



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 05:47 pm BST

PDB ID : 3ZWC  
Title : CRYSTAL STRUCTURE OF RAT PEROXISOMAL MULTIFUNCTIONAL ENZYME TYPE 1 (RPMFE1) COMPLEXED WITH 3S-HYDROXY-DECA NOYL-COA  
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Deposited on : 2011-07-28  
Resolution : 2.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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.

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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

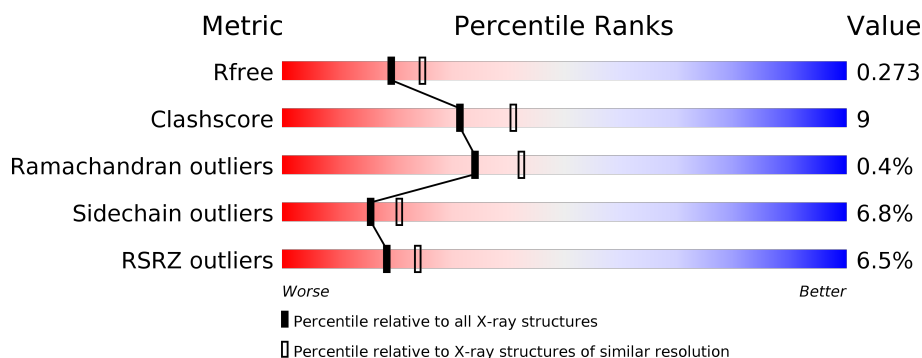
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	742	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>..</div> </div> </div>
1	B	742	<div> <div>7%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>..</div> </div> </div>

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
5	GOL	B	1719	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11720 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 PEROXISOMAL BIFUNCTIONAL ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	725	Total	C	N	O	S	0	0	0
			5562	3553	976	1010	23			
1	B	719	Total	C	N	O	S	0	0	0
			5524	3532	967	1002	23			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P07896
A	-18	GLY	-	expression tag	UNP P07896
A	-17	SER	-	expression tag	UNP P07896
A	-16	SER	-	expression tag	UNP P07896
A	-15	HIS	-	expression tag	UNP P07896
A	-14	HIS	-	expression tag	UNP P07896
A	-13	HIS	-	expression tag	UNP P07896
A	-12	HIS	-	expression tag	UNP P07896
A	-11	HIS	-	expression tag	UNP P07896
A	-10	HIS	-	expression tag	UNP P07896
A	-9	SER	-	expression tag	UNP P07896
A	-8	SER	-	expression tag	UNP P07896
A	-7	GLY	-	expression tag	UNP P07896
A	-6	LEU	-	expression tag	UNP P07896
A	-5	VAL	-	expression tag	UNP P07896
A	-4	PRO	-	expression tag	UNP P07896
A	-3	ARG	-	expression tag	UNP P07896
A	-2	GLY	-	expression tag	UNP P07896
A	-1	SER	-	expression tag	UNP P07896
A	0	HIS	-	expression tag	UNP P07896
B	-19	MET	-	expression tag	UNP P07896
B	-18	GLY	-	expression tag	UNP P07896
B	-17	SER	-	expression tag	UNP P07896
B	-16	SER	-	expression tag	UNP P07896
B	-15	HIS	-	expression tag	UNP P07896

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP P07896
B	-13	HIS	-	expression tag	UNP P07896
B	-12	HIS	-	expression tag	UNP P07896
B	-11	HIS	-	expression tag	UNP P07896
B	-10	HIS	-	expression tag	UNP P07896
B	-9	SER	-	expression tag	UNP P07896
B	-8	SER	-	expression tag	UNP P07896
B	-7	GLY	-	expression tag	UNP P07896
B	-6	LEU	-	expression tag	UNP P07896
B	-5	VAL	-	expression tag	UNP P07896
B	-4	PRO	-	expression tag	UNP P07896
B	-3	ARG	-	expression tag	UNP P07896
B	-2	GLY	-	expression tag	UNP P07896
B	-1	SER	-	expression tag	UNP P07896
B	0	HIS	-	expression tag	UNP P07896

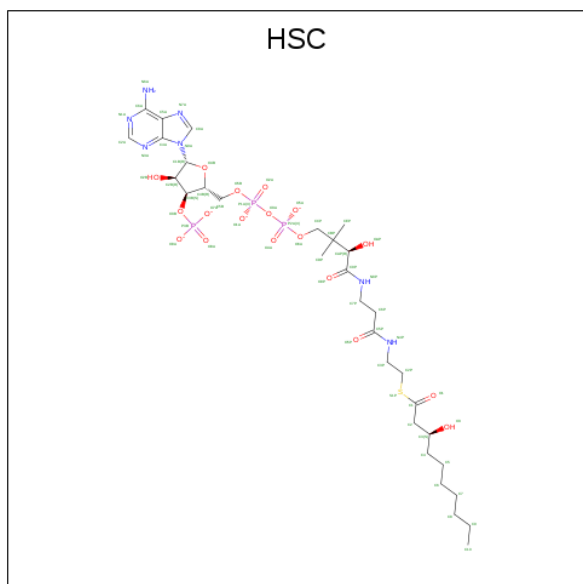
- # NAD
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- The image displays the chemical structure of Nicotinamide Adenine Dinucleotide (NAD), a crucial coenzyme. It is composed of two nucleotides linked by a pyrophosphate bridge. The first nucleotide consists of a nicotinamide ring (colored blue) attached to a ribose sugar (colored green). The second nucleotide consists of an adenine ring (colored blue) attached to a ribose sugar (colored green). The two ribose sugars are linked by a pyrophosphate bridge (colored red). The structure is labeled with various atoms and groups, including NH<sub>2</sub>, N, C, O, P, and H, and is set against a black background.

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is (S)-3-HYDROXYDECANOYL-COA (three-letter code: HSC) (formula:  $C_{31}H_{50}N_7O_{18}P_3S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	
			60	31	7	18	3	1	0
4	B	1	Total	C	N	O	P	S	
			60	31	7	18	3	1	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O		
			6	3	3	0	0

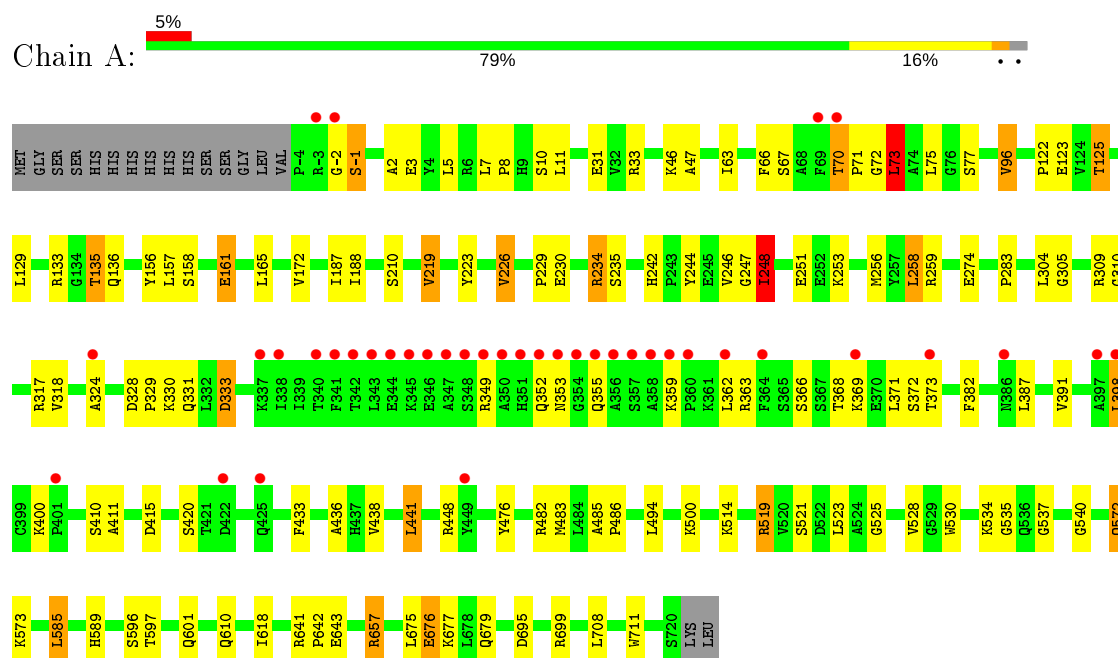
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	231	Total	O		
			231	231	0	0
6	B	174	Total	O		
			174	174	0	0

