



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:06 PM UTC

PDB ID : 3ZWC / pdb_00003zwc
Title : CRYSTAL STRUCTURE OF RAT PEROXISOMAL MULTIFUNCTIONAL ENZYME TYPE 1 (RPMFE1) COMPLEXED WITH 3S-HYDROXY-DECA NOYL-COA
Authors : Kasaragod, P.; Schmitz, W.; Hiltunen, J.K.; Wierenga, R.K.
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

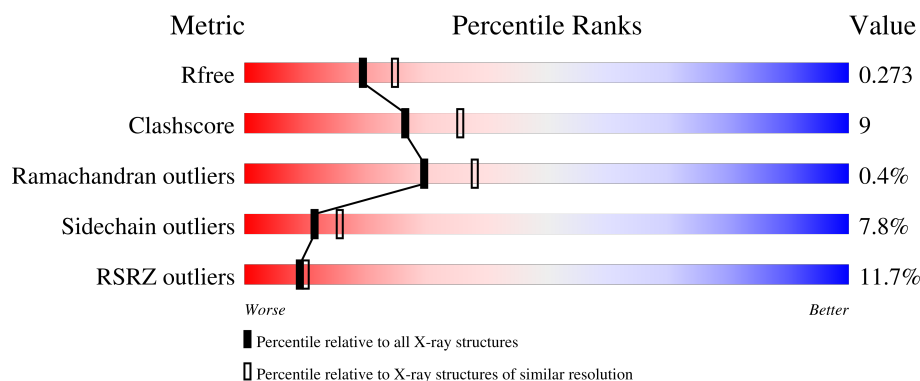
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	742	 12% 78% 17% . .
1	B	742	 11% 73% 21% . .

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:

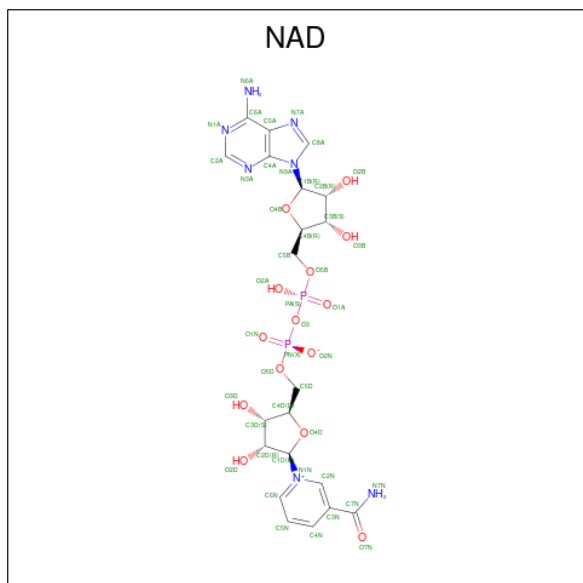
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P07896
A	-18	GLY	-	expression tag	UNP P07896
A	-17	SER	-	expression tag	UNP P07896
A	-16	SER	-	expression tag	UNP P07896
A	-15	HIS	-	expression tag	UNP P07896
A	-14	HIS	-	expression tag	UNP P07896
A	-13	HIS	-	expression tag	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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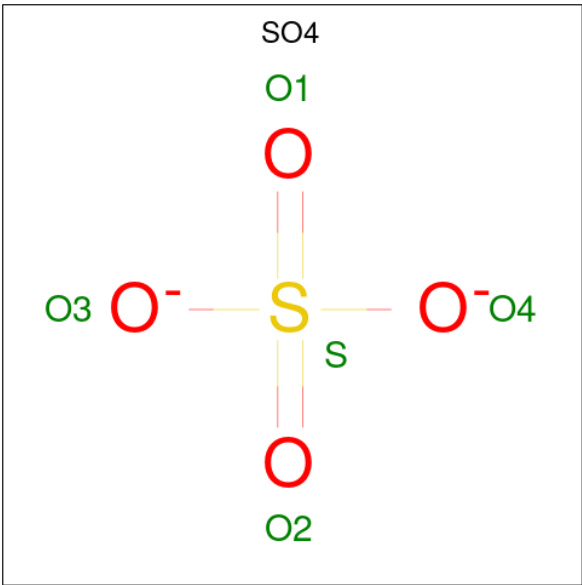
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP P07896
B	-13	HIS	-	expression tag	UNP P07896
B	-12	HIS	-	expression tag	UNP P07896
B	-11	HIS	-	expression tag	UNP P07896
B	-10	HIS	-	expression tag	UNP P07896
B	-9	SER	-	expression tag	UNP P07896
B	-8	SER	-	expression tag	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

