Full wwPDB X-ray Structure Validation Report ⓘ

Jan 6, 2025 – 12:34 pm GMT

PDB ID	:	8PIS
Title	:	Crystal structure of Ser33 in complex with L-Serine
Authors	:	Perrone, S.; Cifuente, J.O.; Marina, A.; Mastrella, L.; Trastoy, B.; Linster, C.L.; Guerin, M.E.
Deposited on	:	2023-06-22
Resolution	:	2.69 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:

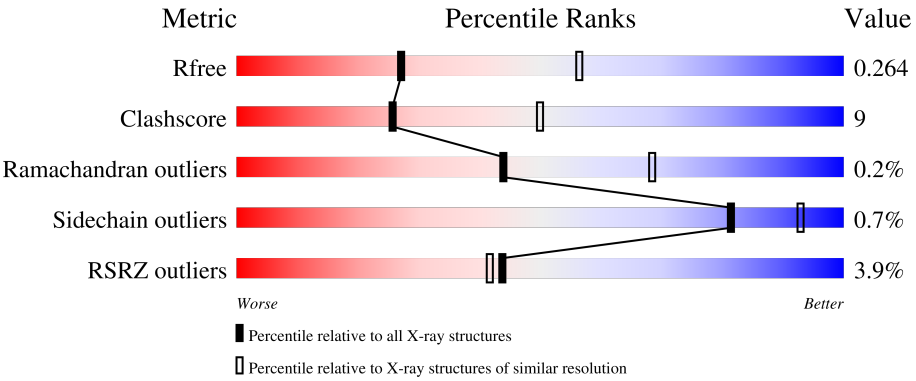
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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 <=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	473	2% 72% 19% 9%
1	B	473	2% 72% 19% 9%
1	C	473	2% 73% 16% 11%
1	D	473	7% 73% 17% 10%
1	E	473	2% 72% 19% 9%

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Mol	Chain	Length	Quality of chain
1	F	473	7% 71% 20% 9%
1	G	473	3% 70% 19% 10%
1	H	473	4% 71% 18% 10%
2	I	10	80% 20%
2	J	10	90% 10%
2	K	10	70% 30%
2	L	10	90% 10%
2	M	10	80% 20%
2	N	10	80% 20%
2	O	10	80% 20%
2	Q	10	90% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SER	E	503	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 26154 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 phosphoglycerate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	1	0
			3209	2032	547	621	9			
1	B	431	Total	C	N	O	S	0	0	0
			3178	2010	549	609	10			
1	C	423	Total	C	N	O	S	0	0	0
			3112	1973	533	597	9			
1	D	428	Total	C	N	O	S	0	0	0
			3076	1950	531	586	9			
1	E	431	Total	C	N	O	S	0	0	0
			3211	2039	551	611	10			
1	F	431	Total	C	N	O	S	0	0	0
			3153	2001	546	596	10			
1	G	426	Total	C	N	O	S	0	0	0
			3123	1987	537	589	10			
1	H	426	Total	C	N	O	S	0	0	0
			3131	1984	541	596	10			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP A0A8H4BZ61
A	-2	SER	-	expression tag	UNP A0A8H4BZ61
A	-1	GLY	-	expression tag	UNP A0A8H4BZ61
A	0	ALA	-	expression tag	UNP A0A8H4BZ61
B	-3	GLY	-	expression tag	UNP A0A8H4BZ61
B	-2	SER	-	expression tag	UNP A0A8H4BZ61
B	-1	GLY	-	expression tag	UNP A0A8H4BZ61
B	0	ALA	-	expression tag	UNP A0A8H4BZ61
C	-3	GLY	-	expression tag	UNP A0A8H4BZ61
C	-2	SER	-	expression tag	UNP A0A8H4BZ61
C	-1	GLY	-	expression tag	UNP A0A8H4BZ61
C	0	ALA	-	expression tag	UNP A0A8H4BZ61
D	-3	GLY	-	expression tag	UNP A0A8H4BZ61

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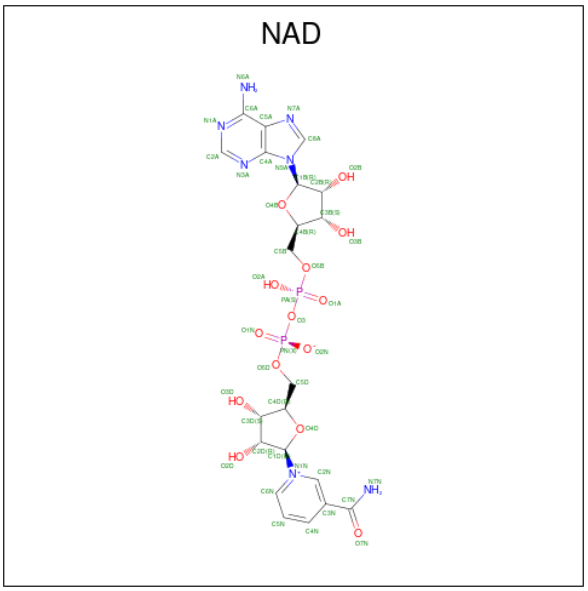
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	SER	-	expression tag	UNP A0A8H4BZ61
D	-1	GLY	-	expression tag	UNP A0A8H4BZ61
D	0	ALA	-	expression tag	UNP A0A8H4BZ61
E	-3	GLY	-	expression tag	UNP A0A8H4BZ61
E	-2	SER	-	expression tag	UNP A0A8H4BZ61
E	-1	GLY	-	expression tag	UNP A0A8H4BZ61
E	0	ALA	-	expression tag	UNP A0A8H4BZ61
F	-3	GLY	-	expression tag	UNP A0A8H4BZ61
F	-2	SER	-	expression tag	UNP A0A8H4BZ61
F	-1	GLY	-	expression tag	UNP A0A8H4BZ61
F	0	ALA	-	expression tag	UNP A0A8H4BZ61
G	-3	GLY	-	expression tag	UNP A0A8H4BZ61
G	-2	SER	-	expression tag	UNP A0A8H4BZ61
G	-1	GLY	-	expression tag	UNP A0A8H4BZ61
G	0	ALA	-	expression tag	UNP A0A8H4BZ61
H	-3	GLY	-	expression tag	UNP A0A8H4BZ61
H	-2	SER	-	expression tag	UNP A0A8H4BZ61
H	-1	GLY	-	expression tag	UNP A0A8H4BZ61
H	0	ALA	-	expression tag	UNP A0A8H4BZ61

- Molecule 2 is a protein called phosphoglycerate dehydrogenase.

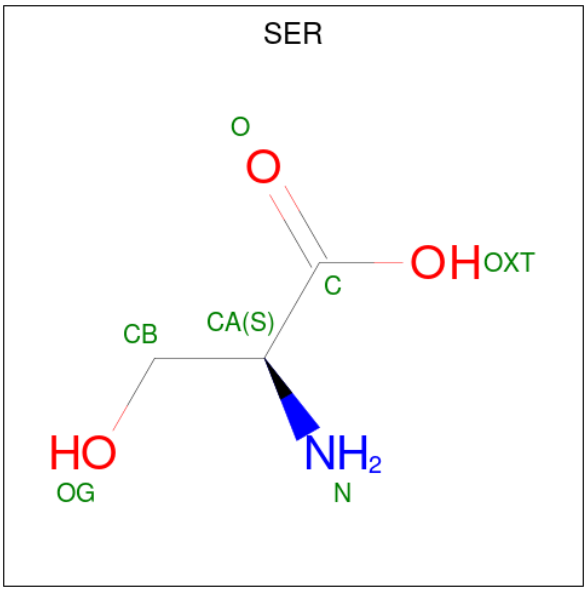
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	8	Total	C	N	O	0	0	0
			40	24	8	8			
2	J	9	Total	C	N	O	0	0	0
			45	27	9	9			
2	K	7	Total	C	N	O	0	0	0
			35	21	7	7			
2	M	8	Total	C	N	O	0	0	0
			40	24	8	8			
2	N	8	Total	C	N	O	0	0	0
			40	24	8	8			
2	O	8	Total	C	N	O	0	0	0
			40	24	8	8			
2	Q	9	Total	C	N	O	0	0	0
			45	27	9	9			
2	L	9	Total	C	N	O	0	0	0
			45	27	9	9			

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is SERINE (three-letter code: SER) (formula: $C_3H_7NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 7 3 1 3	0	0
4	B	1	Total C N O 7 3 1 3	0	0
4	C	1	Total C N O 7 3 1 3	0	0
4	D	1	Total C N O 7 3 1 3	0	0
4	E	1	Total C N O 7 3 1 3	0	0
4	E	1	Total C N O 7 3 1 3	0	0
4	G	1	Total C N O 7 3 1 3	0	0
4	H	1	Total C N O 7 3 1 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	42	Total O 42 42	0	0
5	B	22	Total O 22 22	0	0
5	C	38	Total O 38 38	0	0
5	D	16	Total O 16 16	0	0

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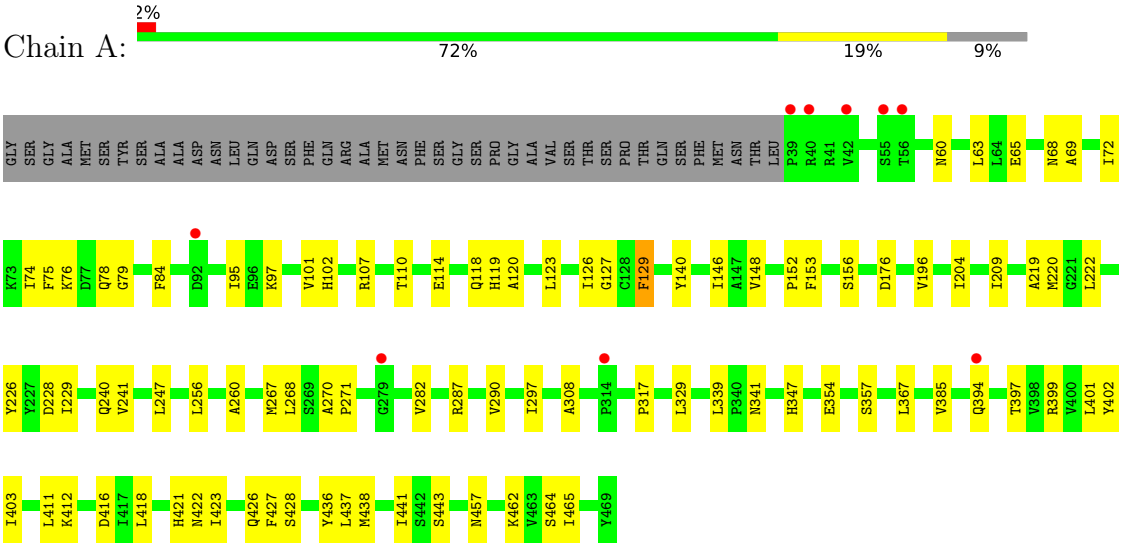
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	31	Total O 31 31	0	0
5	F	20	Total O 20 20	0	0
5	G	27	Total O 27 27	0	0
5	H	24	Total O 24 24	0	0
5	K	1	Total O 1 1	0	0
5	M	1	Total O 1 1	0	0
5	L	1	Total O 1 1	0	0

3 Residue-property plots (i)

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

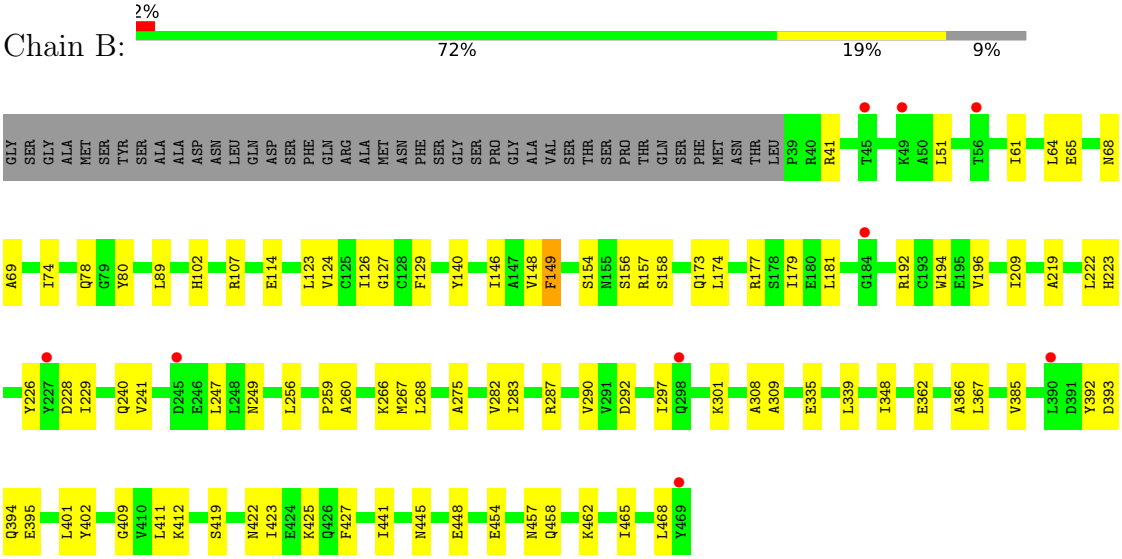
• Molecule 1: phosphoglycerate dehydrogenase

Chain A:



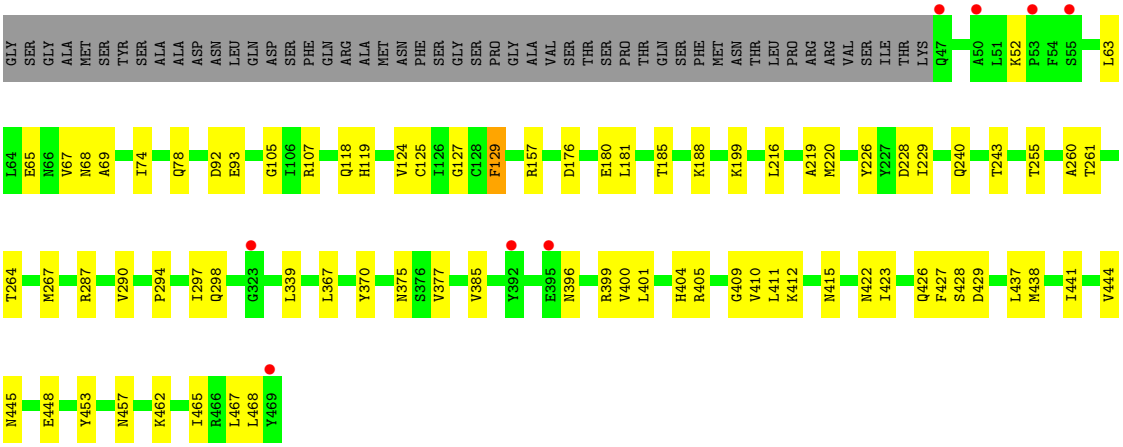
• Molecule 1: phosphoglycerate dehydrogenase

Chain B:



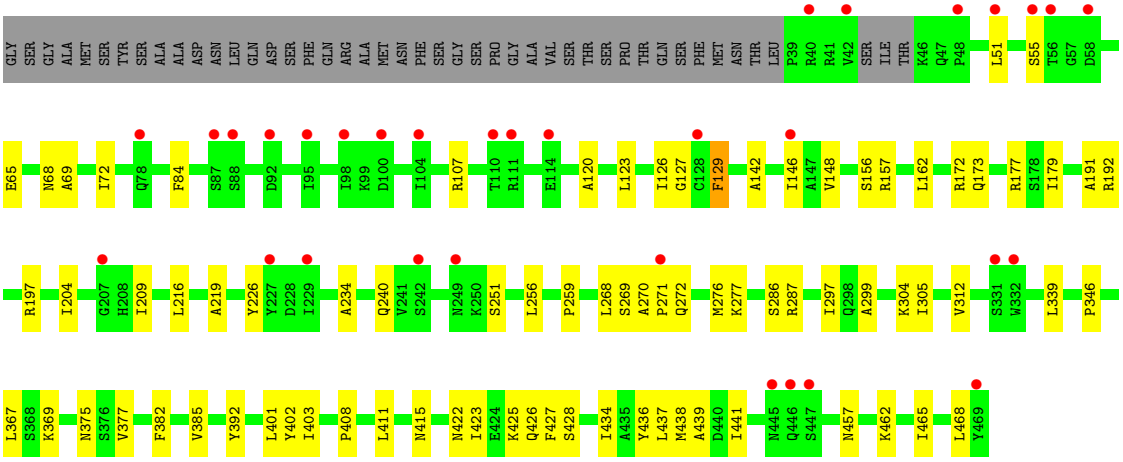
• Molecule 1: phosphoglycerate dehydrogenase