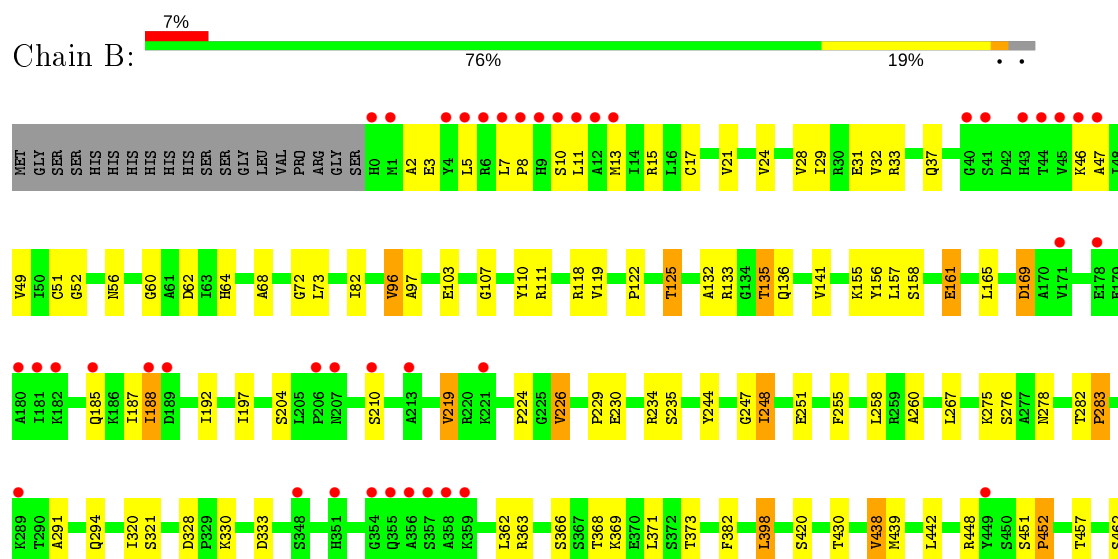
### 3 Residue-property plots

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.

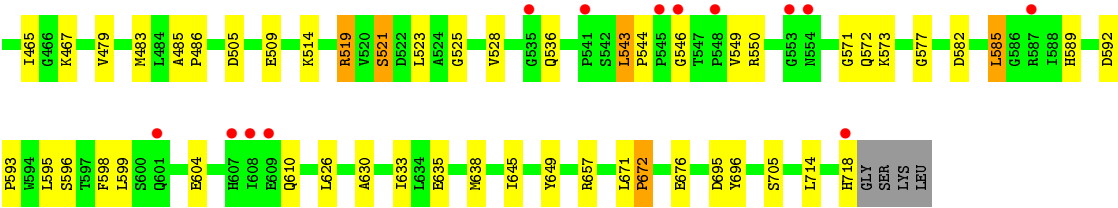
#### • Molecule 1: PEROXISOMAL BIFUNCTIONAL ENZYME



#### • Molecule 1: PEROXISOMAL BIFUNCTIONAL ENZYME







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.57Å 126.51Å 224.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	112.48 – 2.30 44.62 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (112.48-2.30) 99.6 (44.62-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.85 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.231 , 0.280 0.227 , 0.273	Depositor DCC
$R_{free}$ test set	4184 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.1	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11720	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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: GOL, SO4, NAD, HSC

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	0.92	1/5691 (0.0%)	0.87	11/7709 (0.1%)
1	B	0.95	1/5652 (0.0%)	0.89	7/7658 (0.1%)
All	All	0.93	2/11343 (0.0%)	0.88	18/15367 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	17	CYS	CB-SG	7.55	1.95	1.82
1	A	485	ALA	CA-CB	5.13	1.63	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	657	ARG	NE-CZ-NH2	9.49	125.05	120.30
1	A	657	ARG	NE-CZ-NH1	-8.15	116.22	120.30
1	A	234	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	A	234	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	B	649	TYR	CA-CB-CG	-6.89	100.30	113.40
1	A	258	LEU	CB-CG-CD1	6.84	122.63	111.00
1	B	169	ASP	CB-CG-OD1	-6.73	112.24	118.30
1	B	519	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	B	626	LEU	CA-CB-CG	6.18	129.52	115.30
1	B	519	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	A	-2	GLY	N-CA-C	6.00	128.10	113.10
1	A	482	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	A	248	ILE	CA-CB-CG2	5.88	122.66	110.90
1	A	33	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	519	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	B	234	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	33	ARG	NE-CZ-NH2	-5.03	117.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	519	ARG	NE-CZ-NH1	5.03	122.81	120.30