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



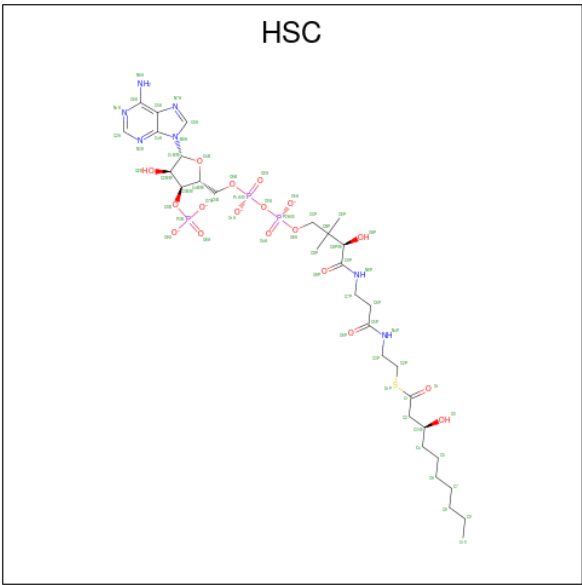
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	B	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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 (CCD ID: HSC) (formula: C₃₁H₅₀N₇O₁₈P₃S).



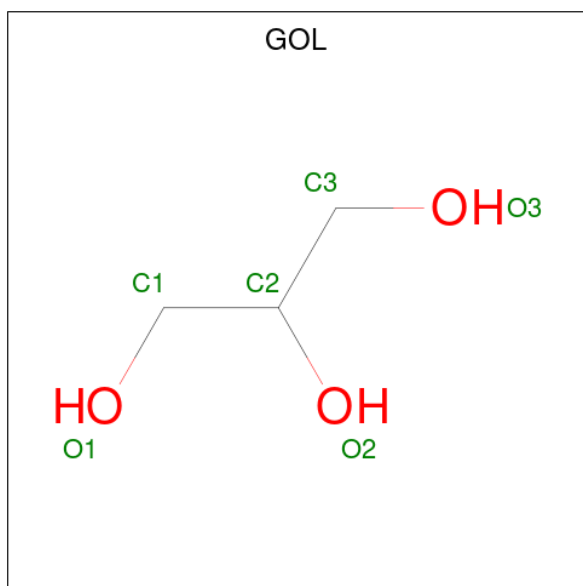
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			60	31	7	18	3	1		

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

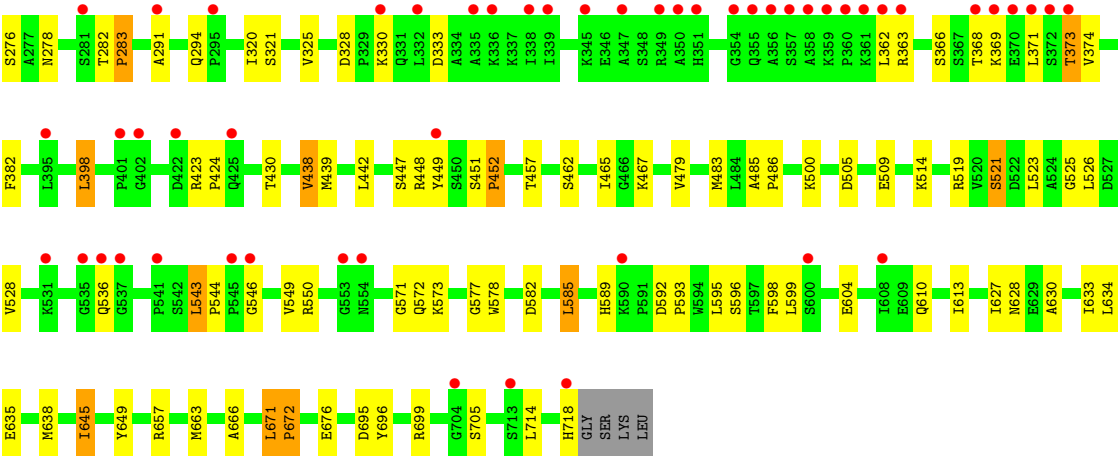
- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.57Å 126.51Å 224.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	112.48 – 2.30 112.47 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (112.48-2.30) 99.6 (112.47-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	30.1	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, HSC, GOL, SO4

