B	352	THR	-	expression tag	UNP B5Z7L9
B	353	ARG	-	expression tag	UNP B5Z7L9
B	354	THR	-	expression tag	UNP B5Z7L9
B	355	GLY	-	expression tag	UNP B5Z7L9
B	356	HIS	-	expression tag	UNP B5Z7L9
B	357	HIS	-	expression tag	UNP B5Z7L9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	358	HIS	-	expression tag	UNP B5Z7L9
B	359	HIS	-	expression tag	UNP B5Z7L9
B	360	HIS	-	expression tag	UNP B5Z7L9
B	361	HIS	-	expression tag	UNP B5Z7L9
B	362	HIS	-	expression tag	UNP B5Z7L9
C	7	GLU	GLY	engineered mutation	UNP B5Z7L9
C	331	LYS	-	expression tag	UNP B5Z7L9
C	332	GLY	-	expression tag	UNP B5Z7L9
C	333	GLU	-	expression tag	UNP B5Z7L9
C	334	LEU	-	expression tag	UNP B5Z7L9
C	335	ASN	-	expression tag	UNP B5Z7L9
C	336	SER	-	expression tag	UNP B5Z7L9
C	337	LYS	-	expression tag	UNP B5Z7L9
C	338	LEU	-	expression tag	UNP B5Z7L9
C	339	GLU	-	expression tag	UNP B5Z7L9
C	340	GLY	-	expression tag	UNP B5Z7L9
C	341	LYS	-	expression tag	UNP B5Z7L9
C	342	PRO	-	expression tag	UNP B5Z7L9
C	343	ILE	-	expression tag	UNP B5Z7L9
C	344	PRO	-	expression tag	UNP B5Z7L9
C	345	ASN	-	expression tag	UNP B5Z7L9
C	346	LEU	-	expression tag	UNP B5Z7L9
C	347	LEU	-	expression tag	UNP B5Z7L9
C	348	GLY	-	expression tag	UNP B5Z7L9
C	349	LEU	-	expression tag	UNP B5Z7L9
C	350	ASP	-	expression tag	UNP B5Z7L9
C	351	SER	-	expression tag	UNP B5Z7L9
C	352	THR	-	expression tag	UNP B5Z7L9
C	353	ARG	-	expression tag	UNP B5Z7L9
C	354	THR	-	expression tag	UNP B5Z7L9
C	355	GLY	-	expression tag	UNP B5Z7L9
C	356	HIS	-	expression tag	UNP B5Z7L9
C	357	HIS	-	expression tag	UNP B5Z7L9
C	358	HIS	-	expression tag	UNP B5Z7L9
C	359	HIS	-	expression tag	UNP B5Z7L9
C	360	HIS	-	expression tag	UNP B5Z7L9
C	361	HIS	-	expression tag	UNP B5Z7L9
C	362	HIS	-	expression tag	UNP B5Z7L9
D	7	GLU	GLY	engineered mutation	UNP B5Z7L9
D	331	LYS	-	expression tag	UNP B5Z7L9
D	332	GLY	-	expression tag	UNP B5Z7L9
D	333	GLU	-	expression tag	UNP B5Z7L9

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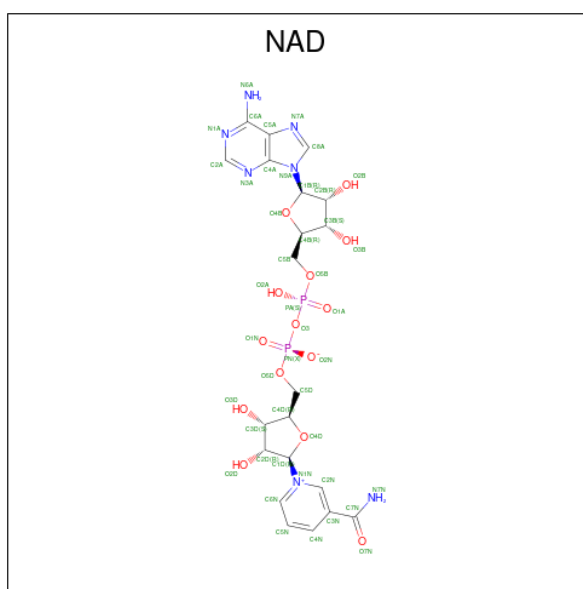
Chain	Residue	Modelled	Actual	Comment	Reference
D	334	LEU	-	expression tag	UNP B5Z7L9
D	335	ASN	-	expression tag	UNP B5Z7L9
D	336	SER	-	expression tag	UNP B5Z7L9
D	337	LYS	-	expression tag	UNP B5Z7L9
D	338	LEU	-	expression tag	UNP B5Z7L9
D	339	GLU	-	expression tag	UNP B5Z7L9
D	340	GLY	-	expression tag	UNP B5Z7L9
D	341	LYS	-	expression tag	UNP B5Z7L9
D	342	PRO	-	expression tag	UNP B5Z7L9
D	343	ILE	-	expression tag	UNP B5Z7L9
D	344	PRO	-	expression tag	UNP B5Z7L9
D	345	ASN	-	expression tag	UNP B5Z7L9
D	346	LEU	-	expression tag	UNP B5Z7L9
D	347	LEU	-	expression tag	UNP B5Z7L9
D	348	GLY	-	expression tag	UNP B5Z7L9
D	349	LEU	-	expression tag	UNP B5Z7L9
D	350	ASP	-	expression tag	UNP B5Z7L9
D	351	SER	-	expression tag	UNP B5Z7L9
D	352	THR	-	expression tag	UNP B5Z7L9
D	353	ARG	-	expression tag	UNP B5Z7L9
D	354	THR	-	expression tag	UNP B5Z7L9
D	355	GLY	-	expression tag	UNP B5Z7L9
D	356	HIS	-	expression tag	UNP B5Z7L9
D	357	HIS	-	expression tag	UNP B5Z7L9
D	358	HIS	-	expression tag	UNP B5Z7L9
D	359	HIS	-	expression tag	UNP B5Z7L9
D	360	HIS	-	expression tag	UNP B5Z7L9
D	361	HIS	-	expression tag	UNP B5Z7L9
D	362	HIS	-	expression tag	UNP B5Z7L9
E	7	GLU	GLY	engineered mutation	UNP B5Z7L9
E	331	LYS	-	expression tag	UNP B5Z7L9
E	332	GLY	-	expression tag	UNP B5Z7L9
E	333	GLU	-	expression tag	UNP B5Z7L9
E	334	LEU	-	expression tag	UNP B5Z7L9
E	335	ASN	-	expression tag	UNP B5Z7L9
E	336	SER	-	expression tag	UNP B5Z7L9
E	337	LYS	-	expression tag	UNP B5Z7L9
E	338	LEU	-	expression tag	UNP B5Z7L9
E	339	GLU	-	expression tag	UNP B5Z7L9
E	340	GLY	-	expression tag	UNP B5Z7L9
E	341	LYS	-	expression tag	UNP B5Z7L9
E	342	PRO	-	expression tag	UNP B5Z7L9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	343	ILE	-	expression tag	UNP B5Z7L9
E	344	PRO	-	expression tag	UNP B5Z7L9
E	345	ASN	-	expression tag	UNP B5Z7L9
E	346	LEU	-	expression tag	UNP B5Z7L9
E	347	LEU	-	expression tag	UNP B5Z7L9
E	348	GLY	-	expression tag	UNP B5Z7L9
E	349	LEU	-	expression tag	UNP B5Z7L9
E	350	ASP	-	expression tag	UNP B5Z7L9
E	351	SER	-	expression tag	UNP B5Z7L9
E	352	THR	-	expression tag	UNP B5Z7L9
E	353	ARG	-	expression tag	UNP B5Z7L9
E	354	THR	-	expression tag	UNP B5Z7L9
E	355	GLY	-	expression tag	UNP B5Z7L9
E	356	HIS	-	expression tag	UNP B5Z7L9
E	357	HIS	-	expression tag	UNP B5Z7L9
E	358	HIS	-	expression tag	UNP B5Z7L9
E	359	HIS	-	expression tag	UNP B5Z7L9
E	360	HIS	-	expression tag	UNP B5Z7L9
E	361	HIS	-	expression tag	UNP B5Z7L9
E	362	HIS	-	expression tag	UNP B5Z7L9

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 44	C 21	N 7	O 14	P 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

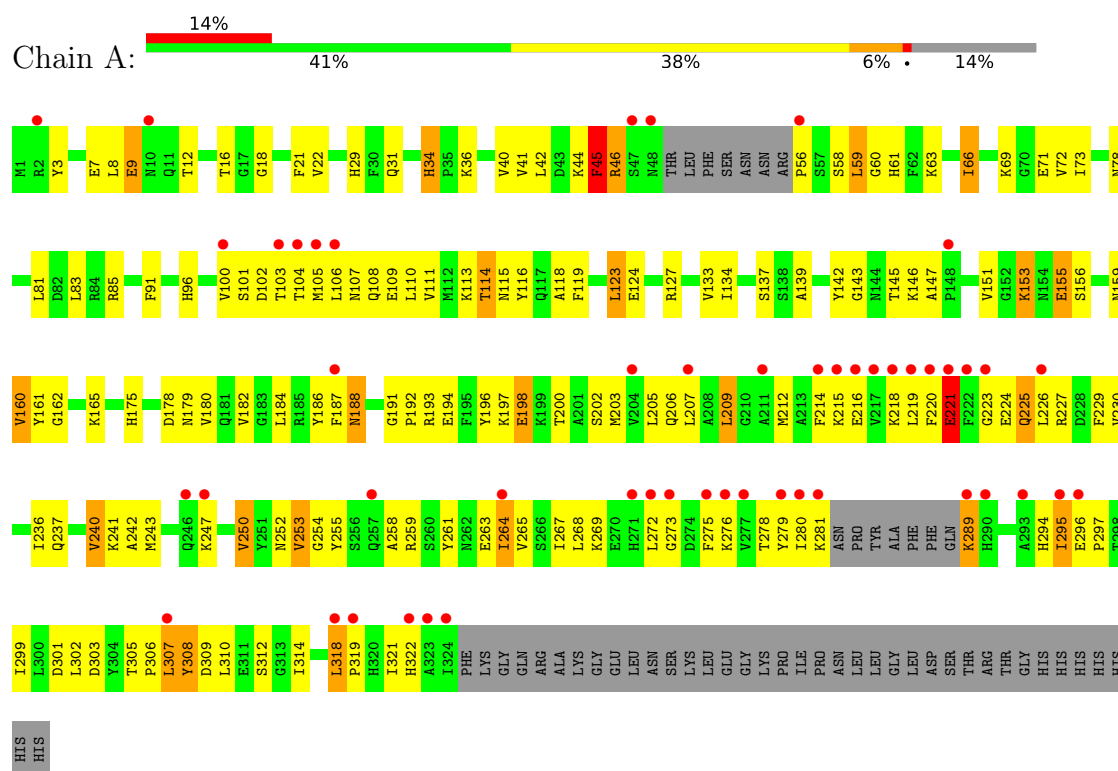
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total	O	0	0
			68	68		
3	B	56	Total	O	0	0
			56	56		
3	C	36	Total	O	0	0
			36	36		
3	D	43	Total	O	0	0
			43	43		
3	E	42	Total	O	0	0
			42	42		

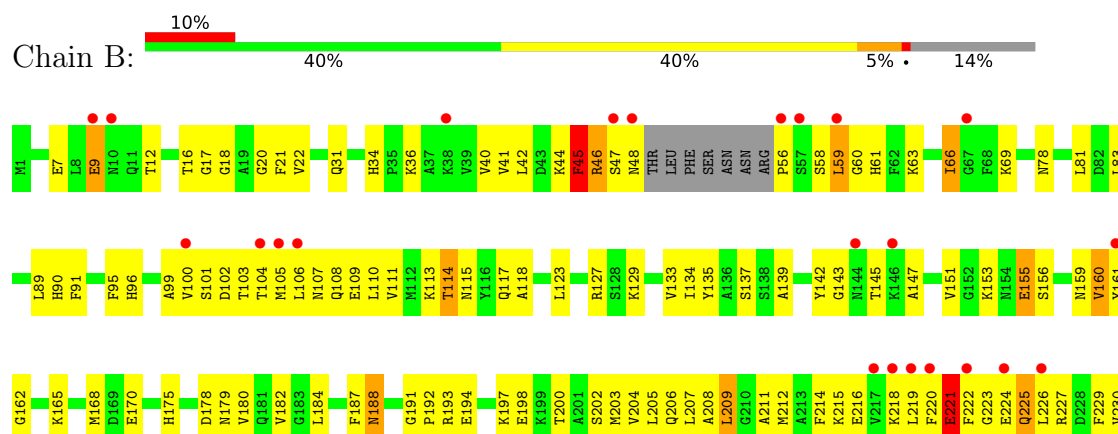
3 Residue-property plots

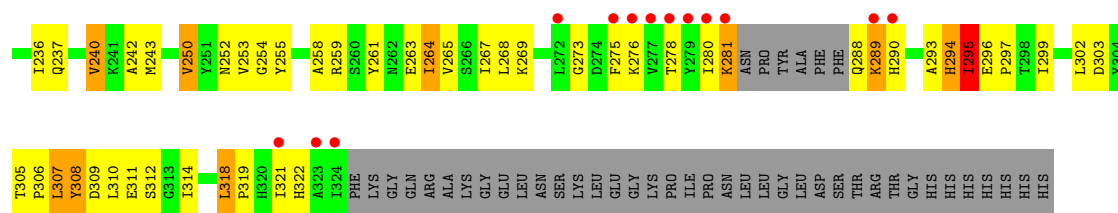
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ADP-L-glycero-D-mannoheptose-6-epimerase