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	5562	0	5667	103	0
1	B	5524	0	5631	103	0
2	A	44	0	26	4	0
2	B	44	0	26	0	0
3	A	10	0	0	0	0
3	B	5	0	0	1	0
4	A	60	0	50	9	0
4	B	60	0	50	8	0
5	B	6	0	8	4	0
6	A	231	0	0	12	0
6	B	174	0	0	15	0
All	All	11720	0	11458	205	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 (205) 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:73:LEU:HD21	1:A:256:MET:HE2	1.32	1.08
1:A:500:LYS:HD3	6:A:2180:HOH:O	1.54	1.04
1:A:253:LYS:HE2	6:A:2067:HOH:O	1.58	1.03
1:B:514:LYS:HE2	6:B:2111:HOH:O	1.60	1.01
1:A:135:THR:HG21	1:A:235:SER:OG	1.71	0.91
5:B:1719:GOL:O3	5:B:1719:GOL:O1	1.83	0.90
1:B:158:SER:OG	1:B:161:GLU:HG2	1.74	0.88
1:A:73:LEU:HD21	1:A:256:MET:CE	2.06	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LEU:CD2	1:A:256:MET:HE2	2.05	0.86
1:A:597:THR:HG23	1:B:382:PHE:HZ	1.42	0.85
1:A:540:GLY:HA3	6:A:2159:HOH:O	1.76	0.84
1:B:135:THR:HG21	1:B:235:SER:OG	1.80	0.81
1:A:73:LEU:CD2	1:A:256:MET:CE	2.59	0.80
1:B:283:PRO:HA	1:B:718:HIS:HE1	1.45	0.80
1:A:597:THR:HG23	1:B:382:PHE:CZ	2.18	0.78
1:A:657:ARG:NH1	6:A:2035:HOH:O	2.12	0.74
1:B:72:GLY:HA3	4:B:1722:HSC:H9A	1.68	0.74
1:B:158:SER:OG	1:B:161:GLU:CG	2.35	0.74
1:A:7:LEU:HG	1:A:8:PRO:HD2	1.68	0.74
1:B:21:VAL:HG12	6:B:2007:HOH:O	1.89	0.72
1:A:67:SER:HB3	1:A:70:THR:OG1	1.90	0.71
1:B:525:GLY:O	1:B:528:VAL:HG22	1.92	0.70
1:B:283:PRO:HA	1:B:718:HIS:CE1	2.27	0.70
1:A:540:GLY:CA	6:A:2159:HOH:O	2.36	0.69
1:A:679:GLN:HG2	6:A:2219:HOH:O	1.91	0.69
1:B:505:ASP:O	1:B:509:GLU:HG3	1.92	0.69
1:A:67:SER:H	1:A:71:PRO:HD3	1.56	0.69
1:B:37:GLN:HB3	6:B:2006:HOH:O	1.93	0.69
1:B:255:PHE:CE2	4:B:1722:HSC:H8	2.27	0.69
1:A:122:PRO:O	1:A:125:THR:HB	1.93	0.68
4:B:1722:HSC:H8A	6:B:2015:HOH:O	1.93	0.68
1:A:96:VAL:HG21	4:A:1724:HSC:HDP	1.74	0.67
1:B:244:TYR:CZ	1:B:248:ILE:HD11	2.29	0.67
1:A:158:SER:OG	1:A:161:GLU:HG3	1.94	0.67
1:B:521:SER:HB2	5:B:1719:GOL:H12	1.77	0.67
1:B:244:TYR:CE1	1:B:248:ILE:HD11	2.29	0.67
1:A:73:LEU:HD22	1:A:256:MET:HE1	1.76	0.67
1:B:133:ARG:HD2	1:B:248:ILE:CG1	2.25	0.67
1:A:72:GLY:C	4:A:1724:HSC:H8	2.17	0.65
1:B:29:ILE:HD12	1:B:73:LEU:HD22	1.78	0.65
1:B:7:LEU:HG	1:B:8:PRO:HD2	1.78	0.65
1:B:122:PRO:O	1:B:125:THR:HB	1.97	0.65
1:A:519:ARG:HD3	1:A:589:HIS:CE1	2.32	0.64
1:A:75:LEU:H	4:A:1724:HSC:H8A	1.61	0.64
1:A:123:GLU:CG	4:A:1724:HSC:H2A	2.28	0.64
1:A:73:LEU:N	4:A:1724:HSC:H8	2.14	0.63
1:B:21:VAL:CG1	6:B:2007:HOH:O	2.47	0.62
1:B:155:LYS:NZ	6:B:2039:HOH:O	2.32	0.62
1:A:514:LYS:HD2	6:A:2148:HOH:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:LEU:HD22	1:B:47:ALA:HB3	1.83	0.60
1:A:133:ARG:HD2	1:A:248:ILE:CG1	2.32	0.60
1:A:597:THR:CG2	1:B:382:PHE:CZ	2.85	0.60
1:A:433:PHE:CE1	1:A:441:LEU:HD13	2.36	0.60
1:A:226:VAL:HG22	1:A:229:PRO:CD	2.33	0.58
1:A:601:GLN:HG3	1:B:382:PHE:CD2	2.39	0.58
1:B:10:SER:HB3	1:B:46:LYS:HG3	1.85	0.58
1:A:597:THR:CG2	1:B:382:PHE:HZ	2.14	0.57
1:B:135:THR:HG22	1:B:251:GLU:OE1	2.03	0.57
1:B:37:GLN:CB	6:B:2006:HOH:O	2.51	0.57
1:A:253:LYS:CE	6:A:2067:HOH:O	2.31	0.57
1:A:135:THR:HB	1:A:251:GLU:OE1	2.05	0.57
1:B:141:VAL:CG2	1:B:197:ILE:HD13	2.34	0.57
1:A:244:TYR:CZ	1:A:248:ILE:HD11	2.40	0.57
1:A:73:LEU:HD22	1:A:256:MET:CE	2.31	0.56
1:A:244:TYR:CZ	1:A:248:ILE:CD1	2.89	0.56
1:B:633:ILE:HG23	1:B:638:MET:HB2	1.86	0.56
1:B:226:VAL:HG22	1:B:229:PRO:CD	2.36	0.56
1:A:641:ARG:HB2	1:A:642:PRO:HD2	1.88	0.56
1:A:411:ALA:HB1	1:A:476:TYR:CE1	2.41	0.55
1:B:118:ARG:HG2	6:B:2044:HOH:O	2.06	0.54
1:A:349:ARG:CG	1:A:352:GLN:HE21	2.21	0.54
1:B:672:PRO:HD3	1:B:705:SER:OG	2.07	0.54
1:B:68:ALA:HB2	1:B:260:ALA:HA	1.89	0.54
1:B:156:TYR:N	1:B:156:TYR:CD1	2.77	0.53
1:A:349:ARG:HG3	1:A:352:GLN:HE21	1.74	0.53
1:A:71:PRO:HD2	1:A:259:ARG:HD2	1.90	0.53
1:B:3:GLU:HG2	1:B:5:LEU:HD13	1.90	0.53
1:B:244:TYR:CZ	1:B:248:ILE:CD1	2.92	0.52
1:A:382:PHE:CE2	2:A:1721:NAD:H8A	2.45	0.52
1:A:156:TYR:CD1	1:A:156:TYR:N	2.77	0.52
1:B:244:TYR:CE1	1:B:248:ILE:CD1	2.93	0.52
1:B:369:LYS:HA	1:B:398:LEU:HD13	1.91	0.52
1:A:244:TYR:CE1	1:A:248:ILE:CD1	2.93	0.52
1:A:494:LEU:HD13	1:A:618:ILE:HG12	1.92	0.52
1:B:267:LEU:HD23	1:B:657:ARG:HG2	1.92	0.52
1:B:582:ASP:HB2	6:B:2132:HOH:O	2.10	0.52
1:A:525:GLY:O	1:A:528:VAL:HG22	2.10	0.51
1:A:369:LYS:HA	1:A:398:LEU:HD13	1.93	0.51
1:B:60:GLY:HA3	4:B:1722:HSC:H2PA	1.92	0.51
1:B:46:LYS:HB2	1:B:188:ILE:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ALA:HA	6:A:2117:HOH:O	2.10	0.51
1:A:483:MET:O	1:A:486:PRO:HD2	2.10	0.51
1:A:2:ALA:HB3	1:A:31:GLU:HB3	1.92	0.50
1:B:96:VAL:HG11	4:B:1722:HSC:HDP	1.93	0.50
1:B:294:GLN:O	1:B:457:THR:HG23	2.11	0.50
1:B:465:ILE:HG13	1:B:467:LYS:HG3	1.93	0.50
1:A:244:TYR:CE1	1:A:248:ILE:HD11	2.47	0.49
1:B:156:TYR:N	1:B:156:TYR:HD1	2.09	0.49
1:A:310:GLY:HA3	1:A:436:ALA:HB3	1.94	0.49
1:B:543:LEU:HD22	1:B:544:PRO:HD2	1.94	0.49
1:A:70:THR:HB	1:A:71:PRO:HD3	1.93	0.49
1:B:451:SER:O	1:B:452:PRO:C	2.51	0.49
1:A:226:VAL:HG22	1:A:229:PRO:HD2	1.93	0.49
1:B:62:ASP:OD2	1:B:64:HIS:HB2	2.13	0.49
1:A:73:LEU:H	4:A:1724:HSC:H7	1.78	0.49
1:B:546:GLY:N	6:B:2124:HOH:O	2.33	0.49
1:B:111:ARG:N	1:B:169:ASP:OD2	2.40	0.49
1:B:13:MET:HA	1:B:49:VAL:O	2.13	0.49
1:B:485:ALA:HB3	1:B:486:PRO:HD3	1.95	0.48
1:A:3:GLU:HG2	1:A:5:LEU:HD13	1.94	0.48
1:A:123:GLU:HG3	4:A:1724:HSC:H2A	1.94	0.48
1:B:97:ALA:HB3	1:B:119:VAL:HG12	1.93	0.48
1:A:10:SER:HB3	1:A:46:LYS:HG3	1.95	0.48
1:A:133:ARG:NE	1:A:248:ILE:HG12	2.28	0.48
1:A:573:LYS:HA	1:A:585:LEU:HD13	1.96	0.48
1:B:136:GLN:NE2	1:B:247:GLY:HA3	2.28	0.47
1:B:671:LEU:HB2	1:B:672:PRO:HD3	1.97	0.47
1:B:604:GLU:O	6:B:2134:HOH:O	2.20	0.47
1:B:714:LEU:HD23	6:B:2173:HOH:O	2.15	0.47
1:A:304:LEU:HD11	1:A:324:ALA:HB1	1.97	0.47
1:A:382:PHE:CD2	2:A:1721:NAD:H8A	2.49	0.47
1:A:420:SER:OG	1:A:420:SER:O	2.33	0.47
1:B:133:ARG:HD2	1:B:248:ILE:HG13	1.97	0.47
1:B:192:ILE:N	3:B:1721:SO4:O2	2.42	0.47
1:B:638:MET:HE3	6:B:2147:HOH:O	2.14	0.47
1:A:133:ARG:CD	1:A:248:ILE:CG1	2.93	0.47
1:B:133:ARG:HD2	1:B:248:ILE:HG12	1.94	0.47
4:B:1722:HSC:HEP	6:B:2007:HOH:O	2.14	0.47
1:B:226:VAL:HG22	1:B:229:PRO:HD2	1.98	0.46
1:B:2:ALA:HB3	1:B:31:GLU:HB3	1.97	0.46
1:A:382:PHE:CZ	2:A:1721:NAD:H2B	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:573:LYS:HA	1:B:585:LEU:HD13	1.97	0.46
1:A:96:VAL:HG11	4:A:1724:HSC:HEP	1.98	0.46
1:A:328:ASP:OD1	1:A:330:LYS:HB2	2.15	0.46
1:A:535:GLY:C	1:A:537:GLY:H	2.19	0.46
1:A:156:TYR:HD1	1:A:156:TYR:N	2.12	0.46
1:A:305:GLY:HA3	2:A:1721:NAD:O5B	2.16	0.46
1:B:595:LEU:HA	1:B:598:PHE:HB3	1.97	0.46
1:B:187:ILE:HD12	1:B:187:ILE:C	2.36	0.46
1:A:73:LEU:CD2	1:A:256:MET:HE1	2.36	0.46
1:A:530:TRP:CE2	1:A:534:LYS:HE2	2.51	0.46
1:B:363:ARG:HH22	1:B:373:THR:HG21	1.81	0.46
1:A:158:SER:OG	1:A:161:GLU:CG	2.63	0.45
1:A:329:PRO:O	1:A:333:ASP:HB2	2.16	0.45
1:A:223:TYR:HB3	1:A:226:VAL:HG13	1.98	0.45
1:B:219:VAL:HG11	1:B:230:GLU:HA	1.98	0.45
1:A:11:LEU:HD22	1:A:47:ALA:HB3	1.97	0.45
1:A:676:GLU:HG3	1:A:677:LYS:N	2.32	0.45
1:B:158:SER:HG	1:B:161:GLU:HG2	1.75	0.45
1:B:571:GLY:HA2	1:B:577:GLY:HA3	1.99	0.45
1:B:521:SER:CB	5:B:1719:GOL:H12	2.45	0.44
1:A:219:VAL:HG11	1:A:230:GLU:HA	1.99	0.44
1:B:110:TYR:HA	1:B:169:ASP:OD2	2.17	0.44
1:B:291:ALA:HB2	1:B:452:PRO:HB3	1.99	0.44
1:A:133:ARG:HD2	1:A:248:ILE:HD11	2.00	0.44
1:A:187:ILE:HD12	1:A:187:ILE:C	2.38	0.44
1:B:420:SER:OG	1:B:420:SER:O	2.36	0.44
1:B:224:PRO:HD2	6:B:2058:HOH:O	2.17	0.44
1:B:635:GLU:HB3	1:B:696:TYR:HB2	1.99	0.44
1:A:349:ARG:HG3	1:A:352:GLN:NE2	2.34	0.43
1:A:400:LYS:HB2	6:A:2115:HOH:O	2.17	0.43
1:B:68:ALA:CB	1:B:260:ALA:HA	2.48	0.43
1:A:66:PHE:HA	1:A:71:PRO:HG3	1.99	0.43
1:A:305:GLY:O	1:A:309:ARG:HG3	2.18	0.43
1:A:363:ARG:HH22	1:A:373:THR:HG21	1.83	0.43
1:A:382:PHE:HB2	1:A:387:LEU:HD23	2.00	0.43
1:A:519:ARG:HD3	1:A:589:HIS:NE2	2.34	0.43
1:B:275:LYS:HG3	4:B:1722:HSC:O2B	2.18	0.43
1:B:73:LEU:O	4:B:1722:HSC:H9	2.18	0.43
1:A:244:TYR:CZ	1:A:248:ILE:HD13	2.52	0.43
1:B:438:VAL:CG1	1:B:439:MET:N	2.82	0.43
1:A:641:ARG:HD3	1:A:643:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:GLU:OE1	1:A:657:ARG:NH2	2.52	0.42
1:A:572:GLN:HE21	1:A:572:GLN:HB3	1.61	0.42
1:B:103:GLU:OE1	1:B:132:ALA:HB3	2.19	0.42
1:B:82:ILE:HG22	1:B:107:GLY:O	2.19	0.42
1:B:320:ILE:CG2	1:B:321:SER:N	2.82	0.42
1:B:438:VAL:HG12	1:B:439:MET:N	2.34	0.42
1:A:540:GLY:C	6:A:2159:HOH:O	2.57	0.42
1:A:353:ASN:HB2	1:A:355:GLN:HG2	2.01	0.42
1:B:430:THR:HB	1:B:442:LEU:HD11	2.02	0.42
1:B:519:ARG:HD3	1:B:589:HIS:CE1	2.55	0.42
1:A:135:THR:CG2	1:A:136:GLN:OE1	2.68	0.42
1:B:244:TYR:CE2	1:B:248:ILE:HD13	2.54	0.42
1:B:462:SER:HA	1:B:465:ILE:HG12	2.02	0.42
1:B:521:SER:HB2	5:B:1719:GOL:C1	2.48	0.41
1:A:136:GLN:NE2	1:A:247:GLY:HA3	2.35	0.41
1:A:708:LEU:HA	1:A:711:TRP:CE2	2.56	0.41
1:A:67:SER:HB3	1:A:70:THR:CB	2.50	0.41
1:B:630:ALA:HB1	1:B:645:ILE:HD13	2.03	0.41
1:B:28:VAL:O	1:B:32:VAL:HG23	2.20	0.41
4:A:1724:HSC:H7A	6:A:2024:HOH:O	2.19	0.41
1:A:129:LEU:HD12	1:A:129:LEU:C	2.41	0.41
1:A:317:ARG:HG3	1:A:318:VAL:HG13	2.03	0.41
1:B:135:THR:CG2	1:B:251:GLU:OE1	2.68	0.41
1:B:52:GLY:HA3	1:B:56:ASN:O	2.20	0.41
1:A:242:HIS:HB3	1:A:246:VAL:HB	2.02	0.40
1:B:328:ASP:OD1	1:B:330:LYS:HB2	2.21	0.40
1:B:15:ARG:HG3	1:B:51:CYS:SG	2.61	0.40
1:B:244:TYR:O	1:B:248:ILE:HB	2.20	0.40
1:B:483:MET:CE	1:B:630:ALA:HB2	2.52	0.40
1:A:387:LEU:O	1:A:391:VAL:HG23	2.21	0.40
1:B:592:ASP:HA	1:B:593:PRO:HD3	1.91	0.40
1:B:479:VAL:HG22	1:B:633:ILE:HG21	2.03	0.40
1:A:415:ASP:OD1	1:A:448:ARG:HB2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	723/742 (97%)	691 (96%)	29 (4%)	3 (0%)	34	42
1	B	717/742 (97%)	679 (95%)	35 (5%)	3 (0%)	34	42
All	All	1440/1484 (97%)	1370 (95%)	64 (4%)	6 (0%)	34	42