Chain C:



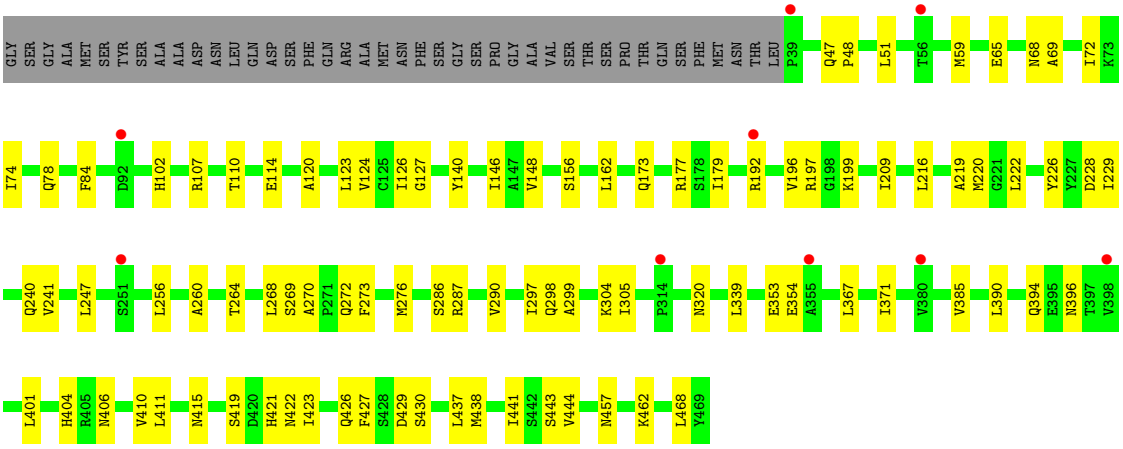
• Molecule 1: phosphoglycerate dehydrogenase

Chain D:



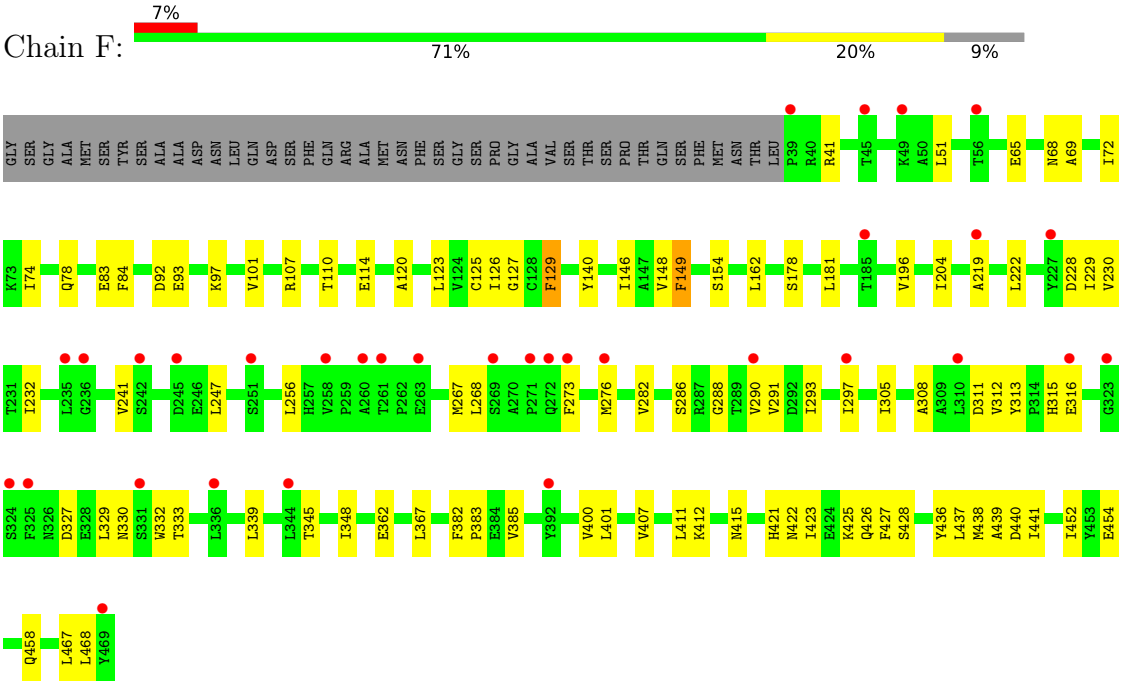
• Molecule 1: phosphoglycerate dehydrogenase

Chain E:



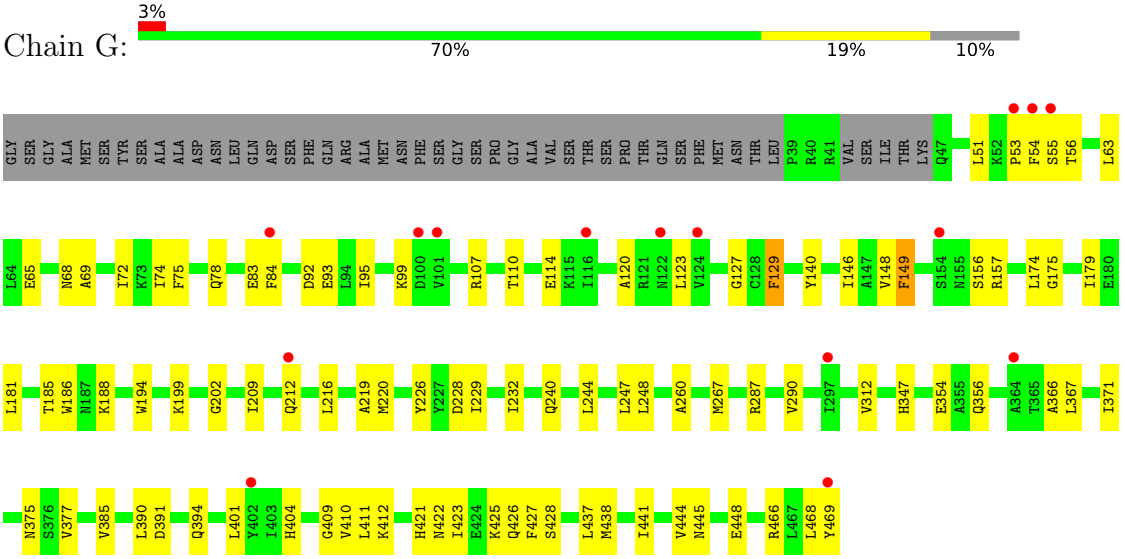
• Molecule 1: phosphoglycerate dehydrogenase

Chain F:



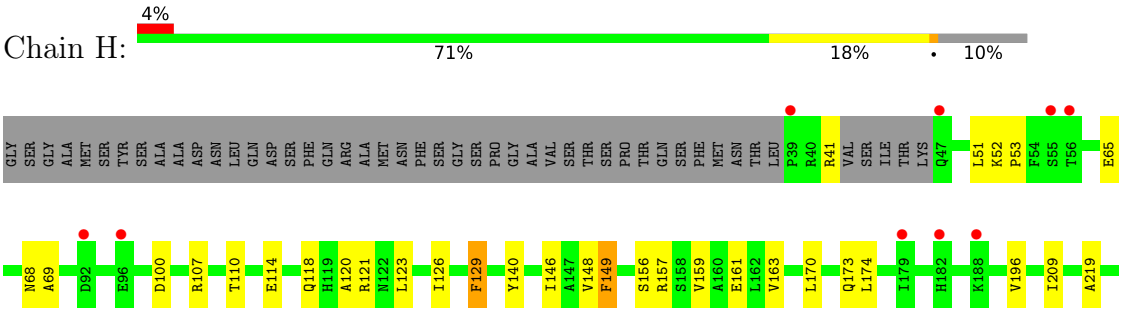
• Molecule 1: phosphoglycerate dehydrogenase

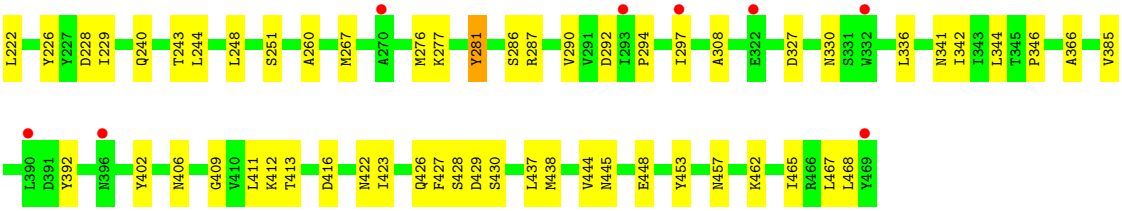
Chain G:



• Molecule 1: phosphoglycerate dehydrogenase

Chain H:





• Molecule 2: phosphoglycerate dehydrogenase

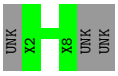
Chain I:

• Molecule 2: phosphoglycerate dehydrogenase

Chain J:

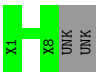
• Molecule 2: phosphoglycerate dehydrogenase

Chain K:



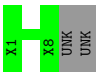
• Molecule 2: phosphoglycerate dehydrogenase

Chain M:



• Molecule 2: phosphoglycerate dehydrogenase

Chain N:



• Molecule 2: phosphoglycerate dehydrogenase

Chain O:

• Molecule 2: phosphoglycerate dehydrogenase

Chain Q:

• Molecule 2: phosphoglycerate dehydrogenase

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	106.11Å 110.73Å 117.03Å 64.42° 65.95° 67.03°	Depositor
Resolution (Å)	43.11 – 2.69 43.11 – 2.69	Depositor EDS
% Data completeness (in resolution range)	97.0 (43.11-2.69) 97.3 (43.11-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.216 , 0.265 0.214 , 0.264	Depositor DCC
R_{free} test set	6021 reflections (5.26%)	wwPDB-VP
Wilson B-factor (Å^2)	43.4	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	26154	wwPDB-VP
Average B, all atoms (Å^2)	48.0	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 70.35 % 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 3.1722e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.33	0/3264	0.55	0/4447
1	B	0.32	0/3232	0.55	0/4405
1	C	0.33	0/3165	0.53	0/4319
1	D	0.31	0/3126	0.53	0/4269
1	E	0.32	0/3267	0.52	0/4446
1	F	0.35	0/3206	0.55	0/4369
1	G	0.33	0/3177	0.54	0/4333
1	H	0.34	0/3184	0.55	0/4338
All	All	0.33	0/25621	0.54	0/34926

There are no bond length outliers.

There are no bond angle outliers.

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	3209	0	3115	69	0
1	B	3178	0	3067	61	0
1	C	3112	0	3021	52	0
1	D	3076	0	2902	64	0
1	E	3211	0	3142	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3153	0	3058	72	0
1	G	3123	0	2999	74	0
1	H	3131	0	3019	61	0
2	I	40	0	10	0	0
2	J	45	0	11	0	0
2	K	35	0	9	0	0
2	L	45	0	12	0	0
2	M	40	0	11	0	0
2	N	40	0	10	0	0
2	O	40	0	10	0	0
2	Q	45	0	12	0	0
3	A	44	0	26	1	0
3	B	44	0	26	1	0
3	C	44	0	26	0	0
3	D	44	0	26	2	0
3	E	44	0	26	1	0
3	F	44	0	26	0	0
3	G	44	0	26	0	0
3	H	44	0	26	0	0
4	A	7	0	4	3	0
4	B	7	0	4	2	0
4	C	7	0	4	3	0
4	D	7	0	4	2	0
4	E	14	0	8	7	0
4	G	7	0	4	3	0
4	H	7	0	4	3	0
5	A	42	0	0	0	0
5	B	22	0	0	2	0
5	C	38	0	0	0	0
5	D	16	0	0	0	0
5	E	31	0	0	0	0
5	F	20	0	0	0	0
5	G	27	0	0	1	0
5	H	24	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
All	All	26154	0	24648	473	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 9.