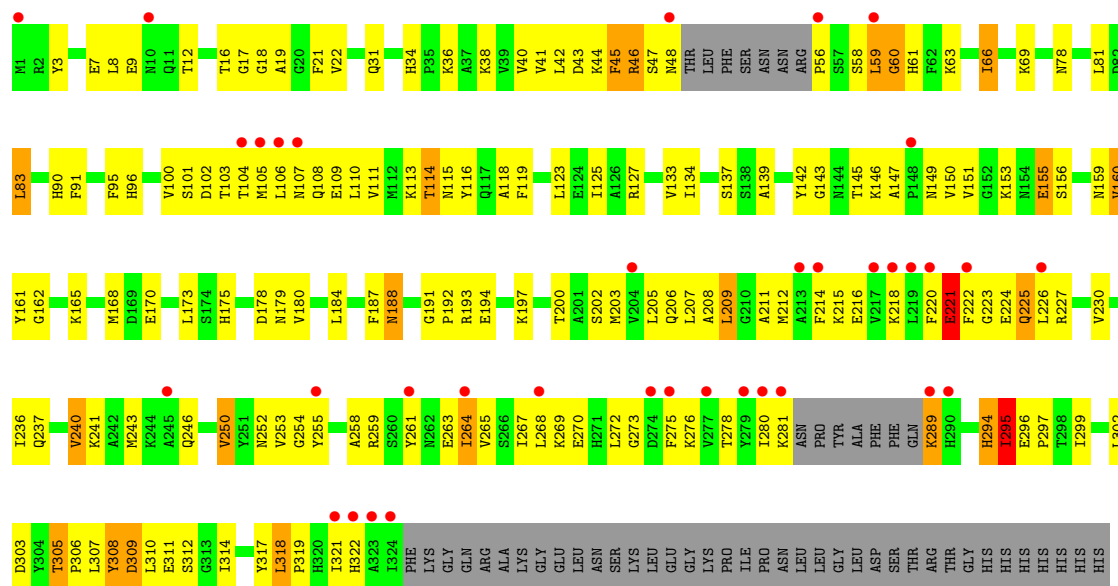


- Molecule 1: ADP-L-glycero-D-mannoheptose-6-epimerase

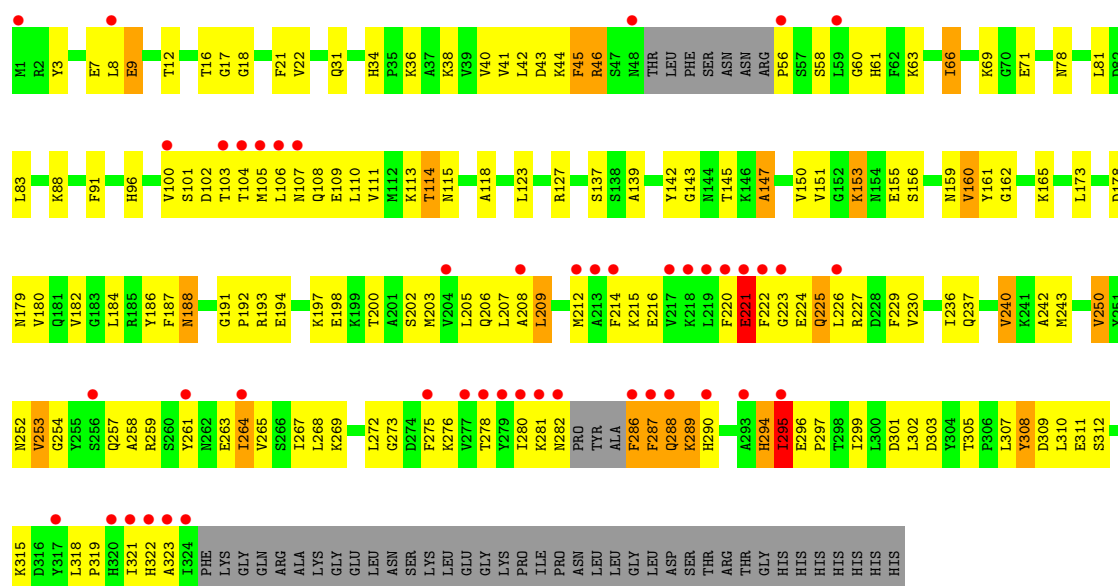




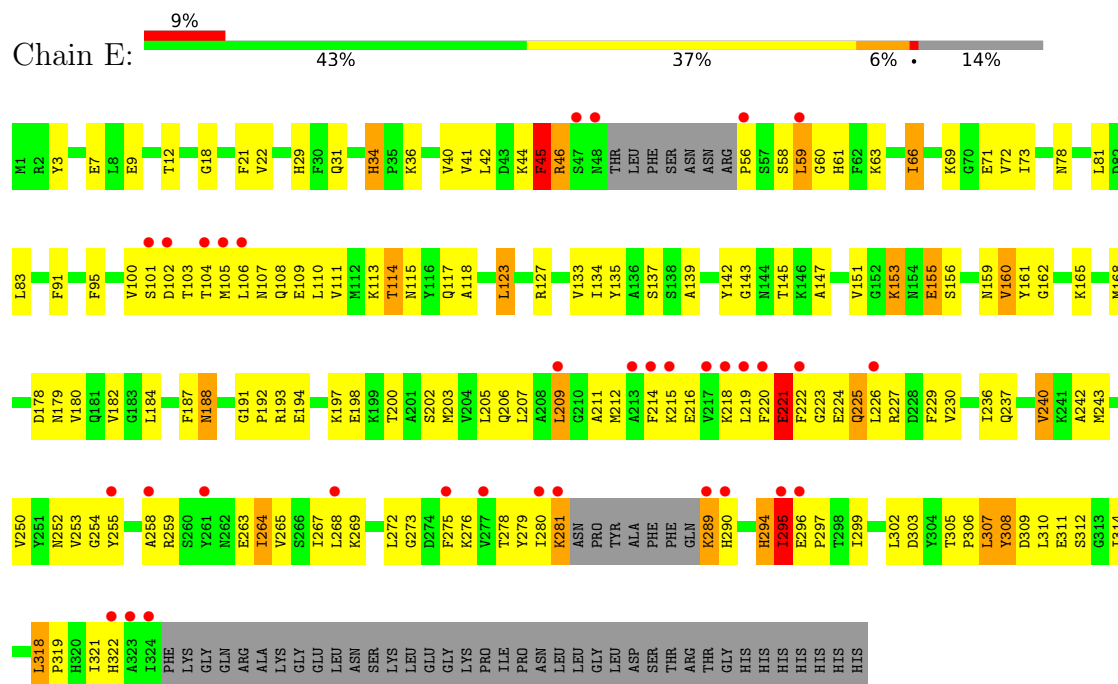
• Molecule 1: ADP-L-glycero-D-mannoheptose-6-epimerase



• Molecule 1: ADP-L-glycero-D-mannoheptose-6-epimerase



● Molecule 1: ADP-L-glycero-D-mannoheptose-6-epimerase



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	130.94Å 106.77Å 152.22Å 90.00° 108.35° 90.00°	Depositor
Resolution (Å)	53.39 – 2.55 53.39 – 2.55	Depositor EDS
% Data completeness (in resolution range)	85.6 (53.39-2.55) 85.6 (53.39-2.55)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.55Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.239 , 0.279 0.239 , 0.276	Depositor DCC
R_{free} test set	2808 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 84.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12913	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.55	0/2532	1.02	16/3415 (0.5%)
1	B	0.55	0/2541	1.02	15/3427 (0.4%)
1	C	0.54	0/2532	1.01	14/3415 (0.4%)
1	D	0.56	0/2573	1.03	17/3470 (0.5%)
1	E	0.52	0/2532	1.01	13/3415 (0.4%)
All	All	0.54	0/12710	1.02	75/17142 (0.4%)

There are no bond length outliers.

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	288	GLN	N-CA-C	7.95	122.58	109.95
1	C	307	LEU	N-CA-C	-7.70	97.80	109.96
1	B	307	LEU	N-CA-C	-7.68	97.82	109.96
1	D	307	LEU	N-CA-C	-7.57	96.93	109.80
1	A	307	LEU	N-CA-C	-7.52	98.08	109.96
1	E	197	LYS	N-CA-C	-7.46	104.17	113.20
1	D	198	GLU	CB-CA-C	-7.44	107.98	116.54
1	A	198	GLU	CB-CA-C	-7.43	108.00	116.54
1	A	294	HIS	N-CA-C	-7.22	97.48	108.67
1	B	198	GLU	CB-CA-C	-7.18	108.28	116.54
1	C	294	HIS	N-CA-C	-7.17	97.55	108.67
1	C	197	LYS	N-CA-C	-7.09	104.62	113.20
1	D	197	LYS	N-CA-C	-7.08	104.63	113.20
1	E	294	HIS	N-CA-C	-7.06	97.72	108.67
1	D	139	ALA	N-CA-C	-6.94	104.80	113.20
1	E	307	LEU	N-CA-C	-6.92	98.04	109.80
1	C	66	ILE	N-CA-C	6.91	118.50	110.62
1	E	198	GLU	CB-CA-C	-6.89	108.61	116.54
1	B	294	HIS	N-CA-C	-6.88	98.01	108.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	294	HIS	N-CA-C	-6.86	98.04	108.67
1	B	197	LYS	N-CA-C	-6.84	104.92	113.20
1	B	66	ILE	N-CA-C	6.84	118.41	110.62
1	C	139	ALA	N-CA-C	-6.74	105.02	113.18
1	A	197	LYS	N-CA-C	-6.71	105.08	113.20
1	E	309	ASP	N-CA-C	-6.59	100.15	110.36
1	B	139	ALA	N-CA-C	-6.43	105.40	113.18
1	A	139	ALA	N-CA-C	-6.36	105.51	113.20
1	B	34	HIS	CA-C-N	6.34	126.03	119.56
1	B	34	HIS	C-N-CA	6.34	126.03	119.56
1	E	139	ALA	N-CA-C	-6.33	105.55	113.20
1	E	66	ILE	N-CA-C	6.25	117.74	110.62
1	A	66	ILE	N-CA-C	6.17	117.66	110.62
1	D	66	ILE	N-CA-C	6.16	117.64	110.62
1	D	34	HIS	CA-C-N	6.13	125.81	119.56
1	D	34	HIS	C-N-CA	6.13	125.81	119.56
1	C	309	ASP	N-CA-C	-6.08	100.93	110.36
1	D	301	ASP	N-CA-C	5.98	119.05	111.69
1	A	309	ASP	N-CA-C	-5.91	101.21	110.36
1	C	34	HIS	CA-C-N	5.85	125.53	119.56
1	C	34	HIS	C-N-CA	5.85	125.53	119.56
1	C	264	ILE	N-CA-C	-5.85	105.03	110.53
1	A	301	ASP	N-CA-C	5.78	118.80	111.69
1	A	264	ILE	N-CA-C	-5.76	105.11	110.53
1	D	264	ILE	N-CA-C	-5.75	105.02	110.42
1	E	34	HIS	CA-C-N	5.73	125.40	119.56
1	E	34	HIS	C-N-CA	5.73	125.40	119.56
1	A	182	VAL	N-CA-C	5.71	115.81	107.37
1	E	295	ILE	N-CA-C	5.68	118.45	112.83
1	D	309	ASP	N-CA-C	-5.65	101.60	110.36
1	A	34	HIS	CA-C-N	5.63	125.30	119.56
1	A	34	HIS	C-N-CA	5.63	125.30	119.56
1	B	309	ASP	N-CA-C	-5.61	101.67	110.36
1	E	45	PHE	N-CA-C	5.59	122.72	110.80
1	A	147	ALA	N-CA-C	-5.58	102.89	110.36
1	C	17	GLY	N-CA-C	-5.47	106.48	114.90
1	A	9	GLU	N-CA-C	5.42	120.25	111.37
1	D	9	GLU	N-CA-C	5.41	120.24	111.37
1	E	264	ILE	N-CA-C	-5.35	105.50	110.53
1	B	182	VAL	N-CA-C	5.34	115.27	107.37
1	C	295	ILE	N-CA-C	5.31	118.08	112.83
1	B	9	GLU	N-CA-C	5.28	120.02	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	8	LEU	N-CA-C	-5.28	105.49	112.24
1	D	182	VAL	N-CA-C	5.27	115.66	107.28
1	B	45	PHE	N-CA-C	5.25	121.97	110.80
1	B	293	ALA	N-CA-C	5.21	117.73	109.96
1	B	295	ILE	N-CA-C	5.20	117.98	112.83
1	C	8	LEU	N-CA-C	-5.20	105.59	112.24
1	E	182	VAL	N-CA-C	5.19	115.53	107.28
1	B	264	ILE	N-CA-C	-5.17	105.56	110.42
1	D	147	ALA	N-CA-C	-5.16	103.44	110.36
1	A	45	PHE	N-CA-C	5.15	121.77	110.80
1	C	147	ALA	N-CA-C	-5.13	103.49	110.36
1	D	295	ILE	N-CA-C	5.12	117.90	112.83
1	A	8	LEU	N-CA-C	-5.10	105.72	112.24
1	C	60	GLY	N-CA-C	-5.01	105.90	112.82

There are no chirality outliers.

There are no planarity outliers.