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-1	SER
1	B	448	ARG
1	B	536	GLN
1	A	73	LEU
1	A	70	THR
1	B	283	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	594/609 (98%)	553 (93%)	41 (7%)	15	20
1	B	590/609 (97%)	551 (93%)	39 (7%)	16	22
All	All	1184/1218 (97%)	1104 (93%)	80 (7%)	16	21

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	SER
1	A	63	ILE
1	A	73	LEU
1	A	77	SER
1	A	96	VAL
1	A	125	THR
1	A	135	THR
1	A	157	LEU
1	A	161	GLU
1	A	165	LEU
1	A	172	VAL
1	A	188	ILE
1	A	210	SER
1	A	219	VAL
1	A	226	VAL
1	A	234	ARG
1	A	248	ILE
1	A	258	LEU
1	A	283	PRO
1	A	331	GLN
1	A	333	ASP
1	A	359	LYS
1	A	362	LEU
1	A	366	SER
1	A	368	THR
1	A	371	LEU
1	A	372	SER
1	A	398	LEU
1	A	410	SER
1	A	438	VAL
1	A	441	LEU
1	A	521	SER
1	A	523	LEU
1	A	572	GLN
1	A	585	LEU
1	A	596	SER
1	A	610	GLN
1	A	675	LEU
1	A	676	GLU
1	A	695	ASP
1	A	699	ARG
1	B	24	VAL
1	B	96	VAL

