



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 06:31 am BST

PDB ID : 1PJS  
Title : The co-crystal structure of CysG, the multifunctional methyltransferase/dehydrogenase/ferrochelatase for siroheme synthesis, in complex with its NAD cofactor  
Authors : Stroupe, M.E.; Leech, H.K.; Daniels, D.S.; Warren, M.J.; Getzoff, E.D.  
Deposited on : 2003-06-03  
Resolution : 2.40 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](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

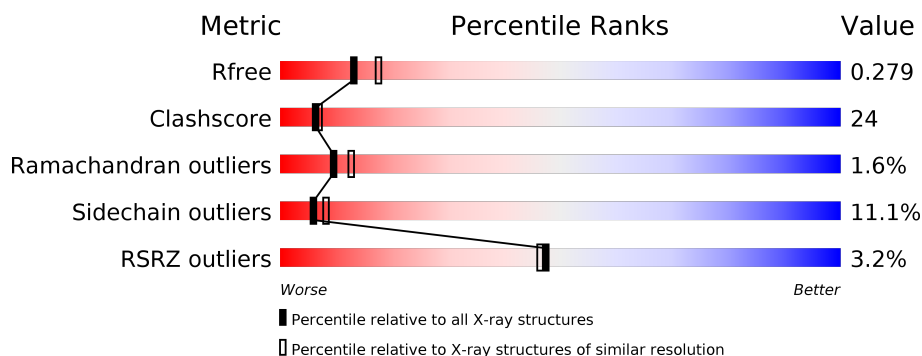
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	457	
1	B	457	

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
3	NAD	A	502	X	-	-	X
4	PGE	A	505	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7310 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.

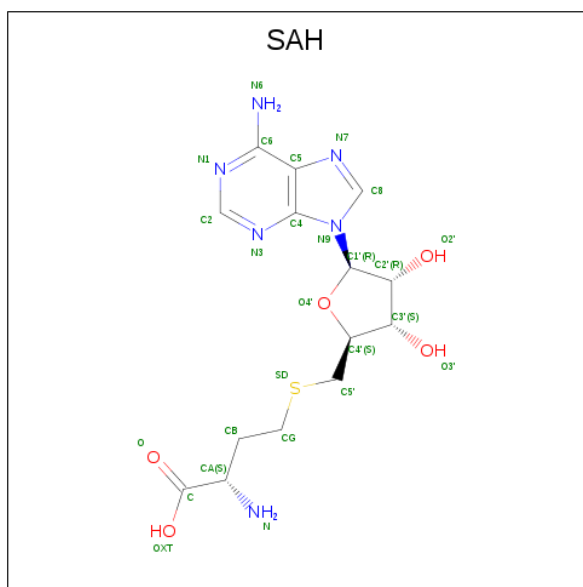
- Molecule 1 is a protein called Siroheme synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	P	S	0	0	0
			3427	2158	614	639	1	15			
1	B	454	Total	C	N	O	P	S	0	0	0
			3506	2205	633	651	1	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	128	SEP	SER	MODIFIED RESIDUE	UNP P25924
B	128	SEP	SER	MODIFIED RESIDUE	UNP P25924

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula:  $C_{14}H_{20}N_6O_5S$ ).



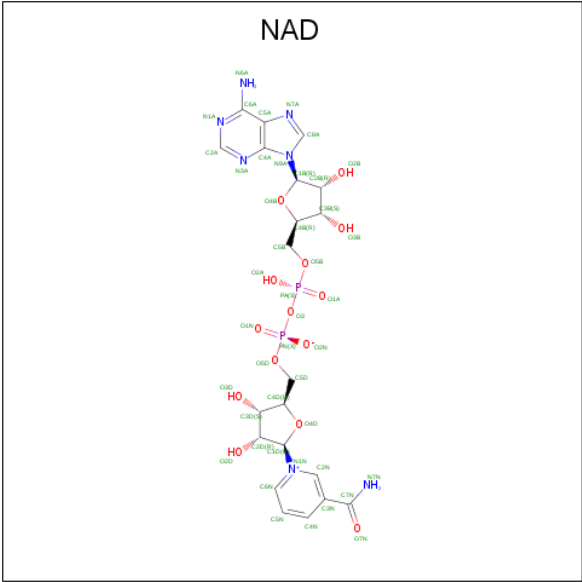
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



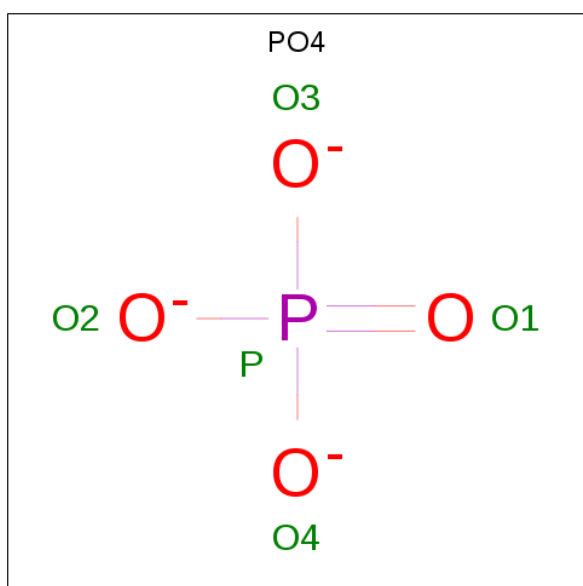
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		

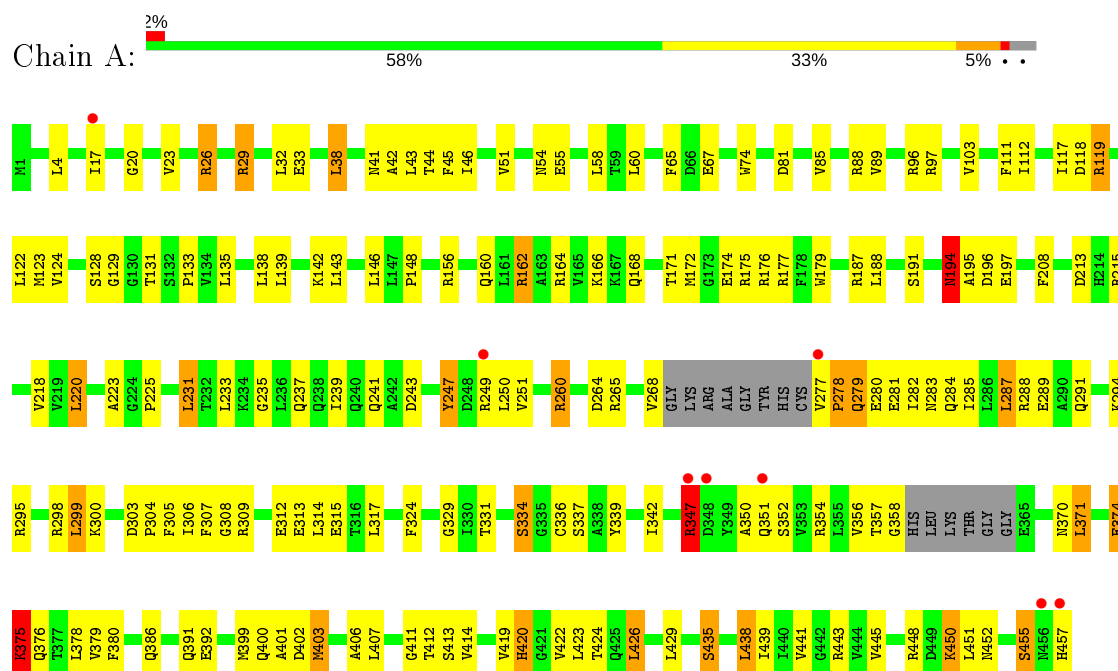
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	98	Total 98	O 98	0	0
6	B	114	Total 114	O 114	0	0

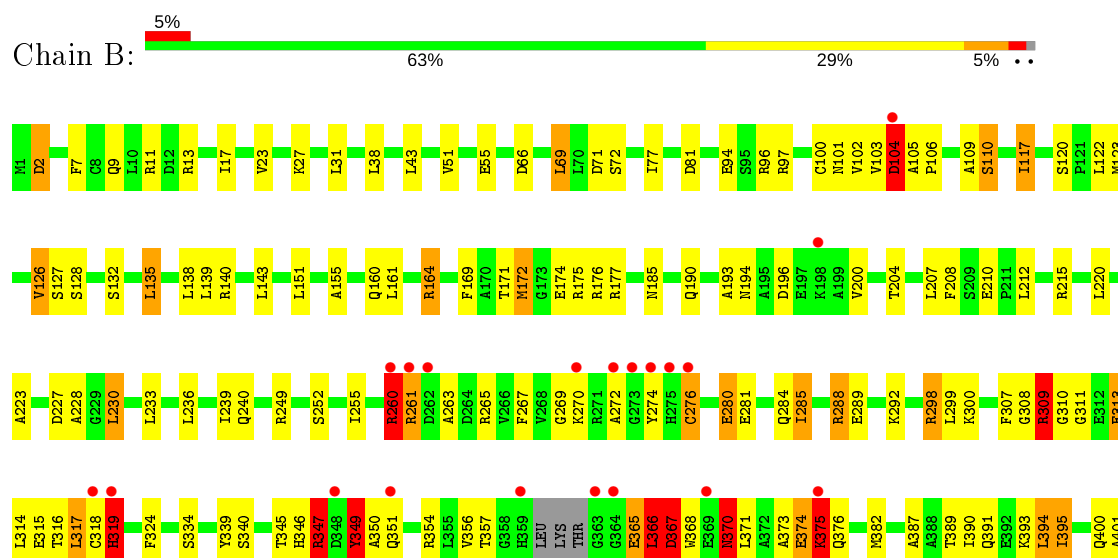
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