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	2480	0	2469	139	0
1	B	2489	0	2477	139	0
1	C	2480	0	2469	141	0
1	D	2519	0	2501	140	0
1	E	2480	0	2469	136	0
2	A	44	0	26	3	0
2	B	44	0	26	6	0
2	C	44	0	26	4	0
2	D	44	0	25	4	0
2	E	44	0	26	5	0
3	A	68	0	0	7	0
3	B	56	0	0	4	0
3	C	36	0	0	5	0
3	D	43	0	0	3	0
3	E	42	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12913	0	12514	684	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (684) 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:C:59:LEU:HD21	1:C:101:SER:CB	1.61	1.31
1:B:59:LEU:CD2	1:B:101:SER:HB3	1.63	1.29
1:B:59:LEU:HD21	1:B:101:SER:CB	1.75	1.17
1:C:59:LEU:HD21	1:C:101:SER:HB3	1.28	1.14
1:C:59:LEU:HD21	1:C:101:SER:HB2	1.39	1.04
1:C:31:GLN:NE2	1:C:69:LYS:H	1.59	0.99
1:A:31:GLN:NE2	1:A:69:LYS:H	1.63	0.95
1:B:31:GLN:NE2	1:B:69:LYS:H	1.64	0.95
1:E:31:GLN:NE2	1:E:69:LYS:H	1.66	0.94
1:D:31:GLN:NE2	1:D:69:LYS:H	1.67	0.93
1:E:212:MET:HE1	1:E:322:HIS:HA	1.52	0.92
1:A:31:GLN:HE22	1:A:69:LYS:H	0.91	0.91
1:C:59:LEU:CD2	1:C:101:SER:HB3	2.01	0.90
1:C:31:GLN:HE22	1:C:69:LYS:N	1.69	0.89
1:C:59:LEU:CD2	1:C:101:SER:CB	2.51	0.88
1:B:59:LEU:N	1:B:59:LEU:HD23	1.89	0.88
1:D:212:MET:HE1	1:D:322:HIS:HA	1.55	0.88
1:E:31:GLN:HE22	1:E:69:LYS:N	1.72	0.87
1:B:31:GLN:HE22	1:B:69:LYS:N	1.72	0.87
1:B:237:GLN:HE22	1:B:305:THR:H	1.22	0.86
1:B:31:GLN:HE22	1:B:69:LYS:H	0.87	0.86
1:A:159:ASN:ND2	1:A:161:TYR:HB3	1.91	0.86
1:C:61:HIS:HD2	1:C:63:LYS:H	1.23	0.86
1:E:61:HIS:HD2	1:E:63:LYS:H	1.23	0.85
1:D:31:GLN:HE22	1:D:69:LYS:N	1.74	0.85
1:C:212:MET:HE1	1:C:322:HIS:HA	1.59	0.85
1:D:159:ASN:ND2	1:D:161:TYR:HB3	1.92	0.85
1:E:237:GLN:HE22	1:E:305:THR:H	1.25	0.84
1:B:61:HIS:HD2	1:B:63:LYS:H	1.22	0.84
1:A:237:GLN:HE22	1:A:305:THR:H	1.26	0.84
1:D:31:GLN:HE22	1:D:69:LYS:H	0.89	0.83
1:A:31:GLN:HE22	1:A:69:LYS:N	1.75	0.83
1:E:100:VAL:H	1:E:115:ASN:HD21	1.26	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:MET:HE1	1:A:322:HIS:HA	1.61	0.82
1:E:159:ASN:ND2	1:E:161:TYR:HB3	1.94	0.82
1:E:296:GLU:HB2	1:E:297:PRO:HD3	1.62	0.81
1:B:212:MET:HE1	1:B:322:HIS:HA	1.63	0.81
1:E:31:GLN:HE22	1:E:69:LYS:H	0.87	0.81
1:C:237:GLN:HE22	1:C:305:THR:H	1.26	0.80
1:A:100:VAL:H	1:A:115:ASN:HD21	1.28	0.80
1:B:100:VAL:H	1:B:115:ASN:HD21	1.26	0.79
1:B:159:ASN:ND2	1:B:161:TYR:HB3	1.97	0.79
1:C:18:GLY:HA3	1:C:41:VAL:HG13	1.64	0.79
1:D:100:VAL:H	1:D:115:ASN:HD21	1.27	0.79
1:D:237:GLN:HE22	1:D:305:THR:H	1.27	0.79
1:E:18:GLY:HA3	1:E:41:VAL:HG13	1.66	0.78
1:A:18:GLY:HA3	1:A:41:VAL:HG13	1.66	0.78
1:C:159:ASN:ND2	1:C:161:TYR:HB3	1.98	0.78
1:A:308:TYR:HA	1:A:312:SER:HB2	1.66	0.77
1:A:61:HIS:HD2	1:A:63:LYS:H	1.33	0.76
1:C:31:GLN:HE22	1:C:69:LYS:H	0.84	0.75
1:C:100:VAL:H	1:C:115:ASN:HD21	1.33	0.75
1:A:59:LEU:HD11	1:A:101:SER:HB2	1.68	0.74
1:D:296:GLU:HB2	1:D:297:PRO:HD3	1.68	0.74
1:C:308:TYR:HA	1:C:312:SER:HB2	1.68	0.74
1:B:308:TYR:HA	1:B:312:SER:HB2	1.70	0.74
1:E:308:TYR:HA	1:E:312:SER:HB2	1.70	0.74
1:D:308:TYR:HA	1:D:312:SER:HB2	1.70	0.73
1:A:34:HIS:HE1	3:A:403:HOH:O	1.71	0.73
1:C:146:LYS:HE2	3:C:393:HOH:O	1.89	0.72
1:D:288:GLN:N	1:D:289:LYS:HZ3	1.88	0.72
1:C:296:GLU:HB2	1:C:297:PRO:HD3	1.70	0.72
1:D:61:HIS:HD2	1:D:63:LYS:H	1.36	0.72
1:B:59:LEU:HD23	1:B:59:LEU:H	1.55	0.72
2:E:2403:NAD:O3D	3:E:384:HOH:O	2.07	0.71
1:D:221:GLU:HA	1:D:281:LYS:HE2	1.73	0.71
1:D:18:GLY:HA3	1:D:41:VAL:HG13	1.72	0.71
1:B:48:ASN:H	1:D:107:ASN:ND2	1.90	0.70
1:E:104:THR:O	1:E:106:LEU:HG	1.90	0.70
1:E:61:HIS:CD2	1:E:63:LYS:H	2.08	0.70
1:E:153:LYS:HE2	1:E:153:LYS:HA	1.74	0.70
1:B:9:GLU:HG3	1:B:36:LYS:HD3	1.74	0.70
1:B:59:LEU:HD21	1:B:101:SER:HB3	0.79	0.69
1:D:236:ILE:O	1:D:240:VAL:HG12	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:GLU:HB2	1:A:297:PRO:HD3	1.74	0.69
1:D:280:ILE:C	1:D:281:LYS:HD2	2.17	0.69
1:B:296:GLU:HB2	1:B:297:PRO:HD3	1.74	0.69
1:C:221:GLU:HA	1:C:281:LYS:HE2	1.74	0.69
1:D:22:VAL:HG22	2:D:2401:NAD:H51N	1.74	0.69
1:E:240:VAL:O	1:E:243:MET:HG2	1.92	0.69
1:E:221:GLU:HA	1:E:281:LYS:HE2	1.73	0.69
1:C:236:ILE:O	1:C:240:VAL:HG12	1.93	0.68
1:E:237:GLN:NE2	1:E:305:THR:H	1.92	0.68
1:A:9:GLU:HG3	1:A:36:LYS:HD3	1.75	0.68
1:B:61:HIS:CD2	1:B:63:LYS:H	2.09	0.68
1:D:104:THR:O	1:D:106:LEU:HG	1.93	0.68
1:B:221:GLU:HA	1:B:281:LYS:HE2	1.76	0.68
1:A:127:ARG:HD2	1:A:178:ASP:HB3	1.75	0.67
1:B:47:SER:HA	1:D:107:ASN:HD21	1.56	0.67
1:C:61:HIS:CD2	1:C:63:LYS:H	2.10	0.67
1:E:29:HIS:HE1	3:E:376:HOH:O	1.77	0.66
1:C:127:ARG:HD2	1:C:178:ASP:HB3	1.76	0.66
1:E:59:LEU:HD11	1:E:101:SER:HB2	1.77	0.66
1:A:240:VAL:O	1:A:243:MET:HG2	1.96	0.66
1:A:61:HIS:CD2	1:A:63:LYS:H	2.14	0.66
1:B:237:GLN:NE2	1:B:305:THR:H	1.92	0.66
1:D:323:ALA:HB2	3:D:400:HOH:O	1.96	0.65
1:B:59:LEU:CD2	1:B:101:SER:CB	2.50	0.65
1:D:257:GLN:HB2	3:D:384:HOH:O	1.95	0.65
1:B:18:GLY:HA3	1:B:41:VAL:HG13	1.78	0.65
1:C:237:GLN:NE2	1:C:305:THR:H	1.95	0.65
1:A:71:GLU:HA	3:A:424:HOH:O	1.97	0.65
1:B:102:ASP:O	1:B:105:MET:HG2	1.98	0.64
1:B:104:THR:O	1:B:106:LEU:HG	1.97	0.64
1:E:179:ASN:ND2	1:E:180:VAL:H	1.95	0.64
1:E:103:THR:HB	1:E:200:THR:CG2	2.28	0.64
1:B:103:THR:HB	1:B:200:THR:CG2	2.28	0.64
1:A:221:GLU:HA	1:A:281:LYS:HE2	1.78	0.64
1:D:102:ASP:O	1:D:105:MET:HG2	1.97	0.64
1:D:287:PHE:C	1:D:289:LYS:HZ3	2.05	0.64
1:C:104:THR:O	1:C:106:LEU:HG	1.98	0.63
1:C:165:LYS:NZ	2:C:2403:NAD:O3D	2.31	0.63
1:E:258:ALA:O	1:E:259:ARG:HD2	1.99	0.63
1:D:9:GLU:HG3	1:D:36:LYS:HD3	1.79	0.63
1:A:289:LYS:HD2	1:A:289:LYS:N	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ASP:O	1:C:105:MET:HG2	1.99	0.63
1:B:288:GLN:N	1:B:289:LYS:HZ3	1.96	0.63
1:E:236:ILE:O	1:E:240:VAL:HG12	1.97	0.63
1:A:102:ASP:O	1:A:105:MET:HG2	1.99	0.63
1:A:159:ASN:HD21	1:A:161:TYR:HB3	1.64	0.63
1:A:103:THR:HB	1:A:200:THR:CG2	2.29	0.62
1:C:109:GLU:O	1:C:113:LYS:HG2	2.00	0.62
1:C:280:ILE:C	1:C:281:LYS:HD2	2.25	0.62
1:A:237:GLN:NE2	1:A:305:THR:H	1.95	0.62
1:E:191:GLY:O	1:E:194:GLU:HG2	1.99	0.62
1:C:22:VAL:CG2	2:C:2403:NAD:H51N	2.29	0.62
1:D:103:THR:HB	1:D:200:THR:CG2	2.29	0.62
1:C:151:VAL:HG23	1:C:252:ASN:ND2	2.15	0.62
1:B:220:PHE:HA	1:B:280:ILE:HG23	1.81	0.62
1:A:104:THR:O	1:A:106:LEU:HG	2.00	0.61
1:D:44:LYS:O	1:D:45:PHE:HB2	1.99	0.61
1:A:280:ILE:C	1:A:281:LYS:HD2	2.25	0.61
1:D:237:GLN:NE2	1:D:305:THR:H	1.97	0.61
1:B:170:GLU:OE1	1:E:69:LYS:HD2	1.99	0.61
1:D:61:HIS:CD2	1:D:63:LYS:H	2.18	0.61
1:C:7:GLU:HG3	1:C:36:LYS:HD2	1.82	0.61
1:A:264:ILE:O	1:A:268:LEU:HB2	2.01	0.61
1:E:34:HIS:HE1	3:E:376:HOH:O	1.84	0.61
1:E:202:SER:O	1:E:206:GLN:HG2	2.01	0.61
1:C:191:GLY:O	1:C:194:GLU:HG2	2.00	0.60
1:C:264:ILE:O	1:C:268:LEU:HB2	2.01	0.60
1:D:286:PHE:C	1:D:288:GLN:H	2.09	0.60
1:E:22:VAL:HG22	2:E:2403:NAD:H51N	1.82	0.60
1:C:44:LYS:O	1:C:45:PHE:HB2	2.01	0.60
1:A:107:ASN:OD1	1:A:110:LEU:HD13	2.01	0.60
1:C:103:THR:HG23	1:C:104:THR:H	1.67	0.60
1:C:149:ASN:HA	3:C:382:HOH:O	2.01	0.60
1:E:137:SER:O	2:E:2403:NAD:H6N	2.01	0.60
1:A:153:LYS:HA	1:A:153:LYS:HE2	1.83	0.60
1:C:7:GLU:CG	1:C:36:LYS:HD2	2.32	0.60
1:C:103:THR:HB	1:C:200:THR:CG2	2.31	0.60
1:D:22:VAL:CG2	2:D:2401:NAD:H51N	2.32	0.60
1:E:280:ILE:C	1:E:281:LYS:HD2	2.26	0.60
1:A:59:LEU:HD11	1:A:101:SER:CB	2.32	0.60
1:C:220:PHE:HA	1:C:280:ILE:HG23	1.83	0.60
1:D:289:LYS:HD2	1:D:289:LYS:N	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:HIS:HE1	3:A:403:HOH:O	1.84	0.60
1:A:103:THR:HB	1:A:200:THR:HG21	1.84	0.60
1:B:113:LYS:HD2	3:B:401:HOH:O	2.01	0.60
1:C:103:THR:HG23	1:C:104:THR:N	2.17	0.60
1:E:264:ILE:O	1:E:268:LEU:HB2	2.02	0.60
1:B:188:ASN:ND2	3:B:390:HOH:O	2.35	0.60
1:B:216:GLU:HG3	1:B:276:LYS:HB3	1.84	0.60
1:D:281:LYS:HD2	1:D:281:LYS:N	2.17	0.60
1:A:236:ILE:O	1:A:240:VAL:HG12	2.02	0.59
1:B:280:ILE:C	1:B:281:LYS:HD2	2.28	0.59
1:C:223:GLY:HA2	1:C:225:GLN:OE1	2.01	0.59
1:B:240:VAL:O	1:B:243:MET:HG2	2.02	0.59
1:A:105:MET:O	1:A:105:MET:HG3	2.02	0.59
1:E:187:PHE:O	1:E:230:VAL:HG12	2.02	0.59
1:A:85:ARG:HD3	3:A:430:HOH:O	2.03	0.59
1:A:263:GLU:O	1:A:267:ILE:HG13	2.02	0.59
1:A:191:GLY:O	1:A:194:GLU:HG2	2.02	0.59
1:E:78:ASN:ND2	1:E:118:ALA:HB2	2.18	0.59
1:A:216:GLU:HG3	1:A:276:LYS:HB3	1.85	0.58
1:A:220:PHE:HA	1:A:280:ILE:HG23	1.85	0.58
1:B:109:GLU:O	1:B:113:LYS:HG2	2.03	0.58
1:E:127:ARG:HD2	1:E:178:ASP:HB3	1.85	0.58
2:B:2401:NAD:O3D	3:B:403:HOH:O	2.04	0.58
1:C:78:ASN:ND2	1:C:118:ALA:HB2	2.18	0.58
1:D:220:PHE:HA	1:D:280:ILE:HG23	1.84	0.58
1:B:179:ASN:ND2	1:B:180:VAL:H	2.02	0.58
1:C:47:SER:HA	1:E:107:ASN:HD21	1.66	0.58
1:E:225:GLN:CD	1:E:225:GLN:H	2.11	0.58
1:C:267:ILE:HD13	1:C:311:GLU:HG3	1.85	0.58
1:D:159:ASN:HD22	1:D:161:TYR:HB3	1.68	0.58
1:A:22:VAL:HG22	2:A:2402:NAD:H51N	1.85	0.58
1:A:225:GLN:H	1:A:225:GLN:CD	2.11	0.58
1:C:237:GLN:NE2	1:C:241:LYS:HZ1	2.01	0.58
1:A:78:ASN:ND2	1:A:118:ALA:HB2	2.18	0.58
1:B:59:LEU:CD2	1:B:59:LEU:N	2.61	0.58
1:C:263:GLU:O	1:C:267:ILE:HG13	2.03	0.58
1:D:153:LYS:HE2	1:D:153:LYS:HA	1.85	0.58
1:E:220:PHE:HA	1:E:280:ILE:HG23	1.86	0.58
1:B:191:GLY:O	1:B:194:GLU:HG2	2.04	0.58
1:D:107:ASN:OD1	1:D:110:LEU:HD13	2.03	0.58
1:A:202:SER:O	1:A:206:GLN:HG2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ILE:O	1:B:240:VAL:HG12	2.03	0.58
1:D:192:PRO:O	1:D:193:ARG:HB2	2.03	0.58
1:D:240:VAL:O	1:D:243:MET:HG2	2.03	0.58
1:C:216:GLU:HG3	1:C:276:LYS:HB3	1.86	0.58
1:A:7:GLU:CG	1:A:36:LYS:HD2	2.34	0.57
1:D:159:ASN:ND2	1:D:162:GLY:H	2.00	0.57
1:E:103:THR:HB	1:E:200:THR:HG21	1.84	0.57
1:C:46:ARG:HA	1:C:58:SER:O	2.03	0.57
1:E:103:THR:HG23	1:E:104:THR:H	1.68	0.57
1:A:7:GLU:HG3	1:A:36:LYS:HD2	1.87	0.57
1:A:44:LYS:O	1:A:45:PHE:HB2	2.03	0.57
1:B:103:THR:HG23	1:B:104:THR:H	1.70	0.57
1:B:159:ASN:HD21	1:B:161:TYR:HB3	1.69	0.57
1:D:46:ARG:HA	1:D:58:SER:O	2.04	0.57
1:B:22:VAL:HG22	2:B:2401:NAD:H51N	1.86	0.57
1:D:202:SER:O	1:D:206:GLN:HG2	2.04	0.57
1:D:258:ALA:O	1:D:259:ARG:HD2	2.04	0.57
1:B:159:ASN:ND2	1:B:162:GLY:H	2.03	0.57
1:C:159:ASN:ND2	1:C:162:GLY:H	2.02	0.57
1:E:44:LYS:O	1:E:45:PHE:HB2	2.03	0.57
1:A:247:LYS:HD3	3:A:426:HOH:O	2.02	0.57
1:B:103:THR:HG23	1:B:104:THR:N	2.19	0.57
1:D:103:THR:HG23	1:D:104:THR:H	1.70	0.57
1:C:153:LYS:HE2	1:C:153:LYS:HA	1.86	0.57
1:A:46:ARG:HA	1:A:58:SER:O	2.05	0.57
1:D:103:THR:HG23	1:D:104:THR:N	2.20	0.56
1:E:103:THR:HG23	1:E:104:THR:N	2.20	0.56
1:B:20:GLY:HA3	2:B:2401:NAD:H52A	1.86	0.56
1:B:127:ARG:HD2	1:B:178:ASP:HB3	1.87	0.56
1:C:269:LYS:HA	1:C:273:GLY:O	2.05	0.56
1:E:9:GLU:HG3	1:E:36:LYS:HD3	1.86	0.56
1:E:46:ARG:HB2	1:E:60:GLY:O	2.06	0.56
1:E:102:ASP:O	1:E:105:MET:HG2	2.04	0.56
1:E:289:LYS:N	1:E:289:LYS:HD2	2.19	0.56
1:C:187:PHE:O	1:C:230:VAL:HG12	2.06	0.56
1:A:109:GLU:O	1:A:113:LYS:HG2	2.04	0.56
1:A:187:PHE:O	1:A:230:VAL:HG12	2.06	0.56
1:C:254:GLY:H	1:C:295:ILE:HD11	1.71	0.56
1:E:203:MET:O	1:E:207:LEU:HG	2.05	0.56
1:C:46:ARG:HB2	1:C:60:GLY:O	2.06	0.56
1:C:225:GLN:H	1:C:225:GLN:CD	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:LEU:C	1:D:42:LEU:HD23	2.30	0.56
1:D:179:ASN:ND2	1:D:180:VAL:H	2.04	0.56
1:D:127:ARG:HD2	1:D:178:ASP:HB3	1.87	0.56
1:E:108:GLN:HG3	1:E:160:VAL:CG1	2.36	0.56
1:E:109:GLU:O	1:E:113:LYS:HG2	2.06	0.56
1:A:159:ASN:HD22	1:A:161:TYR:HB3	1.71	0.55
1:B:103:THR:HB	1:B:200:THR:HG21	1.86	0.55
1:B:187:PHE:O	1:B:230:VAL:HG12	2.07	0.55
1:C:22:VAL:HG22	2:C:2403:NAD:H51N	1.87	0.55
1:C:240:VAL:O	1:C:243:MET:HG2	2.04	0.55
1:E:46:ARG:HA	1:E:58:SER:O	2.06	0.55
1:E:159:ASN:HD21	1:E:161:TYR:HB3	1.70	0.55
1:A:100:VAL:HG22	1:A:115:ASN:ND2	2.22	0.55
1:B:269:LYS:HA	1:B:273:GLY:O	2.07	0.55
1:C:105:MET:O	1:C:105:MET:HG3	2.06	0.55
1:D:108:GLN:HG3	1:D:160:VAL:CG1	2.36	0.55
1:D:159:ASN:HD21	1:D:161:TYR:HB3	1.70	0.55
1:E:216:GLU:HG3	1:E:276:LYS:HB3	1.88	0.55
1:A:103:THR:HG23	1:A:104:THR:H	1.72	0.55
1:B:105:MET:HG3	1:B:105:MET:O	2.06	0.55
1:E:7:GLU:HG3	1:E:36:LYS:HD2	1.87	0.55
1:A:212:MET:HG3	1:A:272:LEU:HD21	1.89	0.55
1:C:258:ALA:O	1:C:259:ARG:HD2	2.07	0.55
1:C:289:LYS:N	1:C:289:LYS:HD2	2.21	0.55
1:D:103:THR:HB	1:D:200:THR:HG21	1.89	0.55
1:C:103:THR:HB	1:C:200:THR:HG21	1.88	0.55
1:C:227:ARG:NH2	1:C:289:LYS:HB2	2.21	0.55
1:E:269:LYS:HA	1:E:273:GLY:O	2.06	0.55
1:B:44:LYS:O	1:B:45:PHE:HB2	2.05	0.55
1:B:225:GLN:CD	1:B:225:GLN:H	2.13	0.55
1:C:12:THR:HB	1:C:91:PHE:HA	1.89	0.55
1:C:295:ILE:HG23	1:C:299:ILE:HG13	1.89	0.55
1:D:7:GLU:CG	1:D:36:LYS:HD2	2.37	0.55
1:E:192:PRO:O	1:E:193:ARG:HB2	2.07	0.55
1:A:103:THR:HG23	1:A:104:THR:N	2.22	0.55
1:E:42:LEU:C	1:E:42:LEU:HD23	2.32	0.55
1:A:142:TYR:O	1:A:145:THR:HG23	2.08	0.54
1:C:90:HIS:HB2	3:C:385:HOH:O	2.06	0.54
1:C:226:LEU:HB3	1:C:258:ALA:HB1	1.89	0.54
1:D:216:GLU:HG3	1:D:276:LYS:HB3	1.88	0.54
1:D:223:GLY:HA2	1:D:225:GLN:OE1	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:264:ILE:O	1:D:268:LEU:HB2	2.07	0.54
1:E:7:GLU:CG	1:E:36:LYS:HD2	2.37	0.54
1:D:191:GLY:O	1:D:194:GLU:HG2	2.07	0.54
1:B:218:LYS:HD2	1:B:218:LYS:C	2.32	0.54
1:B:223:GLY:HA2	1:B:225:GLN:OE1	2.07	0.54
1:D:288:GLN:CA	1:D:289:LYS:HZ3	2.21	0.54
1:E:105:MET:O	1:E:105:MET:HG3	2.07	0.54
1:B:258:ALA:O	1:B:259:ARG:HD2	2.07	0.54
1:B:263:GLU:O	1:B:267:ILE:HG13	2.08	0.54
1:D:226:LEU:HB3	1:D:258:ALA:HB1	1.88	0.54
1:D:269:LYS:HG2	1:D:275:PHE:CE1	2.42	0.54
1:E:226:LEU:HB3	1:E:258:ALA:HB1	1.88	0.54
1:E:281:LYS:HD2	1:E:281:LYS:N	2.22	0.54
1:A:258:ALA:O	1:A:259:ARG:HD2	2.07	0.54
1:B:12:THR:HB	1:B:91:PHE:HA	1.90	0.54
1:B:295:ILE:CG2	1:B:299:ILE:HD11	2.37	0.54
1:D:269:LYS:HA	1:D:273:GLY:O	2.08	0.54
1:E:187:PHE:O	1:E:188:ASN:C	2.51	0.54
1:A:46:ARG:HB2	1:A:60:GLY:O	2.08	0.54
1:B:281:LYS:HD2	1:B:281:LYS:N	2.23	0.54
1:C:125:ILE:HD11	3:C:390:HOH:O	2.06	0.54
1:C:202:SER:O	1:C:206:GLN:HG2	2.08	0.53
1:A:254:GLY:H	1:A:295:ILE:HD11	1.72	0.53
1:C:48:ASN:H	1:E:107:ASN:ND2	2.06	0.53
1:E:22:VAL:CG2	2:E:2403:NAD:H51N	2.38	0.53
1:E:223:GLY:HA2	1:E:225:GLN:OE1	2.08	0.53
1:B:289:LYS:HD2	1:B:289:LYS:N	2.23	0.53
1:A:223:GLY:HA2	1:A:225:GLN:OE1	2.09	0.53
1:B:202:SER:O	1:B:206:GLN:HG2	2.07	0.53
1:C:281:LYS:HD2	1:C:281:LYS:N	2.23	0.53
1:E:151:VAL:HG23	1:E:252:ASN:ND2	2.23	0.53
1:B:254:GLY:H	1:B:295:ILE:HD11	1.73	0.53
1:D:287:PHE:C	1:D:289:LYS:NZ	2.66	0.53
1:E:159:ASN:ND2	1:E:162:GLY:H	2.06	0.53
1:D:78:ASN:ND2	1:D:118:ALA:HB2	2.24	0.53
1:C:3:TYR:CD1	1:C:237:GLN:HG3	2.44	0.53
1:D:78:ASN:HD21	1:D:114:THR:HA	1.74	0.53
1:C:133:VAL:C	1:C:134:ILE:HD12	2.33	0.53
1:E:295:ILE:CG2	1:E:299:ILE:HD11	2.38	0.53
1:B:264:ILE:O	1:B:268:LEU:HB2	2.09	0.53
1:D:254:GLY:H	1:D:295:ILE:HD11	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ARG:HA	1:B:58:SER:O	2.08	0.52
1:E:214:PHE:C	1:E:216:GLU:H	2.16	0.52
1:A:269:LYS:HA	1:A:273:GLY:O	2.09	0.52
1:A:281:LYS:HD2	1:A:281:LYS:N	2.24	0.52
1:D:105:MET:HG3	1:D:105:MET:O	2.08	0.52
1:E:59:LEU:HD11	1:E:101:SER:CB	2.38	0.52
1:A:159:ASN:ND2	1:A:162:GLY:H	2.06	0.52
1:C:267:ILE:HD12	1:C:310:LEU:HG	1.90	0.52
1:D:225:GLN:CD	1:D:225:GLN:H	2.15	0.52
1:E:159:ASN:HD22	1:E:161:TYR:HB3	1.70	0.52
1:C:192:PRO:O	1:C:193:ARG:HB2	2.10	0.52
1:C:214:PHE:C	1:C:216:GLU:H	2.17	0.52
1:C:142:TYR:O	1:C:145:THR:HG23	2.10	0.52
1:C:237:GLN:HE22	1:C:305:THR:N	2.04	0.52
1:E:107:ASN:OD1	1:E:110:LEU:HD13	2.09	0.52
1:E:207:LEU:HD12	1:E:264:ILE:HG21	1.92	0.52
1:C:108:GLN:HG3	1:C:160:VAL:CG1	2.39	0.52