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Mol	Chain	Res	Type
1	B	125	THR
1	B	135	THR
1	B	157	LEU
1	B	161	GLU
1	B	165	LEU
1	B	185	GLN
1	B	188	ILE
1	B	204	SER
1	B	210	SER
1	B	219	VAL
1	B	226	VAL
1	B	248	ILE
1	B	258	LEU
1	B	276	SER
1	B	278	ASN
1	B	282	THR
1	B	333	ASP
1	B	362	LEU
1	B	366	SER
1	B	368	THR
1	B	371	LEU
1	B	398	LEU
1	B	438	VAL
1	B	452	PRO
1	B	521	SER
1	B	523	LEU
1	B	543	LEU
1	B	549	VAL
1	B	550	ARG
1	B	572	GLN
1	B	585	LEU
1	B	596	SER
1	B	599	LEU
1	B	610	GLN
1	B	672	PRO
1	B	676	GLU
1	B	695	ASP

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	294	GLN

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Mol	Chain	Res	Type
1	A	352	GLN
1	A	572	GLN
1	A	589	HIS
1	A	679	GLN
1	B	294	GLN
1	B	331	GLN
1	B	353	ASN
1	B	572	GLN
1	B	589	HIS
1	B	679	GLN
1	B	718	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAD	A	1721	-	42,48,48	1.92	5 (11%)	50,73,73	1.41	6 (12%)
3	SO4	A	1722	-	4,4,4	0.53	0	6,6,6	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	HSC	A	1724	-	53,62,62	1.41	6 (11%)	65,89,89	1.96	13 (20%)
4	HSC	B	1722	-	53,62,62	1.24	5 (9%)	65,89,89	1.63	9 (13%)
3	SO4	A	1723	-	4,4,4	0.22	0	6,6,6	0.28	0
2	NAD	B	1720	-	42,48,48	1.91	5 (11%)	50,73,73	1.37	7 (14%)
5	GOL	B	1719	-	5,5,5	0.20	0	5,5,5	1.26	1 (20%)
3	SO4	B	1721	-	4,4,4	0.22	0	6,6,6	0.84	0

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
4	HSC	A	1724	-	-	22/58/78/78	0/3/3/3
5	GOL	B	1719	-	-	2/4/4/4	-
2	NAD	A	1721	-	-	7/26/62/62	0/5/5/5
2	NAD	B	1720	-	-	7/26/62/62	0/5/5/5
4	HSC	B	1722	-	-	24/58/78/78	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1720	NAD	O7N-C7N	9.37	1.42	1.24
2	A	1721	NAD	O7N-C7N	9.36	1.42	1.24
4	A	1724	HSC	P3B-O8A	5.34	1.67	1.50
4	A	1724	HSC	O4B-C1B	4.48	1.47	1.41
2	A	1721	NAD	C2A-N3A	4.18	1.38	1.32
4	B	1722	HSC	O4B-C1B	3.96	1.46	1.41
2	B	1720	NAD	C2A-N3A	3.84	1.38	1.32
4	B	1722	HSC	P3B-O8A	3.66	1.62	1.50
4	B	1722	HSC	P3B-O3B	3.54	1.66	1.59
2	A	1721	NAD	C2N-N1N	3.50	1.39	1.35
2	B	1720	NAD	C2N-N1N	3.18	1.38	1.35
2	B	1720	NAD	C2A-N1A	2.78	1.39	1.33
2	A	1721	NAD	O4B-C1B	2.63	1.44	1.41
2	A	1721	NAD	C2A-N1A	2.43	1.38	1.33
4	A	1724	HSC	O1-C1	2.40	1.24	1.21
4	A	1724	HSC	P3B-O7A	2.39	1.64	1.54
4	B	1722	HSC	P3B-O7A	2.24	1.63	1.54
4	A	1724	HSC	C1-S1P	2.13	1.81	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1722	HSC	OAP-CAP	2.03	1.46	1.42
4	A	1724	HSC	OAP-CAP	2.02	1.46	1.42
2	B	1720	NAD	PA-O2A	-2.00	1.45	1.55

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1724	HSC	C3-C2-C1	7.42	130.82	113.89
4	A	1724	HSC	O1-C1-S1P	-6.43	114.26	122.61
4	B	1722	HSC	O1-C1-S1P	-6.12	114.67	122.61
2	A	1721	NAD	N3A-C2A-N1A	-5.71	119.76	128.68
2	B	1720	NAD	N3A-C2A-N1A	-5.43	120.19	128.68
4	A	1724	HSC	N3A-C2A-N1A	-5.26	120.46	128.68
4	B	1722	HSC	C2-C1-S1P	4.55	119.26	113.63
4	B	1722	HSC	N3A-C2A-N1A	-4.40	121.79	128.68
4	B	1722	HSC	C3-C2-C1	4.05	123.14	113.89
4	A	1724	HSC	O3-C3-C2	3.65	119.35	109.65
4	A	1724	HSC	O4B-C1B-C2B	-3.60	101.67	106.93
2	B	1720	NAD	PN-O3-PA	-3.23	121.75	132.83
4	A	1724	HSC	O6A-CCP-CBP	3.10	115.54	110.55
4	A	1724	HSC	C2-C1-S1P	3.01	117.36	113.63
4	B	1722	HSC	CEP-CBP-CCP	2.82	112.83	108.23
4	A	1724	HSC	C2P-C3P-N4P	2.79	118.29	112.42
5	B	1719	GOL	C3-C2-C1	-2.70	101.21	111.70
4	A	1724	HSC	C6P-C7P-N8P	-2.60	106.64	111.90
4	B	1722	HSC	CDP-CBP-CCP	-2.54	104.09	108.23
4	A	1724	HSC	C7P-C6P-C5P	-2.49	108.22	112.36
4	B	1722	HSC	O3-C3-C4	-2.47	102.15	109.21
4	B	1722	HSC	O6A-CCP-CBP	2.47	114.52	110.55
2	A	1721	NAD	PN-O3-PA	-2.43	124.48	132.83
2	B	1720	NAD	O3D-C3D-C4D	-2.37	104.20	111.05
4	A	1724	HSC	C2A-N1A-C6A	2.36	122.79	118.75
4	B	1722	HSC	CDP-CBP-CAP	2.34	112.88	108.82
4	A	1724	HSC	CDP-CBP-CCP	-2.31	104.47	108.23
2	B	1720	NAD	C6N-N1N-C2N	-2.26	119.91	121.97
2	A	1721	NAD	O4B-C1B-C2B	-2.18	103.75	106.93
2	B	1720	NAD	O4D-C1D-C2D	-2.17	103.75	106.93
4	A	1724	HSC	C6-C5-C4	-2.15	106.01	113.62
2	A	1721	NAD	O5B-PA-O1A	2.14	117.43	109.07
2	B	1720	NAD	O4B-C1B-C2B	-2.11	103.85	106.93
2	B	1720	NAD	C1B-N9A-C4A	-2.10	122.94	126.64
2	A	1721	NAD	O5B-C5B-C4B	-2.05	101.94	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1721	NAD	O2N-PN-O1N	2.03	122.28	112.24

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1721	NAD	O4D-C1D-N1N-C2N
2	A	1721	NAD	O4D-C1D-N1N-C6N
2	A	1721	NAD	C2D-C1D-N1N-C2N
2	A	1721	NAD	C2D-C1D-N1N-C6N
4	A	1724	HSC	C1-C2-C3-O3
4	A	1724	HSC	C1-C2-C3-C4
4	A	1724	HSC	C5B-O5B-P1A-O1A
4	A	1724	HSC	C5B-O5B-P1A-O2A
4	A	1724	HSC	C3P-C2P-S1P-C1
4	A	1724	HSC	CCP-O6A-P2A-O4A
4	A	1724	HSC	CAP-CBP-CCP-O6A
4	B	1722	HSC	C1-C2-C3-O3
4	B	1722	HSC	C5B-O5B-P1A-O3A
4	B	1722	HSC	CBP-CCP-O6A-P2A
4	B	1722	HSC	N8P-C9P-CAP-OAP
4	B	1722	HSC	C9P-CAP-CBP-CCP
4	B	1722	HSC	C9P-CAP-CBP-CDP
4	B	1722	HSC	C9P-CAP-CBP-CEP
4	B	1722	HSC	OAP-CAP-CBP-CCP
4	B	1722	HSC	OAP-CAP-CBP-CEP
4	B	1722	HSC	CAP-CBP-CCP-O6A
4	B	1722	HSC	CDP-CBP-CCP-O6A
2	B	1720	NAD	O4D-C1D-N1N-C2N
2	B	1720	NAD	O4D-C1D-N1N-C6N
2	B	1720	NAD	C2D-C1D-N1N-C2N
2	B	1720	NAD	C2D-C1D-N1N-C6N
5	B	1719	GOL	C1-C2-C3-O3
4	A	1724	HSC	C6-C7-C8-C9
4	A	1724	HSC	CDP-CBP-CCP-O6A
4	A	1724	HSC	CEP-CBP-CCP-O6A
4	B	1722	HSC	CEP-CBP-CCP-O6A
4	B	1722	HSC	C4-C5-C6-C7
5	B	1719	GOL	O2-C2-C3-O3
4	B	1722	HSC	C5-C6-C7-C8
4	A	1724	HSC	C5-C6-C7-C8
4	B	1722	HSC	O9P-C9P-CAP-OAP