All (473) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:VAL:HG12	1:A:222:LEU:HD21	1.33	1.07
1:D:269:SER:H	1:D:272:GLN:HE21	1.15	0.94
1:E:269:SER:H	1:E:272:GLN:HE21	1.10	0.90
1:E:196:VAL:HG12	1:E:222:LEU:HD21	1.57	0.84
1:D:385:VAL:HG12	1:D:438:MET:HE3	1.62	0.81
1:F:196:VAL:HG12	1:F:222:LEU:HD21	1.64	0.79
1:A:426:GLN:HE21	1:A:437:LEU:HD11	1.48	0.79
1:B:266:LYS:HD3	1:H:243:THR:HG21	1.67	0.76
1:A:219:ALA:HB1	1:C:219:ALA:HB1	1.67	0.75
1:A:196:VAL:HG12	1:A:222:LEU:CD2	2.17	0.74
1:F:267:MET:HG2	1:F:290:VAL:HG13	1.71	0.73
1:F:327:ASP:HA	1:F:330:ASN:O	1.90	0.72
1:F:256:LEU:HD11	1:F:268:LEU:HD12	1.70	0.71
1:A:385:VAL:HG13	1:A:427:PHE:HD2	1.55	0.71
1:E:65:GLU:OE2	1:E:110:THR:N	2.23	0.71
1:G:426:GLN:HE21	1:G:437:LEU:HD11	1.55	0.70
1:C:422:ASN:OD1	4:D:502:SER:N	2.25	0.69
1:G:422:ASN:OD1	4:H:502:SER:N	2.25	0.69
1:F:425:LYS:NZ	1:F:440:ASP:OD2	2.26	0.68
1:H:68:ASN:OD1	1:H:69:ALA:N	2.26	0.68
1:B:223:HIS:ND1	5:B:601:HOH:O	2.25	0.68
1:E:269:SER:H	1:E:272:GLN:NE2	1.89	0.68
1:C:243:THR:HG21	1:G:83:GLU:HG2	1.75	0.68
4:C:502:SER:N	1:D:422:ASN:OD1	2.26	0.68
1:E:219:ALA:HB1	1:G:219:ALA:HB1	1.76	0.68
1:E:415:ASN:HD22	1:F:415:ASN:HD22	1.42	0.67
1:D:65:GLU:OE1	1:D:107:ARG:N	2.26	0.67
1:F:219:ALA:HB1	1:H:219:ALA:HB1	1.77	0.66
1:G:175:GLY:O	1:G:179:ILE:HG12	1.95	0.66
1:F:426:GLN:HE21	1:F:437:LEU:HD11	1.61	0.66
1:C:444:VAL:HG13	1:C:448:GLU:HG3	1.78	0.66
1:G:65:GLU:OE2	1:G:110:THR:N	2.29	0.65
4:A:502:SER:N	1:B:422:ASN:OD1	2.30	0.65
1:E:273:PHE:HD1	1:E:276:MET:HE2	1.61	0.65
1:C:428:SER:HB2	1:C:437:LEU:HD13	1.78	0.64
1:B:256:LEU:HD11	1:B:268:LEU:HD12	1.79	0.64
1:C:68:ASN:OD1	1:C:69:ALA:N	2.30	0.64
1:E:68:ASN:OD1	1:E:69:ALA:N	2.29	0.64
1:A:126:ILE:HB	1:A:148:VAL:HG22	1.80	0.64
1:F:297:ILE:HG23	1:F:339:LEU:HD11	1.79	0.64
1:F:65:GLU:OE2	1:F:110:THR:N	2.30	0.63
1:H:65:GLU:OE1	1:H:107:ARG:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:LEU:HD23	1:D:146:ILE:HD13	1.79	0.63
1:F:68:ASN:OD1	1:F:69:ALA:N	2.32	0.62
1:D:270:ALA:HB3	1:D:271:PRO:HD3	1.81	0.62
1:D:423:ILE:HD13	1:D:441:ILE:HG22	1.81	0.62
1:A:95:ILE:HG23	1:A:119:HIS:ND1	2.14	0.62
1:D:385:VAL:HG13	1:D:427:PHE:CD2	2.34	0.62
1:H:444:VAL:HG13	1:H:448:GLU:HG3	1.81	0.62
1:G:423:ILE:HD13	1:G:441:ILE:HG22	1.81	0.62
1:C:385:VAL:HG13	1:C:427:PHE:CD2	2.35	0.62
1:A:60:ASN:H	1:A:102:HIS:HD2	1.46	0.62
1:A:74:ILE:O	1:A:78:GLN:HG2	2.00	0.62
1:A:385:VAL:HG13	1:A:427:PHE:CD2	2.35	0.61
1:A:416:ASP:OD1	1:B:412:LYS:NZ	2.33	0.61
1:H:118:GLN:HG2	1:H:140:TYR:OH	2.00	0.61
1:H:170:LEU:HB3	1:H:281:TYR:HD2	1.63	0.61
1:A:402:TYR:HD1	1:A:465:ILE:HD13	1.63	0.61
1:F:423:ILE:HD13	1:F:441:ILE:HG22	1.82	0.61
1:H:123:LEU:HD23	1:H:146:ILE:HD13	1.83	0.61
1:C:426:GLN:HE21	1:C:437:LEU:HD11	1.64	0.61
1:A:426:GLN:OE1	1:B:411:LEU:HD23	1.99	0.61
1:E:411:LEU:HD23	1:F:426:GLN:OE1	1.99	0.61
1:E:320:ASN:HD22	1:G:186:TRP:HD1	1.48	0.61
1:E:156:SER:HA	1:E:209:ILE:HG12	1.83	0.61
4:E:503:SER:N	1:F:407:VAL:O	2.34	0.61
1:G:63:LEU:HD21	1:G:75:PHE:HE2	1.65	0.60
1:B:385:VAL:HG13	1:B:427:PHE:CD2	2.36	0.60
1:D:68:ASN:OD1	1:D:69:ALA:N	2.34	0.60
1:E:256:LEU:HD11	1:E:268:LEU:HD12	1.83	0.60
1:A:68:ASN:OD1	1:A:69:ALA:N	2.34	0.60
1:B:226:TYR:CZ	1:B:240:GLN:HB2	2.37	0.60
1:B:74:ILE:O	1:B:78:GLN:HG2	2.01	0.60
1:F:51:LEU:HB3	1:F:468:LEU:HB3	1.84	0.60
1:F:273:PHE:HD1	1:F:276:MET:HE2	1.65	0.60
4:E:502:SER:N	1:F:422:ASN:OD1	2.35	0.59
1:H:65:GLU:OE2	1:H:110:THR:N	2.33	0.59
1:E:51:LEU:HB3	1:E:468:LEU:HB3	1.85	0.59
1:C:297:ILE:HG23	1:C:339:LEU:HD11	1.84	0.59
1:E:422:ASN:OD1	4:E:503:SER:N	2.35	0.59
1:G:385:VAL:HG13	1:G:427:PHE:CD2	2.37	0.59
1:A:76:LYS:HD3	1:E:298:GLN:NE2	2.18	0.58
1:B:158:SER:O	1:D:172:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:502:SER:N	1:H:422:ASN:OD1	2.36	0.58
1:G:371:ILE:O	1:G:466:ARG:NH2	2.35	0.58
1:A:411:LEU:HD13	4:A:502:SER:HB3	1.85	0.58
1:B:219:ALA:HB1	1:D:219:ALA:HB1	1.86	0.58
1:G:68:ASN:OD1	1:G:69:ALA:N	2.35	0.58
1:E:123:LEU:HD23	1:E:146:ILE:HD13	1.84	0.58
1:D:173:GLN:HG3	1:D:177:ARG:NH1	2.19	0.58
1:E:47:GLN:HG3	1:E:48:PRO:HD2	1.85	0.58
1:A:114:GLU:O	1:A:118:GLN:HG3	2.04	0.57
1:B:196:VAL:HG12	1:B:222:LEU:HD21	1.85	0.57
1:F:315:HIS:H	1:F:330:ASN:HD21	1.52	0.57
1:D:226:TYR:CZ	1:D:240:GLN:HB2	2.39	0.57
1:B:423:ILE:HD13	1:B:441:ILE:HG22	1.87	0.57
1:G:232:ILE:HG12	1:H:41:ARG:HG2	1.85	0.57
1:G:426:GLN:OE1	1:H:411:LEU:HD13	2.05	0.57
1:C:243:THR:HG21	1:G:83:GLU:CG	2.33	0.56
1:F:228:ASP:OD1	1:F:229:ILE:N	2.38	0.56
1:G:385:VAL:HG12	1:G:438:MET:SD	2.46	0.56
1:H:453:TYR:HD1	1:H:467:LEU:HD13	1.71	0.56
1:B:68:ASN:OD1	1:B:69:ALA:N	2.38	0.56
1:E:385:VAL:HG13	1:E:427:PHE:CD2	2.41	0.56
1:B:65:GLU:OE1	1:B:107:ARG:N	2.34	0.56
1:E:74:ILE:O	1:E:78:GLN:HG2	2.05	0.56
1:B:393:ASP:O	1:B:395:GLU:N	2.39	0.56
1:D:428:SER:HB2	1:D:437:LEU:HD13	1.88	0.56
1:G:444:VAL:HG13	1:G:448:GLU:HG3	1.88	0.56
1:B:64:LEU:HD22	1:B:89:LEU:HD13	1.86	0.56
1:B:445:ASN:OD1	1:B:448:GLU:HG2	2.06	0.56
1:D:408:PRO:HA	4:D:502:SER:OG	2.06	0.56
1:B:228:ASP:OD1	1:B:229:ILE:N	2.39	0.55
1:D:256:LEU:HD11	1:D:268:LEU:HD12	1.88	0.55
1:D:403:ILE:HD13	1:D:436:TYR:CD1	2.41	0.55
1:E:220:MET:HE1	1:G:216:LEU:HD22	1.88	0.55
1:H:170:LEU:HB3	1:H:281:TYR:CD2	2.41	0.55
1:G:202:GLY:HA2	1:G:247:LEU:HD11	1.88	0.55
1:D:127:GLY:HA3	1:D:367:LEU:HD11	1.88	0.55
1:H:426:GLN:HG3	1:H:437:LEU:HD11	1.89	0.55
1:B:149:PHE:CD2	1:B:366:ALA:HB1	2.42	0.55
1:D:385:VAL:HG13	1:D:427:PHE:HD2	1.69	0.55
1:H:100:ASP:OD1	1:H:121:ARG:NH2	2.40	0.55
1:A:256:LEU:HD11	1:A:268:LEU:HD12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:TYR:HD1	1:C:467:LEU:HD23	1.71	0.55
1:G:127:GLY:HA3	1:G:367:LEU:HD11	1.89	0.55
1:A:65:GLU:OE2	1:A:110:THR:N	2.40	0.55
1:H:385:VAL:HG13	1:H:427:PHE:CD2	2.42	0.55
1:G:51:LEU:HB3	1:G:468:LEU:HB3	1.89	0.54
1:E:415:ASN:HD21	1:E:426:GLN:HE22	1.56	0.54
1:F:92:ASP:OD1	1:F:93:GLU:N	2.41	0.54
1:C:415:ASN:ND2	1:D:415:ASN:OD1	2.41	0.54
1:E:228:ASP:OD1	1:E:229:ILE:N	2.41	0.54
1:E:297:ILE:HG23	1:E:339:LEU:HD11	1.88	0.54
1:G:445:ASN:OD1	1:G:448:GLU:HG2	2.07	0.54
1:F:154:SER:OG	1:F:362:GLU:OE1	2.26	0.54
1:F:316:GLU:HA	1:F:329:LEU:HD21	1.91	0.53
1:E:102:HIS:O	1:E:124:VAL:HG22	2.09	0.53
1:E:179:ILE:HG12	1:G:179:ILE:HD12	1.90	0.53
1:G:65:GLU:OE1	1:G:107:ARG:HB2	2.07	0.53
1:H:244:LEU:O	1:H:248:LEU:HG	2.08	0.53
1:E:404:HIS:CD2	1:E:410:VAL:HG11	2.44	0.53
1:G:226:TYR:CZ	1:G:240:GLN:HB2	2.43	0.53
1:E:320:ASN:ND2	1:G:188:LYS:H	2.06	0.53
1:B:297:ILE:HG23	1:B:339:LEU:HD11	1.91	0.53
1:D:297:ILE:HG23	1:D:339:LEU:HD11	1.89	0.53
1:D:426:GLN:HG3	1:D:439:ALA:HB2	1.91	0.53
1:E:241:VAL:HG21	1:E:247:LEU:HB2	1.91	0.53
1:A:127:GLY:HA3	1:A:367:LEU:HD11	1.91	0.52
1:C:423:ILE:HD13	1:C:441:ILE:HG22	1.89	0.52
1:F:120:ALA:HB1	1:F:123:LEU:HB2	1.92	0.52
1:D:276:MET:O	1:D:304:LYS:NZ	2.30	0.52
1:C:74:ILE:O	1:C:78:GLN:HG2	2.10	0.52
1:C:411:LEU:HD23	1:D:426:GLN:OE1	2.09	0.52
1:E:426:GLN:HG3	1:E:437:LEU:HD11	1.91	0.52
1:F:426:GLN:NE2	1:F:437:LEU:HD11	2.24	0.52
1:C:65:GLU:OE1	1:C:107:ARG:N	2.40	0.52
1:D:191:ALA:O	1:D:192:ARG:HB2	2.09	0.52
1:F:454:GLU:O	1:F:458:GLN:HG2	2.09	0.52
1:A:120:ALA:HB1	1:A:123:LEU:HB2	1.92	0.52
1:C:404:HIS:CD2	1:C:410:VAL:HG11	2.44	0.52
1:C:426:GLN:OE1	1:D:411:LEU:HD13	2.10	0.52
1:F:126:ILE:HB	1:F:148:VAL:HG22	1.92	0.52
1:G:401:LEU:CD2	1:G:438:MET:HG2	2.40	0.52
1:E:457:ASN:HA	1:E:462:LYS:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:ASN:HA	1:A:462:LYS:HD3	1.92	0.51
1:G:260:ALA:HB2	1:G:287:ARG:HG3	1.93	0.51
1:G:391:ASP:HB2	1:G:394:GLN:HG3	1.92	0.51
1:E:260:ALA:HB2	1:E:287:ARG:HG3	1.93	0.51
1:C:226:TYR:CZ	1:C:240:GLN:HB2	2.46	0.51
1:G:114:GLU:HG3	1:G:140:TYR:CZ	2.46	0.51
1:H:228:ASP:OD1	1:H:229:ILE:N	2.43	0.51
1:B:123:LEU:HD23	1:B:146:ILE:HD13	1.92	0.51
1:B:156:SER:HA	1:B:209:ILE:HG12	1.92	0.51
1:F:74:ILE:O	1:F:78:GLN:HG2	2.10	0.51
1:F:114:GLU:HG3	1:F:140:TYR:CZ	2.46	0.51
1:B:127:GLY:HA3	1:B:367:LEU:HD11	1.92	0.51
1:A:156:SER:HA	1:A:209:ILE:HG12	1.93	0.51
1:E:196:VAL:CG1	1:E:222:LEU:HD21	2.35	0.51
1:F:273:PHE:CD1	1:F:276:MET:HE2	2.45	0.51
1:H:51:LEU:HB3	1:H:468:LEU:HB3	1.93	0.51
1:H:428:SER:HB2	1:H:437:LEU:HD13	1.92	0.51
1:B:114:GLU:HG3	1:B:140:TYR:CZ	2.46	0.51
1:C:401:LEU:O	1:C:465:ILE:HD12	2.11	0.51
1:A:422:ASN:OD1	4:B:502:SER:N	2.44	0.51
1:E:65:GLU:OE1	1:E:107:ARG:HB2	2.10	0.51
1:A:394[B]:GLN:NE2	1:A:397:THR:OG1	2.43	0.50
1:C:385:VAL:HG12	1:C:438:MET:SD	2.52	0.50
1:G:428:SER:HB2	1:G:437:LEU:HD13	1.92	0.50
1:G:404:HIS:CD2	1:G:410:VAL:HG11	2.45	0.50
1:D:426:GLN:NE2	1:D:437:LEU:HD11	2.27	0.50
1:F:282:VAL:O	1:F:308:ALA:HA	2.11	0.50
1:A:403:ILE:HD12	1:A:464:SER:OG	2.12	0.50
1:F:256:LEU:HD13	1:F:290:VAL:HG12	1.94	0.50
1:A:63:LEU:HD21	1:A:75:PHE:HE2	1.77	0.50
1:F:241:VAL:HG21	1:F:247:LEU:HB2	1.94	0.50
1:B:266:LYS:NZ	1:B:292:ASP:OD1	2.35	0.49
1:E:354:GLU:OE2	1:G:199:LYS:NZ	2.41	0.49
1:A:228:ASP:OD1	1:A:229:ILE:N	2.45	0.49
1:E:226:TYR:CZ	1:E:240:GLN:HB2	2.47	0.49
1:G:129:PHE:N	1:G:129:PHE:CD1	2.80	0.49
1:A:317:PRO:HD3	1:A:329:LEU:HD21	1.93	0.49
1:G:53:PRO:HB2	1:G:56:THR:CB	2.42	0.49
1:G:228:ASP:OD1	1:G:229:ILE:N	2.46	0.49
1:G:409:GLY:O	1:G:412:LYS:HB3	2.13	0.49
1:C:453:TYR:CD1	1:C:467:LEU:HD23	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ASN:H	1:A:102:HIS:CD2	2.27	0.49
1:A:220:MET:HG2	1:C:220:MET:HE3	1.94	0.49
1:A:423:ILE:HB	4:B:502:SER:HA	1.95	0.49
1:B:51:LEU:HB3	1:B:468:LEU:HB3	1.94	0.49
1:B:385:VAL:HA	1:B:427:PHE:HE2	1.77	0.49
1:H:297:ILE:HD11	1:H:336:LEU:HB2	1.95	0.49
1:F:178:SER:HA	1:H:344:LEU:O	2.13	0.49
1:H:120:ALA:HB1	1:H:123:LEU:HB2	1.95	0.49
1:G:129:PHE:N	1:G:129:PHE:HD1	2.11	0.49
1:H:260:ALA:HB2	1:H:287:ARG:HG3	1.95	0.49
1:A:427:PHE:HD1	1:B:427:PHE:HB2	1.78	0.48
1:D:156:SER:HA	1:D:209:ILE:HG12	1.94	0.48
1:C:228:ASP:OD1	1:C:229:ILE:N	2.46	0.48
1:E:423:ILE:HB	4:E:503:SER:HA	1.94	0.48
1:D:126:ILE:HB	1:D:148:VAL:HG22	1.96	0.48
1:D:426:GLN:HE21	1:D:437:LEU:HD11	1.77	0.48
1:F:276:MET:CE	1:F:305:ILE:HD11	2.43	0.48
1:G:423:ILE:HB	4:H:502:SER:HA	1.95	0.48
1:F:83:GLU:OE1	1:F:97:LYS:HE2	2.13	0.48
1:F:327:ASP:OD1	1:F:333:THR:N	2.47	0.48
1:E:197:ARG:HB2	1:G:157:ARG:NH2	2.29	0.48
1:F:65:GLU:OE1	1:F:107:ARG:HB2	2.13	0.48
1:A:418:LEU:HD22	1:A:441:ILE:HD13	1.95	0.48
1:E:276:MET:O	1:E:304:LYS:NZ	2.34	0.48
1:G:312:VAL:HG12	1:G:347:HIS:CD2	2.48	0.48
1:A:226:TYR:CZ	1:A:240:GLN:HB2	2.49	0.48
1:A:428:SER:HB2	1:A:437:LEU:HD13	1.96	0.48
1:C:457:ASN:HA	1:C:462:LYS:HD3	1.96	0.48
1:F:97:LYS:O	1:F:101:VAL:HG23	2.14	0.48
1:H:445:ASN:OD1	1:H:448:GLU:HG2	2.13	0.48
1:G:156:SER:HA	1:G:209:ILE:HG12	1.95	0.48
1:B:402:TYR:HD1	1:B:465:ILE:HD13	1.79	0.48
1:C:181:LEU:HD23	1:C:185:THR:O	2.14	0.48
1:D:65:GLU:HB3	1:D:107:ARG:HD3	1.95	0.48
1:D:204:ILE:HB	1:D:256:LEU:HD23	1.95	0.47
1:D:259:PRO:HD3	3:D:501:NAD:H51A	1.94	0.47