1:E:78:ASN:HD21	1:E:114:THR:HA	1.74	0.52
1:B:78:ASN:HD21	1:B:114:THR:HA	1.74	0.52
1:A:226:LEU:HB3	1:A:258:ALA:HB1	1.92	0.52
1:E:267:ILE:HD13	1:E:311:GLU:HG3	1.92	0.52
1:B:137:SER:HA	1:B:165:LYS:HD2	1.92	0.51
1:D:267:ILE:HD13	1:D:311:GLU:HG3	1.92	0.51
1:D:108:GLN:HG3	1:D:160:VAL:HG11	1.91	0.51
1:B:269:LYS:HG2	1:B:275:PHE:CE1	2.46	0.51
1:D:212:MET:HG3	1:D:272:LEU:HD21	1.91	0.51
1:E:295:ILE:HG23	1:E:299:ILE:HG13	1.91	0.51
1:B:100:VAL:HG22	1:B:115:ASN:ND2	2.24	0.51
1:A:237:GLN:HE22	1:A:305:THR:N	2.04	0.51
1:A:237:GLN:NE2	1:A:241:LYS:HZ1	2.08	0.51
1:D:7:GLU:HG3	1:D:36:LYS:HD2	1.91	0.51
1:D:214:PHE:C	1:D:216:GLU:H	2.18	0.51
1:E:12:THR:HB	1:E:91:PHE:HA	1.92	0.51
1:B:153:LYS:HE2	1:B:153:LYS:HA	1.91	0.51
1:D:69:LYS:O	1:D:69:LYS:HG3	2.11	0.51
1:D:142:TYR:O	1:D:145:THR:HG23	2.10	0.51
1:A:12:THR:HB	1:A:91:PHE:HA	1.93	0.51
1:B:78:ASN:ND2	1:B:118:ALA:HB2	2.25	0.51
1:E:269:LYS:HG2	1:E:275:PHE:CE1	2.45	0.51
1:D:109:GLU:O	1:D:113:LYS:HG2	2.10	0.51
1:A:179:ASN:ND2	1:A:180:VAL:H	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:PHE:O	1:B:188:ASN:C	2.54	0.51
1:C:187:PHE:O	1:C:188:ASN:C	2.54	0.51
1:C:319:PRO:O	1:C:322:HIS:HB2	2.11	0.51
1:C:212:MET:HG3	1:C:272:LEU:HD21	1.91	0.50
1:D:151:VAL:HG23	1:D:252:ASN:ND2	2.26	0.50
1:D:295:ILE:CG2	1:D:299:ILE:HD11	2.40	0.50
1:A:187:PHE:O	1:A:188:ASN:C	2.52	0.50
1:A:295:ILE:HG23	1:A:299:ILE:HG13	1.93	0.50
1:B:237:GLN:HE22	1:B:305:THR:N	2.01	0.50
1:C:9:GLU:HG3	1:C:36:LYS:HD3	1.93	0.50
1:C:218:LYS:C	1:C:218:LYS:HD2	2.37	0.50
1:B:7:GLU:HG3	1:B:36:LYS:HD2	1.93	0.50
1:D:286:PHE:N	1:D:286:PHE:CD2	2.78	0.50
1:B:42:LEU:C	1:B:42:LEU:HD23	2.36	0.50
1:B:214:PHE:C	1:B:216:GLU:H	2.19	0.50
1:C:56:PRO:HA	1:C:104:THR:OG1	2.11	0.50
1:D:12:THR:HB	1:D:91:PHE:HA	1.94	0.50
1:D:267:ILE:HD12	1:D:310:LEU:HG	1.94	0.50
1:A:42:LEU:HD23	1:A:42:LEU:C	2.37	0.49
1:A:214:PHE:C	1:A:216:GLU:H	2.20	0.49
1:B:165:LYS:NZ	2:B:2401:NAD:O3D	2.43	0.49
1:D:151:VAL:HG11	1:D:250:VAL:HG22	1.93	0.49
1:B:192:PRO:O	1:B:193:ARG:HB2	2.12	0.49
1:C:134:ILE:HD12	1:C:134:ILE:N	2.28	0.49
1:E:307:LEU:HB2	1:E:308:TYR:CD2	2.47	0.49
1:B:142:TYR:O	1:B:145:THR:HG23	2.12	0.49
1:A:56:PRO:HA	1:A:104:THR:OG1	2.13	0.49
1:D:208:ALA:O	1:D:212:MET:HG3	2.12	0.49
1:E:267:ILE:HD12	1:E:310:LEU:HG	1.94	0.49
1:D:187:PHE:O	1:D:188:ASN:C	2.54	0.49
1:A:78:ASN:HD21	1:A:114:THR:HA	1.76	0.49
1:B:151:VAL:HG11	1:B:250:VAL:HG22	1.94	0.49
1:D:17:GLY:CA	2:D:2401:NAD:H4B	2.42	0.49
1:D:46:ARG:HB2	1:D:60:GLY:O	2.12	0.49
1:B:17:GLY:CA	2:B:2401:NAD:H4B	2.43	0.49
1:B:175:HIS:HE1	1:E:71:GLU:OE2	1.95	0.49
1:C:295:ILE:CG2	1:C:299:ILE:HD11	2.43	0.49
1:E:108:GLN:HG3	1:E:160:VAL:HG11	1.93	0.49
1:B:7:GLU:CG	1:B:36:LYS:HD2	2.42	0.49
1:B:108:GLN:HG3	1:B:160:VAL:CG1	2.43	0.49
1:D:295:ILE:HG23	1:D:299:ILE:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:LEU:C	1:C:42:LEU:HD23	2.38	0.49
1:C:46:ARG:HB3	1:E:108:GLN:HB3	1.95	0.49
1:C:214:PHE:C	1:C:216:GLU:N	2.71	0.49
1:C:255:TYR:HD1	1:C:306:PRO:HB2	1.78	0.49
1:E:133:VAL:C	1:E:134:ILE:HD12	2.38	0.49
1:A:242:ALA:HA	1:A:302:LEU:HD22	1.95	0.49
1:C:108:GLN:HG3	1:C:160:VAL:HG11	1.95	0.49
1:C:179:ASN:ND2	1:C:180:VAL:H	2.11	0.49
1:B:208:ALA:O	1:B:212:MET:HG3	2.13	0.48
1:C:203:MET:O	1:C:207:LEU:HG	2.13	0.48
1:A:192:PRO:O	1:A:193:ARG:HB2	2.13	0.48
1:B:46:ARG:HB3	1:D:108:GLN:HB3	1.93	0.48
1:B:267:ILE:HD12	1:B:310:LEU:HG	1.95	0.48
1:D:221:GLU:OE2	1:D:282:ASN:N	2.46	0.48
1:D:187:PHE:O	1:D:230:VAL:HG12	2.13	0.48
1:D:227:ARG:NH2	1:D:289:LYS:HB2	2.28	0.48
1:E:69:LYS:O	1:E:69:LYS:HG3	2.13	0.48
1:A:218:LYS:HD2	1:A:218:LYS:C	2.38	0.48
1:A:225:GLN:H	1:A:225:GLN:NE2	2.11	0.48
1:A:269:LYS:HG2	1:A:275:PHE:CE1	2.49	0.48
1:C:78:ASN:HD21	1:C:114:THR:HA	1.79	0.48
1:E:104:THR:O	1:E:106:LEU:N	2.47	0.48
1:E:134:ILE:HD12	1:E:134:ILE:N	2.29	0.48
1:B:63:LYS:O	1:B:66:ILE:HG12	2.13	0.48
1:C:159:ASN:HD22	1:C:161:TYR:HB3	1.75	0.48
1:E:214:PHE:C	1:E:216:GLU:N	2.70	0.48
1:E:263:GLU:O	1:E:267:ILE:HG13	2.14	0.48
1:A:124:GLU:OE1	1:D:88:LYS:HE2	2.13	0.48
1:B:207:LEU:HD12	1:B:264:ILE:HG21	1.96	0.48
1:B:255:TYR:HD1	1:B:306:PRO:HB2	1.79	0.47
1:C:207:LEU:HD12	1:C:264:ILE:HG21	1.97	0.47
1:D:237:GLN:HE22	1:D:305:THR:N	2.04	0.47
1:D:230:VAL:HB	1:D:254:GLY:HA2	1.96	0.47
1:A:203:MET:HG3	1:A:261:TYR:CE1	2.49	0.47
1:B:214:PHE:C	1:B:216:GLU:N	2.72	0.47
1:A:319:PRO:O	1:A:322:HIS:HB2	2.14	0.47
1:E:63:LYS:O	1:E:66:ILE:HG12	2.14	0.47
1:D:173:LEU:HD21	1:D:250:VAL:HG13	1.97	0.47
1:A:71:GLU:OE2	1:C:175:HIS:HE1	1.98	0.47
1:C:159:ASN:HD21	1:C:161:TYR:HB3	1.74	0.47
1:D:104:THR:O	1:D:106:LEU:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLN:HG3	1:A:160:VAL:CG1	2.44	0.47
1:A:175:HIS:HE1	1:D:71:GLU:OE2	1.97	0.47
1:C:155:GLU:H	1:C:155:GLU:HG2	1.44	0.47
1:C:269:LYS:HG2	1:C:275:PHE:CE1	2.49	0.47
1:D:203:MET:HG3	1:D:261:TYR:CE1	2.49	0.47
1:D:286:PHE:C	1:D:288:GLN:N	2.73	0.47
1:E:212:MET:HG3	1:E:272:LEU:HD21	1.96	0.47
1:E:230:VAL:HB	1:E:254:GLY:HA2	1.96	0.47
1:E:294:HIS:NE2	1:E:296:GLU:HG3	2.29	0.47
1:A:111:VAL:O	1:A:115:ASN:HB2	2.15	0.47
1:C:295:ILE:HG23	1:C:295:ILE:O	2.13	0.47
1:D:296:GLU:HB2	1:D:297:PRO:CD	2.41	0.47
1:E:165:LYS:NZ	2:E:2403:NAD:O3D	2.46	0.47
1:A:3:TYR:CD1	1:A:237:GLN:HG3	2.50	0.47
1:B:143:GLY:HA3	1:B:156:SER:O	2.15	0.47
1:C:107:ASN:O	1:C:111:VAL:HG23	2.15	0.47
1:B:227:ARG:HB2	1:B:229:PHE:CZ	2.50	0.47
1:C:209:LEU:CD1	1:C:321:ILE:HG23	2.45	0.47
1:D:295:ILE:HG23	1:D:295:ILE:O	2.15	0.47
1:E:3:TYR:CD1	1:E:237:GLN:HG3	2.50	0.47
1:E:72:VAL:HG12	1:E:73:ILE:N	2.30	0.47
1:A:69:LYS:HD2	1:C:170:GLU:OE1	2.15	0.46
1:B:147:ALA:HB2	1:B:290:HIS:O	2.15	0.46
1:B:203:MET:O	1:B:207:LEU:HG	2.16	0.46
1:B:69:LYS:O	1:B:69:LYS:HG3	2.15	0.46
1:E:100:VAL:N	1:E:115:ASN:HD21	2.04	0.46
1:B:46:ARG:HB2	1:B:60:GLY:O	2.15	0.46
1:B:133:VAL:C	1:B:134:ILE:HD12	2.41	0.46
1:E:295:ILE:HG23	1:E:295:ILE:O	2.15	0.46
1:B:226:LEU:HB3	1:B:258:ALA:HB1	1.95	0.46
1:C:109:GLU:HG3	1:C:113:LYS:HE2	1.97	0.46
1:D:263:GLU:O	1:D:267:ILE:HG13	2.15	0.46
1:A:295:ILE:CG2	1:A:299:ILE:HD11	2.46	0.46
1:B:203:MET:HG3	1:B:261:TYR:CE1	2.50	0.46
1:E:254:GLY:H	1:E:295:ILE:HD11	1.79	0.46
1:B:159:ASN:HD22	1:B:161:TYR:HB3	1.80	0.46
1:C:107:ASN:OD1	1:C:110:LEU:HD13	2.15	0.46
1:A:165:LYS:NZ	2:A:2402:NAD:O3D	2.45	0.46
1:A:267:ILE:HD12	1:A:310:LEU:HG	1.98	0.46
1:B:111:VAL:O	1:B:115:ASN:HB2	2.16	0.46
1:B:134:ILE:HD12	1:B:134:ILE:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:GLU:CB	1:D:297:PRO:HD3	2.41	0.46
1:C:69:LYS:HG3	1:C:69:LYS:O	2.16	0.45
1:E:59:LEU:HG	1:E:101:SER:HB3	1.98	0.45
1:A:101:SER:OG	1:A:103:THR:HG22	2.15	0.45
1:B:202:SER:OG	1:B:204:VAL:HG22	2.16	0.45
1:E:225:GLN:H	1:E:225:GLN:NE2	2.14	0.45
1:A:137:SER:O	2:A:2402:NAD:H6N	2.16	0.45
1:A:225:GLN:NE2	1:A:225:GLN:N	2.64	0.45
1:B:230:VAL:HB	1:B:254:GLY:HA2	1.98	0.45
1:D:143:GLY:HA3	1:D:156:SER:O	2.17	0.45
1:C:230:VAL:HB	1:C:254:GLY:HA2	1.98	0.45
1:C:296:GLU:HB2	1:C:297:PRO:CD	2.43	0.45
1:E:143:GLY:HA3	1:E:156:SER:O	2.17	0.45
1:A:72:VAL:HG12	1:A:73:ILE:N	2.31	0.45
1:C:215:LYS:O	1:C:275:PHE:HB2	2.16	0.45
1:E:319:PRO:O	1:E:322:HIS:HB2	2.16	0.45
1:B:16:THR:OG1	1:B:96:HIS:HA	2.17	0.45
1:B:48:ASN:H	1:D:107:ASN:HD22	1.61	0.45
1:D:294:HIS:NE2	1:D:296:GLU:HG3	2.31	0.45
1:E:242:ALA:HA	1:E:302:LEU:HD22	1.99	0.45
1:A:214:PHE:C	1:A:216:GLU:N	2.74	0.45
1:B:108:GLN:HG3	1:B:160:VAL:HG11	1.97	0.45
1:B:267:ILE:HD13	1:B:311:GLU:HG3	1.99	0.45
1:E:72:VAL:CG1	1:E:73:ILE:N	2.79	0.45
1:E:265:VAL:HG13	1:E:275:PHE:CE2	2.52	0.45
1:A:104:THR:O	1:A:106:LEU:N	2.50	0.45
1:A:137:SER:HA	1:A:165:LYS:HD2	1.99	0.45
1:B:218:LYS:HD2	1:B:219:LEU:N	2.32	0.45
1:B:307:LEU:HB2	1:B:308:TYR:CD2	2.52	0.45
1:C:95:PHE:HA	1:C:134:ILE:O	2.17	0.45
1:D:214:PHE:C	1:D:216:GLU:N	2.73	0.44
1:A:230:VAL:HB	1:A:254:GLY:HA2	1.99	0.44
1:B:155:GLU:H	1:B:155:GLU:HG2	1.43	0.44
1:C:83:LEU:HB3	3:C:390:HOH:O	2.16	0.44
1:A:116:TYR:O	1:A:119:PHE:HB3	2.17	0.44
1:B:295:ILE:HG23	1:B:299:ILE:HG13	1.98	0.44
1:D:221:GLU:CD	1:D:282:ASN:H	2.26	0.44
1:A:59:LEU:HG	1:A:101:SER:HB3	1.99	0.44
1:B:105:MET:HE1	1:B:159:ASN:HB2	2.00	0.44
1:B:151:VAL:HG23	1:B:252:ASN:ND2	2.33	0.44
1:D:100:VAL:HG22	1:D:115:ASN:ND2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:VAL:HG22	1:E:115:ASN:ND2	2.31	0.44
1:E:218:LYS:C	1:E:218:LYS:HD2	2.42	0.44
1:A:151:VAL:HG23	1:A:252:ASN:ND2	2.32	0.44
1:A:307:LEU:HB2	1:A:308:TYR:CD2	2.52	0.44
1:B:104:THR:O	1:B:106:LEU:N	2.50	0.44
1:D:3:TYR:CD1	1:D:237:GLN:HG3	2.53	0.44
1:D:302:LEU:O	1:D:303:ASP:HB3	2.17	0.44
1:E:113:LYS:O	1:E:117:GLN:HB3	2.18	0.44
1:D:319:PRO:O	1:D:322:HIS:HB2	2.18	0.44
1:C:63:LYS:O	1:C:66:ILE:HG12	2.17	0.44
1:C:143:GLY:HA3	1:C:156:SER:O	2.18	0.44
1:E:265:VAL:O	1:E:269:LYS:HG3	2.18	0.44
1:A:69:LYS:HG3	1:A:69:LYS:O	2.18	0.44
1:A:237:GLN:HE21	1:A:241:LYS:NZ	2.16	0.44
1:B:294:HIS:NE2	1:B:296:GLU:HG3	2.31	0.44
1:C:111:VAL:O	1:C:115:ASN:HB2	2.18	0.44
1:C:220:PHE:O	1:C:221:GLU:C	2.61	0.44
1:D:286:PHE:O	1:D:288:GLN:N	2.49	0.44
1:B:215:LYS:O	1:B:275:PHE:HB2	2.18	0.43
1:B:261:TYR:O	1:B:265:VAL:HG23	2.18	0.43
1:B:319:PRO:O	1:B:322:HIS:HB2	2.18	0.43
1:E:123:LEU:HD12	1:E:123:LEU:HA	1.86	0.43
1:E:314:ILE:O	1:E:318:LEU:HB2	2.18	0.43
1:A:255:TYR:HD1	1:A:306:PRO:HB2	1.83	0.43
1:C:119:PHE:CG	1:C:168:MET:HE3	2.53	0.43
1:D:207:LEU:HD12	1:D:264:ILE:HG21	2.01	0.43
1:E:209:LEU:CD1	1:E:321:ILE:HG23	2.48	0.43
1:E:237:GLN:HE22	1:E:305:THR:N	2.03	0.43
1:C:237:GLN:HE21	1:C:241:LYS:NZ	2.16	0.43
1:D:56:PRO:HA	1:D:104:THR:OG1	2.18	0.43
1:E:56:PRO:HA	1:E:104:THR:OG1	2.18	0.43
1:E:225:GLN:NE2	1:E:225:GLN:N	2.67	0.43
1:B:56:PRO:HA	1:B:104:THR:OG1	2.17	0.43
1:C:150:VAL:HG22	1:C:294:HIS:CB	2.48	0.43
1:D:203:MET:O	1:D:207:LEU:HG	2.18	0.43
1:E:179:ASN:ND2	1:E:180:VAL:N	2.65	0.43
1:E:111:VAL:O	1:E:115:ASN:HB2	2.18	0.43
1:B:314:ILE:O	1:B:318:LEU:HB2	2.18	0.43
1:C:100:VAL:HG22	1:C:115:ASN:ND2	2.34	0.43
1:C:104:THR:O	1:C:106:LEU:N	2.51	0.43
1:E:9:GLU:HA	1:E:36:LYS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:268:LEU:HD12	1:E:268:LEU:HA	1.84	0.43
1:A:295:ILE:HG23	1:A:295:ILE:O	2.19	0.43
1:B:242:ALA:HA	1:B:302:LEU:HD22	2.01	0.43
1:D:137:SER:HA	1:D:165:LYS:HD2	2.01	0.43
1:D:215:LYS:O	1:D:275:PHE:HB2	2.18	0.43
1:E:302:LEU:O	1:E:303:ASP:HB3	2.19	0.43
1:A:63:LYS:O	1:A:66:ILE:HG12	2.18	0.43
1:C:208:ALA:O	1:C:212:MET:HG3	2.19	0.43
1:D:220:PHE:O	1:D:221:GLU:C	2.62	0.43
1:E:211:ALA:O	1:E:215:LYS:HA	2.19	0.43
1:B:90:HIS:HB2	3:B:417:HOH:O	2.17	0.43
1:E:227:ARG:HB2	1:E:229:PHE:CZ	2.54	0.43
1:E:310:LEU:O	1:E:314:ILE:HG13	2.19	0.43
1:A:227:ARG:HB2	1:A:229:PHE:CZ	2.54	0.43
1:E:255:TYR:HD1	1:E:306:PRO:HB2	1.83	0.43
1:A:123:LEU:HD12	1:A:123:LEU:HA	1.86	0.42
1:C:225:GLN:H	1:C:225:GLN:NE2	2.17	0.42
1:A:72:VAL:CG1	1:A:73:ILE:N	2.81	0.42
1:A:151:VAL:HG11	1:A:250:VAL:HG22	2.01	0.42
1:E:220:PHE:O	1:E:221:GLU:C	2.62	0.42
1:B:225:GLN:H	1:B:225:GLN:NE2	2.17	0.42
1:E:296:GLU:HB2	1:E:297:PRO:CD	2.37	0.42
1:A:220:PHE:O	1:A:221:GLU:C	2.63	0.42
1:B:216:GLU:OE1	1:B:276:LYS:HD3	2.18	0.42
1:D:111:VAL:O	1:D:115:ASN:HB2	2.19	0.42
1:D:209:LEU:CD1	1:D:321:ILE:HG23	2.49	0.42
1:E:142:TYR:O	1:E:145:THR:HG23	2.19	0.42
1:D:100:VAL:N	1:D:115:ASN:HD21	2.04	0.42
2:D:2401:NAD:H52A	3:D:379:HOH:O	2.19	0.42
1:A:133:VAL:C	1:A:134:ILE:HD12	2.44	0.42
1:A:237:GLN:NE2	1:A:241:LYS:NZ	2.67	0.42
1:B:220:PHE:O	1:B:221:GLU:C	2.62	0.42
1:C:270:GLU:HG2	1:C:270:GLU:O	2.20	0.42
1:D:107:ASN:O	1:D:111:VAL:HG23	2.20	0.42
1:D:147:ALA:HB2	1:D:290:HIS:O	2.19	0.42
1:E:147:ALA:HB2	1:E:290:HIS:O	2.18	0.42
1:E:227:ARG:NH2	1:E:289:LYS:HB2	2.34	0.42
1:B:48:ASN:N	1:D:107:ASN:ND2	2.65	0.42
1:B:296:GLU:CB	1:B:297:PRO:HD3	2.47	0.42
1:C:173:LEU:HD21	1:C:250:VAL:HG13	2.01	0.42
1:C:261:TYR:O	1:C:265:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:ARG:HB2	1:D:229:PHE:CZ	2.55	0.42
1:D:295:ILE:O	1:D:299:ILE:HG13	2.20	0.42
1:A:216:GLU:OE1	1:A:276:LYS:HD3	2.19	0.42
1:B:9:GLU:HA	1:B:36:LYS:HB3	2.02	0.42
1:C:246:GLN:HE21	1:C:246:GLN:HB2	1.66	0.42
1:D:16:THR:OG1	1:D:96:HIS:HA	2.19	0.42
1:A:9:GLU:HA	1:A:36:LYS:HB3	2.01	0.42
1:A:134:ILE:HD12	1:A:134:ILE:N	2.34	0.42
1:C:237:GLN:NE2	1:C:241:LYS:NZ	2.66	0.42
1:D:12:THR:HA	1:D:38:LYS:HB2	2.02	0.42
1:A:127:ARG:HD3	3:A:371:HOH:O	2.18	0.41
1:A:302:LEU:O	1:A:303:ASP:HB3	2.20	0.41
1:C:211:ALA:O	1:C:215:LYS:HA	2.20	0.41
1:E:107:ASN:O	1:E:111:VAL:HG23	2.20	0.41
1:A:314:ILE:O	1:A:318:LEU:HB2	2.19	0.41
1:D:265:VAL:HG13	1:D:275:PHE:CE2	2.55	0.41
1:B:135:TYR:CD1	1:B:168:MET:HE2	2.55	0.41
1:C:272:LEU:HD13	1:C:318:LEU:HD21	2.01	0.41
1:A:215:LYS:O	1:A:275:PHE:HB2	2.20	0.41
1:A:268:LEU:HD12	1:A:268:LEU:HA	1.86	0.41
1:B:95:PHE:HA	1:B:134:ILE:O	2.21	0.41
1:B:211:ALA:O	1:B:215:LYS:HA	2.20	0.41
1:E:216:GLU:OE1	1:E:276:LYS:HD3	2.20	0.41
1:D:63:LYS:O	1:D:66:ILE:HG12	2.20	0.41
1:D:150:VAL:HG22	1:D:294:HIS:CB	2.51	0.41
1:A:143:GLY:HA3	1:A:156:SER:O	2.20	0.41
1:B:209:LEU:CD1	1:B:321:ILE:HG23	2.50	0.41
1:C:12:THR:HA	1:C:38:LYS:HB2	2.02	0.41
1:A:108:GLN:HG3	1:A:160:VAL:HG11	2.01	0.41
1:A:296:GLU:HB2	1:A:297:PRO:CD	2.46	0.41
1:C:265:VAL:HG13	1:C:275:PHE:CE2	2.56	0.41
1:C:294:HIS:NE2	1:C:296:GLU:HG3	2.35	0.41
1:D:186:TYR:HD1	1:D:253:VAL:CG1	2.33	0.41
1:A:16:THR:OG1	1:A:96:HIS:HA	2.20	0.41
1:A:155:GLU:H	1:A:155:GLU:HG2	1.47	0.41
1:A:209:LEU:CD1	1:A:321:ILE:HG23	2.51	0.41
1:A:265:VAL:O	1:A:269:LYS:HG3	2.20	0.41
1:D:225:GLN:H	1:D:225:GLN:NE2	2.19	0.41
1:D:268:LEU:HD12	1:D:268:LEU:HA	1.89	0.41
1:A:7:GLU:HG2	1:A:36:LYS:HD2	2.02	0.41
1:A:146:LYS:HE2	3:A:374:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:MET:O	1:A:207:LEU:HG	2.21	0.41
1:B:302:LEU:O	1:B:303:ASP:HB3	2.21	0.41
1:C:302:LEU:O	1:C:303:ASP:HB3	2.21	0.41
1:D:7:GLU:HG2	1:D:36:LYS:HD2	2.02	0.41
1:D:101:SER:OG	1:D:103:THR:HG22	2.20	0.41
1:D:242:ALA:HA	1:D:302:LEU:HD22	2.02	0.41
1:D:294:HIS:NE2	1:D:296:GLU:CG	2.84	0.41
1:D:315:LYS:O	1:D:319:PRO:HD3	2.21	0.41
1:B:99:ALA:O	2:B:2401:NAD:H8A	2.21	0.41
1:C:16:THR:OG1	1:C:96:HIS:HA	2.21	0.41
1:C:19:ALA:HB3	1:C:43:ASP:CG	2.46	0.41
1:C:137:SER:HA	1:C:165:LYS:HD2	2.03	0.41
1:A:78:ASN:OD1	1:A:114:THR:HB	2.21	0.40
1:B:107:ASN:O	1:B:111:VAL:HG23	2.20	0.40
1:C:31:GLN:NE2	1:C:69:LYS:N	2.44	0.40
1:C:59:LEU:HD12	2:C:2403:NAD:O1A	2.21	0.40
1:C:116:TYR:O	1:C:119:PHE:HB3	2.21	0.40
1:C:317:TYR:CD2	1:C:321:ILE:HD11	2.57	0.40
1:E:135:TYR:CD1	1:E:168:MET:HE2	2.56	0.40
1:E:294:HIS:NE2	1:E:296:GLU:CG	2.84	0.40
1:A:100:VAL:HG22	1:A:115:ASN:HD21	1.86	0.40
1:B:107:ASN:OD1	1:B:110:LEU:HD13	2.21	0.40
1:D:101:SER:CB	1:D:103:THR:HG22	2.52	0.40
1:D:109:GLU:HG2	1:D:110:LEU:HD12	2.02	0.40
1:E:207:LEU:HD12	1:E:264:ILE:CG2	2.51	0.40
1:A:186:TYR:HD1	1:A:253:VAL:CG1	2.34	0.40
1:A:196:TYR:C	1:A:198:GLU:H	2.29	0.40
1:A:261:TYR:O	1:A:265:VAL:HG23	2.21	0.40
1:B:89:LEU:O	1:B:129:LYS:HE3	2.21	0.40
1:C:314:ILE:O	1:C:318:LEU:HB2	2.21	0.40
1:A:219:LEU:O	1:A:279:TYR:HA	2.21	0.40
1:D:42:LEU:HD23	1:D:43:ASP:N	2.36	0.40
1:B:113:LYS:O	1:B:117:GLN:HB3	2.22	0.40
1:E:95:PHE:HA	1:E:134:ILE:O	2.21	0.40
1:E:155:GLU:H	1:E:155:GLU:HG2	1.45	0.40
1:E:219:LEU:O	1:E:279:TYR:HA	2.21	0.40