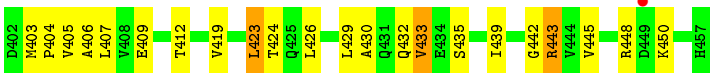
#### • Molecule 1: Siroheme synthase



#### • Molecule 1: Siroheme synthase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.12Å 120.69Å 130.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.58 – 2.40 22.58 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.7 (22.58-2.40) 95.6 (22.58-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 2.41Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.239 , 0.281 0.236 , 0.279	Depositor DCC
$R_{free}$ test set	3603 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.9	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7310	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.59% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PO4, SAH, PGE, NAD, SEP

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	0.42	1/3470 (0.0%)	0.78	8/4696 (0.2%)
1	B	0.44	0/3553	0.90	15/4807 (0.3%)
All	All	0.43	1/7023 (0.0%)	0.84	23/9503 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	374	GLU	CB-CG	5.10	1.61	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	263	ALA	N-CA-C	-10.59	82.42	111.00
1	B	309	ARG	N-CA-C	10.14	138.38	111.00
1	B	374	GLU	N-CA-C	9.09	135.53	111.00
1	B	104	ASP	N-CA-CB	8.94	126.70	110.60
1	B	366	LEU	N-CA-C	8.62	134.26	111.00
1	A	375	LYS	CA-CB-CG	-7.90	96.03	113.40
1	B	365	GLU	N-CA-C	7.70	131.78	111.00
1	B	374	GLU	CA-C-N	-7.18	101.40	117.20
1	A	374	GLU	CA-C-N	-7.15	101.47	117.20
1	A	308	GLY	N-CA-C	-6.66	96.44	113.10
1	B	260	ARG	N-CA-C	6.65	128.94	111.00
1	A	194	ASN	N-CA-C	-6.32	93.93	111.00
1	B	104	ASP	N-CA-C	-6.22	94.20	111.00
1	A	375	LYS	N-CA-CB	5.96	121.33	110.60
1	B	370	ASN	N-CA-C	-5.83	95.25	111.00
1	B	375	LYS	N-CA-C	-5.73	95.52	111.00
1	B	274	TYR	N-CA-C	5.67	126.30	111.00
1	A	374	GLU	N-CA-C	5.43	125.65	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	347	ARG	N-CA-C	5.30	125.31	111.00
1	B	104	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	347	ARG	N-CA-C	5.09	124.73	111.00
1	A	374	GLU	C-N-CA	5.01	134.24	121.70
1	B	319	HIS	N-CA-CB	5.01	119.61	110.60

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	3427	0	3466	198	0
1	B	3506	0	3538	174	1
2	A	26	0	19	0	0
2	B	26	0	19	0	0
3	A	44	0	26	12	0
3	B	44	0	26	4	1
4	A	20	0	26	10	0
5	B	5	0	0	1	0
6	A	98	0	0	6	0
6	B	114	0	0	3	0
All	All	7310	0	7120	344	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (344) 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)
3:A:502:NAD:C1D	3:A:502:NAD:N1N	1.71	1.48
1:A:128:SEP:OG	1:A:128:SEP:CB	1.64	1.46
1:B:128:SEP:CB	1:B:128:SEP:OG	1.67	1.42
1:A:307:PHE:H	1:B:345:THR:HG21	0.92	1.05
1:A:351:GLN:OE1	1:B:309:ARG:NH2	1.94	1.01