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	1.15	7/5691 (0.1%)	1.12	16/7709 (0.2%)
1	B	1.16	8/5652 (0.1%)	1.18	21/7658 (0.3%)
All	All	1.16	15/11343 (0.1%)	1.15	37/15367 (0.2%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	705	SER	C-O	-10.00	1.19	1.23
1	A	485	ALA	CA-CB	7.26	1.63	1.53
1	B	645	ILE	CA-CB	-6.66	1.46	1.54
1	A	701	VAL	CA-C	5.93	1.60	1.52
1	B	666	ALA	N-CA	5.90	1.53	1.46
1	A	143	GLY	C-O	5.63	1.30	1.23
1	B	228	ALA	CA-CB	-5.48	1.46	1.53
1	B	226	VAL	CA-CB	5.28	1.60	1.54
1	B	627	ILE	CA-CB	5.12	1.61	1.54
1	A	132	ALA	N-CA	-5.08	1.39	1.46
1	B	628	ASN	N-CA	5.07	1.52	1.46
1	B	135	THR	CA-C	5.07	1.59	1.52
1	A	509	GLU	C-O	-5.05	1.18	1.24
1	B	109	HIS	N-CA	5.03	1.52	1.46
1	A	719	GLY	N-CA	5.00	1.48	1.44

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	649	TYR	CA-CB-CG	-7.55	100.30	113.90
1	A	226	VAL	CB-CA-C	7.49	120.02	110.96
1	A	24	VAL	CB-CA-C	7.23	119.71	110.96
1	A	248	ILE	CA-CB-CG2	7.15	122.66	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	373	THR	N-CA-C	6.55	118.30	111.03
1	B	226	VAL	N-CA-C	6.55	118.25	108.23
1	B	232	CYS	N-CA-C	-6.51	104.27	111.82
1	A	657	ARG	NE-CZ-NH2	6.50	125.05	119.20
1	B	93	ILE	N-CA-C	6.33	116.73	107.37
1	B	578	TRP	N-CA-C	-6.33	103.91	111.69
1	B	136	GLN	N-CA-C	-6.30	105.25	113.12
1	A	-2	GLY	N-CA-C	6.30	128.10	113.18
1	A	325	VAL	N-CA-C	6.18	116.77	107.75
1	B	671	LEU	CA-C-N	-6.14	112.53	119.28
1	B	671	LEU	C-N-CA	-6.14	112.53	119.28
1	B	96	VAL	CB-CA-C	6.08	119.64	110.63
1	B	325	VAL	N-CA-C	6.07	116.61	108.11
1	B	193	GLU	CA-C-N	-6.02	113.44	120.12
1	B	193	GLU	C-N-CA	-6.02	113.44	120.12
1	A	76	GLY	N-CA-C	-5.98	105.55	112.73
1	A	73	LEU	N-CA-C	5.97	123.52	110.80
1	A	227	LEU	N-CA-C	5.85	117.33	111.07
1	B	634	LEU	N-CA-C	-5.77	104.44	112.45
1	B	699	ARG	N-CA-C	5.75	117.55	111.28
1	B	244	TYR	N-CA-C	5.61	117.84	111.11
1	A	578	TRP	N-CA-C	-5.50	104.92	111.69
1	B	138	LEU	CA-C-N	-5.43	114.02	119.56
1	B	138	LEU	C-N-CA	-5.43	114.02	119.56
1	B	374	VAL	N-CA-C	5.36	117.18	109.51
1	B	60	GLY	N-CA-C	-5.36	105.47	111.63
1	A	649	TYR	CA-CB-CG	-5.33	104.30	113.90
1	A	375	ASP	N-CA-C	5.28	117.79	111.71
1	A	657	ARG	NE-CZ-NH1	-5.28	116.22	121.50
1	B	153	SER	N-CA-C	-5.14	107.56	113.88
1	A	72	GLY	N-CA-C	5.12	125.31	113.18
1	A	75	LEU	CA-C-N	5.08	125.62	119.98
1	A	75	LEU	C-N-CA	5.08	125.62	119.98