There are no symmetry-related clashes.

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	304/362 (84%)	267 (88%)	31 (10%)	6 (2%)	6	6
1	B	305/362 (84%)	269 (88%)	29 (10%)	7 (2%)	5	4
1	C	304/362 (84%)	268 (88%)	29 (10%)	7 (2%)	5	4
1	D	308/362 (85%)	271 (88%)	29 (9%)	8 (3%)	4	3
1	E	304/362 (84%)	267 (88%)	30 (10%)	7 (2%)	5	4
All	All	1525/1810 (84%)	1342 (88%)	148 (10%)	35 (2%)	5	4

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	PHE
1	A	221	GLU
1	B	45	PHE
1	B	221	GLU
1	C	45	PHE
1	C	221	GLU
1	D	45	PHE
1	D	221	GLU
1	E	45	PHE
1	E	221	GLU
1	A	21	PHE
1	B	21	PHE
1	C	21	PHE
1	D	21	PHE
1	D	46	ARG
1	D	287	PHE
1	E	21	PHE
1	E	308	TYR
1	A	46	ARG
1	A	188	ASN
1	A	308	TYR

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Mol	Chain	Res	Type
1	B	188	ASN
1	B	308	TYR
1	C	46	ARG
1	C	188	ASN
1	C	222	PHE
1	C	308	TYR
1	D	308	TYR
1	E	46	ARG
1	E	188	ASN
1	B	46	ARG
1	B	222	PHE
1	D	188	ASN
1	D	222	PHE
1	E	222	PHE

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	268/313 (86%)	246 (92%)	22 (8%)	10	14
1	B	269/313 (86%)	247 (92%)	22 (8%)	10	14
1	C	268/313 (86%)	245 (91%)	23 (9%)	10	13
1	D	272/313 (87%)	250 (92%)	22 (8%)	11	15
1	E	268/313 (86%)	245 (91%)	23 (9%)	10	13
All	All	1345/1565 (86%)	1233 (92%)	112 (8%)	10	14