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:PHE:N	1:B:345:THR:HG21	1.76	0.99
1:B:101:ASN:OD1	1:B:103:VAL:HG23	1.65	0.96
1:B:374:GLU:HG2	1:B:375:LYS:N	1.82	0.94
1:B:270:LYS:HG2	1:B:276:CYS:SG	2.07	0.94
1:A:374:GLU:HG2	1:A:375:LYS:N	1.81	0.93
1:A:374:GLU:CG	1:A:375:LYS:N	2.32	0.92
1:A:407:LEU:HD22	1:A:439:ILE:HG12	1.52	0.90
1:B:349:TYR:N	1:B:349:TYR:HD1	1.69	0.90
1:B:407:LEU:HD21	1:B:439:ILE:HG12	1.55	0.88
1:A:374:GLU:HG3	1:A:376:GLN:H	1.37	0.88
1:A:370:ASN:ND2	1:B:370:ASN:CG	2.29	0.86
1:B:260:ARG:O	1:B:260:ARG:HG3	1.75	0.86
1:A:284:GLN:HA	1:A:287:LEU:HD21	1.58	0.85
1:A:354:ARG:NH2	1:B:354:ARG:NH2	2.25	0.84
1:A:213:ASP:OD1	1:A:215:ARG:HG2	1.78	0.83
1:B:101:ASN:OD1	1:B:103:VAL:CG2	2.26	0.82
1:A:124:VAL:HG22	1:B:126:VAL:HG13	1.58	0.82
1:B:349:TYR:H	1:B:349:TYR:HD1	0.87	0.82
1:B:374:GLU:CG	1:B:375:LYS:N	2.42	0.82
3:A:502:NAD:C1D	3:A:502:NAD:C2N	2.57	0.82
1:B:227:ASP:HB3	1:B:230:LEU:HD22	1.61	0.82
1:B:367:ASP:OD1	1:B:367:ASP:N	2.12	0.82
1:B:171:THR:HG22	1:B:174:GLU:OE1	1.80	0.81
1:A:29:ARG:O	1:A:33:GLU:HG3	1.81	0.80
1:A:351:GLN:CD	1:B:309:ARG:HH22	1.86	0.79
1:A:351:GLN:NE2	1:B:309:ARG:HH22	1.79	0.79
1:A:374:GLU:HG3	1:A:376:GLN:N	1.98	0.79
1:B:281:GLU:O	1:B:285:ILE:HG12	1.84	0.78
1:A:176:ARG:HH22	1:A:260:ARG:HH21	1.30	0.77
1:A:399:MET:HE2	1:A:423:LEU:HD11	1.66	0.77
1:A:307:PHE:H	1:B:345:THR:CG2	1.86	0.77
6:A:583:HOH:O	1:B:309:ARG:HG3	1.84	0.77
1:A:279:GLN:HG3	1:A:309:ARG:HD3	1.69	0.75
1:B:443:ARG:CG	1:B:443:ARG:HH21	2.00	0.75
1:B:220:LEU:HD21	1:B:310:GLY:HA3	1.70	0.74
1:B:117:ILE:HD12	1:B:143:LEU:HB2	1.70	0.74
1:B:391:GLN:O	1:B:395:ILE:HG12	1.88	0.73
1:A:81:ASP:HB3	3:A:502:NAD:O5D	1.90	0.72
1:A:356:VAL:HG12	1:A:357:THR:N	2.05	0.72
1:A:419:VAL:HG21	1:A:429:LEU:HB3	1.72	0.72
1:A:67:GLU:HG2	1:A:96:ARG:NH2	2.05	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:GLU:HG3	1:B:376:GLN:H	1.54	0.71
1:B:288:ARG:HG2	1:B:288:ARG:HH11	1.55	0.71
1:A:402:ASP:HA	1:A:422:VAL:HG11	1.72	0.71
1:B:346:HIS:CE1	1:B:347:ARG:HG2	2.24	0.71
1:B:409:GLU:HB2	1:B:433:VAL:CG1	2.21	0.71
1:A:176:ARG:NH2	1:A:243:ASP:OD1	2.24	0.71
1:A:278:PRO:HD2	1:A:281:GLU:OE2	1.90	0.71
3:B:504:NAD:O1N	3:B:504:NAD:H52A	1.91	0.70
1:B:104:ASP:HB3	3:B:504:NAD:N7N	2.06	0.70
1:B:407:LEU:CD2	1:B:439:ILE:HG12	2.19	0.70
1:A:67:GLU:HG2	1:A:96:ARG:HH22	1.57	0.70
1:A:176:ARG:HH22	1:A:260:ARG:NH2	1.89	0.69
1:A:171:THR:OG1	1:A:174:GLU:HG3	1.92	0.69
1:A:283:ASN:O	1:A:287:LEU:HD22	1.92	0.69
1:A:351:GLN:HE22	1:B:309:ARG:HH22	1.38	0.69
1:B:419:VAL:CG1	1:B:429:LEU:HD22	2.23	0.69
1:A:112:ILE:CD1	1:A:129:GLY:HA2	2.23	0.68
1:A:233:LEU:HD23	1:B:233:LEU:HD12	1.74	0.68
3:A:502:NAD:O1A	6:A:604:HOH:O	2.11	0.68
1:B:51:VAL:O	1:B:55:GLU:HG2	1.93	0.68
1:A:142:LYS:NZ	4:A:505:PGE:H12	2.09	0.68
1:B:310:GLY:HA2	1:B:313:GLU:HG3	1.76	0.68
1:A:124:VAL:HG22	1:B:126:VAL:CG1	2.24	0.67
1:A:374:GLU:HG2	1:A:375:LYS:CA	2.25	0.67
1:A:225:PRO:CG	1:A:412:THR:HG21	2.24	0.67
1:A:370:ASN:HD21	1:B:370:ASN:CG	1.98	0.67
1:B:374:GLU:HG2	1:B:375:LYS:CA	2.25	0.66
1:B:160:GLN:O	1:B:161:LEU:HD23	1.94	0.66
1:A:85:VAL:HG21	3:A:502:NAD:N6A	2.10	0.66
1:A:401:ALA:O	1:A:422:VAL:CG1	2.44	0.66
1:B:309:ARG:HG2	6:B:621:HOH:O	1.96	0.65
1:B:135:LEU:HA	1:B:138:LEU:HD12	1.78	0.65
1:A:279:GLN:CG	1:A:309:ARG:HD3	2.26	0.65
1:B:373:ALA:O	1:B:374:GLU:HB2	1.96	0.65
1:A:400:GLN:HG2	1:A:402:ASP:OD2	1.97	0.64
1:A:249:ARG:HG3	1:A:249:ARG:HH11	1.61	0.64
1:B:100:CYS:H	1:B:110:SER:HB2	1.61	0.64
1:A:220:LEU:HD12	1:A:298:ARG:HB3	1.80	0.64
1:A:194:ASN:O	1:A:196:ASP:N	2.30	0.64
1:A:223:ALA:HB2	1:A:299:LEU:CD2	2.28	0.63
1:A:351:GLN:HB3	1:B:357:THR:OG1	1.97	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:VAL:HG23	3:B:504:NAD:O2N	1.98	0.63
1:B:404:PRO:HB2	1:B:445:VAL:HB	1.82	0.62
1:A:287:LEU:CD2	1:A:287:LEU:H	2.13	0.62
1:A:251:VAL:HG11	1:A:299:LEU:HD13	1.82	0.62
1:B:280:GLU:O	1:B:284:GLN:HG2	1.99	0.62
1:B:354:ARG:NH2	1:B:370:ASN:O	2.31	0.62
1:B:196:ASP:O	1:B:200:VAL:HG23	2.00	0.61
1:A:146:LEU:C	1:A:146:LEU:HD23	2.21	0.61
1:A:284:GLN:HA	1:A:287:LEU:CD2	2.30	0.61
1:A:399:MET:CE	1:A:423:LEU:HD11	2.29	0.61
1:B:164:ARG:HD2	1:B:208:PHE:CE2	2.35	0.61
1:B:220:LEU:HD21	1:B:310:GLY:CA	2.30	0.61
1:A:356:VAL:CG1	1:A:357:THR:N	2.64	0.61
1:A:370:ASN:ND2	1:B:370:ASN:HA	2.16	0.60
1:A:237:GLN:O	1:A:241:GLN:HG2	2.01	0.60
1:A:370:ASN:HD22	1:B:370:ASN:CG	2.03	0.60
1:B:239:ILE:HD11	1:B:299:LEU:HD21	1.83	0.60
1:B:104:ASP:HB3	3:B:504:NAD:H72N	1.66	0.60
1:A:112:ILE:HD12	1:A:129:GLY:HA2	1.83	0.59
1:A:380:PHE:O	1:A:438:LEU:HD23	2.02	0.59
1:A:356:VAL:CG1	1:A:357:THR:H	2.15	0.59
1:B:102:VAL:HG23	1:B:109:ALA:HB2	1.83	0.59
1:B:122:LEU:HD13	1:B:123:MET:N	2.18	0.59
1:A:401:ALA:O	1:A:422:VAL:HG12	2.02	0.59
1:A:225:PRO:HG2	1:A:412:THR:HG21	1.83	0.59
1:A:41:ASN:OD1	1:A:65:PHE:HA	2.03	0.59
1:B:340:SER:O	1:B:448:ARG:HG3	2.02	0.59
1:A:162:ARG:HG3	6:B:605:HOH:O	2.02	0.59
4:A:506:PGE:H42	1:B:139:LEU:HD21	1.85	0.59
1:B:177:ARG:NH2	1:B:212:LEU:HD23	2.18	0.59
1:A:450:LYS:O	1:A:451:LEU:HD23	2.02	0.58
1:B:66:ASP:O	1:B:69:LEU:HB2	2.03	0.58
1:B:284:GLN:O	1:B:288:ARG:HB2	2.03	0.58
1:B:374:GLU:HG3	1:B:376:GLN:N	2.18	0.58
1:B:375:LYS:HG2	1:B:375:LYS:O	2.03	0.58
1:A:283:ASN:O	1:A:287:LEU:CD2	2.51	0.58
1:A:288:ARG:O	1:A:291:GLN:HB2	2.04	0.58
1:B:117:ILE:HD12	1:B:143:LEU:CB	2.32	0.58
1:B:350:ALA:HA	1:B:375:LYS:HG2	1.84	0.58
1:A:315:GLU:HB2	1:B:450:LYS:HD3	1.86	0.58
1:A:370:ASN:HD22	1:B:370:ASN:ND2	2.03	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:MET:HE1	1:B:442:GLY:HA2	1.85	0.57
1:A:455:SER:HB3	1:A:457:HIS:H	1.70	0.57
1:A:122:LEU:HD22	1:B:127:SER:O	2.04	0.57
1:A:305:PHE:O	1:B:345:THR:HG22	2.05	0.57
3:A:502:NAD:O2A	6:A:595:HOH:O	2.18	0.56
1:A:85:VAL:HG22	1:A:88:ARG:HH12	1.70	0.56
1:B:349:TYR:N	1:B:349:TYR:CD1	2.43	0.56
1:A:85:VAL:HG21	3:A:502:NAD:H61A	1.71	0.56
1:B:228:ALA:HA	1:B:255:ILE:CD1	2.36	0.56
1:A:139:LEU:HD21	4:A:505:PGE:H5	1.87	0.56
1:A:117:ILE:HD13	1:A:143:LEU:CB	2.36	0.56
1:A:401:ALA:O	1:A:422:VAL:HG11	2.06	0.56
1:A:399:MET:HE2	1:A:423:LEU:CD1	2.36	0.55
1:B:443:ARG:HG2	1:B:443:ARG:HH21	1.70	0.55
1:B:354:ARG:HH12	1:B:370:ASN:HB3	1.71	0.55
1:B:419:VAL:HG12	1:B:429:LEU:HD22	1.88	0.55
1:A:420:HIS:N	1:A:420:HIS:ND1	2.53	0.55
1:B:102:VAL:HG23	1:B:109:ALA:CB	2.37	0.55
1:A:280:GLU:HA	1:A:283:ASN:HD22	1.72	0.55
1:A:176:ARG:HD3	1:A:295:ARG:HH11	1.71	0.55
1:A:142:LYS:HZ2	4:A:505:PGE:H12	1.71	0.55
4:A:506:PGE:H42	1:B:139:LEU:CD2	2.37	0.55
1:B:409:GLU:HB2	1:B:433:VAL:HG12	1.86	0.55
1:A:223:ALA:HB2	1:A:299:LEU:HD22	1.89	0.54
1:A:279:GLN:HG3	1:A:309:ARG:CD	2.37	0.54
1:B:285:ILE:HG23	1:B:288:ARG:HH22	1.72	0.54
1:A:260:ARG:O	1:A:265:ARG:NH2	2.41	0.54
1:B:443:ARG:NH2	1:B:443:ARG:CG	2.66	0.54
1:A:131:THR:HG22	1:B:155:ALA:O	2.07	0.54
1:A:42:ALA:HA	3:A:502:NAD:N3A	2.22	0.54
1:B:366:LEU:HD12	1:B:366:LEU:H	1.73	0.54
1:A:370:ASN:ND2	1:B:370:ASN:OD1	2.41	0.54
1:B:288:ARG:CG	1:B:288:ARG:HH11	2.19	0.54
1:A:356:VAL:HG12	1:A:357:THR:H	1.70	0.53
1:A:309:ARG:HE	1:A:312:GLU:CD	2.12	0.53
1:B:100:CYS:H	1:B:110:SER:CB	2.21	0.53
1:B:285:ILE:HG23	1:B:288:ARG:NH2	2.24	0.53
1:A:406:ALA:C	1:A:407:LEU:HD23	2.28	0.53
1:B:117:ILE:CD1	1:B:143:LEU:HB2	2.39	0.53
1:B:288:ARG:HD3	6:B:612:HOH:O	2.08	0.53
1:A:117:ILE:CD1	1:A:143:LEU:HB2	2.39	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:LEU:CD1	1:A:298:ARG:HB3	2.38	0.53
1:A:391:GLN:HE22	1:A:424:THR:HA	1.73	0.53
1:B:122:LEU:C	1:B:122:LEU:HD13	2.29	0.53
1:A:225:PRO:HG3	1:A:412:THR:HG21	1.91	0.53
1:A:44:THR:O	3:A:502:NAD:O2B	2.27	0.53