1:G:411:LEU:HD13	4:G:502:SER:HB3	1.96	0.47
1:H:457:ASN:HA	1:H:462:LYS:HD3	1.96	0.47
1:C:127:GLY:HA3	1:C:367:LEU:HD11	1.96	0.47
1:C:445:ASN:OD1	1:C:448:GLU:HG2	2.13	0.47
1:B:126:ILE:HB	1:B:148:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:125:CYS:SG	1:F:367:LEU:HD22	2.54	0.47
1:A:354:GLU:OE2	1:C:199:LYS:NZ	2.42	0.47
1:E:216:LEU:HD22	1:G:220:MET:HE1	1.96	0.47
1:E:273:PHE:HD1	1:E:276:MET:CE	2.26	0.47
1:F:276:MET:HE3	1:F:305:ILE:HD11	1.96	0.47
1:B:192:ARG:HD3	1:B:194:TRP:HZ2	1.79	0.47
1:D:402:TYR:HD1	1:D:465:ILE:HD13	1.79	0.47
1:F:428:SER:HB2	1:F:437:LEU:HD13	1.95	0.47
1:F:228:ASP:OD2	1:F:232:ILE:HD11	2.14	0.47
1:A:72:ILE:HD11	1:A:84:PHE:CD1	2.48	0.47
1:D:269:SER:H	1:D:272:GLN:NE2	1.98	0.47
1:F:196:VAL:CG1	1:F:222:LEU:HD21	2.37	0.47
1:G:95:ILE:O	1:G:99:LYS:HG3	2.14	0.47
1:G:427:PHE:HB2	1:H:427:PHE:CD1	2.49	0.47
1:H:129:PHE:N	1:H:129:PHE:HD1	2.13	0.47
1:A:222:LEU:HD23	1:A:222:LEU:N	2.29	0.47
1:B:179:ILE:HG12	1:D:179:ILE:HG12	1.97	0.47
1:C:409:GLY:O	1:C:412:LYS:HB3	2.15	0.47
1:B:457:ASN:HA	1:B:462:LYS:HD3	1.96	0.47
1:C:294:PRO:O	1:C:298:GLN:HG3	2.15	0.47
1:E:390:LEU:HD22	1:E:394:GLN:OE1	2.15	0.47
1:E:396:ASN:HB3	1:E:444:VAL:H	1.80	0.47
1:H:173:GLN:HG2	1:H:341:ASN:ND2	2.30	0.46
1:F:273:PHE:HA	1:F:276:MET:HE2	1.98	0.46
1:D:375:ASN:OD1	1:D:377:VAL:HG22	2.15	0.46
4:E:502:SER:HA	1:F:423:ILE:HB	1.97	0.46
1:G:385:VAL:HG13	1:G:427:PHE:HD2	1.78	0.46
1:H:402:TYR:HD1	1:H:465:ILE:HD12	1.81	0.46
1:B:409:GLY:O	1:B:412:LYS:HB3	2.15	0.46
1:E:385:VAL:HG12	1:E:438:MET:SD	2.56	0.46
1:H:126:ILE:HB	1:H:148:VAL:HG22	1.97	0.46
1:E:114:GLU:HG3	1:E:140:TYR:CZ	2.50	0.46
1:E:162:LEU:HD11	1:G:174:LEU:HD21	1.98	0.46
1:E:299:ALA:HB1	1:E:305:ILE:HG12	1.97	0.46
1:G:123:LEU:HD23	1:G:146:ILE:HD13	1.97	0.46
1:H:129:PHE:N	1:H:129:PHE:CD1	2.83	0.46
1:H:413:THR:O	1:H:416:ASP:HB3	2.15	0.46
1:A:241:VAL:HG21	1:A:247:LEU:HB2	1.98	0.46
1:B:192:ARG:HD3	1:B:194:TRP:CZ2	2.51	0.46
1:B:454:GLU:O	1:B:458:GLN:HG2	2.15	0.46
1:C:92:ASP:OD1	1:C:93:GLU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:427:PHE:HB2	1:H:427:PHE:HD1	1.81	0.46
1:D:299:ALA:HB1	1:D:305:ILE:HG12	1.98	0.46
1:F:385:VAL:HG13	1:F:427:PHE:CD2	2.50	0.46
1:F:382:PHE:CD2	1:F:383:PRO:HD2	2.51	0.46
1:H:226:TYR:CZ	1:H:240:GLN:HB2	2.51	0.46
1:A:426:GLN:HE21	1:A:437:LEU:CD1	2.23	0.45
1:E:126:ILE:HB	1:E:148:VAL:HG22	1.97	0.45
1:H:149:PHE:CD2	1:H:366:ALA:HB1	2.51	0.45
1:B:61:ILE:HD13	1:B:80:TYR:HB3	1.97	0.45
1:B:154:SER:OG	1:B:362:GLU:OE1	2.34	0.45
1:G:421:HIS:CE1	1:G:444:VAL:HG22	2.50	0.45
3:A:501:NAD:O3B	1:B:41:ARG:NH2	2.40	0.45
4:A:502:SER:HA	1:B:423:ILE:HB	1.98	0.45
1:B:385:VAL:HA	1:B:427:PHE:CE2	2.52	0.45
1:C:63:LEU:HD13	1:C:67:VAL:HG21	1.97	0.45
1:E:127:GLY:HA3	1:E:367:LEU:HD11	1.98	0.45
1:E:196:VAL:HG12	1:E:222:LEU:CD2	2.39	0.45
1:D:287:ARG:HA	1:D:287:ARG:HD3	1.78	0.45
1:F:400:VAL:HA	1:F:467:LEU:HD23	1.99	0.45
1:D:286:SER:OG	1:D:287:ARG:N	2.46	0.45
1:E:423:ILE:HD13	1:E:441:ILE:HG22	1.98	0.45
1:D:157:ARG:HH12	1:D:216:LEU:HD21	1.82	0.45
1:E:264:THR:HG23	1:E:290:VAL:HG13	1.98	0.45
1:F:421:HIS:CE1	1:F:452:ILE:HD11	2.51	0.45
1:H:149:PHE:N	1:H:149:PHE:CD1	2.85	0.45
1:H:308:ALA:O	1:H:342:ILE:HA	2.17	0.45
1:B:196:VAL:CG1	1:B:222:LEU:HD21	2.47	0.44
1:H:156:SER:HA	1:H:209:ILE:HG12	1.99	0.44
1:F:288:GLY:HA3	1:F:313:TYR:O	2.17	0.44
1:G:426:GLN:NE2	1:G:437:LEU:HD11	2.27	0.44
1:G:120:ALA:HB1	1:G:123:LEU:HB2	1.98	0.44
1:G:356:GLN:NE2	5:G:603:HOH:O	2.49	0.44
1:H:114:GLU:O	1:H:118:GLN:HG3	2.18	0.44
1:E:353:GLU:HG3	1:G:194:TRP:CZ3	2.53	0.44
1:H:251:SER:O	1:H:277:LYS:HD3	2.18	0.44
1:E:419:SER:HB3	1:F:412:LYS:HD2	2.00	0.44
1:H:327:ASP:HA	1:H:330:ASN:O	2.18	0.44
1:A:260:ALA:HB2	1:A:287:ARG:HG3	2.00	0.44
1:A:347:HIS:O	1:C:188:LYS:HE2	2.18	0.44
1:B:401:LEU:O	1:B:465:ILE:HD12	2.18	0.44
1:E:59:MET:HE2	1:E:371:ILE:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:GLN:O	1:E:177:ARG:HG2	2.18	0.44
1:F:72:ILE:HD11	1:F:84:PHE:CD1	2.53	0.44
1:B:259:PRO:HD3	3:B:501:NAD:H51A	2.00	0.43
1:B:267:MET:HG2	1:B:290:VAL:HG13	1.99	0.43
1:B:425:LYS:NZ	5:B:604:HOH:O	2.51	0.43
1:C:267:MET:HG2	1:C:290:VAL:HG13	2.00	0.43
1:C:375:ASN:OD1	1:C:377:VAL:HG22	2.18	0.43
1:E:286:SER:OG	1:E:287:ARG:N	2.51	0.43
1:G:74:ILE:O	1:G:78:GLN:HG2	2.18	0.43
1:A:297:ILE:HG23	1:A:339:LEU:HD11	1.99	0.43
1:D:457:ASN:HA	1:D:462:LYS:HD3	2.00	0.43
1:G:92:ASP:OD1	1:G:93:GLU:N	2.51	0.43
1:H:286:SER:OG	1:H:287:ARG:N	2.47	0.43
1:B:174:LEU:HD21	1:D:162:LEU:HD11	1.99	0.43
1:C:118:GLN:HE21	1:C:119:HIS:CE1	2.37	0.43
1:D:401:LEU:O	1:D:465:ILE:HD12	2.18	0.43
1:D:428:SER:HB2	1:D:437:LEU:CD1	2.47	0.43
1:F:149:PHE:CD1	1:F:149:PHE:N	2.86	0.43
1:G:54:PHE:O	1:G:55:SER:C	2.56	0.43
1:G:149:PHE:N	1:G:149:PHE:HD1	2.16	0.43
1:H:267:MET:HG2	1:H:290:VAL:HG13	2.00	0.43
1:D:142:ALA:HB1	1:D:434:ILE:HD13	2.01	0.43
1:E:264:THR:CG2	1:E:290:VAL:HG22	2.47	0.43
1:D:129:PHE:HD1	1:D:129:PHE:N	2.16	0.43
1:F:229:ILE:HG13	1:F:230:VAL:HG23	2.01	0.43
1:F:426:GLN:HG3	1:F:439:ALA:HB2	2.00	0.43
1:H:196:VAL:CG1	1:H:222:LEU:HD21	2.48	0.43
1:H:409:GLY:O	1:H:412:LYS:HB3	2.19	0.43
1:A:412:LYS:HD2	1:B:419:SER:HB3	2.00	0.43
1:B:181:LEU:HD21	1:D:346:PRO:HB3	2.01	0.43
1:H:292:ASP:OD1	1:H:294:PRO:HD2	2.18	0.43
1:A:97:LYS:O	1:A:101:VAL:HG23	2.19	0.43
1:C:385:VAL:HG13	1:C:427:PHE:HD2	1.81	0.43
1:C:400:VAL:HG22	1:C:467:LEU:HD11	2.00	0.43
1:D:269:SER:O	1:D:270:ALA:C	2.57	0.43
1:E:429:ASP:OD1	1:F:425:LYS:HG2	2.19	0.43
1:F:204:ILE:HB	1:F:256:LEU:HD23	2.01	0.43
1:G:149:PHE:N	1:G:149:PHE:CD1	2.86	0.43
1:A:267:MET:HG2	1:A:290:VAL:HG13	2.01	0.43
1:B:102:HIS:O	1:B:124:VAL:HG22	2.19	0.43
1:A:401:LEU:HD22	1:A:436:TYR:OH	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:PHE:N	1:B:149:PHE:CD1	2.87	0.43
1:D:129:PHE:N	1:D:129:PHE:CD1	2.86	0.43
1:E:406:ASN:ND2	1:E:430:SER:HB2	2.34	0.43
1:E:415:ASN:ND2	1:F:415:ASN:HD22	2.14	0.43
1:F:123:LEU:HD23	1:F:146:ILE:HD13	2.01	0.43
1:F:316:GLU:CA	1:F:329:LEU:HD21	2.47	0.43
1:A:385:VAL:HG12	1:A:438:MET:SD	2.59	0.43
1:B:301:LYS:HE3	1:B:335:GLU:OE2	2.19	0.43
1:B:348:ILE:H	1:B:348:ILE:HG13	1.72	0.43
1:E:120:ALA:HB1	1:E:123:LEU:HB2	2.01	0.43
1:G:385:VAL:HA	1:G:427:PHE:HE2	1.84	0.43
1:H:281:TYR:CD1	1:H:281:TYR:N	2.87	0.43
1:A:196:VAL:O	1:A:222:LEU:HD22	2.19	0.42
1:C:129:PHE:CD1	1:C:129:PHE:N	2.87	0.42
1:C:399:ARG:HD3	1:C:438:MET:HE2	2.01	0.42
1:D:369:LYS:HE2	1:D:375:ASN:HD22	1.84	0.42
1:D:382:PHE:HZ	1:D:403:ILE:HD12	1.84	0.42
1:E:423:ILE:H	4:E:503:SER:HA	1.84	0.42
1:F:311:ASP:OD1	1:F:345:THR:OG1	2.28	0.42
1:F:348:ILE:H	1:F:348:ILE:HG13	1.73	0.42
1:A:79:GLY:HA2	1:E:270:ALA:HB3	2.00	0.42
1:F:127:GLY:HA3	1:F:367:LEU:HD11	2.01	0.42
1:F:162:LEU:HD11	1:H:174:LEU:HD21	2.01	0.42
1:A:399:ARG:HD3	1:A:438:MET:HE2	2.01	0.42
1:A:457:ASN:OD1	1:A:462:LYS:HE2	2.19	0.42
1:E:72:ILE:HD11	1:E:84:PHE:CD1	2.54	0.42
1:F:401:LEU:HD22	1:F:436:TYR:OH	2.19	0.42
1:G:148:VAL:C	1:G:149:PHE:HD1	2.22	0.42
1:A:120:ALA:HB1	1:A:123:LEU:CB	2.50	0.42
1:A:204:ILE:HB	1:A:256:LEU:HD23	2.01	0.42
1:D:259:PRO:HD2	3:D:501:NAD:C8A	2.50	0.42
1:G:72:ILE:HD11	1:G:84:PHE:CD1	2.55	0.42
1:G:244:LEU:O	1:G:248:LEU:HG	2.18	0.42
1:H:406:ASN:ND2	1:H:430:SER:HB2	2.34	0.42
4:C:502:SER:HA	1:D:423:ILE:HB	2.02	0.42
1:A:129:PHE:N	1:A:129:PHE:CD1	2.88	0.42
1:B:173:GLN:O	1:B:177:ARG:HG2	2.19	0.42
1:C:129:PHE:N	1:C:129:PHE:HD1	2.18	0.42
1:C:429:ASP:OD1	1:D:425:LYS:HG2	2.20	0.42
1:G:427:PHE:HD1	1:H:427:PHE:HB2	1.85	0.42
1:A:114:GLU:HG3	1:A:140:TYR:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LEU:HD23	1:A:146:ILE:HD13	2.02	0.42
1:C:261:THR:OG1	1:C:264:THR:HG23	2.19	0.42
3:E:501:NAD:O3B	1:F:41:ARG:NH2	2.41	0.42
1:A:65:GLU:OE1	1:A:107:ARG:HB2	2.20	0.42
1:B:249:ASN:ND2	1:B:275:ALA:O	2.53	0.42
1:B:283:ILE:HG12	1:B:309:ALA:HB3	2.01	0.42
1:C:411:LEU:HD13	4:C:502:SER:HB3	2.02	0.42
1:G:390:LEU:HD22	1:G:394:GLN:OE1	2.20	0.42
1:C:176:ASP:O	1:C:180:GLU:HG3	2.19	0.41
1:C:260:ALA:HB2	1:C:287:ARG:HG3	2.02	0.41
1:F:286:SER:O	1:F:312:VAL:HG11	2.20	0.41
1:A:129:PHE:N	1:A:129:PHE:HD1	2.18	0.41
1:B:282:VAL:O	1:B:308:ALA:HA	2.20	0.41
1:E:197:ARG:HB2	1:G:157:ARG:HH21	1.85	0.41
1:G:149:PHE:CD2	1:G:366:ALA:HB1	2.55	0.41
1:A:226:TYR:CE2	1:A:240:GLN:HB2	2.54	0.41
1:E:421:HIS:HD2	1:E:443:SER:O	2.04	0.41
1:G:267:MET:HG2	1:G:290:VAL:HG13	2.03	0.41
1:A:426:GLN:NE2	1:A:437:LEU:HD11	2.26	0.41
1:C:52:LYS:O	1:C:468:LEU:HA	2.20	0.41
1:G:149:PHE:HD2	1:G:366:ALA:HB1	1.86	0.41
1:A:270:ALA:HB3	1:A:271:PRO:HD3	2.03	0.41
1:D:286:SER:O	1:D:312:VAL:HG11	2.20	0.41
4:E:503:SER:HB3	1:F:411:LEU:HD13	2.03	0.41
1:G:181:LEU:HD23	1:G:185:THR:O	2.21	0.41
1:C:125:CYS:SG	1:C:367:LEU:HD22	2.61	0.41
1:H:52:LYS:HA	1:H:53:PRO:HD3	1.94	0.41
1:H:385:VAL:HG12	1:H:438:MET:HE3	2.03	0.41
1:D:382:PHE:CZ	1:D:403:ILE:HD12	2.56	0.41
1:H:157:ARG:NE	1:H:161:GLU:OE2	2.50	0.41
1:A:68:ASN:ND2	1:A:357:SER:HA	2.36	0.41
1:A:421:HIS:HD2	1:A:443:SER:O	2.04	0.41
1:D:51:LEU:HB3	1:D:468:LEU:HB3	2.02	0.41
1:F:385:VAL:HG12	1:F:438:MET:SD	2.60	0.41
1:C:105:GLY:HA2	1:C:127:GLY:O	2.20	0.41
1:D:120:ALA:HB1	1:D:123:LEU:HB2	2.02	0.41
1:D:251:SER:O	1:D:277:LYS:HD3	2.21	0.41
1:E:199:LYS:NZ	1:G:354:GLU:OE2	2.51	0.41
1:E:401:LEU:CD2	1:E:438:MET:HG2	2.51	0.41
1:F:181:LEU:HD21	1:H:346:PRO:HB3	2.03	0.41
1:F:291:VAL:HG12	1:F:293:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:375:ASN:OD1	1:G:377:VAL:HG22	2.21	0.41
1:A:152:PRO:HG2	1:A:153:PHE:CD2	2.55	0.41
1:A:176:ASP:OD2	1:A:341:ASN:N	2.54	0.41
1:A:196:VAL:CG1	1:A:222:LEU:HD21	2.25	0.41
1:A:282:VAL:O	1:A:308:ALA:HA	2.21	0.41
1:H:248:LEU:O	1:H:276:MET:HA	2.21	0.41
1:H:411:LEU:HG	4:H:502:SER:HB3	2.02	0.41
1:C:124:VAL:HG12	1:C:370:TYR:HE2	1.85	0.40
1:B:241:VAL:HG21	1:B:247:LEU:HB2	2.03	0.40
1:B:260:ALA:HB2	1:B:287:ARG:HG3	2.04	0.40
1:C:157:ARG:HH12	1:C:216:LEU:HD21	1.87	0.40
1:D:72:ILE:HD11	1:D:84:PHE:CD1	2.56	0.40
1:D:226:TYR:OH	1:D:234:ALA:HB2	2.20	0.40
1:G:425:LYS:HG2	1:H:429:ASP:OD1	2.21	0.40
1:H:159:VAL:O	1:H:163:VAL:HG23	2.21	0.40
1:D:402:TYR:HB3	1:D:437:LEU:HB3	2.04	0.40
1:E:192:ARG:HA	1:E:192:ARG:HD2	1.48	0.40
4:G:502:SER:HA	1:H:423:ILE:HB	2.03	0.40
1:B:157:ARG:HH21	1:D:197:ARG:HB2	1.86	0.40
1:E:226:TYR:CE2	1:E:240:GLN:HB2	2.56	0.40
1:F:129:PHE:N	1:F:129:PHE:CD1	2.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	430/473 (91%)	413 (96%)	17 (4%)	0	100	100
1	B	429/473 (91%)	413 (96%)	14 (3%)	2 (0%)	25	49
1	C	421/473 (89%)	398 (94%)	22 (5%)	1 (0%)	44	68
1	D	424/473 (90%)	410 (97%)	12 (3%)	2 (0%)	25	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	429/473 (91%)	410 (96%)	19 (4%)	0	100	100
1	F	429/473 (91%)	412 (96%)	17 (4%)	0	100	100
1	G	422/473 (89%)	408 (97%)	14 (3%)	0	100	100
1	H	422/473 (89%)	408 (97%)	13 (3%)	1 (0%)	44	68
All	All	3406/3784 (90%)	3272 (96%)	128 (4%)	6 (0%)	44	68