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	104	0
1	B	5524	0	5631	108	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	211	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 (211) 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:500:LYS:HD3	6:A:2180:HOH:O	1.54	1.04
1:A:73:LEU:HD21	1:A:256:MET:HE2	1.34	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:O1	5:B:1719:GOL:O3	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
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:A:73:LEU:CD2	1:A:256:MET:HE2	2.10	0.82
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:A:73:LEU:HD22	1:A:256:MET:HE1	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:72:GLY:C	4:A:1724:HSC:H8	2.17	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:67:SER:H	1:A:71:PRO:HD3	1.56	0.69
1:A:679:GLN:HG2	6:A:2219:HOH:O	1.91	0.69
1:B:37:GLN:HB3	6:B:2006:HOH:O	1.93	0.69
1:B:505:ASP:O	1:B:509:GLU:HG3	1.92	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:B:133:ARG:HD2	1:B:248:ILE:CG1	2.25	0.67
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
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:B:663:MET:HA	1:B:663:MET:HE2	1.83	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:73:LEU:CD2	1:A:256:MET:HE1	2.30	0.56
1:A:411:ALA:HB1	1:A:476:TYR:CE1	2.41	0.55
1:A:73:LEU:HD22	1:A:256:MET:CE	2.31	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:451:SER:O	1:B:452:PRO:C	2.51	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:CD1	1:B:156:TYR:N	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:N	1:A:156:TYR:CD1	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:A:663:MET:HA	1:A:663:MET:HE2	1.91	0.51
1:A:535:GLY:C	1:A:537:GLY:H	2.19	0.51
1:B:46:LYS:HB2	1:B:188:ILE:HD11	1.91	0.51
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:B:187:ILE:C	1:B:187:ILE:HD12	2.36	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:187:ILE:C	1:A:187:ILE:HD12	2.38	0.49
1:B:13:MET:HA	1:B:49:VAL:O	2.13	0.49
1:B:111:ARG:N	1:B:169:ASP:OD2	2.40	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: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
1:A:540:GLY:C	6:A:2159:HOH:O	2.57	0.47
4:B:1722:HSC:HEP	6:B:2007:HOH:O	2.14	0.47
1:B:2:ALA:HB3	1:B:31:GLU:HB3	1.97	0.46
1:B:226:VAL:HG22	1:B:229:PRO:HD2	1.98	0.46
1:A:382:PHE:CZ	2:A:1721:NAD:H2B	2.50	0.46
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:156:TYR:N	1:A:156:TYR:HD1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LEU:C	1:A:129:LEU:HD12	2.41	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: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:A:135:THR:HG21	1:A:235:SER:HG	1.75	0.45
1:A:626:LEU:HD23	1:A:626:LEU:C	2.42	0.44
1:B:521:SER:CB	5:B:1719:GOL:H12	2.45	0.44
1:B:423:ARG:O	1:B:424:PRO:C	2.60	0.44
1:B:483:MET:HE3	1:B:630:ALA:HB2	2.00	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: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
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:353:ASN:HB2	1:A:355:GLN:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:447:SER:C	1:B:449:TYR:H	2.28	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:42:ASP:OD1	1:B:44:THR:OG1	2.31	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:447:SER:C	1:B:449:TYR:N	2.79	0.40
1:B:479:VAL:HG22	1:B:633:ILE:HG21	2.03	0.40
1:B:592:ASP:HA	1:B:593:PRO:HD3	1.91	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%)	30	38
1	B	717/742 (97%)	679 (95%)	35 (5%)	3 (0%)	30	38
All	All	1440/1484 (97%)	1370 (95%)	64 (4%)	6 (0%)	30	38