1:B:318:CYS:HB2	1:B:324:PHE:HE2	1.74	0.53
1:A:164:ARG:HD2	1:A:208:PHE:CE2	2.44	0.52
3:A:502:NAD:C6N	3:A:502:NAD:C1D	2.74	0.52
1:A:277:VAL:O	1:A:282:ILE:HG13	2.10	0.52
1:A:314:LEU:HD23	1:A:317:LEU:HD12	1.92	0.52
1:A:370:ASN:HD21	1:B:370:ASN:CA	2.22	0.52
1:B:2:ASP:OD2	1:B:2:ASP:N	2.42	0.52
1:A:191:SER:O	1:A:194:ASN:O	2.27	0.52
1:A:371:LEU:O	1:A:378:LEU:HD11	2.10	0.52
1:A:117:ILE:HD13	1:A:143:LEU:HB2	1.92	0.52
1:A:287:LEU:H	1:A:287:LEU:HD23	1.75	0.52
1:B:236:LEU:C	1:B:236:LEU:HD23	2.30	0.52
1:B:317:LEU:C	1:B:319:HIS:H	2.13	0.52
1:B:368:TRP:CD1	1:B:393:LYS:HD3	2.45	0.52
1:B:443:ARG:HG3	1:B:443:ARG:HH21	1.73	0.51
1:B:171:THR:HG23	1:B:174:GLU:HB2	1.92	0.51
1:B:298:ARG:NH1	1:B:300:LYS:HD3	2.24	0.51
1:A:347:ARG:NH2	1:B:315:GLU:OE2	2.44	0.51
1:B:311:GLY:O	1:B:315:GLU:HG2	2.11	0.51
1:B:17:ILE:HD11	1:B:31:LEU:HD22	1.92	0.51
1:B:401:ALA:HB1	1:B:424:THR:CG2	2.41	0.50
1:A:401:ALA:HB1	1:A:424:THR:HG23	1.93	0.50
1:A:402:ASP:CA	1:A:422:VAL:HG11	2.39	0.50
1:B:443:ARG:HG3	1:B:443:ARG:NH2	2.26	0.50
1:B:346:HIS:ND1	1:B:347:ARG:HG2	2.25	0.50
1:A:175:ARG:O	1:A:179:TRP:CD1	2.64	0.49
1:A:337:SER:HB2	1:A:342:ILE:O	2.11	0.49
1:A:306:ILE:HA	1:B:345:THR:HG22	1.93	0.49
1:A:303:ASP:HB2	1:A:329:GLY:O	2.12	0.49
1:B:339:TYR:CD2	1:B:412:THR:HA	2.47	0.49
1:A:370:ASN:HD21	1:B:370:ASN:HA	1.78	0.49
1:A:399:MET:HE3	1:A:441:VAL:CG1	2.42	0.49
1:A:264:ASP:O	1:A:265:ARG:HG3	2.12	0.49
1:A:419:VAL:HG23	1:A:429:LEU:HD13	1.93	0.49
1:A:139:LEU:CD2	4:A:505:PGE:H5	2.43	0.49
1:B:177:ARG:CZ	1:B:212:LEU:HD23	2.43	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ASN:HD22	1:B:207:LEU:HD21	1.76	0.49
1:B:300:LYS:HE3	1:B:308:GLY:O	2.13	0.49
1:A:67:GLU:CG	1:A:96:ARG:HH22	2.25	0.48
1:A:177:ARG:CZ	1:A:213:ASP:HB3	2.43	0.48
1:B:103:VAL:HG12	1:B:103:VAL:O	2.14	0.48
1:B:405:VAL:HG12	1:B:406:ALA:N	2.27	0.48
1:A:23:VAL:CG1	1:A:103:VAL:HG11	2.42	0.48
1:B:220:LEU:CD2	1:B:310:GLY:HA3	2.42	0.48
1:A:96:ARG:HH11	1:A:96:ARG:HG3	1.78	0.48
1:B:307:PHE:CE2	1:B:357:THR:OG1	2.61	0.48
1:A:279:GLN:HA	1:A:282:ILE:HD12	1.94	0.48
1:B:71:ASP:OD1	1:B:96:ARG:NH2	2.47	0.48
1:A:287:LEU:N	1:A:287:LEU:HD23	2.29	0.48
1:B:101:ASN:CG	1:B:103:VAL:HG23	2.33	0.48
1:B:228:ALA:HA	1:B:255:ILE:HD11	1.95	0.48
1:A:435:SER:HB2	6:A:588:HOH:O	2.13	0.48
1:A:51:VAL:O	1:A:55:GLU:HG3	2.13	0.48
1:A:303:ASP:OD1	1:A:304:PRO:HD2	2.14	0.47
1:A:400:GLN:O	1:A:403:MET:HB2	2.13	0.47
1:B:354:ARG:HD2	1:B:356:VAL:CG2	2.44	0.47
1:A:85:VAL:O	1:A:89:VAL:HG23	2.13	0.47
1:A:339:TYR:CD2	1:A:412:THR:HA	2.48	0.47
1:B:260:ARG:O	1:B:261:ARG:HB2	2.14	0.47
1:A:422:VAL:HG12	1:A:423:LEU:N	2.30	0.47
1:B:374:GLU:CG	1:B:376:GLN:H	2.24	0.47
1:A:336:CYS:SG	1:A:411:GLY:HA3	2.55	0.47
1:A:44:THR:HG22	1:A:45:PHE:N	2.30	0.47
1:A:135:LEU:O	1:A:139:LEU:HG	2.15	0.47
1:B:387:ALA:HB1	1:B:426:LEU:HD22	1.96	0.47
1:A:166:LYS:HG3	1:A:175:ARG:NH1	2.29	0.46
1:A:407:LEU:HD22	1:A:439:ILE:CG1	2.35	0.46
1:A:142:LYS:HZ3	4:A:505:PGE:H12	1.76	0.46
1:A:406:ALA:O	1:A:407:LEU:HD23	2.15	0.46
1:B:309:ARG:CD	1:B:309:ARG:N	2.77	0.46
1:A:17:ILE:HG13	1:A:38:LEU:HD21	1.96	0.46
1:B:357:THR:HG23	1:B:382:MET:CE	2.45	0.46
1:A:371:LEU:HD23	1:A:378:LEU:HD22	1.97	0.46
1:A:118:ASP:O	1:A:119:ARG:HD3	2.14	0.46
1:A:445:VAL:O	1:A:445:VAL:HG12	2.15	0.46
1:A:156:ARG:O	1:A:160:GLN:HG3	2.15	0.46
1:A:162:ARG:HG2	6:A:539:HOH:O	2.14	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:VAL:CG1	1:A:438:LEU:HD21	2.46	0.46
1:A:277:VAL:O	1:A:282:ILE:CG1	2.64	0.46
4:A:506:PGE:H4	4:A:506:PGE:O4	2.16	0.46
1:B:169:PHE:O	1:B:175:ARG:HD3	2.15	0.46
1:A:374:GLU:HG3	1:A:375:LYS:N	2.25	0.45
1:B:172:MET:SD	1:B:175:ARG:NH2	2.85	0.45
1:B:390:ILE:O	1:B:394:LEU:HB2	2.16	0.45
1:B:128:SEP:HB3	1:B:132:SER:H	1.79	0.45
1:B:368:TRP:CE3	1:B:371:LEU:HD12	2.51	0.45
1:A:300:LYS:NZ	1:A:313:GLU:OE2	2.49	0.45
1:A:331:THR:HG22	1:A:334:SER:HB2	1.98	0.45
1:A:379:VAL:HG12	1:A:438:LEU:HD21	1.98	0.45
1:A:148:PRO:HD3	4:A:506:PGE:H2	1.97	0.45
1:B:401:ALA:HB1	1:B:424:THR:HG21	1.98	0.45
1:B:171:THR:CG2	1:B:174:GLU:HB2	2.45	0.45
1:B:140:ARG:NH1	5:B:507:PO4:O4	2.50	0.45
1:A:350:ALA:HA	1:A:375:LYS:O	2.16	0.44
1:A:117:ILE:HD13	1:A:143:LEU:HB3	1.98	0.44
1:A:281:GLU:O	1:A:285:ILE:HG13	2.17	0.44
1:A:309:ARG:O	1:A:313:GLU:HG3	2.17	0.44
1:A:414:VAL:CG1	1:B:193:ALA:O	2.66	0.44
1:A:218:VAL:O	1:A:324:PHE:HA	2.17	0.44
1:B:139:LEU:O	1:B:143:LEU:HG	2.15	0.44
1:B:171:THR:HG23	1:B:174:GLU:H	1.82	0.44
1:B:236:LEU:HD21	1:B:240:GLN:OE1	2.17	0.44
1:B:281:GLU:O	1:B:285:ILE:CG1	2.61	0.44
1:A:177:ARG:NH1	1:A:213:ASP:HB3	2.33	0.44
1:B:267:PHE:CZ	1:B:269:GLY:HA3	2.53	0.44
1:A:122:LEU:HD13	1:A:123:MET:N	2.33	0.44
1:B:204:THR:O	1:B:207:LEU:HB2	2.17	0.44
1:B:400:GLN:O	1:B:403:MET:HB2	2.18	0.44
1:B:9:GLN:HE22	1:B:11:ARG:HE	1.64	0.44
1:B:31:LEU:HD23	1:B:38:LEU:HD13	1.99	0.44
1:A:29:ARG:CG	1:A:29:ARG:HH21	2.30	0.44
1:A:168:GLN:O	1:A:168:GLN:OE1	2.36	0.44
1:A:268:VAL:HG11	1:A:282:ILE:CD1	2.48	0.44
1:A:407:LEU:HA	1:A:438:LEU:O	2.18	0.44
1:B:101:ASN:OD1	1:B:103:VAL:HG21	2.14	0.44
1:B:260:ARG:O	1:B:261:ARG:CB	2.63	0.44
1:A:112:ILE:HG13	1:B:7:PHE:HB2	2.00	0.43
1:A:306:ILE:HA	1:B:345:THR:CG2	2.48	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:TRP:NE1	1:B:393:LYS:HD3	2.34	0.43
1:B:105:ALA:HA	1:B:106:PRO:HD2	1.90	0.43
1:B:407:LEU:HD13	1:B:430:ALA:HA	2.00	0.43
1:A:139:LEU:HD21	4:A:505:PGE:C5	2.48	0.43
1:A:32:LEU:HD11	1:A:58:LEU:HD23	2.00	0.43
1:A:391:GLN:HB3	1:A:426:LEU:HD13	2.00	0.43
1:B:164:ARG:HD2	1:B:208:PHE:CZ	2.53	0.43
1:A:357:THR:HG22	1:A:358:GLY:N	2.34	0.43
1:A:414:VAL:HG13	1:B:194:ASN:HA	2.00	0.43
1:A:176:ARG:NH1	1:A:241:GLN:O	2.51	0.43
1:A:45:PHE:CE1	1:A:60:LEU:HD22	2.53	0.43
1:A:74:TRP:NE1	1:B:97:ARG:HG2	2.33	0.43
1:B:169:PHE:HB2	1:B:175:ARG:HG2	2.01	0.43
1:B:27:LYS:HG2	1:B:77:ILE:HG21	2.01	0.43
1:A:247:TYR:H	1:A:247:TYR:HD2	1.67	0.43
1:A:231:LEU:O	1:B:233:LEU:HD13	2.18	0.43
1:A:97:ARG:NE	1:B:72:SER:HA	2.33	0.43
1:B:423:LEU:O	1:B:423:LEU:HD23	2.19	0.42
1:B:9:GLN:OE1	1:B:11:ARG:HG3	2.19	0.42
1:A:250:LEU:HD23	1:A:250:LEU:HA	1.81	0.42
1:A:448:ARG:O	1:A:452:ASN:HB2	2.19	0.42
1:A:374:GLU:HG2	1:A:375:LYS:HA	2.00	0.42
1:B:430:ALA:C	1:B:432:GLN:H	2.23	0.42
1:A:128:SEP:O1P	1:A:133:PRO:HA	2.20	0.42
1:A:314:LEU:HD23	1:A:317:LEU:CD1	2.50	0.42
1:A:378:LEU:HB2	1:A:441:VAL:HB	2.01	0.42
1:A:374:GLU:CG	1:A:375:LYS:CA	2.94	0.42
1:A:391:GLN:HG3	1:A:392:GLU:N	2.34	0.42
1:A:379:VAL:HG13	1:A:438:LEU:HD22	2.01	0.42
1:A:20:GLY:O	1:A:46:ILE:HG23	2.19	0.41
1:A:81:ASP:CB	3:A:502:NAD:H4D	2.51	0.41
1:B:368:TRP:CE3	1:B:368:TRP:HA	2.55	0.41
1:A:162:ARG:NH1	6:A:584:HOH:O	2.52	0.41
1:A:356:VAL:HG21	1:A:371:LEU:HD21	2.02	0.41
1:A:352:SER:OG	1:B:356:VAL:HG22	2.20	0.41
1:A:278:PRO:O	1:A:282:ILE:HG13	2.21	0.41
1:A:289:GLU:O	1:A:294:LYS:HB2	2.21	0.41
1:B:220:LEU:HD22	1:B:314:LEU:HD11	2.02	0.41
1:B:223:ALA:HB2	1:B:299:LEU:HD22	2.01	0.41
1:B:288:ARG:NH1	1:B:288:ARG:CG	2.80	0.41
1:B:448:ARG:HG2	1:B:448:ARG:O	2.19	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:GLU:CG	1:A:376:GLN:H	2.21	0.41
1:A:235:GLY:O	1:A:239:ILE:HG23	2.20	0.41
1:A:81:ASP:HB2	3:A:502:NAD:H4D	2.02	0.41
1:A:23:VAL:HG11	1:A:103:VAL:HG11	2.03	0.41
1:A:314:LEU:CD2	1:A:317:LEU:HD12	2.50	0.41
1:B:404:PRO:HG2	1:B:443:ARG:HA	2.03	0.41
1:A:370:ASN:HD21	1:B:370:ASN:CB	2.33	0.40
1:A:26:ARG:H	1:A:26:ARG:HG2	1.55	0.40
1:B:171:THR:CG2	1:B:174:GLU:HG3	2.52	0.40
1:B:270:LYS:H	1:B:270:LYS:HG3	1.62	0.40
1:B:350:ALA:O	1:B:351:GLN:CG	2.69	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:LYS:NZ	3:B:504:NAD:O1A[3_455]	2.16	0.04