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Mol	Chain	Res	Type	Atoms
4	B	1722	HSC	OAP-CAP-CBP-CDP
4	B	1722	HSC	P1A-O3A-P2A-O4A
4	A	1724	HSC	O4B-C4B-C5B-O5B
4	A	1724	HSC	O1-C1-S1P-C2P
4	A	1724	HSC	P2A-O3A-P1A-O5B
4	A	1724	HSC	C2-C1-S1P-C2P
2	A	1721	NAD	C5D-O5D-PN-O3
4	A	1724	HSC	CCP-O6A-P2A-O3A
2	B	1720	NAD	C5D-O5D-PN-O3
4	A	1724	HSC	C7-C8-C9-C10
4	A	1724	HSC	CCP-O6A-P2A-O5A
4	B	1722	HSC	C1-C2-C3-C4
4	B	1722	HSC	C5B-O5B-P1A-O1A
4	B	1722	HSC	S1P-C2P-C3P-N4P
2	B	1720	NAD	O4B-C4B-C5B-O5B
4	B	1722	HSC	P1A-O3A-P2A-O5A
4	B	1722	HSC	C4B-C5B-O5B-P1A
4	B	1722	HSC	C3-C4-C5-C6
2	A	1721	NAD	O4B-C4B-C5B-O5B
4	B	1722	HSC	C3P-C2P-S1P-C1
4	A	1724	HSC	C3-C4-C5-C6
4	A	1724	HSC	C3B-C4B-C5B-O5B
4	A	1724	HSC	C5B-O5B-P1A-O3A
2	B	1720	NAD	PA-O3-PN-O1N
4	A	1724	HSC	CBP-CCP-O6A-P2A
2	A	1721	NAD	C5B-O5B-PA-O1A

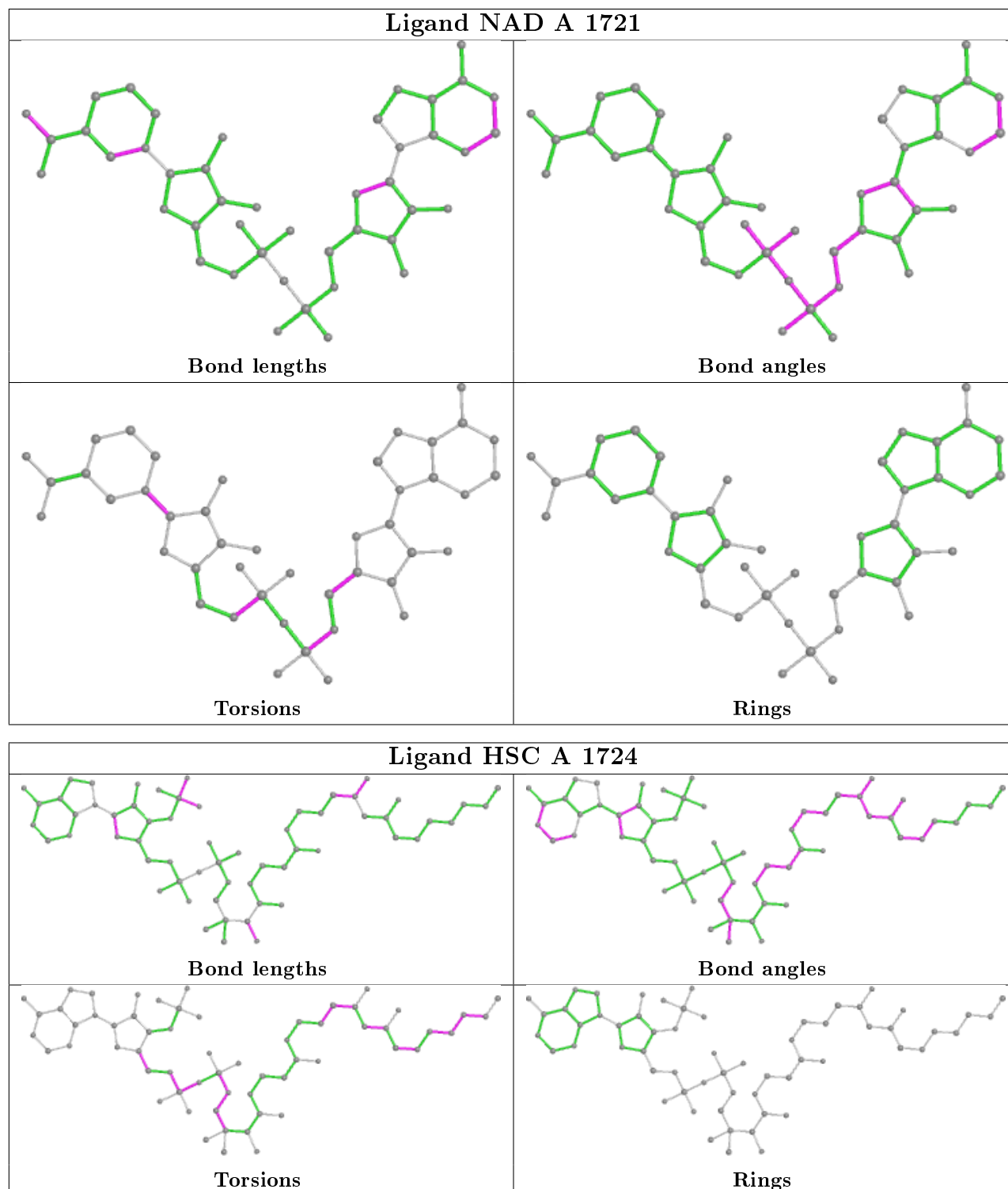
There are no ring outliers.