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	394	GLN
1	C	396	ASN
1	B	392	TYR
1	D	55	SER
1	H	392	TYR
1	D	392	TYR

5.3.2 Protein sidechains (i)

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	335/402 (83%)	334 (100%)	1 (0%)	91	97
1	B	326/402 (81%)	324 (99%)	2 (1%)	84	94
1	C	321/402 (80%)	318 (99%)	3 (1%)	75	90
1	D	298/402 (74%)	297 (100%)	1 (0%)	91	97
1	E	334/402 (83%)	334 (100%)	0	100	100
1	F	320/402 (80%)	317 (99%)	3 (1%)	75	90
1	G	312/402 (78%)	308 (99%)	4 (1%)	65	85
1	H	318/402 (79%)	315 (99%)	3 (1%)	75	90
All	All	2564/3216 (80%)	2547 (99%)	17 (1%)	81	93

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	PHE
1	B	129	PHE
1	B	149	PHE
1	C	129	PHE
1	C	255	THR
1	C	405	ARG
1	D	129	PHE
1	F	129	PHE
1	F	149	PHE
1	F	332	TRP
1	G	129	PHE
1	G	149	PHE
1	G	212	GLN
1	G	469	TYR
1	H	129	PHE
1	H	149	PHE
1	H	281	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	HIS
1	A	426	GLN
1	B	119	HIS
1	C	119	HIS
1	C	415	ASN
1	C	421	HIS
1	C	426	GLN
1	D	85	HIS
1	D	272	GLN
1	D	415	ASN
1	D	421	HIS
1	E	272	GLN
1	E	298	GLN
1	E	320	ASN
1	E	415	ASN
1	E	421	HIS
1	F	119	HIS
1	F	330	ASN
1	F	372	ASN
1	G	356	GLN
1	H	119	HIS
1	H	134	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

16 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	$\#\|Z\| > 2$
3	NAD	E	501	-	42,48,48	0.56	0	50,73,73	0.72	1 (2%)
4	SER	B	502	-	5,6,6	1.06	1 (20%)	5,7,7	1.86	2 (40%)
3	NAD	B	501	-	42,48,48	0.55	0	50,73,73	0.68	1 (2%)
3	NAD	D	501	-	42,48,48	0.56	0	50,73,73	0.58	1 (2%)
4	SER	D	502	-	5,6,6	1.54	1 (20%)	5,7,7	1.21	0
4	SER	C	502	-	5,6,6	1.06	1 (20%)	5,7,7	1.80	2 (40%)
4	SER	A	502	-	5,6,6	0.98	1 (20%)	5,7,7	1.72	2 (40%)
4	SER	H	502	-	5,6,6	0.99	1 (20%)	5,7,7	1.59	2 (40%)
3	NAD	C	501	-	42,48,48	0.50	0	50,73,73	0.64	1 (2%)
3	NAD	A	501	-	42,48,48	0.58	0	50,73,73	0.66	1 (2%)
4	SER	E	502	-	5,6,6	1.29	1 (20%)	5,7,7	0.89	0
4	SER	G	502	-	5,6,6	1.01	1 (20%)	5,7,7	1.77	2 (40%)
4	SER	E	503	-	5,6,6	1.29	1 (20%)	5,7,7	1.28	0
3	NAD	F	501	-	42,48,48	0.57	0	50,73,73	0.61	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAD	G	501	-	42,48,48	0.57	0	50,73,73	0.63	1 (2%)
3	NAD	H	501	-	42,48,48	0.56	0	50,73,73	0.66	1 (2%)

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
3	NAD	E	501	-	-	7/26/62/62	0/5/5/5
4	SER	B	502	-	-	0/6/6/6	-
3	NAD	B	501	-	-	7/26/62/62	0/5/5/5
3	NAD	D	501	-	-	7/26/62/62	0/5/5/5
4	SER	D	502	-	-	0/6/6/6	-
4	SER	C	502	-	-	0/6/6/6	-
4	SER	A	502	-	-	1/6/6/6	-
4	SER	H	502	-	-	4/6/6/6	-
3	NAD	C	501	-	-	7/26/62/62	0/5/5/5
3	NAD	A	501	-	-	7/26/62/62	0/5/5/5
4	SER	E	502	-	-	0/6/6/6	-
4	SER	G	502	-	-	0/6/6/6	-
4	SER	E	503	-	-	3/6/6/6	-
3	NAD	F	501	-	-	7/26/62/62	0/5/5/5
3	NAD	G	501	-	-	7/26/62/62	0/5/5/5
3	NAD	H	501	-	-	7/26/62/62	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	502	SER	OXT-C	-2.96	1.20	1.30
4	E	502	SER	OXT-C	-2.49	1.22	1.30
4	E	503	SER	OXT-C	-2.41	1.22	1.30
4	C	502	SER	OXT-C	-2.28	1.23	1.30
4	B	502	SER	OXT-C	-2.20	1.23	1.30
4	G	502	SER	OXT-C	-2.15	1.23	1.30
4	A	502	SER	OXT-C	-2.08	1.23	1.30
4	H	502	SER	OXT-C	-2.08	1.23	1.30

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	502	SER	OXT-C-O	-3.42	116.33	124.09
4	C	502	SER	OXT-C-O	-3.21	116.80	124.09
4	G	502	SER	OXT-C-O	-3.08	117.09	124.09
4	H	502	SER	OXT-C-O	-2.88	117.54	124.09
4	A	502	SER	OXT-C-O	-2.81	117.72	124.09
4	G	502	SER	OXT-C-CA	2.47	121.80	113.38
3	B	501	NAD	C5A-C6A-N6A	2.46	124.09	120.35
3	A	501	NAD	C5A-C6A-N6A	2.44	124.05	120.35
4	A	502	SER	OXT-C-CA	2.42	121.64	113.38
3	G	501	NAD	C5A-C6A-N6A	2.38	123.96	120.35
4	C	502	SER	OXT-C-CA	2.36	121.44	113.38
3	F	501	NAD	C5A-C6A-N6A	2.35	123.92	120.35
3	D	501	NAD	C5A-C6A-N6A	2.31	123.86	120.35
3	E	501	NAD	C5A-C6A-N6A	2.31	123.86	120.35
4	B	502	SER	OXT-C-CA	2.26	121.09	113.38
3	C	501	NAD	C5A-C6A-N6A	2.24	123.76	120.35
3	H	501	NAD	C5A-C6A-N6A	2.24	123.75	120.35
4	H	502	SER	OXT-C-CA	2.01	120.23	113.38

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	NAD	O4D-C1D-N1N-C2N
3	A	501	NAD	O4D-C1D-N1N-C6N
3	A	501	NAD	C2D-C1D-N1N-C2N
3	A	501	NAD	C2D-C1D-N1N-C6N
3	B	501	NAD	O4D-C1D-N1N-C2N
3	B	501	NAD	O4D-C1D-N1N-C6N
3	B	501	NAD	C2D-C1D-N1N-C2N
3	B	501	NAD	C2D-C1D-N1N-C6N
3	C	501	NAD	O4D-C1D-N1N-C2N
3	C	501	NAD	O4D-C1D-N1N-C6N
3	C	501	NAD	C2D-C1D-N1N-C2N
3	C	501	NAD	C2D-C1D-N1N-C6N
3	D	501	NAD	O4D-C1D-N1N-C2N
3	D	501	NAD	O4D-C1D-N1N-C6N
3	D	501	NAD	C2D-C1D-N1N-C2N
3	D	501	NAD	C2D-C1D-N1N-C6N
3	E	501	NAD	O4D-C1D-N1N-C2N
3	E	501	NAD	O4D-C1D-N1N-C6N
3	E	501	NAD	C2D-C1D-N1N-C2N
3	E	501	NAD	C2D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
3	F	501	NAD	O4D-C1D-N1N-C2N
3	F	501	NAD	O4D-C1D-N1N-C6N
3	F	501	NAD	C2D-C1D-N1N-C2N
3	F	501	NAD	C2D-C1D-N1N-C6N
3	G	501	NAD	O4D-C1D-N1N-C2N
3	G	501	NAD	O4D-C1D-N1N-C6N
3	G	501	NAD	C2D-C1D-N1N-C2N
3	G	501	NAD	C2D-C1D-N1N-C6N
3	H	501	NAD	O4D-C1D-N1N-C2N
3	H	501	NAD	O4D-C1D-N1N-C6N
3	H	501	NAD	C2D-C1D-N1N-C2N
3	H	501	NAD	C2D-C1D-N1N-C6N
4	E	503	SER	O-C-CA-CB
4	E	503	SER	OXT-C-CA-CB
4	H	502	SER	O-C-CA-CB
4	H	502	SER	OXT-C-CA-CB
4	H	502	SER	OXT-C-CA-N
3	G	501	NAD	PN-O3-PA-O1A
4	H	502	SER	O-C-CA-N
3	A	501	NAD	PN-O3-PA-O1A
3	D	501	NAD	PN-O3-PA-O1A
3	A	501	NAD	PN-O3-PA-O2A
3	B	501	NAD	PN-O3-PA-O2A
3	C	501	NAD	PN-O3-PA-O1A
3	C	501	NAD	PN-O3-PA-O2A
3	D	501	NAD	PN-O3-PA-O2A
3	E	501	NAD	PN-O3-PA-O1A
3	E	501	NAD	PN-O3-PA-O2A
3	F	501	NAD	PN-O3-PA-O1A
3	F	501	NAD	PN-O3-PA-O2A
3	G	501	NAD	PN-O3-PA-O2A
3	H	501	NAD	PN-O3-PA-O2A
3	E	501	NAD	O4B-C4B-C5B-O5B
3	H	501	NAD	O4B-C4B-C5B-O5B
3	B	501	NAD	O4B-C4B-C5B-O5B
3	F	501	NAD	O4B-C4B-C5B-O5B
4	E	503	SER	OXT-C-CA-N
3	B	501	NAD	PN-O3-PA-O1A
3	H	501	NAD	PN-O3-PA-O1A
3	D	501	NAD	O4B-C4B-C5B-O5B
4	A	502	SER	OXT-C-CA-N
3	A	501	NAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
3	C	501	NAD	O4B-C4B-C5B-O5B
3	G	501	NAD	O4B-C4B-C5B-O5B

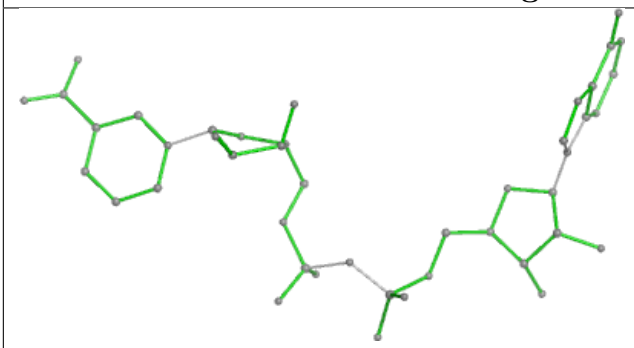
There are no ring outliers.