## 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	436/457 (95%)	408 (94%)	23 (5%)	5 (1%)	14	20
1	B	449/457 (98%)	416 (93%)	24 (5%)	9 (2%)	7	9
All	All	885/914 (97%)	824 (93%)	47 (5%)	14 (2%)	9	13

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	ALA
1	A	347	ARG

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	375	LYS
1	B	309	ARG
1	B	375	LYS
1	B	272	ALA
1	B	367	ASP
1	B	104	ASP
1	B	347	ARG
1	B	349	TYR
1	B	366	LEU
1	A	450	LYS
1	B	319	HIS
1	A	278	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	363/372 (98%)	330 (91%)	33 (9%)	9	14
1	B	369/372 (99%)	321 (87%)	48 (13%)	4	4
All	All	732/744 (98%)	651 (89%)	81 (11%)	6	8

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	26	ARG
1	A	29	ARG
1	A	38	LEU
1	A	43	LEU
1	A	54	ASN
1	A	111	PHE
1	A	119	ARG
1	A	138	LEU
1	A	162	ARG
1	A	172	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	187	ARG
1	A	188	LEU
1	A	194	ASN
1	A	197	GLU
1	A	220	LEU
1	A	231	LEU
1	A	247	TYR
1	A	260	ARG
1	A	279	GLN
1	A	287	LEU
1	A	299	LEU
1	A	334	SER
1	A	371	LEU
1	A	386	GLN
1	A	403	MET
1	A	413	SER
1	A	420	HIS
1	A	426	LEU
1	A	435	SER
1	A	438	LEU
1	A	443	ARG
1	A	455	SER
1	B	2	ASP
1	B	13	ARG
1	B	43	LEU
1	B	69	LEU
1	B	81	ASP
1	B	94	GLU
1	B	104	ASP
1	B	110	SER
1	B	117	ILE
1	B	120	SER
1	B	126	VAL
1	B	135	LEU
1	B	151	LEU
1	B	164	ARG
1	B	172	MET
1	B	176	ARG
1	B	190	GLN
1	B	210	GLU
1	B	215	ARG
1	B	230	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	249	ARG
1	B	252	SER
1	B	260	ARG
1	B	261	ARG
1	B	265	ARG
1	B	276	CYS
1	B	280	GLU
1	B	285	ILE
1	B	288	ARG
1	B	289	GLU
1	B	298	ARG
1	B	313	GLU
1	B	316	THR
1	B	317	LEU
1	B	319	HIS
1	B	334	SER
1	B	347	ARG
1	B	349	TYR
1	B	365	GLU
1	B	367	ASP
1	B	370	ASN
1	B	389	THR
1	B	394	LEU
1	B	395	ILE
1	B	423	LEU
1	B	433	VAL
1	B	435	SER
1	B	443	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	GLN
1	A	194	ASN
1	A	238	GLN
1	A	279	GLN
1	A	370	ASN
1	A	431	GLN
1	A	432	GLN
1	B	54	ASN
1	B	190	GLN
1	B	241	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	351	GLN
1	B	385	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	SEP	B	128	1	8,9,10	3.29	4 (50%)	8,12,14	6.68	5 (62%)
1	SEP	A	128	1	8,9,10	3.08	3 (37%)	8,12,14	4.77	5 (62%)

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
1	SEP	B	128	1	-	2/5/8/10	-
1	SEP	A	128	1	-	1/5/8/10	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	128	SEP	OG-CB	5.78	1.67	1.44
1	B	128	SEP	CA-N	-5.23	1.32	1.48
1	A	128	SEP	CA-N	-5.09	1.32	1.48
1	A	128	SEP	OG-CB	5.02	1.64	1.44
1	A	128	SEP	P-OG	4.29	1.74	1.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	128	SEP	P-OG	4.05	1.73	1.60
1	B	128	SEP	P-O1P	2.11	1.57	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	128	SEP	OG-CB-CA	14.92	122.67	108.14
1	B	128	SEP	P-OG-CB	10.23	146.47	118.30
1	A	128	SEP	P-OG-CB	8.87	142.73	118.30
1	A	128	SEP	OG-CB-CA	8.42	116.34	108.14
1	A	128	SEP	O3P-P-OG	-4.00	96.10	106.73
1	B	128	SEP	O3P-P-OG	-3.54	97.31	106.73
1	B	128	SEP	O3P-P-O2P	3.12	119.55	107.64
1	A	128	SEP	O3P-P-O2P	3.06	119.33	107.64
1	B	128	SEP	OG-P-O1P	-2.26	100.14	106.47
1	A	128	SEP	OG-P-O1P	-2.03	100.78	106.47

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	128	SEP	N-CA-CB-OG
1	B	128	SEP	CA-CB-OG-P
1	A	128	SEP	CA-CB-OG-P

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	128	SEP	2	0
1	A	128	SEP	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

7 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	SAH	A	501	-	21,28,28	1.38	1 (4%)	20,40,40	1.51	2 (10%)
4	PGE	A	506	-	9,9,9	2.05	2 (22%)	8,8,8	1.64	3 (37%)
5	PO4	B	507	-	4,4,4	1.59	0	6,6,6	0.67	0
4	PGE	A	505	-	9,9,9	2.10	2 (22%)	8,8,8	1.49	3 (37%)
2	SAH	B	503	-	21,28,28	1.47	1 (4%)	20,40,40	1.55	2 (10%)
3	NAD	A	502	-	42,48,48	2.26	12 (28%)	50,73,73	1.66	10 (20%)
3	NAD	B	504	-	42,48,48	2.23	11 (26%)	50,73,73	1.79	10 (20%)

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	SAH	A	501	-	-	0/7/31/31	0/3/3/3
4	PGE	A	506	-	-	2/7/7/7	-
4	PGE	A	505	-	-	2/7/7/7	-
2	SAH	B	503	-	-	0/7/31/31	0/3/3/3
3	NAD	A	502	-	4/4/11/11	6/26/62/62	0/5/5/5
3	NAD	B	504	-	-	4/26/62/62	0/5/5/5