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%)	548 (92%)	46 (8%)	12	16
1	B	590/609 (97%)	544 (92%)	46 (8%)	11	16
All	All	1184/1218 (97%)	1092 (92%)	92 (8%)	11	16

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	SER
1	A	7	LEU
1	A	24	VAL
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

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Mol	Chain	Res	Type
1	A	161	GLU
1	A	165	LEU
1	A	172	VAL
1	A	185	GLN
1	A	188	ILE
1	A	210	SER
1	A	219	VAL
1	A	226	VAL
1	A	234	ARG
1	A	245	GLU
1	A	248	ILE
1	A	258	LEU
1	A	283	PRO
1	A	333	ASP
1	A	355	GLN
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	526	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	5	LEU
1	B	7	LEU
1	B	24	VAL
1	B	31	GLU
1	B	96	VAL
1	B	125	THR

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Mol	Chain	Res	Type
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	245	GLU
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	500	LYS
1	B	521	SER
1	B	523	LEU
1	B	526	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	613	ILE
1	B	672	PRO
1	B	676	GLU
1	B	695	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	242	HIS
1	A	294	GLN
1	A	331	GLN
1	A	352	GLN
1	A	536	GLN
1	A	572	GLN
1	A	589	HIS
1	A	679	GLN
1	B	94	GLN
1	B	242	HIS
1	B	294	GLN
1	B	353	ASN
1	B	536	GLN
1	B	572	GLN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HSC	B	1722	-	60,62,62	1.92	8 (13%)	83,89,89	1.76	16 (19%)
3	SO4	A	1723	-	4,4,4	0.33	0	6,6,6	0.29	0
2	NAD	A	1721	-	46,48,48	2.06	7 (15%)	64,73,73	1.82	16 (25%)
5	GOL	B	1719	-	5,5,5	0.20	0	5,5,5	1.35	1 (20%)
4	HSC	A	1724	-	60,62,62	2.51	11 (18%)	83,89,89	2.05	20 (24%)
3	SO4	A	1722	-	4,4,4	0.62	0	6,6,6	0.61	0
2	NAD	B	1720	-	46,48,48	1.86	5 (10%)	64,73,73	1.78	14 (21%)
3	SO4	B	1721	-	4,4,4	0.33	0	6,6,6	0.74	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
2	NAD	A	1721	-	-	8/30/62/62	0/5/5/5
5	GOL	B	1719	-	-	2/4/4/4	-
4	HSC	A	1724	-	-	22/62/78/78	0/3/3/3
2	NAD	B	1720	-	-	7/30/62/62	0/5/5/5
4	HSC	B	1722	-	-	24/62/78/78	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1724	HSC	P2A-O3A	13.13	1.73	1.59
2	B	1720	NAD	O7N-C7N	9.65	1.42	1.24
2	A	1721	NAD	O7N-C7N	9.64	1.42	1.24
4	B	1722	HSC	P2A-O3A	9.05	1.69	1.59
4	A	1724	HSC	P1A-O3A	7.76	1.67	1.59
4	B	1722	HSC	P1A-O3A	5.89	1.65	1.59
4	A	1724	HSC	C2-C1	5.60	1.62	1.51
4	A	1724	HSC	P3B-O8A	5.56	1.67	1.50
2	A	1721	NAD	PA-O3	5.20	1.65	1.59
4	B	1722	HSC	C2-C1	4.36	1.60	1.51
2	A	1721	NAD	PN-O3	3.87	1.63	1.59
2	A	1721	NAD	C2N-N1N	3.86	1.39	1.35
4	B	1722	HSC	P3B-O8A	3.82	1.62	1.50
4	B	1722	HSC	P3B-O3B	3.69	1.66	1.59
2	B	1720	NAD	C2N-N1N	3.51	1.38	1.35
2	B	1720	NAD	C2A-N1A	2.90	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1724	HSC	C5A-N7A	-2.85	1.33	1.39
2	A	1721	NAD	C2A-N3A	2.76	1.38	1.33
4	B	1722	HSC	C5A-N7A	-2.63	1.34	1.39
2	A	1721	NAD	C2A-N1A	2.53	1.38	1.33
4	A	1724	HSC	O1-C1	2.51	1.24	1.21
4	A	1724	HSC	P3B-O7A	2.49	1.64	1.54
2	B	1720	NAD	C2A-N3A	2.45	1.38	1.33
4	B	1722	HSC	P3B-O7A	2.34	1.63	1.54
4	A	1724	HSC	O4B-C1B	2.30	1.47	1.42
4	A	1724	HSC	C1B-N9A	2.28	1.52	1.46
2	A	1721	NAD	C8A-N7A	2.14	1.35	1.31
4	A	1724	HSC	C1-S1P	2.13	1.81	1.76
4	B	1722	HSC	OAP-CAP	2.11	1.46	1.42
4	A	1724	HSC	OAP-CAP	2.09	1.46	1.42
2	B	1720	NAD	PA-O2A	-2.03	1.45	1.55