12 monomers are involved in 28 short contacts:

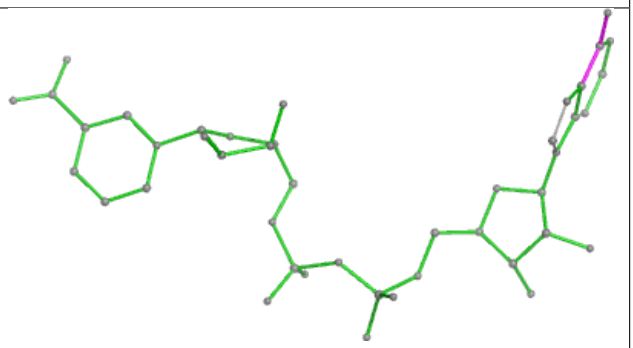
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	501	NAD	1	0
4	B	502	SER	2	0
3	B	501	NAD	1	0
3	D	501	NAD	2	0
4	D	502	SER	2	0
4	C	502	SER	3	0
4	A	502	SER	3	0
4	H	502	SER	3	0
3	A	501	NAD	1	0
4	E	502	SER	2	0
4	G	502	SER	3	0
4	E	503	SER	5	0

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 then 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.

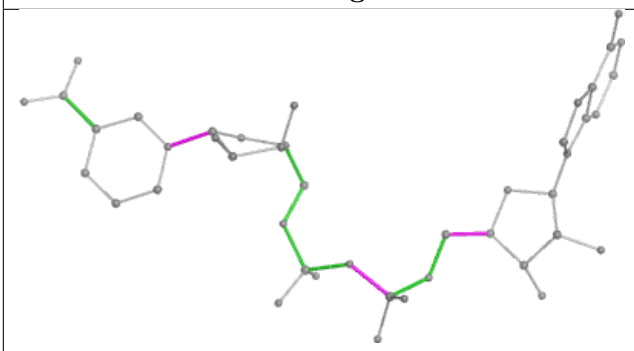
Ligand NAD E 501



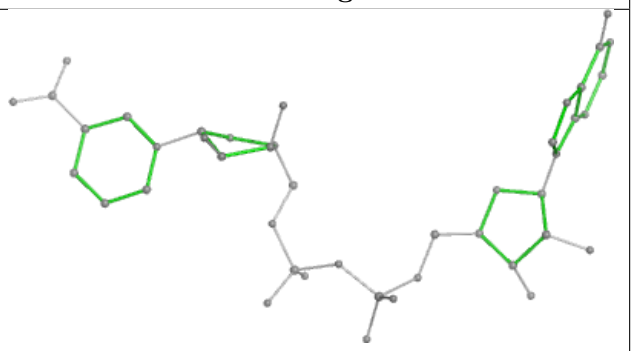
Bond lengths



Bond angles

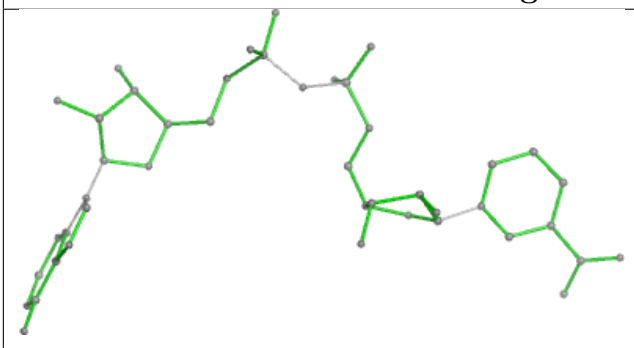


Torsions

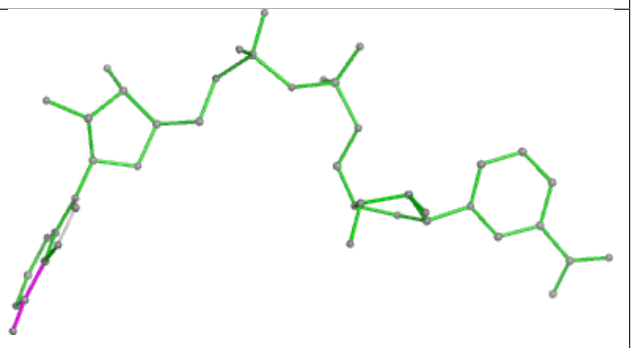


Rings

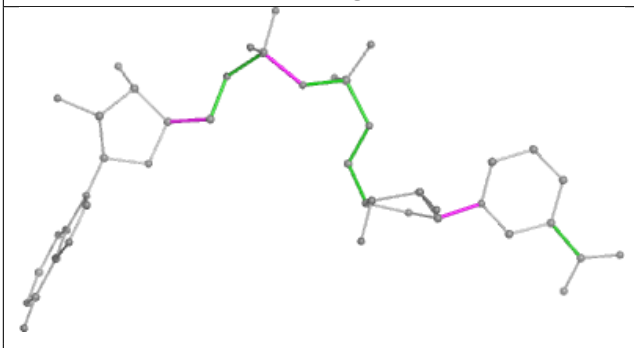
Ligand NAD B 501



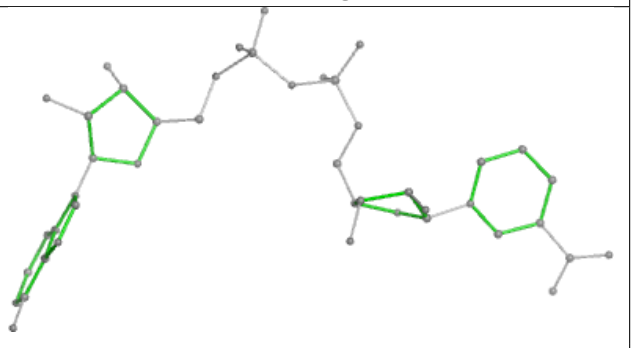
Bond lengths



Bond angles

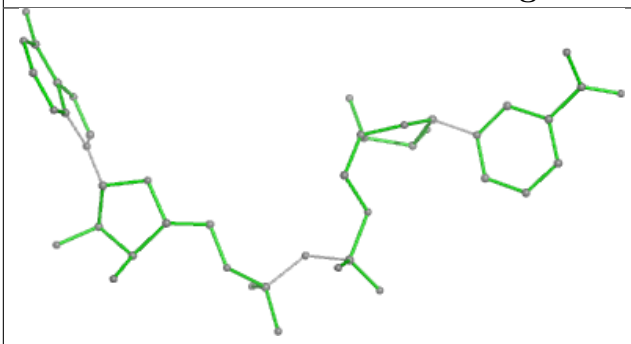


Torsions

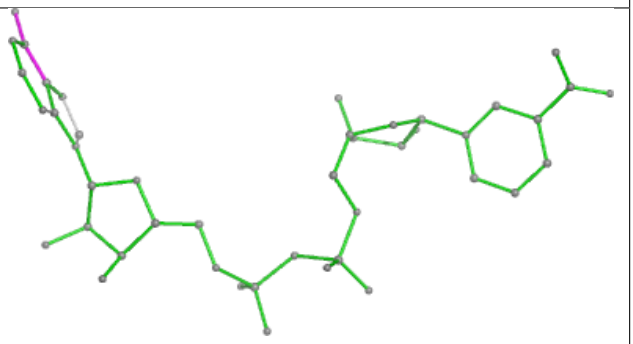


Rings

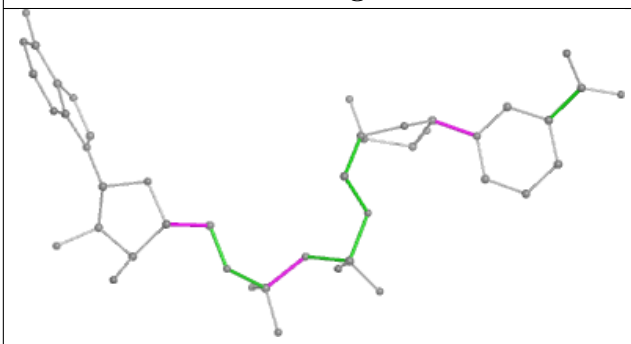
Ligand NAD D 501



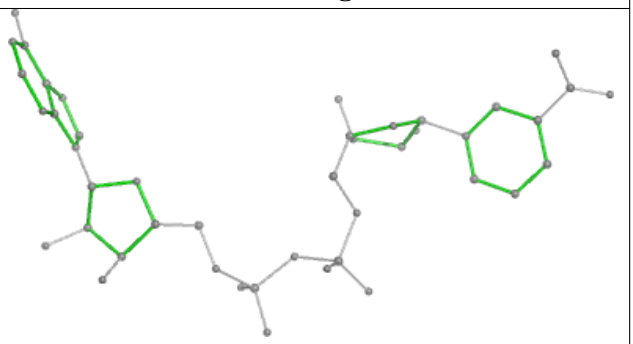
Bond lengths



Bond angles

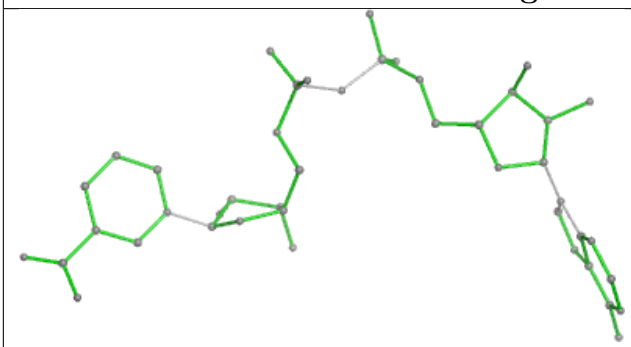


Torsions

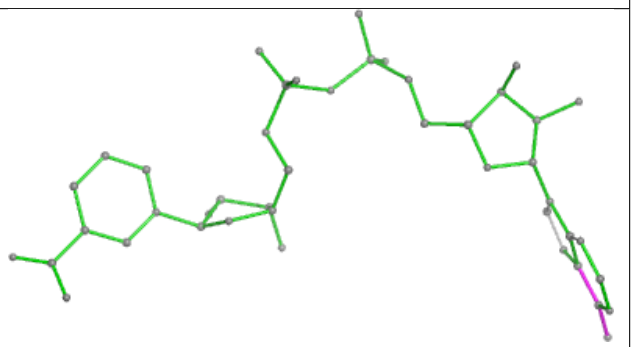


Rings

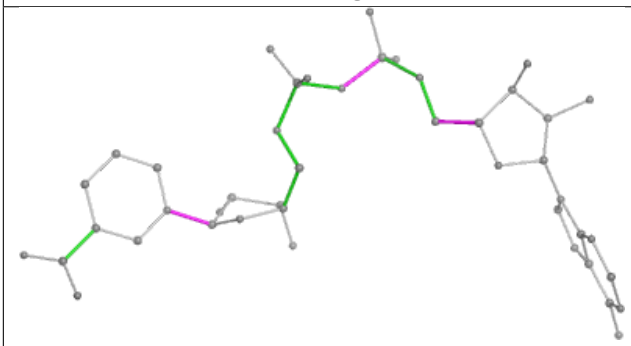
Ligand NAD C 501



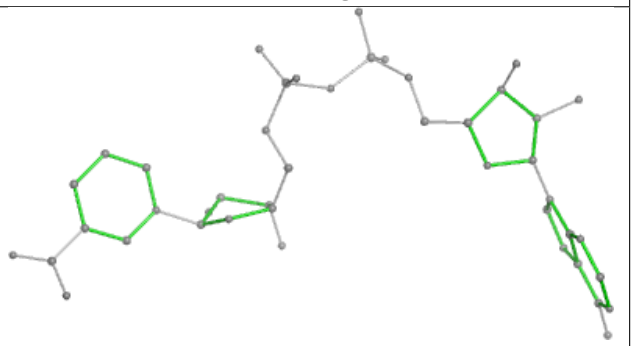
Bond lengths



Bond angles

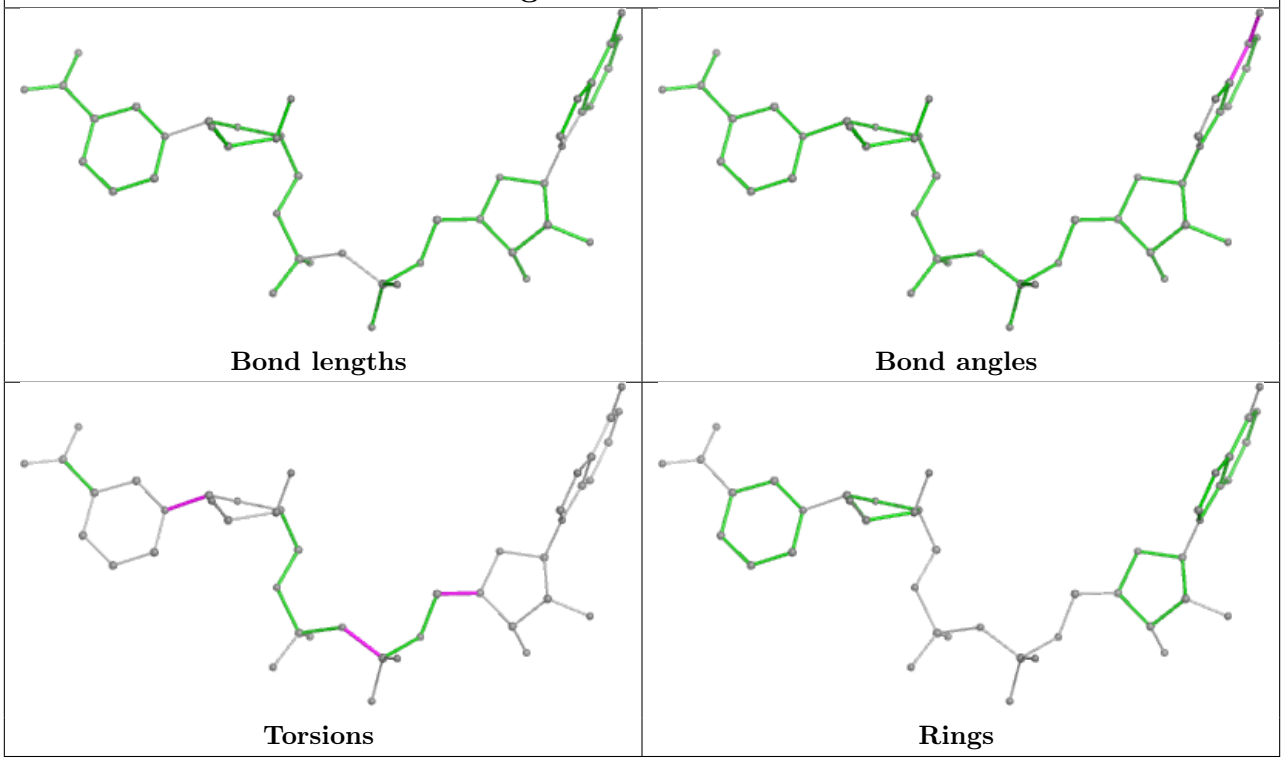


Torsions

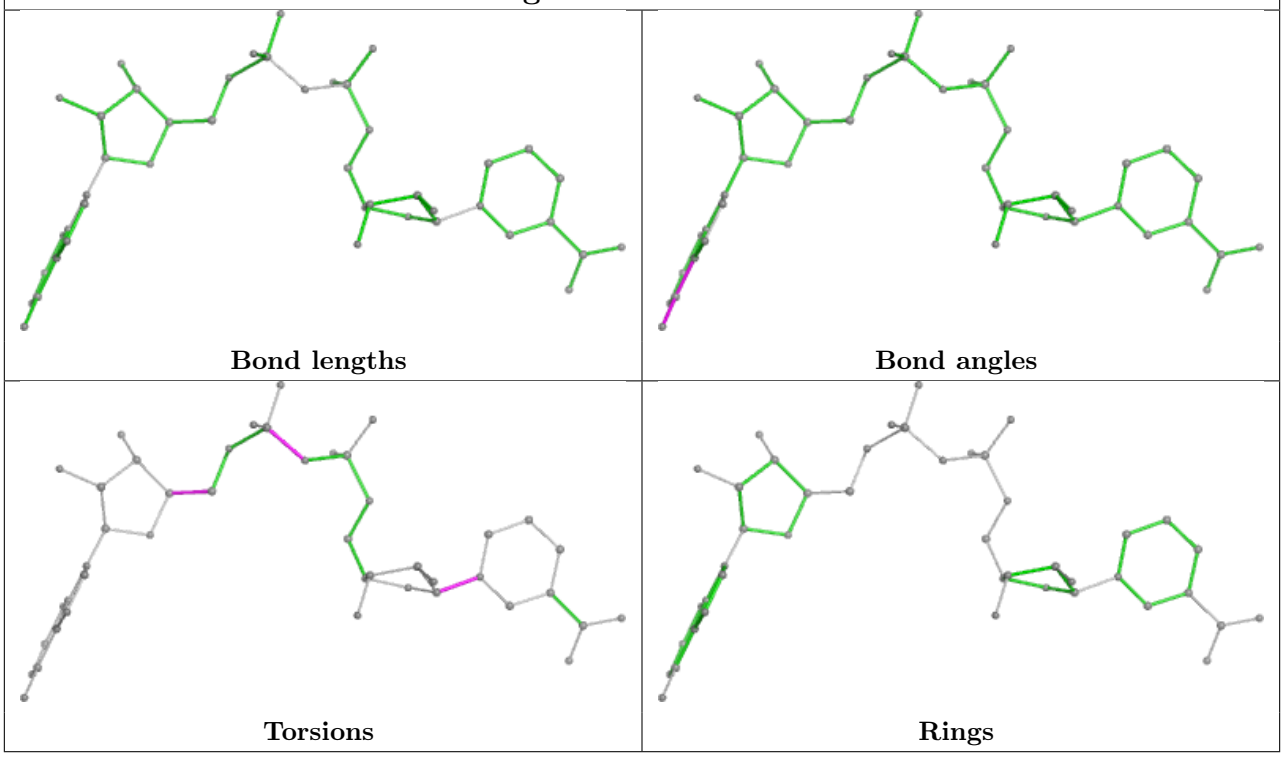


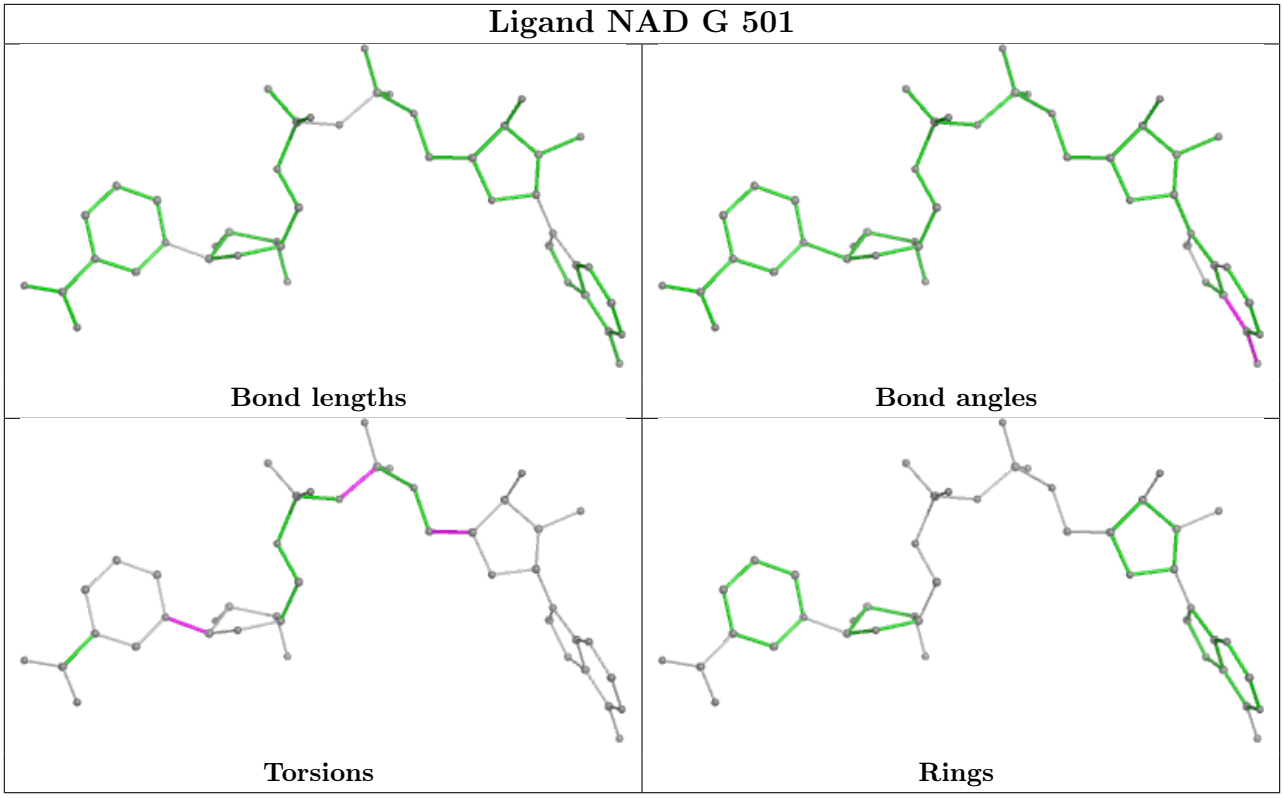
Rings

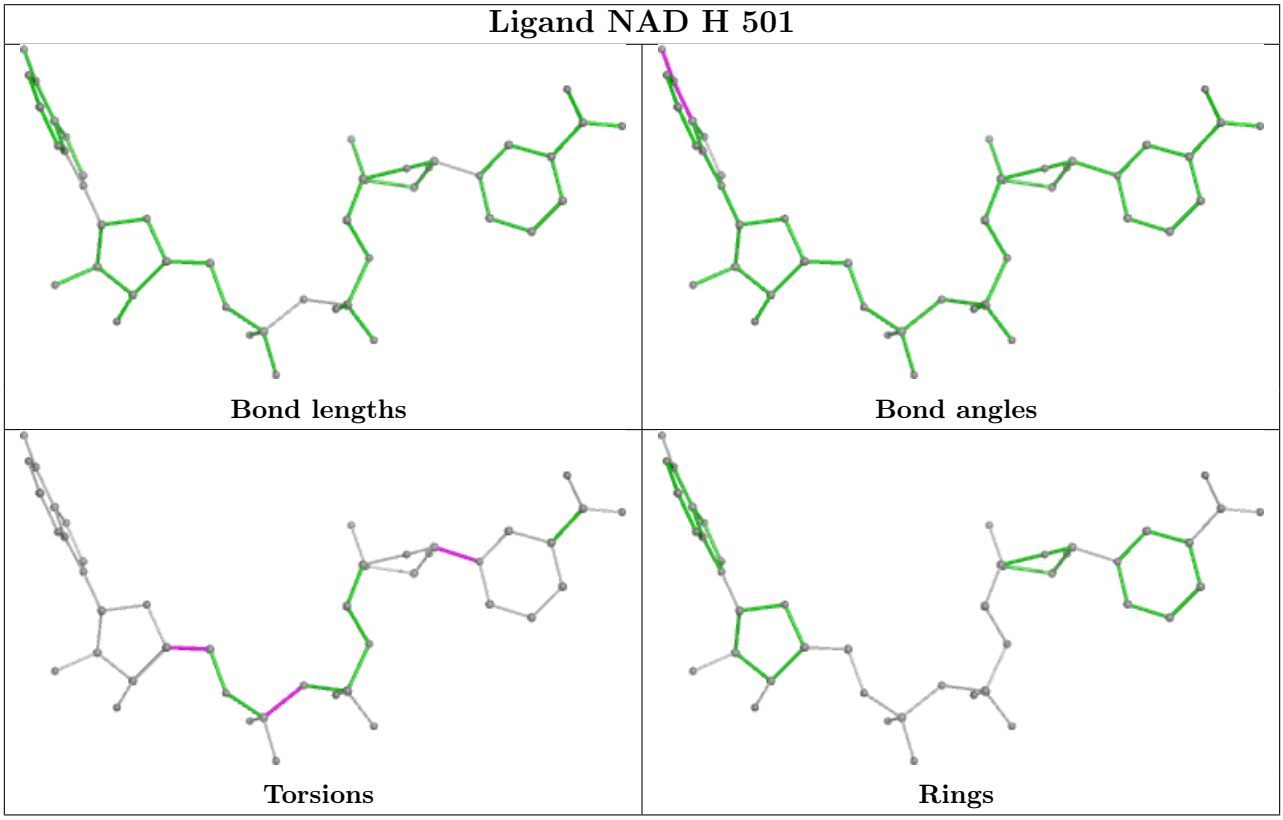
Ligand NAD A 501



Ligand NAD F 501







5.7 Other polymers

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, 95^{th} 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	431/473 (91%)	0.14	9 (2%)	63	63	21, 38, 67, 90	1 (0%)
1	B	431/473 (91%)	0.23	9 (2%)	63	63	27, 43, 73, 108	0
1	C	423/473 (89%)	0.24	8 (1%)	66	65	21, 43, 73, 101	0
1	D	428/473 (90%)	0.78	32 (7%)	22	20	31, 57, 87, 115	0
1	E	431/473 (91%)	0.16	9 (2%)	63	63	25, 41, 70, 90	0
1	F	431/473 (91%)	0.52	33 (7%)	21	19	24, 48, 75, 99	0
1	G	426/473 (90%)	0.43	15 (3%)	47	45	23, 47, 77, 98	0
1	H	426/473 (90%)	0.35	17 (3%)	43	41	28, 46, 77, 101	0
2	I	0/10	-	-			-	-
2	J	0/10	-	-			-	-
2	K	0/10	-	-			-	-
2	L	0/10	-	-			-	-
2	M	0/10	-	-			-	-
2	N	0/10	-	-			-	-
2	O	0/10	-	-			-	-
2	Q	0/10	-	-			-	-
All	All	3427/3864 (88%)	0.36	132 (3%)	44	42	21, 45, 77, 115	1 (0%)

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	260	ALA	4.9
1	D	55	SER	4.1
1	E	56	THR	3.9
1	D	56	THR	3.8
1	D	271	PRO	3.8
1	E	314	PRO	3.7
1	B	245	ASP	3.7
1	F	290	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	92	ASP	3.6
1	F	325	PHE	3.5
1	H	55	SER	3.5
1	B	56	THR	3.4
1	F	39	PRO	3.3
1	B	390	LEU	3.2
1	A	55	SER	3.2
1	D	469	TYR	3.2
1	F	331	SER	3.1
1	D	331	SER	3.1
1	A	39	PRO	3.1
1	H	92	ASP	3.0
1	G	84	PHE	3.0