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	504	NAD	C3N-C7N	-7.38	1.39	1.50
3	A	502	NAD	C3N-C7N	-7.11	1.39	1.50
3	A	502	NAD	O7N-C7N	6.82	1.37	1.24
3	B	504	NAD	O7N-C7N	6.65	1.36	1.24
2	B	503	SAH	O4'-C1'	5.93	1.49	1.41
2	A	501	SAH	O4'-C1'	5.42	1.48	1.41
3	B	504	NAD	PN-O5D	-4.79	1.39	1.59
3	A	502	NAD	O4D-C1D	4.76	1.47	1.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	505	PGE	O3-C4	-4.27	1.23	1.42
3	B	504	NAD	C2D-C3D	-4.16	1.42	1.53
4	A	506	PGE	O3-C4	-4.04	1.24	1.42
3	A	502	NAD	O4B-C1B	4.01	1.46	1.41
3	A	502	NAD	PN-O5D	-3.84	1.43	1.59
4	A	505	PGE	O4-C6	-3.63	1.23	1.42
4	A	506	PGE	O4-C6	-3.58	1.23	1.42
3	A	502	NAD	C5B-C4B	3.12	1.61	1.51
3	B	504	NAD	C3B-C4B	3.09	1.60	1.53
3	A	502	NAD	PN-O2N	-2.57	1.43	1.55
3	B	504	NAD	C2N-C3N	-2.54	1.35	1.39
3	B	504	NAD	PA-O2A	-2.39	1.44	1.55
3	A	502	NAD	C2A-N3A	2.26	1.35	1.32
3	A	502	NAD	O5D-C5D	-2.24	1.36	1.44
3	B	504	NAD	PN-O2N	-2.21	1.44	1.55
3	A	502	NAD	PA-O2A	-2.20	1.45	1.55
3	B	504	NAD	C6N-C5N	-2.18	1.33	1.38
3	B	504	NAD	O5B-C5B	2.15	1.53	1.44
3	A	502	NAD	PA-O5B	2.09	1.67	1.59
3	B	504	NAD	PN-O1N	-2.09	1.43	1.50
3	A	502	NAD	C5A-N7A	-2.03	1.32	1.39

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	503	SAH	N3-C2-N1	-5.36	120.30	128.68
3	B	504	NAD	N3A-C2A-N1A	-5.34	120.34	128.68
2	A	501	SAH	N3-C2-N1	-5.28	120.43	128.68
3	B	504	NAD	O4D-C1D-C2D	5.17	114.48	106.93
3	A	502	NAD	N3A-C2A-N1A	-5.00	120.87	128.68
3	B	504	NAD	C5D-C4D-C3D	-4.98	96.51	115.18
3	A	502	NAD	C3N-C2N-N1N	3.61	123.96	120.43
3	A	502	NAD	C6N-N1N-C2N	-3.21	119.05	121.97
3	B	504	NAD	PN-O3-PA	-3.16	121.97	132.83
3	A	502	NAD	C3B-C2B-C1B	3.01	105.51	100.98
3	A	502	NAD	C3N-C7N-N7N	3.01	121.36	117.75
3	A	502	NAD	O5D-C5D-C4D	2.93	119.09	108.99
3	B	504	NAD	C2D-C3D-C4D	2.90	108.28	102.64
4	A	506	PGE	O3-C5-C6	2.78	122.27	110.07
4	A	506	PGE	O3-C4-C3	2.45	121.44	110.39
3	A	502	NAD	O3D-C3D-C4D	-2.36	104.22	111.05
4	A	505	PGE	O3-C5-C6	2.35	120.38	110.07

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	503	SAH	C3'-C2'-C1'	2.32	104.48	100.98
3	B	504	NAD	C1B-N9A-C4A	-2.32	122.57	126.64
4	A	506	PGE	O2-C3-C4	2.28	120.66	110.39
3	B	504	NAD	O4B-C1B-C2B	2.25	110.21	106.93
3	B	504	NAD	O2D-C2D-C1D	-2.23	102.62	110.85
3	B	504	NAD	PN-O5D-C5D	-2.22	108.69	121.68
3	A	502	NAD	O5B-C5B-C4B	2.12	116.28	108.99
3	A	502	NAD	O4D-C1D-C2D	-2.11	103.85	106.93
4	A	505	PGE	O2-C3-C4	2.08	119.79	110.39
4	A	505	PGE	O3-C4-C3	2.08	119.78	110.39
3	B	504	NAD	O7N-C7N-N7N	-2.06	119.65	122.58
2	A	501	SAH	C3'-C2'-C1'	2.03	104.04	100.98
3	A	502	NAD	O7N-C7N-N7N	-2.03	119.70	122.58

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	502	NAD	C3D
3	A	502	NAD	C2D
3	A	502	NAD	C4D
3	A	502	NAD	C1D

All (14) torsion outliers are listed below:

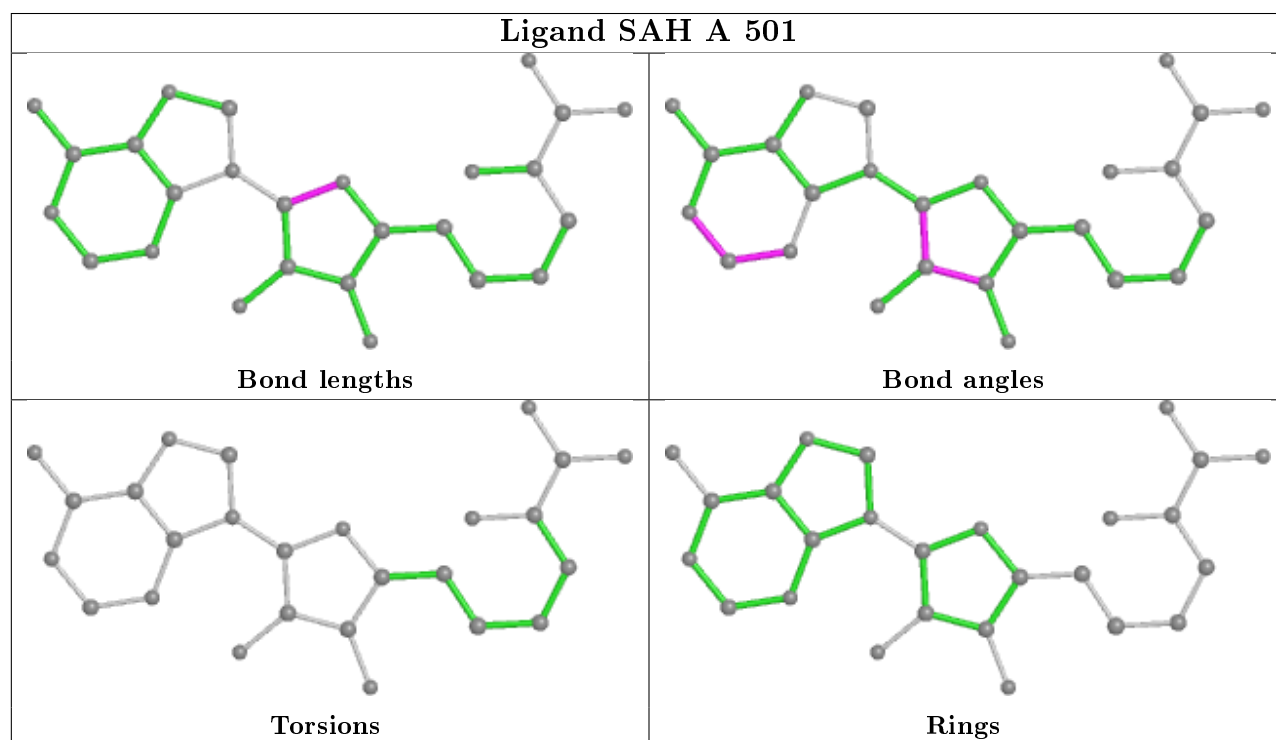
Mol	Chain	Res	Type	Atoms
3	A	502	NAD	C3D-C4D-C5D-O5D
3	A	502	NAD	C2D-C1D-N1N-C2N
3	A	502	NAD	C2D-C1D-N1N-C6N
3	B	504	NAD	O4B-C4B-C5B-O5B
3	B	504	NAD	O4D-C4D-C5D-O5D
3	B	504	NAD	C3D-C4D-C5D-O5D
3	B	504	NAD	O4D-C1D-N1N-C2N
3	A	502	NAD	O4D-C4D-C5D-O5D
4	A	505	PGE	O2-C3-C4-O3
4	A	506	PGE	O2-C3-C4-O3
4	A	506	PGE	C6-C5-O3-C4
3	A	502	NAD	O4B-C4B-C5B-O5B
3	A	502	NAD	C4B-C5B-O5B-PA
4	A	505	PGE	C6-C5-O3-C4