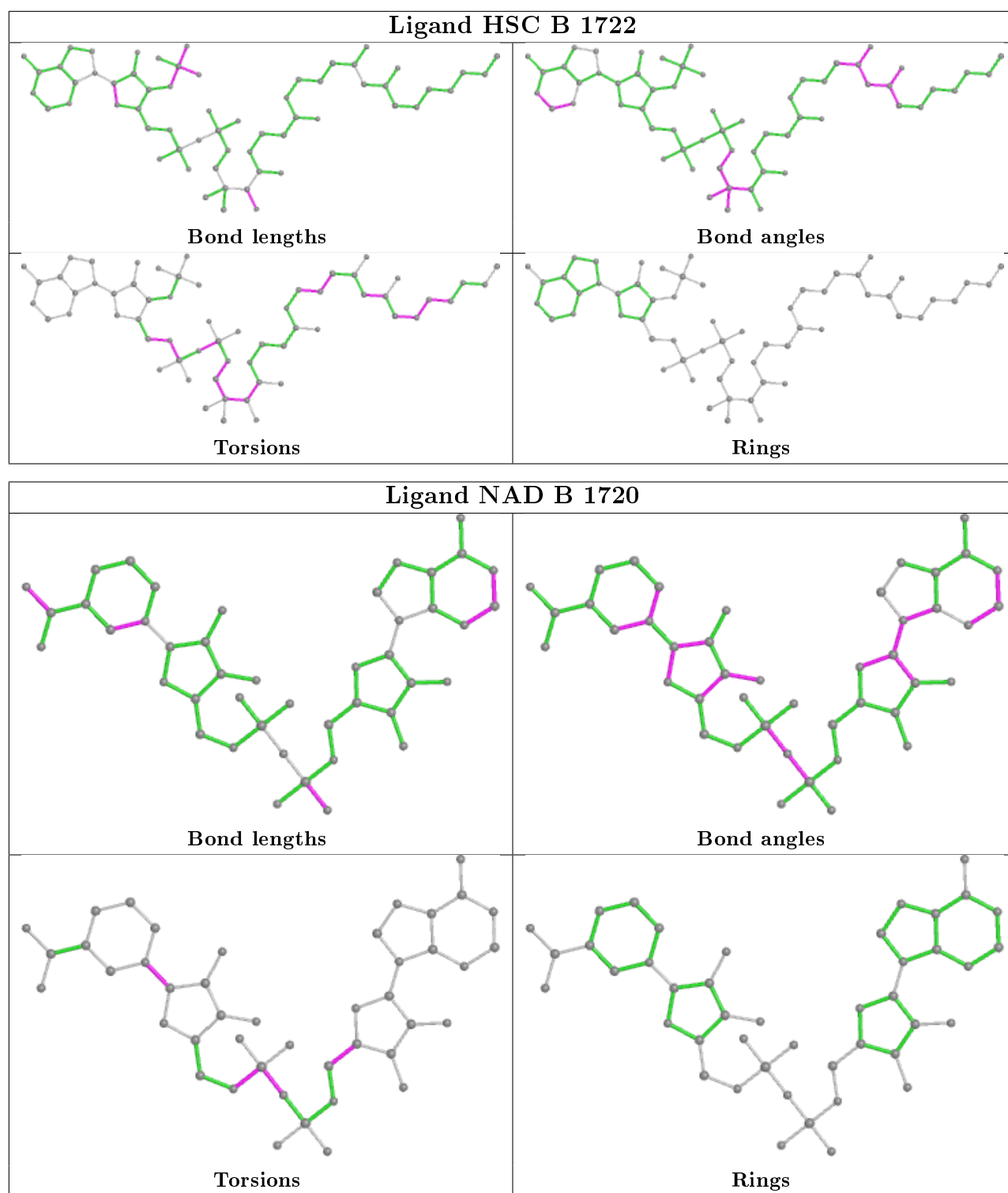
5 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1721	NAD	4	0
4	A	1724	HSC	9	0
4	B	1722	HSC	8	0
5	B	1719	GOL	4	0
3	B	1721	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	725/742 (97%)	0.28	39 (5%) 25 32	9, 31, 62, 99	0
1	B	719/742 (96%)	0.16	55 (7%) 13 18	10, 32, 62, 96	0
All	All	1444/1484 (97%)	0.22	94 (6%) 18 24	9, 32, 62, 99	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	356	ALA	7.6
1	A	350	ALA	6.7
1	A	354	GLY	5.7
1	A	351	HIS	5.6
1	A	352	GLN	5.5
1	B	43	HIS	5.0
1	B	354	GLY	4.8
1	A	357	SER	4.7
1	A	69	PHE	4.7
1	B	0	HIS	4.7
1	B	358	ALA	4.6
1	B	178	GLU	4.5
1	B	45	VAL	4.5
1	B	449	TYR	4.5
1	A	348	SER	4.4
1	B	718	HIS	4.4
1	B	185	GLN	4.4
1	B	5	LEU	4.3
1	B	8	PRO	4.2
1	A	341	PHE	4.1
1	B	44	THR	4.1
1	B	541	PRO	4.1
1	A	70	THR	4.1
1	B	356	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	4	TYR	3.9
1	B	608	ILE	3.8
1	B	180	ALA	3.7
1	B	535	GLY	3.7
1	B	545	PRO	3.7
1	A	355	GLN	3.5
1	A	347	ALA	3.5
1	A	364	PHE	3.5
1	B	207	ASN	3.4
1	B	553	GLY	3.4
1	B	40	GLY	3.3
1	A	349	ARG	3.3
1	A	359	LYS	3.3
1	B	351	HIS	3.3
1	B	171	VAL	3.3
1	A	338	ILE	3.2
1	A	337	LYS	3.1
1	A	345	LYS	3.1
1	B	10	SER	3.1
1	A	-2	GLY	3.1
1	B	609	GLU	3.1
1	A	398	LEU	3.0
1	B	13	MET	2.9
1	A	342	THR	2.9
1	A	360	PRO	2.9
1	A	362	LEU	2.9
1	A	353	ASN	2.9
1	A	425	GLN	2.9
1	B	601	GLN	2.9
1	B	7	LEU	2.8
1	B	6	ARG	2.8
1	B	554	ASN	2.8
1	B	206	PRO	2.7
1	B	9	HIS	2.7
1	A	358	ALA	2.6
1	B	188	ILE	2.6
1	B	12	ALA	2.6
1	A	346	GLU	2.5
1	A	369	LYS	2.5
1	B	221	LYS	2.5
1	B	181	ILE	2.5
1	B	546	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	397	ALA	2.4
1	B	1	MET	2.3
1	A	386	ASN	2.3
1	A	-3	ARG	2.3
1	B	213	ALA	2.3
1	B	189	ASP	2.2
1	A	449	TYR	2.2
1	A	401	PRO	2.2
1	B	182	LYS	2.2
1	B	607	HIS	2.2
1	A	324	ALA	2.2
1	B	11	LEU	2.2
1	B	348	SER	2.2
1	B	355	GLN	2.2
1	B	210	SER	2.1
1	B	548	PRO	2.1
1	A	343	LEU	2.1
1	A	422	ASP	2.1
1	A	340	THR	2.1
1	B	357	SER	2.1
1	B	46	LYS	2.0
1	B	359	LYS	2.0
1	A	373	THR	2.0
1	B	47	ALA	2.0
1	A	344	GLU	2.0
1	B	41	SER	2.0
1	B	289	LYS	2.0
1	B	587	ARG	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 carbohydrates in this entry.

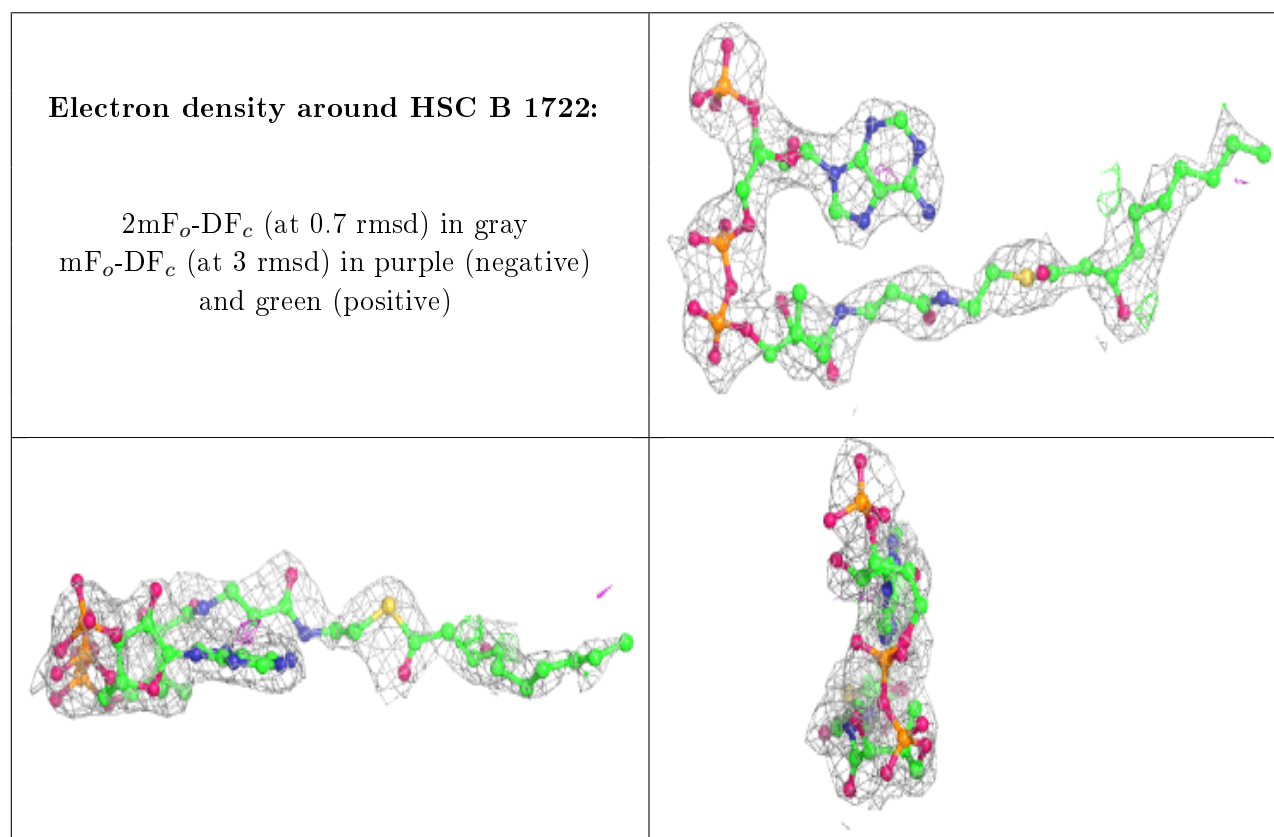
## 6.4 Ligands [i](#)