1	H	322	GLU	3.0
1	A	40	ARG	2.9
1	D	42	VAL	2.9
1	D	78	GLN	2.9
1	D	100	ASP	2.9
1	D	114	GLU	2.9
1	G	55	SER	2.9
1	D	40	ARG	2.8
1	E	192	ARG	2.8
1	C	55	SER	2.8
1	A	314	PRO	2.8
1	G	116	ILE	2.7
1	F	45	THR	2.7
1	G	402	TYR	2.7
1	F	245	ASP	2.7
1	F	56	THR	2.7
1	H	332	TRP	2.7
1	F	242	SER	2.6
1	B	227	TYR	2.6
1	D	87	SER	2.5
1	D	207	GLY	2.5
1	F	251	SER	2.5
1	C	469	TYR	2.5
1	E	92	ASP	2.5
1	F	324	SER	2.5
1	G	469	TYR	2.5
1	H	47	GLN	2.4
1	F	271	PRO	2.4
1	H	188	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	98	ILE	2.4
1	G	154	SER	2.4
1	D	249	ASN	2.4
1	B	45	THR	2.4
1	F	261	THR	2.3
1	H	390	LEU	2.3
1	D	146	ILE	2.3
1	E	355	ALA	2.3
1	F	219	ALA	2.3
1	H	293	ILE	2.3
1	H	469	TYR	2.3
1	D	128	CYS	2.3
1	F	297	ILE	2.3
1	D	227	TYR	2.3
1	F	227	TYR	2.3
1	C	395	GLU	2.3
1	A	42	VAL	2.3
1	F	236	GLY	2.3
1	F	336	LEU	2.3
1	F	344	LEU	2.3
1	B	469	TYR	2.3
1	D	445	ASN	2.3
1	G	100	ASP	2.3
1	C	53	PRO	2.3
1	B	298	GLN	2.3
1	F	258	VAL	2.3
1	G	212	GLN	2.3
1	B	49	LYS	2.2
1	G	54	PHE	2.2
1	H	179	ILE	2.2
1	E	39	PRO	2.2
1	D	92	ASP	2.2
1	E	380	VAL	2.2
1	D	95	ILE	2.2
1	C	323	GLY	2.2
1	F	323	GLY	2.2
1	G	53	PRO	2.2
1	H	56	THR	2.2
1	G	101	VAL	2.2
1	F	310	LEU	2.2
1	D	48	PRO	2.2
1	D	104	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	446	GLN	2.2
1	F	273	PHE	2.2
1	F	49	LYS	2.2
1	G	364	ALA	2.2
1	H	270	ALA	2.2
1	D	111	ARG	2.2
1	D	88	SER	2.1
1	H	182	HIS	2.1
1	G	124	VAL	2.1
1	H	297	ILE	2.1
1	A	279	GLY	2.1
1	D	332	TRP	2.1
1	F	263	GLU	2.1
1	A	56	THR	2.1
1	F	185	THR	2.1
1	F	269	SER	2.1
1	C	47	GLN	2.1
1	D	229	ILE	2.1
1	E	398	VAL	2.1
1	F	469	TYR	2.1
1	D	51	LEU	2.1
1	F	235	LEU	2.1
1	H	96	GLU	2.1
1	E	251	SER	2.1
1	F	276	MET	2.1
1	F	392	TYR	2.1
1	B	184	GLY	2.1
1	F	316	GLU	2.1
1	D	447	SER	2.1
1	D	58	ASP	2.1
1	C	50	ALA	2.1
1	D	110	THR	2.0
1	G	297	ILE	2.0
1	F	272	GLN	2.0
1	C	392	TYR	2.0
1	H	39	PRO	2.0
1	A	394[A]	GLN	2.0
1	D	242	SER	2.0
1	G	122	ASN	2.0
1	H	396	ASN	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)

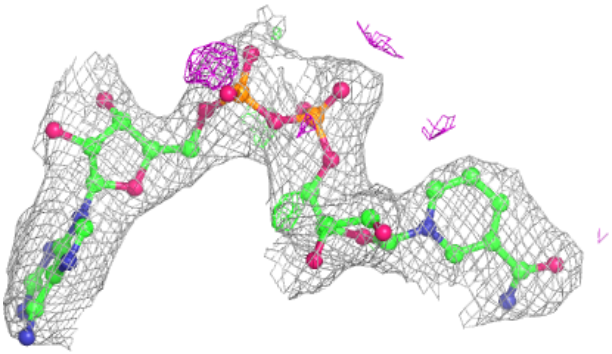
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

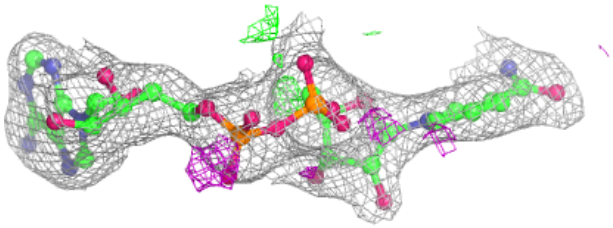
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SER	E	502	7/7	0.77	0.19	34,41,52,57	0
4	SER	E	503	7/7	0.79	0.16	34,38,52,60	0
4	SER	D	502	7/7	0.81	0.23	44,54,70,70	0
4	SER	G	502	7/7	0.82	0.20	31,41,60,66	0
4	SER	H	502	7/7	0.86	0.17	32,43,48,61	0
4	SER	B	502	7/7	0.87	0.15	37,41,55,56	0
4	SER	C	502	7/7	0.88	0.12	37,46,56,63	0
4	SER	A	502	7/7	0.89	0.17	28,41,48,59	0
3	NAD	D	501	44/44	0.89	0.12	32,50,69,78	0
3	NAD	F	501	44/44	0.90	0.12	27,47,68,77	0
3	NAD	G	501	44/44	0.92	0.09	24,48,58,64	0
3	NAD	E	501	44/44	0.94	0.08	24,39,48,53	0
3	NAD	C	501	44/44	0.94	0.08	24,34,44,52	0
3	NAD	B	501	44/44	0.94	0.09	23,35,44,48	0
3	NAD	H	501	44/44	0.94	0.08	25,36,47,55	0
3	NAD	A	501	44/44	0.95	0.08	20,33,44,54	0