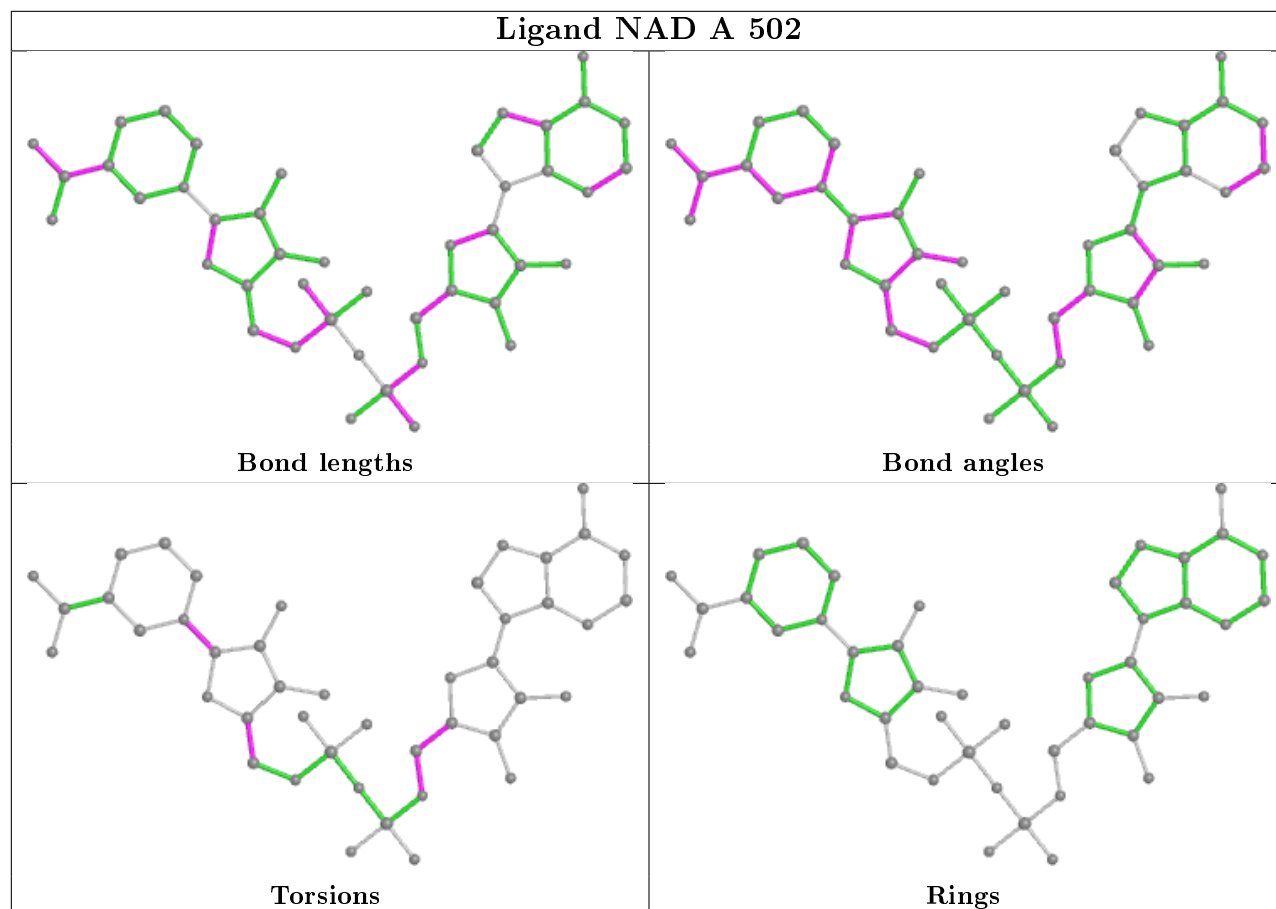
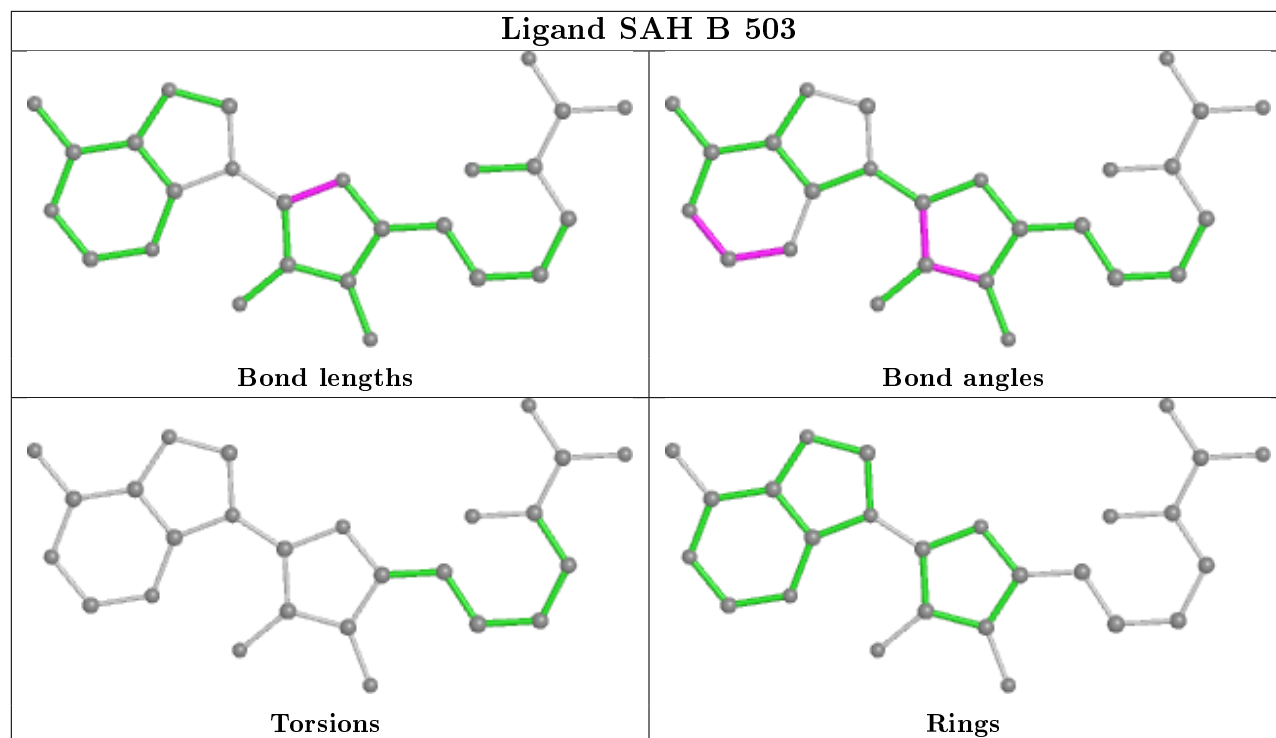
There are no ring outliers.

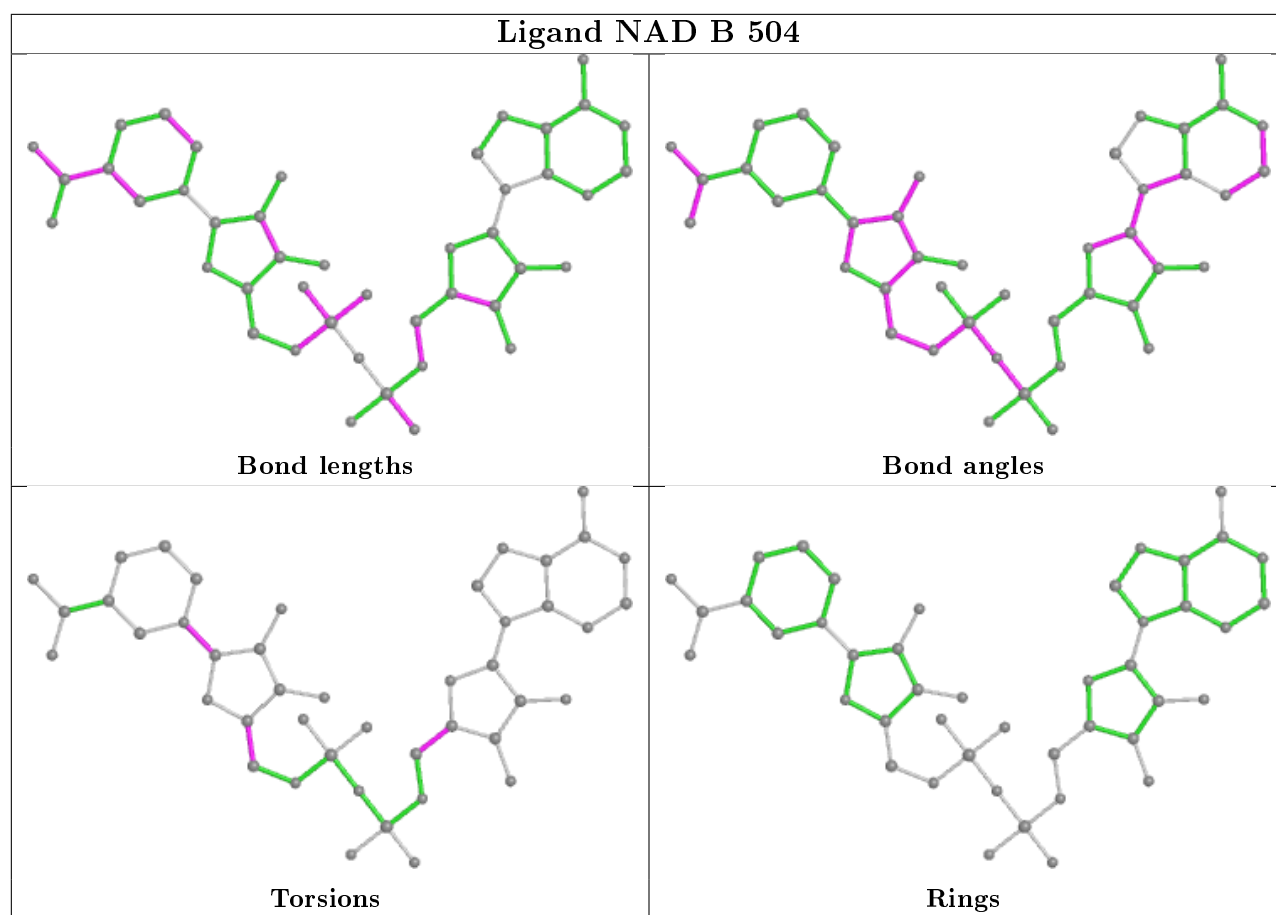
5 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	506	PGE	4	0
5	B	507	PO4	1	0
4	A	505	PGE	6	0
3	A	502	NAD	12	0
3	B	504	NAD	4	1