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	VAL
1	A	59	LEU
1	A	81	LEU
1	A	83	LEU
1	A	114	THR

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Mol	Chain	Res	Type
1	A	123	LEU
1	A	153	LYS
1	A	155	GLU
1	A	160	VAL
1	A	184	LEU
1	A	205	LEU
1	A	209	LEU
1	A	221	GLU
1	A	224	GLU
1	A	225	GLN
1	A	240	VAL
1	A	250	VAL
1	A	253	VAL
1	A	278	THR
1	A	289	LYS
1	A	295	ILE
1	A	318	LEU
1	B	40	VAL
1	B	59	LEU
1	B	81	LEU
1	B	83	LEU
1	B	114	THR
1	B	123	LEU
1	B	155	GLU
1	B	160	VAL
1	B	184	LEU
1	B	205	LEU
1	B	209	LEU
1	B	221	GLU
1	B	224	GLU
1	B	225	GLN
1	B	240	VAL
1	B	250	VAL
1	B	253	VAL
1	B	278	THR
1	B	281	LYS
1	B	289	LYS
1	B	295	ILE
1	B	318	LEU
1	C	40	VAL
1	C	59	LEU
1	C	81	LEU

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Mol	Chain	Res	Type
1	C	83	LEU
1	C	114	THR
1	C	123	LEU
1	C	155	GLU
1	C	160	VAL
1	C	184	LEU
1	C	205	LEU
1	C	209	LEU
1	C	221	GLU
1	C	224	GLU
1	C	225	GLN
1	C	240	VAL
1	C	250	VAL
1	C	253	VAL
1	C	278	THR
1	C	289	LYS
1	C	295	ILE
1	C	305	THR
1	C	309	ASP
1	C	318	LEU
1	D	40	VAL
1	D	81	LEU
1	D	83	LEU
1	D	114	THR
1	D	123	LEU
1	D	153	LYS
1	D	155	GLU
1	D	160	VAL
1	D	184	LEU
1	D	205	LEU
1	D	209	LEU
1	D	221	GLU
1	D	224	GLU
1	D	225	GLN
1	D	240	VAL
1	D	250	VAL
1	D	253	VAL
1	D	278	THR
1	D	286	PHE
1	D	289	LYS
1	D	295	ILE
1	D	318	LEU

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Mol	Chain	Res	Type
1	E	40	VAL
1	E	59	LEU
1	E	81	LEU
1	E	83	LEU
1	E	114	THR
1	E	123	LEU
1	E	153	LYS
1	E	155	GLU
1	E	160	VAL
1	E	184	LEU
1	E	205	LEU
1	E	209	LEU
1	E	221	GLU
1	E	224	GLU
1	E	225	GLN
1	E	240	VAL
1	E	250	VAL
1	E	253	VAL
1	E	278	THR
1	E	281	LYS
1	E	289	LYS
1	E	295	ILE
1	E	318	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	11	GLN
1	A	29	HIS
1	A	31	GLN
1	A	34	HIS
1	A	61	HIS
1	A	78	ASN
1	A	115	ASN
1	A	117	GLN
1	A	159	ASN
1	A	175	HIS
1	A	179	ASN
1	A	225	GLN
1	A	237	GLN
1	A	239	ASN

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Mol	Chain	Res	Type
1	A	246	GLN
1	A	257	GLN
1	A	262	ASN
1	A	271	HIS
1	A	292	GLN
1	B	10	ASN
1	B	11	GLN
1	B	31	GLN
1	B	34	HIS
1	B	61	HIS
1	B	115	ASN
1	B	117	GLN
1	B	121	ASN
1	B	159	ASN
1	B	175	HIS
1	B	179	ASN
1	B	225	GLN
1	B	237	GLN
1	B	239	ASN
1	B	246	GLN
1	B	257	GLN
1	B	262	ASN
1	B	271	HIS
1	B	292	GLN
1	C	11	GLN
1	C	31	GLN
1	C	61	HIS
1	C	78	ASN
1	C	115	ASN
1	C	121	ASN
1	C	159	ASN
1	C	175	HIS
1	C	179	ASN
1	C	225	GLN
1	C	237	GLN
1	C	239	ASN
1	C	246	GLN
1	C	257	GLN
1	C	262	ASN
1	C	271	HIS
1	C	292	GLN
1	D	10	ASN

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Mol	Chain	Res	Type
1	D	11	GLN
1	D	31	GLN
1	D	61	HIS
1	D	78	ASN
1	D	107	ASN
1	D	115	ASN
1	D	121	ASN
1	D	159	ASN
1	D	177	ASN
1	D	179	ASN
1	D	225	GLN
1	D	237	GLN
1	D	239	ASN
1	D	246	GLN
1	D	257	GLN
1	D	262	ASN
1	D	271	HIS
1	D	292	GLN
1	E	10	ASN
1	E	11	GLN
1	E	31	GLN
1	E	34	HIS
1	E	61	HIS
1	E	78	ASN
1	E	115	ASN
1	E	121	ASN
1	E	159	ASN
1	E	177	ASN
1	E	179	ASN
1	E	225	GLN
1	E	237	GLN
1	E	239	ASN
1	E	246	GLN
1	E	257	GLN
1	E	262	ASN
1	E	271	HIS
1	E	290	HIS
1	E	292	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	B	2401	-	46,48,48	1.54	8 (17%)	64,73,73	1.80	13 (20%)
2	NAD	A	2402	-	46,48,48	1.41	7 (15%)	64,73,73	1.67	13 (20%)
2	NAD	C	2403	-	46,48,48	1.33	6 (13%)	64,73,73	1.76	13 (20%)
2	NAD	E	2403	-	46,48,48	1.34	9 (19%)	64,73,73	1.76	14 (21%)
2	NAD	D	2401	-	46,48,48	1.40	9 (19%)	64,73,73	1.83	14 (21%)

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	B	2401	-	-	10/30/62/62	0/5/5/5
2	NAD	A	2402	-	-	7/30/62/62	0/5/5/5
2	NAD	C	2403	-	-	5/30/62/62	0/5/5/5
2	NAD	E	2403	-	-	6/30/62/62	0/5/5/5
2	NAD	D	2401	-	-	4/30/62/62	0/5/5/5

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2401	NAD	O3D-C3D	5.47	1.56	1.43
2	E	2403	NAD	C2N-N1N	5.09	1.40	1.35
2	B	2401	NAD	C2N-N1N	5.04	1.40	1.35
2	C	2403	NAD	C2N-N1N	4.97	1.40	1.35
2	A	2402	NAD	C2N-N1N	4.92	1.40	1.35
2	D	2401	NAD	C2N-N1N	4.89	1.40	1.35
2	A	2402	NAD	O3D-C3D	3.87	1.52	1.43
2	D	2401	NAD	C5A-N7A	-3.20	1.33	1.39
2	E	2403	NAD	C5A-N7A	-3.15	1.33	1.39
2	C	2403	NAD	C5A-N7A	-3.15	1.33	1.39
2	B	2401	NAD	C5A-N7A	-3.02	1.33	1.39
2	A	2402	NAD	C5A-N7A	-2.98	1.33	1.39
2	D	2401	NAD	O3D-C3D	-2.94	1.35	1.43
2	E	2403	NAD	O4D-C1D	2.67	1.44	1.40
2	C	2403	NAD	O4D-C1D	2.64	1.44	1.40
2	D	2401	NAD	O4D-C1D	2.59	1.44	1.40
2	A	2402	NAD	O4D-C1D	2.56	1.44	1.40
2	B	2401	NAD	O4D-C1D	2.55	1.44	1.40
2	A	2402	NAD	C6N-N1N	2.36	1.40	1.35
2	A	2402	NAD	C8A-N9A	-2.34	1.33	1.37
2	C	2403	NAD	C6N-N1N	2.33	1.40	1.35
2	C	2403	NAD	C8A-N9A	-2.30	1.33	1.37
2	D	2401	NAD	C6N-N1N	2.30	1.40	1.35
2	B	2401	NAD	C6N-N1N	2.29	1.40	1.35
2	E	2403	NAD	C6N-N1N	2.28	1.40	1.35
2	B	2401	NAD	C8A-N9A	-2.27	1.33	1.37
2	D	2401	NAD	PN-O3	2.23	1.61	1.59
2	D	2401	NAD	C8A-N9A	-2.21	1.33	1.37
2	D	2401	NAD	PA-O3	2.19	1.61	1.59
2	E	2403	NAD	PN-O3	2.18	1.61	1.59
2	E	2403	NAD	C8A-N9A	-2.16	1.33	1.37
2	B	2401	NAD	PN-O3	2.12	1.61	1.59
2	E	2403	NAD	C3N-C7N	2.12	1.53	1.50
2	A	2402	NAD	C4A-N9A	-2.05	1.33	1.37
2	B	2401	NAD	PA-O3	2.05	1.61	1.59
2	E	2403	NAD	PA-O3	2.04	1.61	1.59
2	E	2403	NAD	C4A-N9A	-2.03	1.33	1.37
2	D	2401	NAD	C4A-N9A	-2.03	1.33	1.37
2	C	2403	NAD	PN-O3	2.01	1.61	1.59

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2403	NAD	C5A-C4A-N3A	-5.50	119.14	126.72
2	D	2401	NAD	C5A-C4A-N3A	-5.45	119.21	126.72
2	A	2402	NAD	C5A-C4A-N3A	-5.37	119.33	126.72
2	C	2403	NAD	C5A-C4A-N3A	-5.36	119.34	126.72
2	B	2401	NAD	C5A-C4A-N3A	-5.32	119.39	126.72
2	C	2403	NAD	O3D-C3D-C2D	5.20	128.47	111.82
2	D	2401	NAD	O3D-C3D-C2D	5.04	127.99	111.82
2	D	2401	NAD	N3A-C2A-N1A	-4.56	121.67	128.58
2	B	2401	NAD	N3A-C2A-N1A	-4.54	121.71	128.58
2	E	2403	NAD	O3D-C3D-C2D	4.54	126.36	111.82
2	A	2402	NAD	N3A-C2A-N1A	-4.52	121.74	128.58
2	E	2403	NAD	N3A-C2A-N1A	-4.50	121.77	128.58
2	C	2403	NAD	N3A-C2A-N1A	-4.48	121.80	128.58
2	B	2401	NAD	O3D-C3D-C2D	4.40	125.94	111.82
2	B	2401	NAD	C4B-O4B-C1B	-3.91	100.83	109.47
2	A	2402	NAD	N3A-C4A-N9A	3.85	133.71	127.17
2	E	2403	NAD	N3A-C4A-N9A	3.79	133.62	127.17
2	C	2403	NAD	N3A-C4A-N9A	3.76	133.56	127.17
2	D	2401	NAD	O4B-C1B-C2B	-3.71	98.67	106.62
2	B	2401	NAD	N3A-C4A-N9A	3.67	133.42	127.17
2	D	2401	NAD	N3A-C4A-N9A	3.66	133.38	127.17
2	E	2403	NAD	C2A-N3A-C4A	3.65	120.75	111.83
2	D	2401	NAD	C2A-N3A-C4A	3.61	120.65	111.83
2	B	2401	NAD	C2A-N3A-C4A	3.56	120.53	111.83
2	A	2402	NAD	C2A-N3A-C4A	3.55	120.50	111.83
2	C	2403	NAD	C2A-N3A-C4A	3.51	120.40	111.83
2	A	2402	NAD	O3D-C3D-C2D	3.35	122.55	111.82
2	D	2401	NAD	C4B-O4B-C1B	-3.28	102.22	109.47
2	B	2401	NAD	O3D-C3D-C4D	3.23	120.37	111.08
2	D	2401	NAD	C4D-O4D-C1D	-3.15	107.04	109.92
2	B	2401	NAD	C4D-O4D-C1D	-3.11	107.08	109.92
2	D	2401	NAD	N9A-C8A-N7A	-3.09	109.56	113.94
2	D	2401	NAD	C4A-C5A-N7A	-3.09	107.05	110.58
2	A	2402	NAD	N9A-C8A-N7A	-3.05	109.61	113.94
2	D	2401	NAD	C5A-N7A-C8A	3.03	108.22	103.45
2	E	2403	NAD	N9A-C8A-N7A	-3.00	109.68	113.94
2	C	2403	NAD	N9A-C8A-N7A	-2.99	109.70	113.94
2	B	2401	NAD	O4B-C1B-C2B	-2.97	100.26	106.62
2	C	2403	NAD	C4D-O4D-C1D	-2.94	107.24	109.92
2	B	2401	NAD	N9A-C8A-N7A	-2.90	109.81	113.94
2	A	2402	NAD	C4D-O4D-C1D	-2.88	107.29	109.92
2	C	2403	NAD	C5A-N7A-C8A	2.86	107.95	103.45
2	B	2401	NAD	C4A-C5A-N7A	-2.86	107.31	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2403	NAD	C4A-C5A-N7A	-2.84	107.33	110.58
2	E	2403	NAD	C5A-N7A-C8A	2.83	107.90	103.45
2	B	2401	NAD	C5A-N7A-C8A	2.82	107.88	103.45
2	E	2403	NAD	C4A-C5A-N7A	-2.80	107.38	110.58
2	A	2402	NAD	C5A-N7A-C8A	2.78	107.83	103.45
2	A	2402	NAD	C4A-C5A-N7A	-2.78	107.40	110.58
2	E	2403	NAD	C4D-O4D-C1D	-2.66	107.49	109.92
2	C	2403	NAD	O4B-C1B-C2B	-2.57	101.11	106.62
2	E	2403	NAD	O4B-C1B-C2B	-2.57	101.12	106.62
2	C	2403	NAD	C6N-N1N-C2N	-2.49	119.76	121.88
2	E	2403	NAD	C6N-N1N-C2N	-2.45	119.79	121.88
2	A	2402	NAD	O4B-C1B-C2B	-2.39	101.50	106.62
2	E	2403	NAD	C3N-C7N-N7N	-2.39	114.80	117.74
2	E	2403	NAD	C4B-O4B-C1B	-2.38	104.21	109.47
2	D	2401	NAD	C6N-N1N-C2N	-2.36	119.87	121.88
2	B	2401	NAD	C3N-C7N-N7N	-2.36	114.83	117.74
2	E	2403	NAD	O4B-C1B-N9A	2.35	112.61	108.09
2	A	2402	NAD	C4A-N9A-C8A	2.35	108.20	105.74
2	C	2403	NAD	C4B-O4B-C1B	-2.14	104.74	109.47
2	C	2403	NAD	C4A-N9A-C8A	2.09	107.93	105.74
2	A	2402	NAD	C4B-O4B-C1B	-2.08	104.87	109.47
2	A	2402	NAD	C3N-C7N-N7N	-2.07	115.19	117.74
2	D	2401	NAD	O4B-C1B-N9A	2.05	112.03	108.09
2	D	2401	NAD	C3N-C7N-N7N	-2.05	115.21	117.74

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2402	NAD	C5B-O5B-PA-O1A
2	A	2402	NAD	C5D-O5D-PN-O3
2	A	2402	NAD	C5D-O5D-PN-O2N
2	B	2401	NAD	C5B-O5B-PA-O2A
2	B	2401	NAD	C5B-O5B-PA-O3
2	B	2401	NAD	C5D-O5D-PN-O2N
2	C	2403	NAD	C5D-O5D-PN-O3
2	C	2403	NAD	C5D-O5D-PN-O1N
2	C	2403	NAD	C5D-O5D-PN-O2N
2	D	2401	NAD	C5D-O5D-PN-O3
2	D	2401	NAD	C5D-O5D-PN-O1N
2	D	2401	NAD	C5D-O5D-PN-O2N
2	E	2403	NAD	C5D-O5D-PN-O3