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1724	HSC	C3-C2-C1	7.61	130.82	113.86
4	A	1724	HSC	O1-C1-S1P	-6.62	114.26	122.68
4	B	1722	HSC	O1-C1-S1P	-6.30	114.67	122.68
2	A	1721	NAD	N3A-C2A-N1A	-5.83	119.76	128.58
2	B	1720	NAD	N3A-C2A-N1A	-5.55	120.19	128.58
4	A	1724	HSC	N3A-C2A-N1A	-5.37	120.46	128.58
4	A	1724	HSC	C5A-C4A-N3A	-5.17	119.60	126.72
4	B	1722	HSC	C5A-C4A-N3A	-4.92	119.95	126.72
4	B	1722	HSC	C2-C1-S1P	4.52	119.26	113.56
4	B	1722	HSC	N3A-C2A-N1A	-4.48	121.79	128.58
2	B	1720	NAD	N9A-C8A-N7A	-4.37	107.74	113.94
4	B	1722	HSC	C3-C2-C1	4.16	123.14	113.86
2	A	1721	NAD	O3-PN-O1N	-4.15	98.23	110.70
2	A	1721	NAD	C5A-C4A-N3A	-4.10	121.07	126.72
2	B	1720	NAD	C5A-C4A-N3A	-4.04	121.16	126.72
2	A	1721	NAD	N9A-C8A-N7A	-3.99	108.28	113.94
4	B	1722	HSC	N3A-C4A-N9A	3.89	133.78	127.17
2	B	1720	NAD	O2N-PN-O3	3.75	117.41	107.27
4	A	1724	HSC	O3-C3-C2	3.75	119.35	109.64
4	A	1724	HSC	N3A-C4A-N9A	3.74	133.53	127.17
2	B	1720	NAD	C5A-N7A-C8A	3.70	109.26	103.45
4	A	1724	HSC	C2A-N3A-C4A	3.62	120.67	111.83
2	A	1721	NAD	C2A-N3A-C4A	3.47	120.30	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1720	NAD	C2A-N3A-C4A	3.42	120.18	111.83
4	B	1722	HSC	C2A-N3A-C4A	3.40	120.12	111.83
2	B	1720	NAD	C4D-O4D-C1D	3.23	112.89	109.92
4	A	1724	HSC	O6A-CCP-CBP	3.10	115.54	110.55
2	B	1720	NAD	N3A-C4A-N9A	3.07	132.38	127.17
2	A	1721	NAD	N3A-C4A-N9A	3.05	132.36	127.17
4	A	1724	HSC	C2-C1-S1P	3.01	117.36	113.56
4	B	1722	HSC	N9A-C8A-N7A	-2.98	109.71	113.94
2	A	1721	NAD	O2A-PA-O3	2.96	115.27	107.27
4	A	1724	HSC	C5A-N7A-C8A	2.91	108.03	103.45