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	442/457 (96%)	0.11	8 (1%) 68 66	18, 40, 61, 81	0
1	B	453/457 (99%)	0.11	21 (4%) 32 31	15, 35, 66, 84	0
All	All	895/914 (97%)	0.11	29 (3%) 47 46	15, 37, 62, 84	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	274	TYR	6.2
1	A	277	VAL	6.1
1	B	276	CYS	5.4
1	B	359	HIS	4.5
1	A	457	HIS	4.5
1	B	262	ASP	4.2
1	A	456	ASN	3.9
1	A	351	GLN	3.8
1	B	364	GLY	3.6
1	B	318	CYS	3.2
1	A	348	ASP	3.1
1	B	375	LYS	3.0
1	B	348	ASP	3.0
1	B	198	LYS	2.9
1	B	272	ALA	2.9
1	B	369	GLU	2.9
1	B	363	GLY	2.7
1	B	275	HIS	2.5
1	A	249	ARG	2.4
1	B	260	ARG	2.4
1	B	261	ARG	2.4
1	B	273	GLY	2.4
1	B	351	GLN	2.4
1	A	347	ARG	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	319	HIS	2.2
1	A	17	ILE	2.1
1	B	104	ASP	2.1
1	B	270	LYS	2.1
1	B	449	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	SEP	A	128	10/11	0.77	0.28	37,44,57,57	0
1	SEP	B	128	10/11	0.87	0.17	36,43,54,55	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

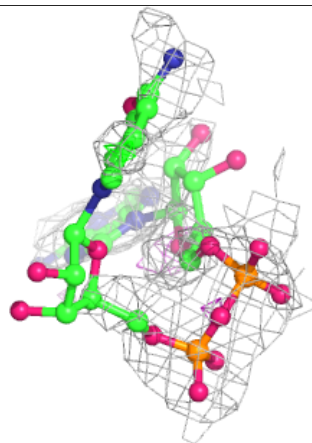
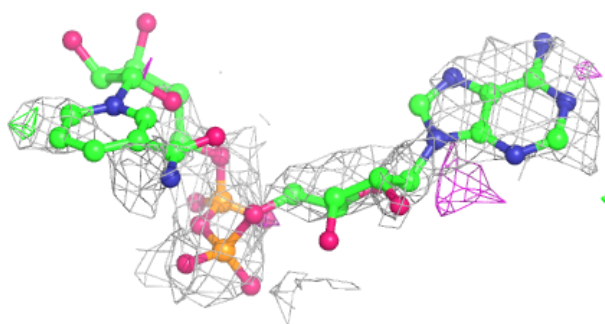
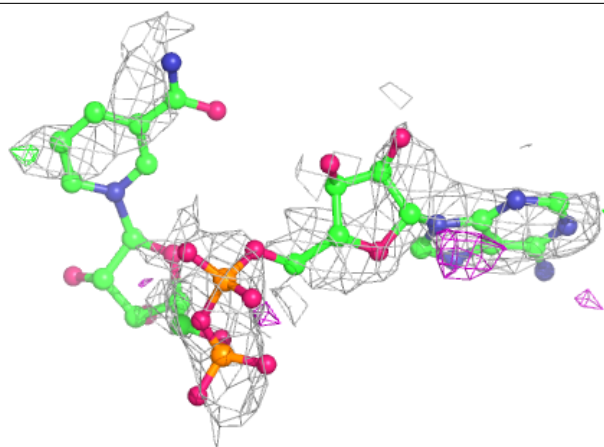
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAD	A	502	44/44	0.59	0.48	101,111,113,113	0
3	NAD	B	504	44/44	0.68	0.35	62,84,100,101	0
4	PGE	A	506	10/10	0.74	0.22	79,80,81,81	0
4	PGE	A	505	10/10	0.87	0.26	51,52,53,54	0
2	SAH	A	501	26/26	0.91	0.13	38,42,45,46	0
5	PO4	B	507	5/5	0.97	0.09	49,50,51,53	0
2	SAH	B	503	26/26	0.97	0.09	19,27,28,31	0

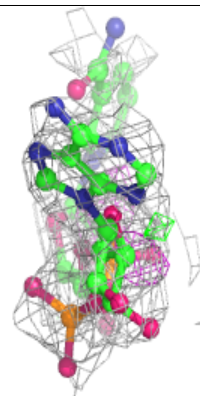
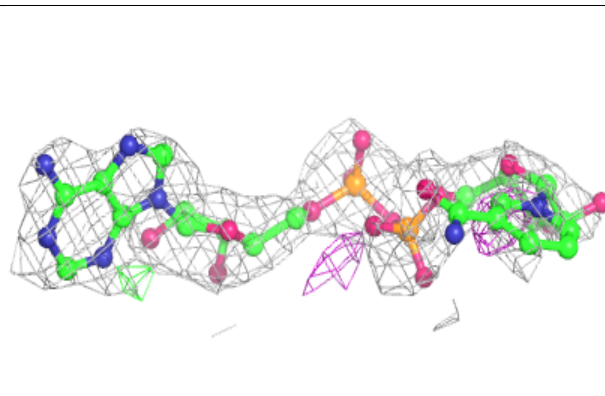
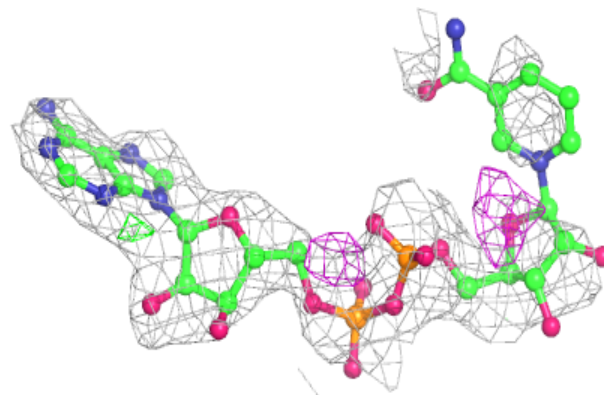
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAD A 502:**

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

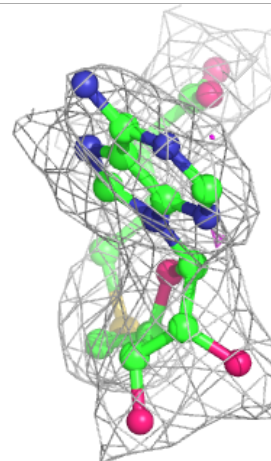
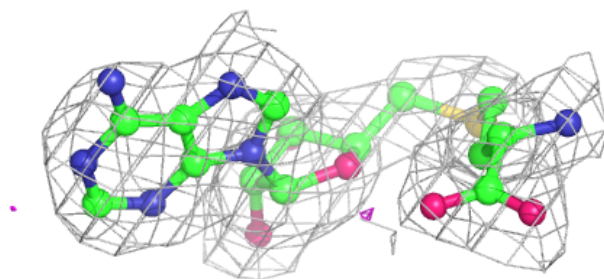
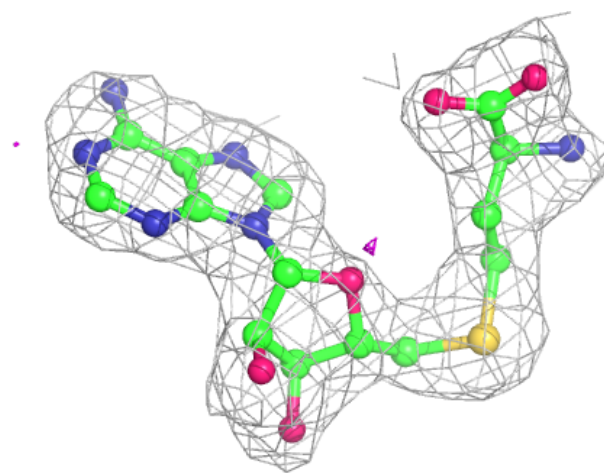
**Electron density around NAD B 504:**

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



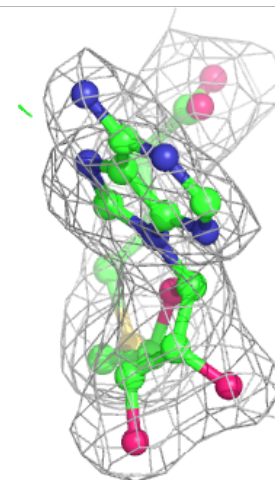
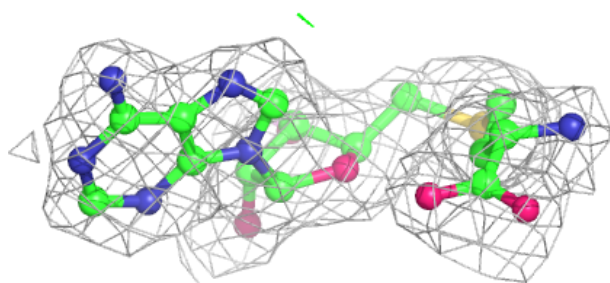
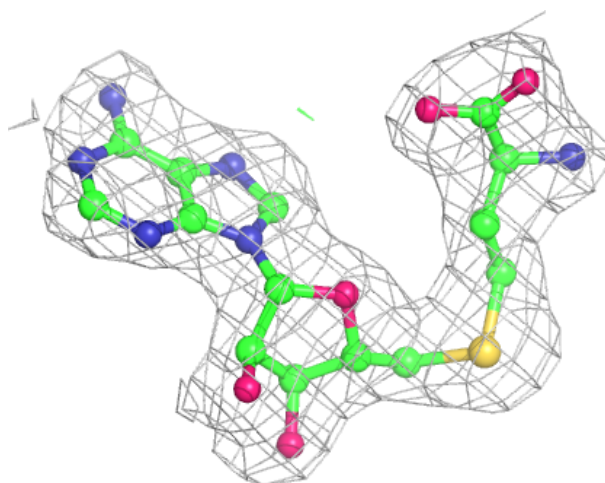
**Electron density around SAH A 501:**

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



**Electron density around SAH B 503:**

$2mF_o-DF_c$  (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.