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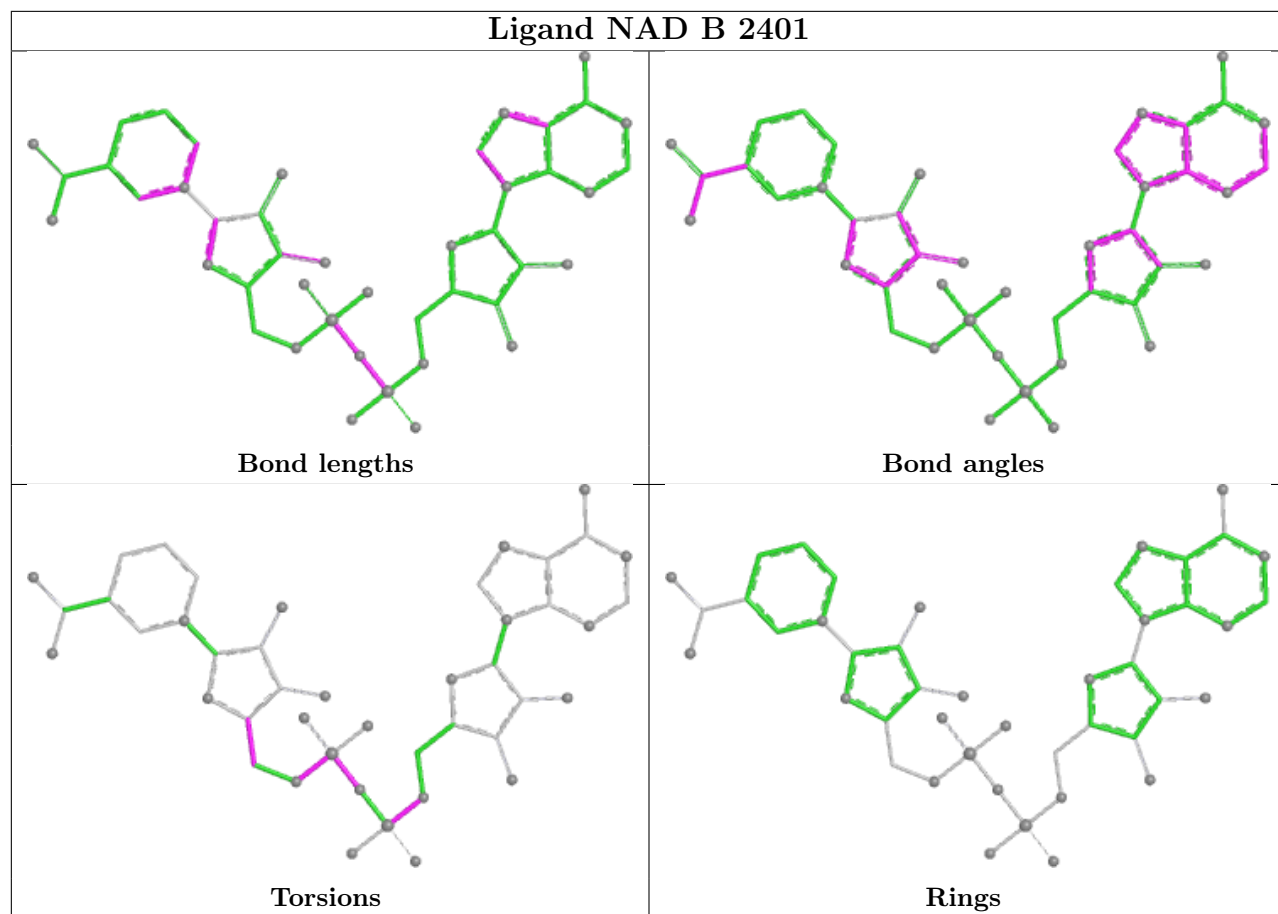
Mol	Chain	Res	Type	Atoms
2	E	2403	NAD	C5D-O5D-PN-O1N
2	E	2403	NAD	C5D-O5D-PN-O2N
2	B	2401	NAD	O4D-C4D-C5D-O5D
2	C	2403	NAD	PN-O3-PA-O5B
2	E	2403	NAD	PN-O3-PA-O5B
2	B	2401	NAD	C3D-C4D-C5D-O5D
2	A	2402	NAD	C5D-O5D-PN-O1N
2	B	2401	NAD	C5B-O5B-PA-O1A
2	B	2401	NAD	C5D-O5D-PN-O3
2	B	2401	NAD	C5D-O5D-PN-O1N
2	A	2402	NAD	PA-O3-PN-O2N
2	D	2401	NAD	PA-O3-PN-O2N
2	B	2401	NAD	PA-O3-PN-O2N
2	A	2402	NAD	PA-O3-PN-O1N
2	C	2403	NAD	PA-O3-PN-O1N
2	E	2403	NAD	PA-O3-PN-O1N
2	E	2403	NAD	PA-O3-PN-O2N
2	B	2401	NAD	PA-O3-PN-O1N
2	A	2402	NAD	O4B-C4B-C5B-O5B

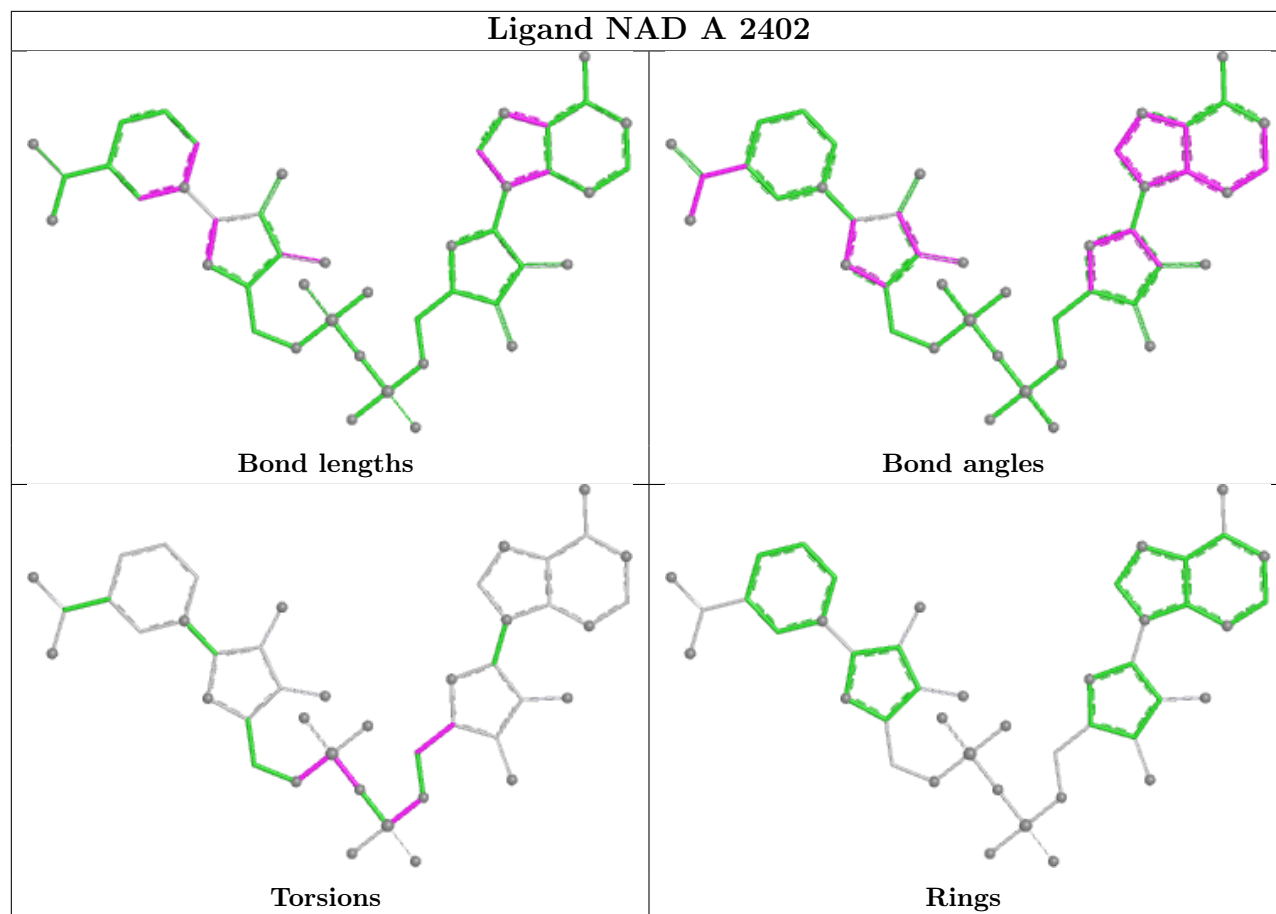
There are no ring outliers.

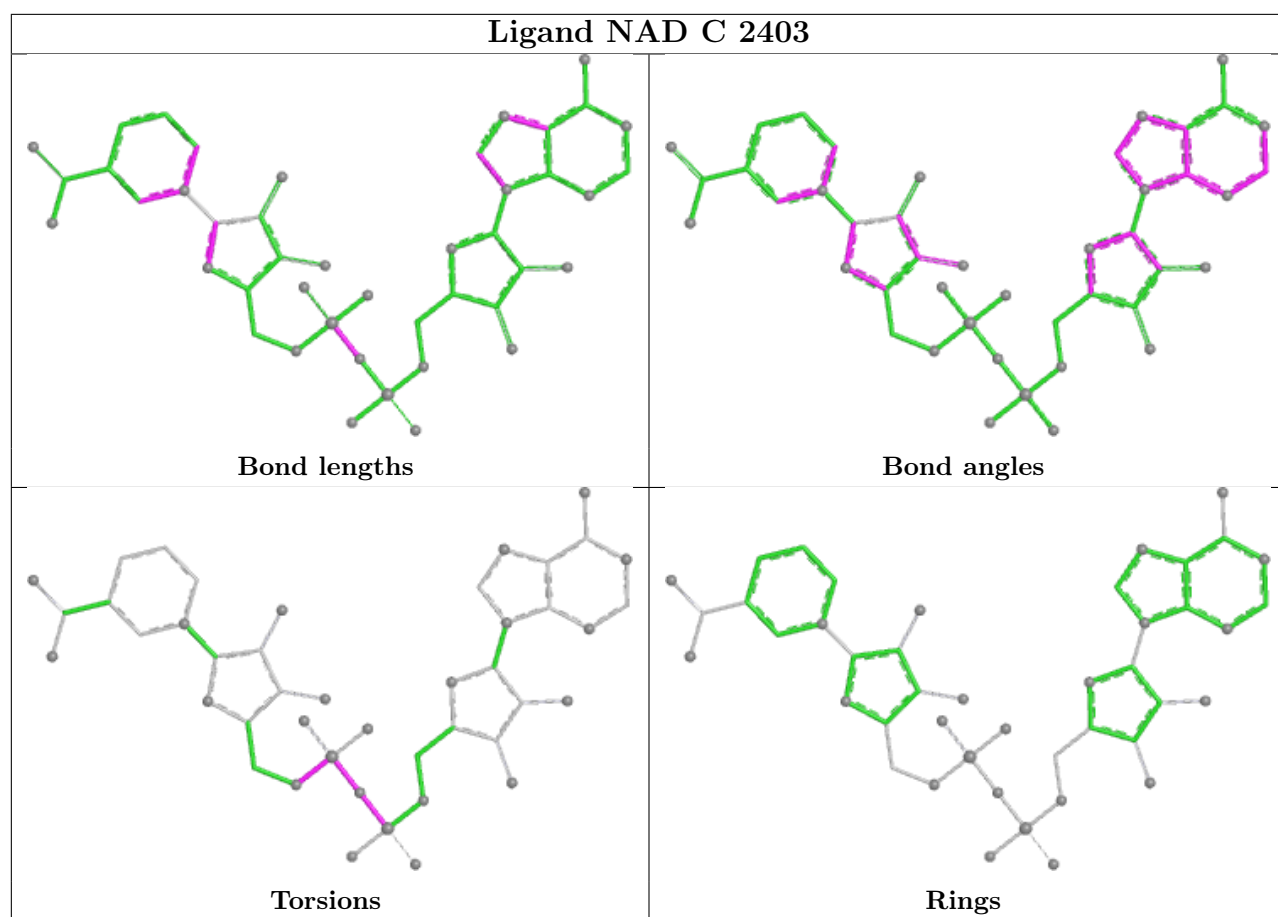
5 monomers are involved in 22 short contacts:

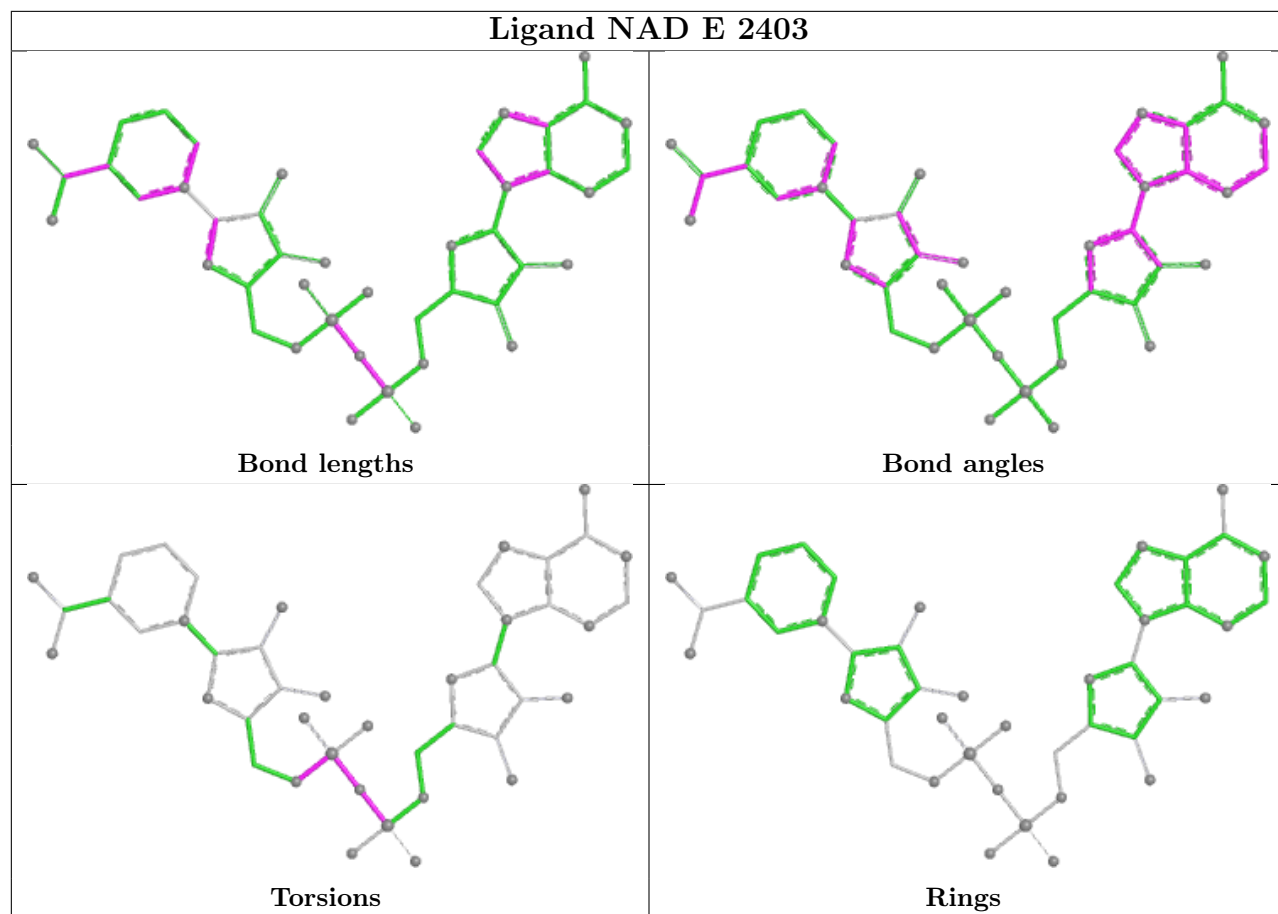
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2401	NAD	6	0
2	A	2402	NAD	3	0
2	C	2403	NAD	4	0
2	E	2403	NAD	5	0
2	D	2401	NAD	4	0

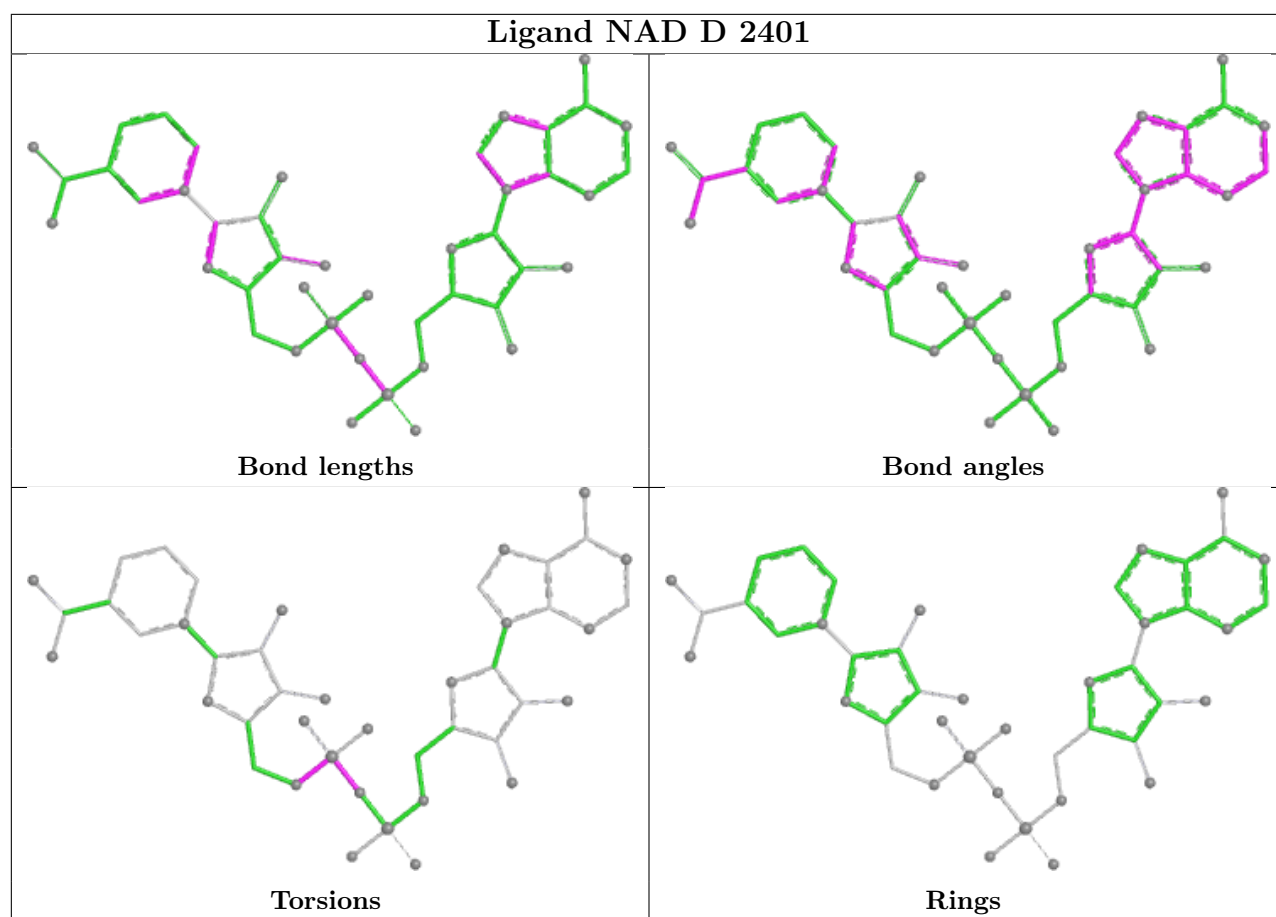
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