4	A	1724	HSC	O1-C1-C2	2.90	128.29	123.74
2	A	1721	NAD	C5A-N7A-C8A	2.89	107.99	103.45
5	B	1719	GOL	C3-C2-C1	-2.89	101.21	111.80
4	A	1724	HSC	N9A-C8A-N7A	-2.83	109.92	113.94
4	A	1724	HSC	C2P-C3P-N4P	2.81	118.29	112.41
4	B	1722	HSC	CEP-CBP-CCP	2.79	112.83	108.22
4	A	1724	HSC	C4A-C5A-N7A	-2.77	107.42	110.58
4	B	1722	HSC	O3-C3-C4	-2.70	102.15	109.35
2	B	1720	NAD	O3-PN-O1N	-2.65	102.75	110.70
4	B	1722	HSC	C5A-N7A-C8A	2.64	107.60	103.45
2	B	1720	NAD	C4A-N9A-C8A	2.56	108.43	105.74
2	A	1721	NAD	C4A-N9A-C8A	2.55	108.42	105.74
4	B	1722	HSC	C4A-N9A-C8A	2.55	108.41	105.74
4	A	1724	HSC	C6P-C7P-N8P	-2.52	106.64	112.00
4	A	1724	HSC	C7P-C6P-C5P	-2.51	108.22	112.39
4	B	1722	HSC	CDP-CBP-CCP	-2.50	104.09	108.22
2	B	1720	NAD	C2B-C1B-N9A	2.47	119.45	113.30
4	A	1724	HSC	C2A-N1A-C6A	2.47	122.79	118.73
4	B	1722	HSC	O6A-CCP-CBP	2.47	114.52	110.55
4	B	1722	HSC	CDP-CBP-CAP	2.41	112.88	108.77
2	A	1721	NAD	O4B-C1B-N9A	2.40	112.69	108.09
2	B	1720	NAD	O3D-C3D-C4D	-2.39	104.20	111.08
4	A	1724	HSC	O4B-C1B-C2B	-2.31	101.67	106.62
2	B	1720	NAD	C6N-N1N-C2N	-2.31	119.91	121.88
4	A	1724	HSC	CDP-CBP-CCP	-2.28	104.47	108.22
2	A	1721	NAD	O3-PA-O1A	-2.25	103.95	110.70
4	B	1722	HSC	C4A-C5A-N7A	-2.24	108.02	110.58
2	B	1720	NAD	C4A-C5A-N7A	-2.18	108.09	110.58
2	A	1721	NAD	O5B-PA-O1A	2.14	117.43	108.94
2	A	1721	NAD	O2N-PN-O1N	2.11	122.28	112.44
2	A	1721	NAD	O2N-PN-O3	2.08	112.89	107.27
2	A	1721	NAD	O5B-C5B-C4B	-2.07	101.94	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1721	NAD	C5B-C4B-C3B	-2.06	107.80	115.21
4	A	1724	HSC	C6-C5-C4	-2.02	106.01	113.62