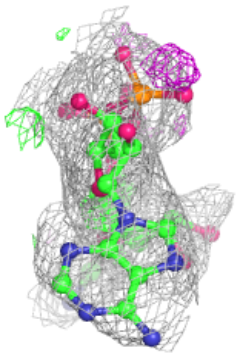
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

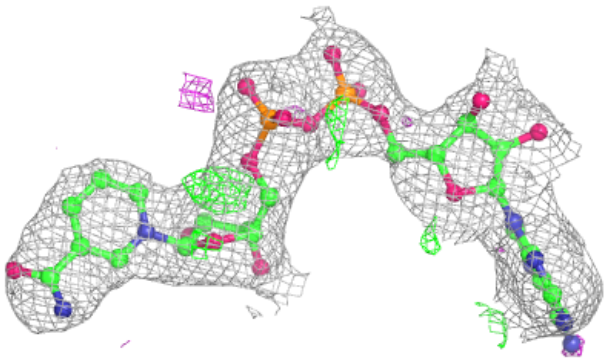


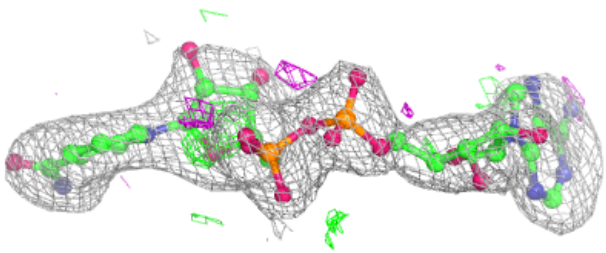


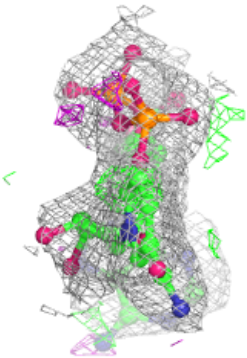


Electron density around NAD F 501:

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

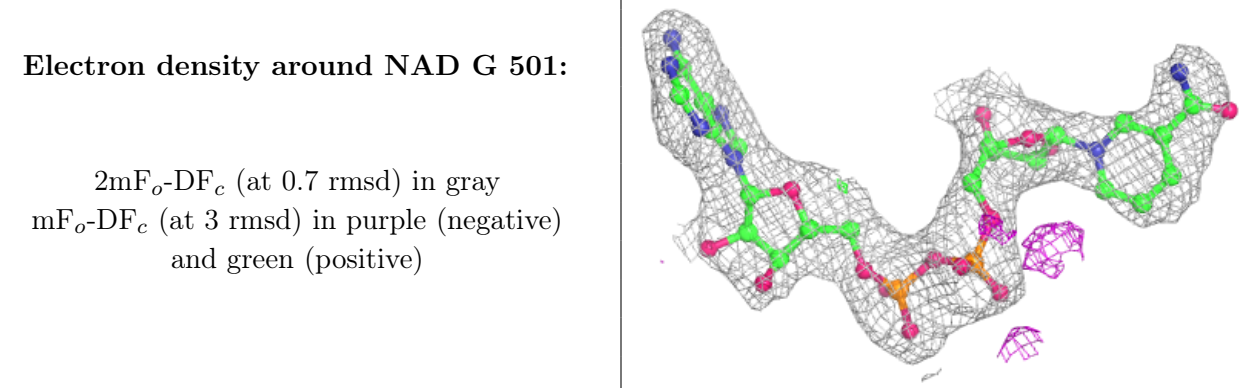


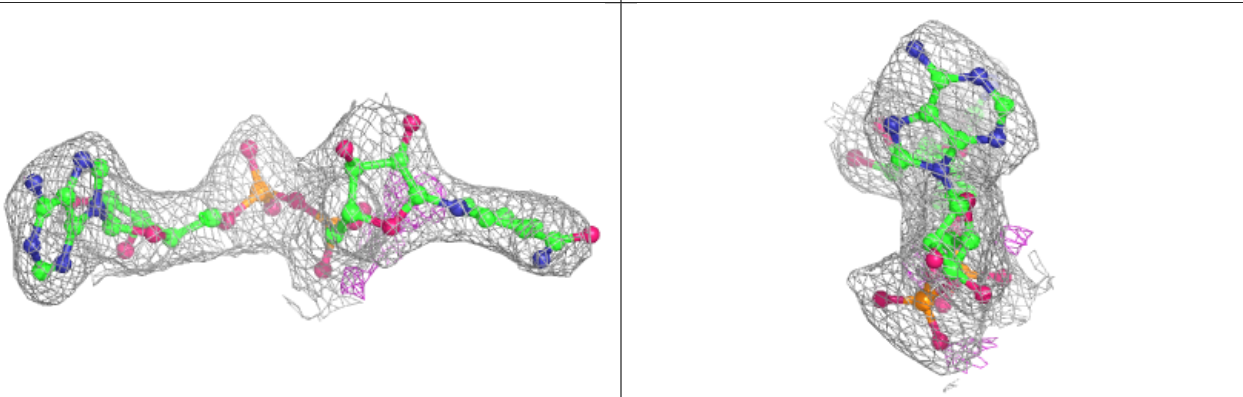




Electron density around NAD G 501:

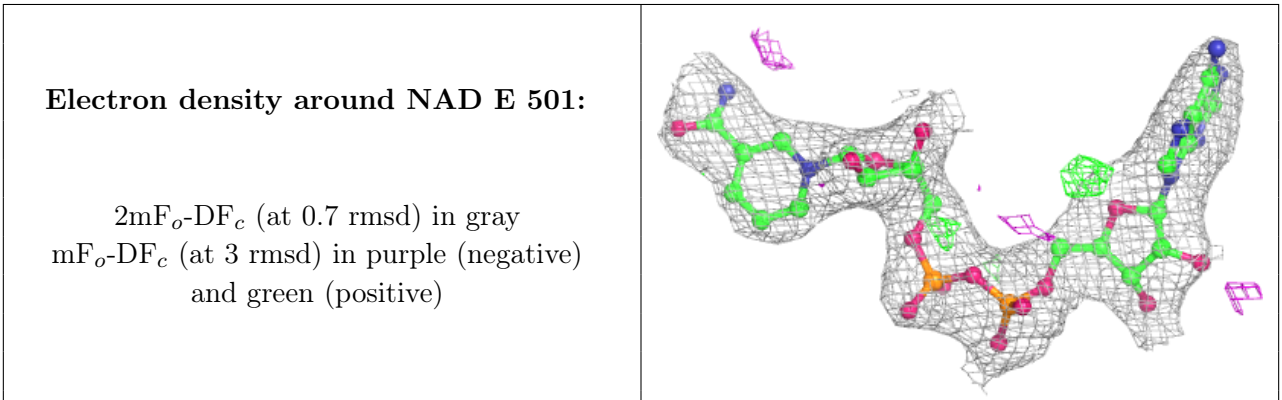
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

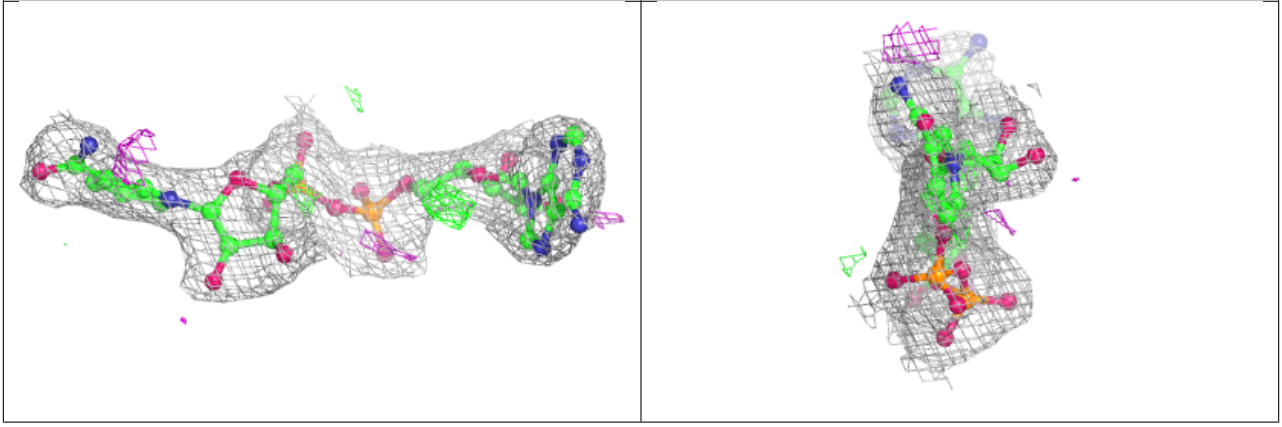




Electron density around NAD E 501:

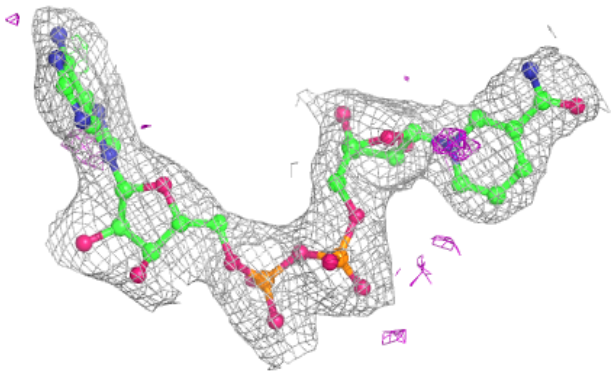
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

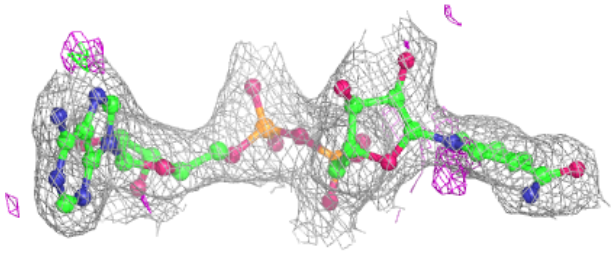


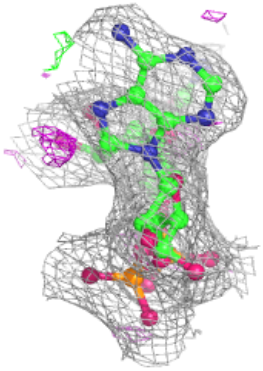


Electron density around NAD C 501:

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

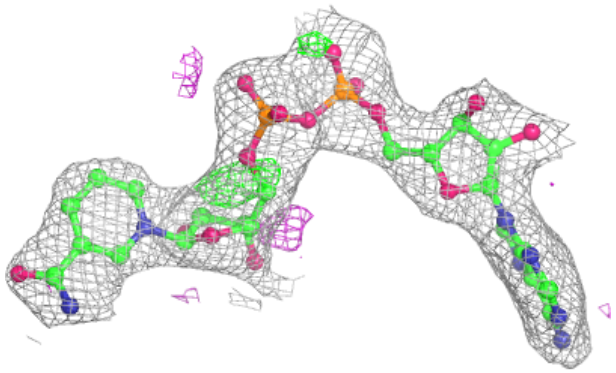


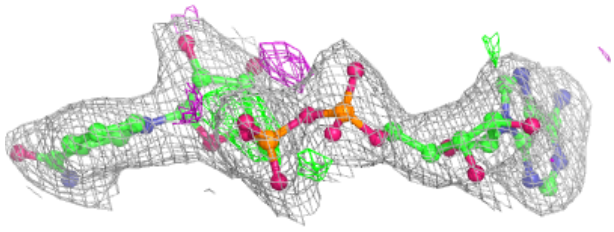


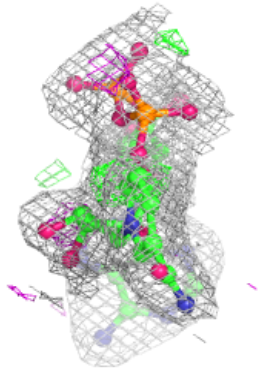


Electron density around NAD B 501:

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

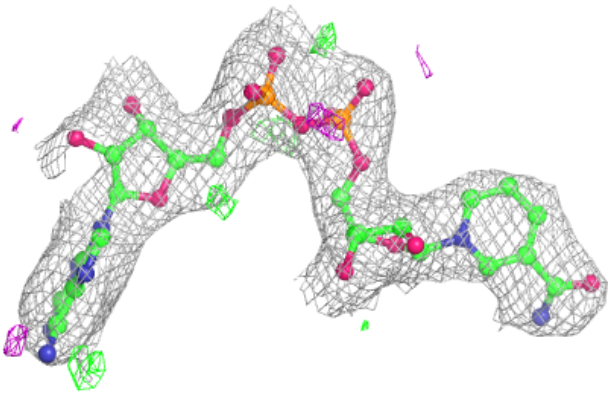


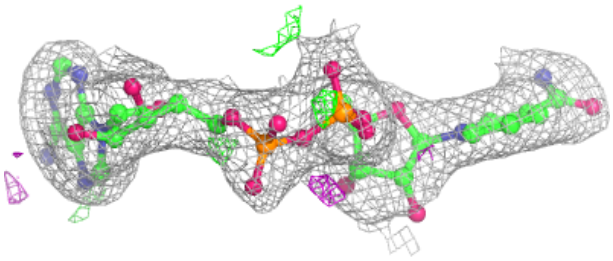


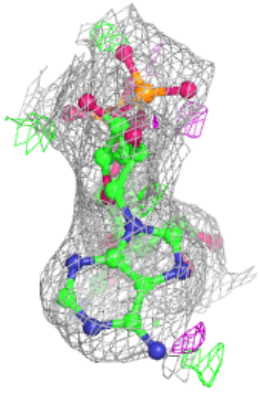


Electron density around NAD H 501:

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

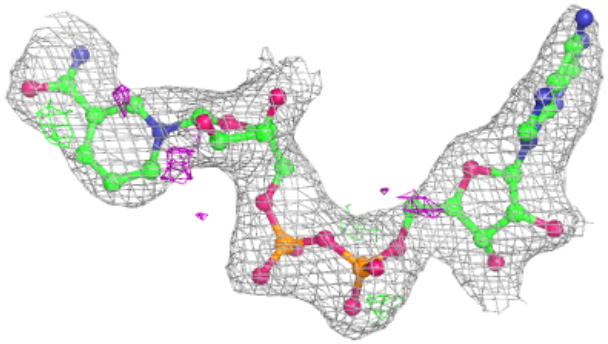


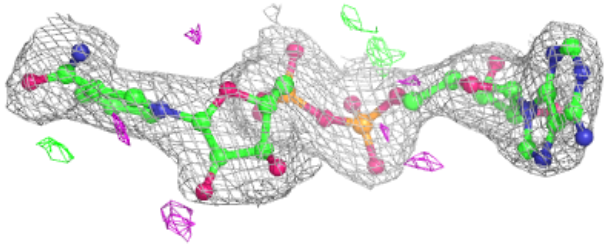


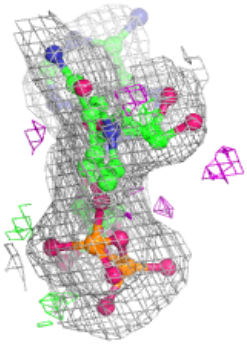


Electron density around NAD A 501:

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







6.5 Other polymers (i)

There are no such residues in this entry.