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( $\text{\AA}^2$ )	Q<0.9
3	SO4	B	1721	5/5	0.81	0.19	69,70,74,75	0
4	HSC	B	1722	60/60	0.84	0.19	56,76,83,83	0
3	SO4	A	1723	5/5	0.84	0.24	79,82,82,84	0
4	HSC	A	1724	60/60	0.84	0.18	24,62,79,81	0
5	GOL	B	1719	6/6	0.87	0.18	43,47,48,50	0
2	NAD	A	1721	44/44	0.91	0.14	33,42,49,52	0
2	NAD	B	1720	44/44	0.97	0.10	24,33,41,42	0
3	SO4	A	1722	5/5	0.98	0.09	27,31,32,35	0

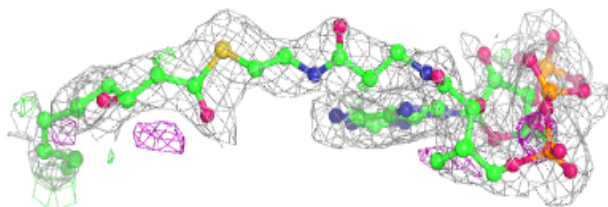
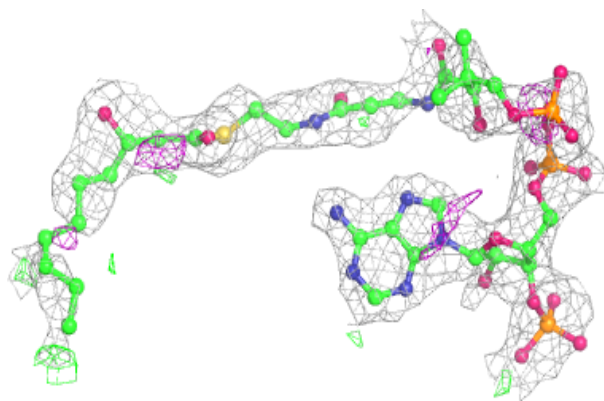
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



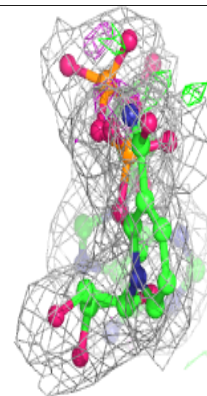
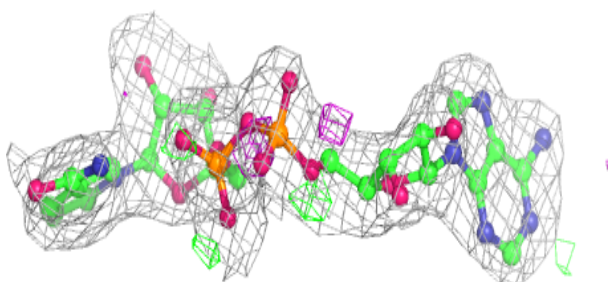
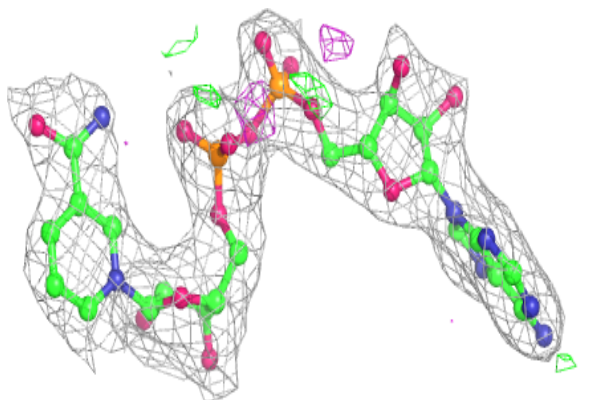


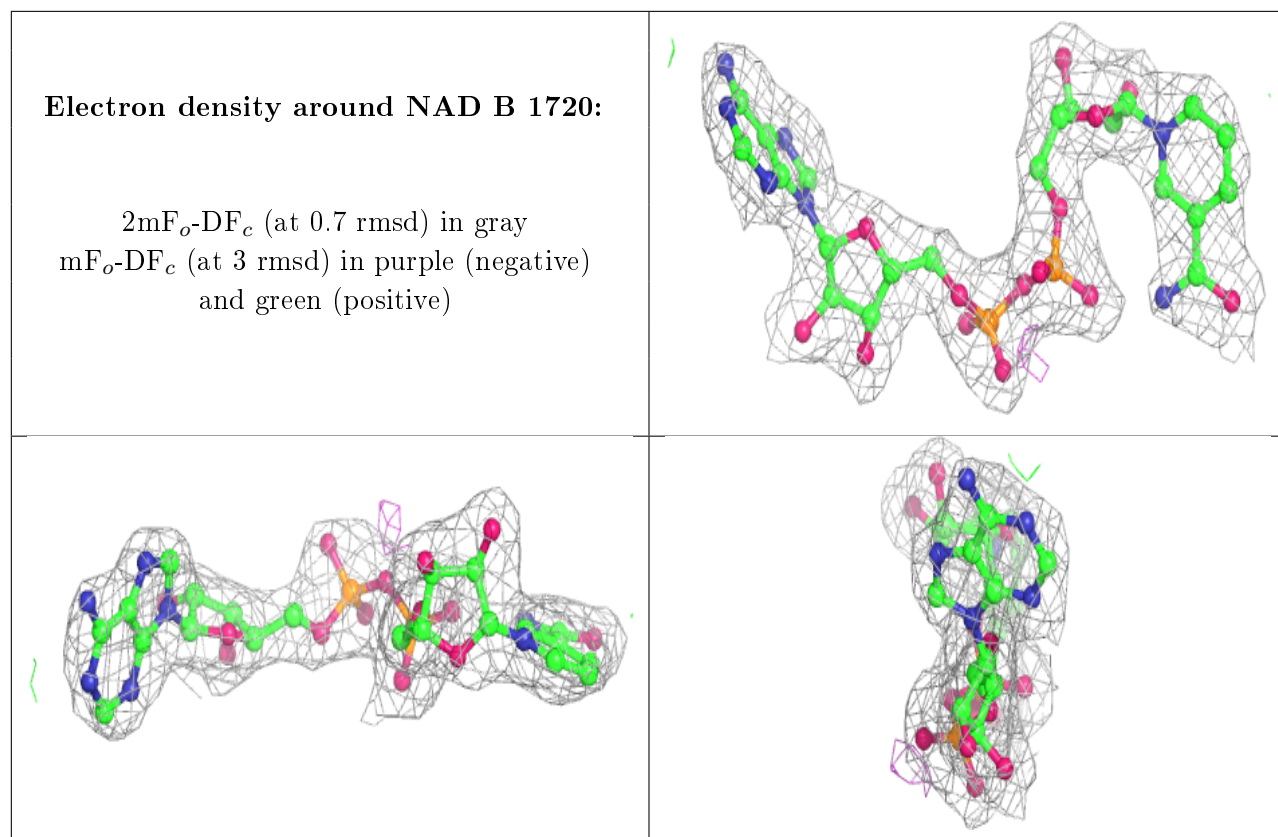
**Electron density around HSC A 1724:**

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

**Electron density around NAD A 1721:**

$2mF_o-DF_c$  (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.