6.1 Protein, DNA and RNA chains

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	310/362 (85%)	0.88	50 (16%) 4 4	27, 46, 86, 100	0
1	B	311/362 (85%)	0.84	36 (11%) 9 8	26, 46, 87, 100	0
1	C	310/362 (85%)	0.76	36 (11%) 9 8	29, 48, 87, 102	0
1	D	314/362 (86%)	0.90	46 (14%) 6 5	27, 47, 88, 101	0
1	E	310/362 (85%)	0.86	34 (10%) 10 10	30, 48, 87, 101	0
All	All	1555/1810 (85%)	0.85	202 (12%) 7 6	26, 47, 88, 102	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	104	THR	5.8
1	D	222	PHE	5.7
1	B	56	PRO	5.3
1	A	218	LYS	5.2
1	D	324	ILE	4.9
1	D	261	TYR	4.8
1	E	324	ILE	4.7
1	D	277	VAL	4.6
1	A	106	LEU	4.6
1	D	104	THR	4.4
1	D	219	LEU	4.3
1	C	222	PHE	4.2
1	A	219	LEU	4.2
1	D	218	LYS	4.2
1	E	106	LEU	4.1
1	A	104	THR	4.1
1	A	56	PRO	4.0
1	B	222	PHE	3.9
1	D	220	PHE	3.9
1	E	222	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	217	VAL	3.9
1	D	106	LEU	3.9
1	A	222	PHE	3.8
1	D	223	GLY	3.8
1	D	280	ILE	3.8
1	B	324	ILE	3.8
1	C	219	LEU	3.8
1	A	323	ALA	3.7
1	D	48	ASN	3.7
1	D	290	HIS	3.7
1	E	226	LEU	3.7
1	C	217	VAL	3.6
1	A	211	ALA	3.6
1	B	217	VAL	3.6
1	A	275	PHE	3.6
1	C	106	LEU	3.6
1	B	48	ASN	3.6
1	E	220	PHE	3.6
1	B	224	GLU	3.6
1	B	289	LYS	3.6
1	A	277	VAL	3.5
1	B	105	MET	3.5
1	C	105	MET	3.5
1	D	56	PRO	3.5
1	D	323	ALA	3.4
1	D	213	ALA	3.4
1	A	279	TYR	3.4
1	D	278	THR	3.4
1	A	223	GLY	3.4
1	E	323	ALA	3.4
1	A	103	THR	3.3
1	A	105	MET	3.3
1	D	275	PHE	3.3
1	A	214	PHE	3.3
1	E	47	SER	3.3
1	E	101	SER	3.2
1	E	105	MET	3.2
1	A	324	ILE	3.2
1	B	10	ASN	3.2
1	D	279	TYR	3.2
1	C	104	THR	3.2
1	B	57	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	275	PHE	3.1
1	C	226	LEU	3.1
1	A	272	LEU	3.1
1	B	219	LEU	3.1
1	E	48	ASN	3.1
1	B	323	ALA	3.1
1	D	287	PHE	3.1
1	A	247	LYS	3.1
1	A	220	PHE	3.1
1	A	273	GLY	3.1
1	E	104	THR	3.0
1	D	105	MET	3.0
1	A	290	HIS	3.0
1	D	282	ASN	3.0
1	C	59	LEU	3.0
1	C	264	ILE	3.0
1	E	56	PRO	3.0
1	D	226	LEU	3.0
1	D	288	GLN	3.0
1	E	296	GLU	2.9
1	A	319	PRO	2.9
1	A	280	ILE	2.9
1	B	106	LEU	2.9
1	B	275	PHE	2.9
1	B	290	HIS	2.9
1	A	226	LEU	2.9
1	C	204	VAL	2.9
1	A	281	LYS	2.9
1	C	218	LYS	2.9
1	A	215	LYS	2.8
1	A	322	HIS	2.8
1	C	277	VAL	2.8
1	C	220	PHE	2.8
1	E	295	ILE	2.8
1	E	277	VAL	2.8
1	C	280	ILE	2.8
1	D	221	GLU	2.8
1	A	10	ASN	2.7
1	A	100	VAL	2.7
1	C	323	ALA	2.7
1	E	281	LYS	2.7
1	B	321	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	277	VAL	2.7
1	A	289	LYS	2.6
1	B	280	ILE	2.6
1	C	56	PRO	2.6
1	B	47	SER	2.6
1	C	289	LYS	2.6
1	B	278	THR	2.6
1	B	276	LYS	2.6
1	C	321	ILE	2.6
1	A	221	GLU	2.6
1	C	290	HIS	2.6
1	C	324	ILE	2.6
1	D	281	LYS	2.6
1	C	214	PHE	2.5
1	E	59	LEU	2.5
1	E	219	LEU	2.5
1	D	204	VAL	2.5
1	E	280	ILE	2.5
1	B	272	LEU	2.5
1	C	48	ASN	2.5
1	D	217	VAL	2.5
1	C	213	ALA	2.5
1	E	209	LEU	2.4
1	C	275	PHE	2.4
1	B	281	LYS	2.4
1	B	59	LEU	2.4
1	C	255	TYR	2.4
1	C	279	TYR	2.4
1	A	48	ASN	2.4
1	D	103	THR	2.4
1	B	38	LYS	2.4
1	D	321	ILE	2.4
1	C	261	TYR	2.4
1	D	286	PHE	2.4
1	B	67	GLY	2.3
1	B	279	TYR	2.3
1	A	307	LEU	2.3
1	A	187	PHE	2.3
1	C	10	ASN	2.3
1	E	213	ALA	2.3
1	D	320	HIS	2.3
1	E	322	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	276	LYS	2.3
1	E	214	PHE	2.3
1	B	100	VAL	2.3
1	D	322	HIS	2.3
1	A	207	LEU	2.3
1	B	226	LEU	2.3
1	D	295	ILE	2.3
1	C	1	MET	2.3
1	D	100	VAL	2.3
1	A	148	PRO	2.3
1	D	293	ALA	2.2
1	E	261	TYR	2.3
1	A	246	GLN	2.2
1	A	295	ILE	2.2
1	E	289	LYS	2.2
1	E	102	ASP	2.2
1	A	216	GLU	2.2
1	D	107	ASN	2.2
1	B	161	TYR	2.2
1	B	146	LYS	2.2
1	D	59	LEU	2.2
1	A	47	SER	2.2
1	D	264	ILE	2.2
1	C	245	ALA	2.2
1	E	218	LYS	2.2
1	E	290	HIS	2.2
1	D	8	LEU	2.2
1	A	204	VAL	2.2
1	C	322	HIS	2.2
1	B	9	GLU	2.2
1	B	218	LYS	2.2
1	B	220	PHE	2.2
1	B	144	ASN	2.1
1	C	107	ASN	2.1
1	A	2	ARG	2.1
1	C	148	PRO	2.1
1	C	281	LYS	2.1
1	E	215	LYS	2.1
1	A	271	HIS	2.1
1	C	268	LEU	2.1
1	A	264	ILE	2.1
1	E	255	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	1	MET	2.1
1	D	212	MET	2.1
1	A	257	GLN	2.1
1	E	217	VAL	2.1
1	D	317	TYR	2.1
1	D	214	PHE	2.1
1	A	318	LEU	2.1
1	C	274	ASP	2.1
1	D	208	ALA	2.0
1	E	258	ALA	2.0
1	A	293	ALA	2.0
1	A	296	GLU	2.0
1	E	268	LEU	2.0
1	D	256	SER	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

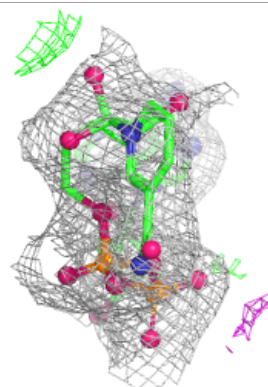
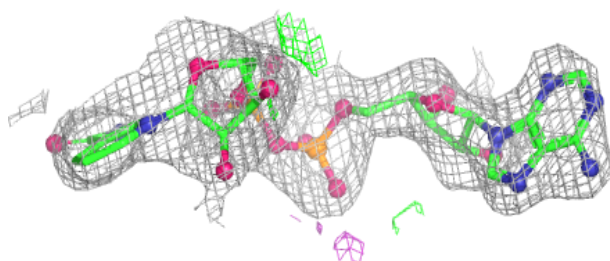
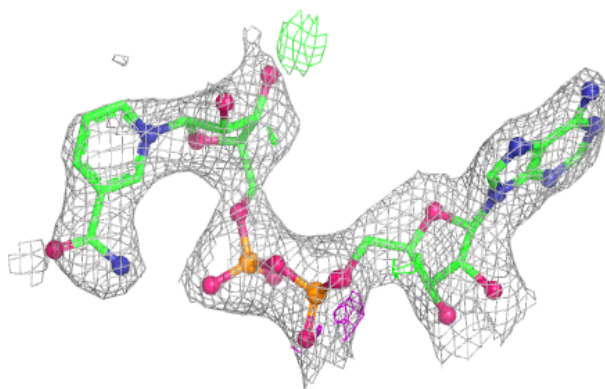
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	C	2403	44/44	0.94	0.10	40,51,62,63	0
2	NAD	D	2401	44/44	0.94	0.08	27,35,45,49	0
2	NAD	E	2403	44/44	0.94	0.09	43,47,57,58	0
2	NAD	B	2401	44/44	0.95	0.09	35,39,51,53	0
2	NAD	A	2402	44/44	0.96	0.09	30,35,44,49	0

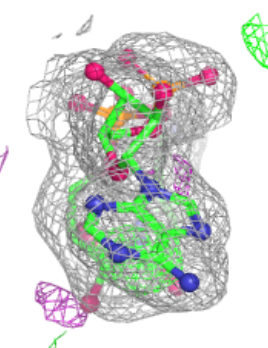
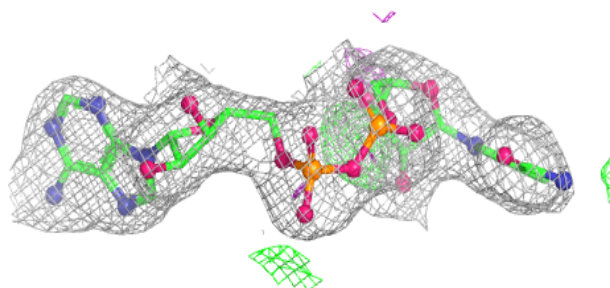
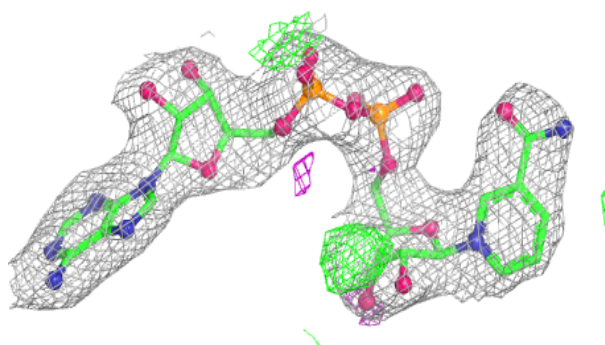
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD C 2403:

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

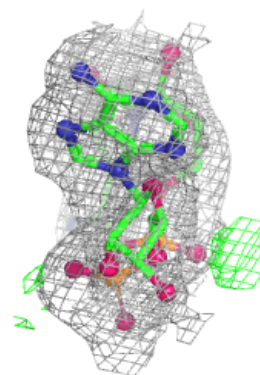
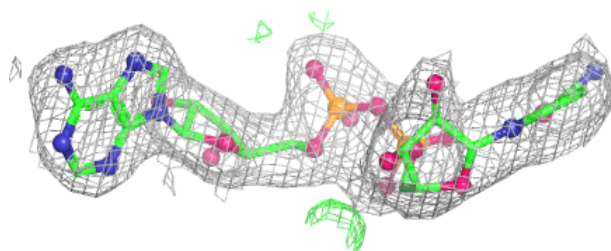
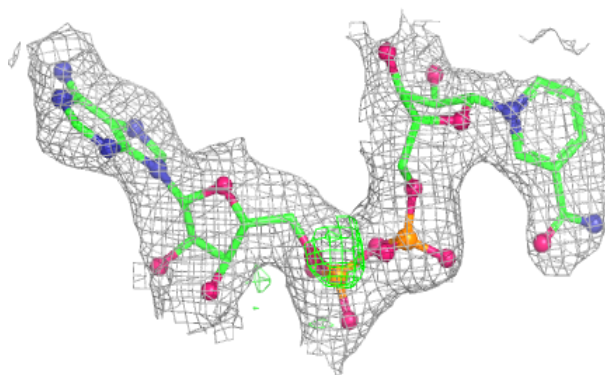
**Electron density around NAD D 2401:**

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

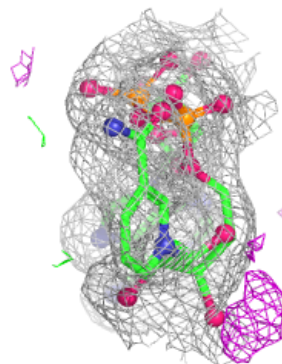
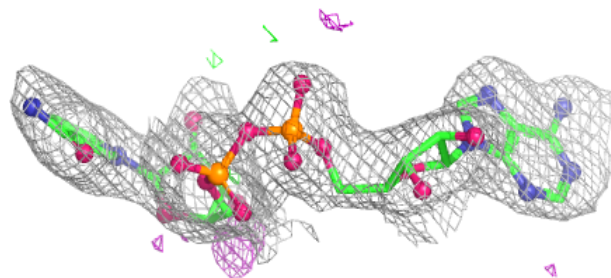
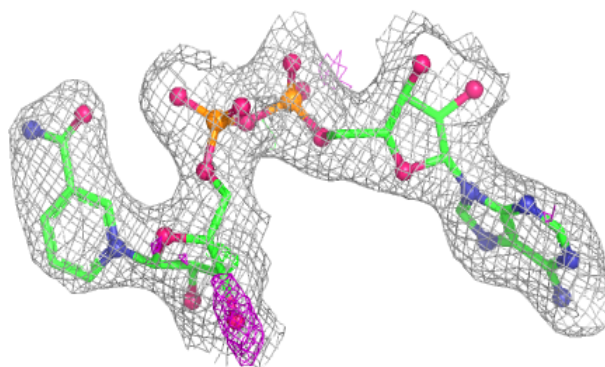


Electron density around NAD E 2403:

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

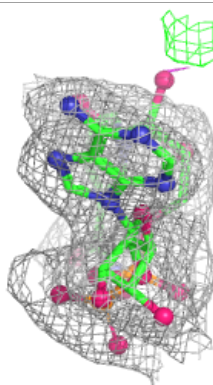
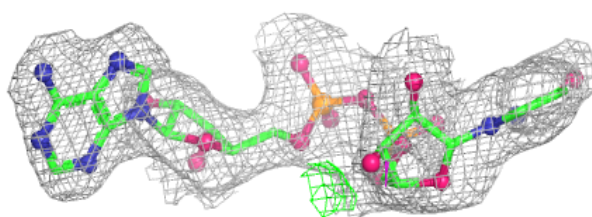
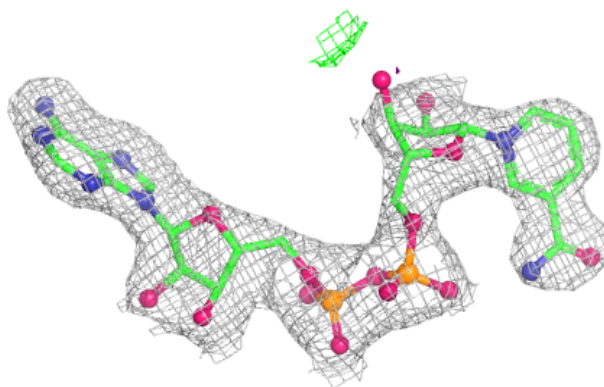
**Electron density around NAD B 2401:**

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



Electron density around NAD A 2402:

$2mF_o-DF_c$ (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.