There are no chirality outliers.

All (63) 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
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
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	C5B-O5B-P1A-O3A
4	A	1724	HSC	C3P-C2P-S1P-C1
4	A	1724	HSC	CCP-O6A-P2A-O3A
4	A	1724	HSC	CCP-O6A-P2A-O4A
4	A	1724	HSC	CAP-CBP-CCP-O6A
4	A	1724	HSC	CDP-CBP-CCP-O6A
4	A	1724	HSC	CEP-CBP-CCP-O6A
4	B	1722	HSC	C1-C2-C3-O3
4	B	1722	HSC	C5B-O5B-P1A-O1A
4	B	1722	HSC	C5B-O5B-P1A-O3A
4	B	1722	HSC	C3P-C2P-S1P-C1
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
4	B	1722	HSC	CEP-CBP-CCP-O6A
5	B	1719	GOL	C1-C2-C3-O3
4	A	1724	HSC	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
5	B	1719	GOL	O2-C2-C3-O3
4	B	1722	HSC	C4-C5-C6-C7
4	B	1722	HSC	C5-C6-C7-C8
4	A	1724	HSC	C5-C6-C7-C8
4	A	1724	HSC	O4B-C4B-C5B-O5B
4	B	1722	HSC	OAP-CAP-CBP-CDP
4	B	1722	HSC	P1A-O3A-P2A-O4A
4	A	1724	HSC	O1-C1-S1P-C2P
4	A	1724	HSC	P2A-O3A-P1A-O5B
4	B	1722	HSC	C1-C2-C3-C4
4	A	1724	HSC	C2-C1-S1P-C2P
4	B	1722	HSC	S1P-C2P-C3P-N4P
4	A	1724	HSC	C7-C8-C9-C10
2	A	1721	NAD	C5B-O5B-PA-O1A
2	A	1721	NAD	C5D-O5D-PN-O3
2	B	1720	NAD	C5D-O5D-PN-O3
4	A	1724	HSC	CCP-O6A-P2A-O5A
4	B	1722	HSC	P1A-O3A-P2A-O5A
4	B	1722	HSC	C3-C4-C5-C6
4	A	1724	HSC	C3-C4-C5-C6
4	B	1722	HSC	O9P-C9P-CAP-OAP
2	B	1720	NAD	O4B-C4B-C5B-O5B
4	B	1722	HSC	C4B-C5B-O5B-P1A
2	A	1721	NAD	O4B-C4B-C5B-O5B
2	A	1721	NAD	C2B-C1B-N9A-C8A
2	B	1720	NAD	PA-O3-PN-O1N
4	A	1724	HSC	CBP-CCP-O6A-P2A
4	A	1724	HSC	C3B-C4B-C5B-O5B

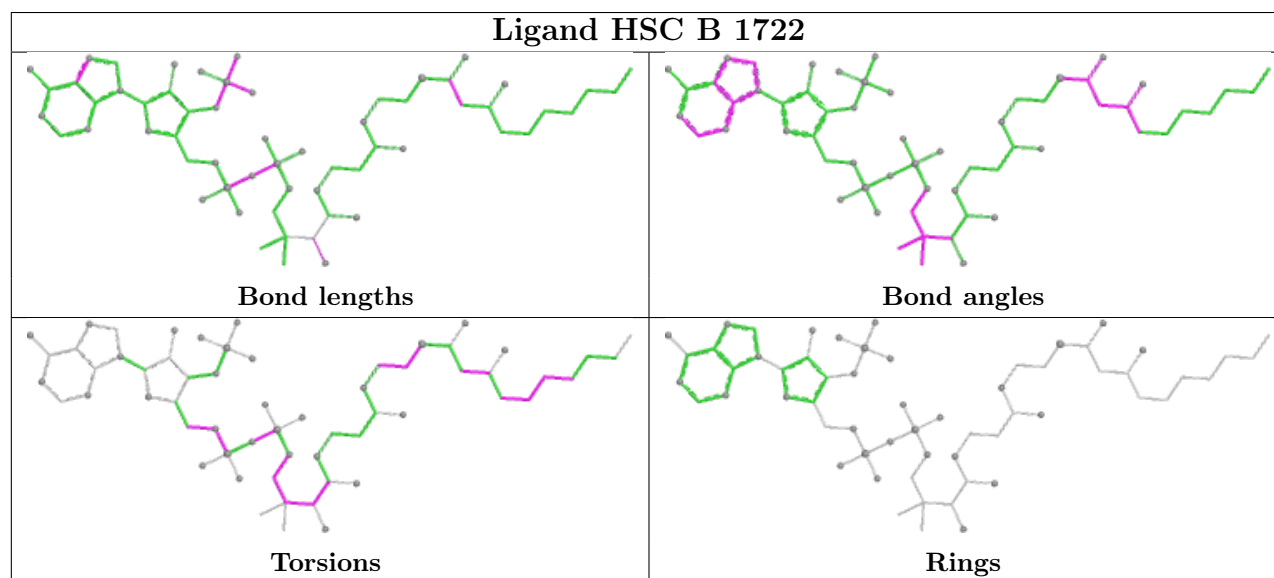
There are no ring outliers.

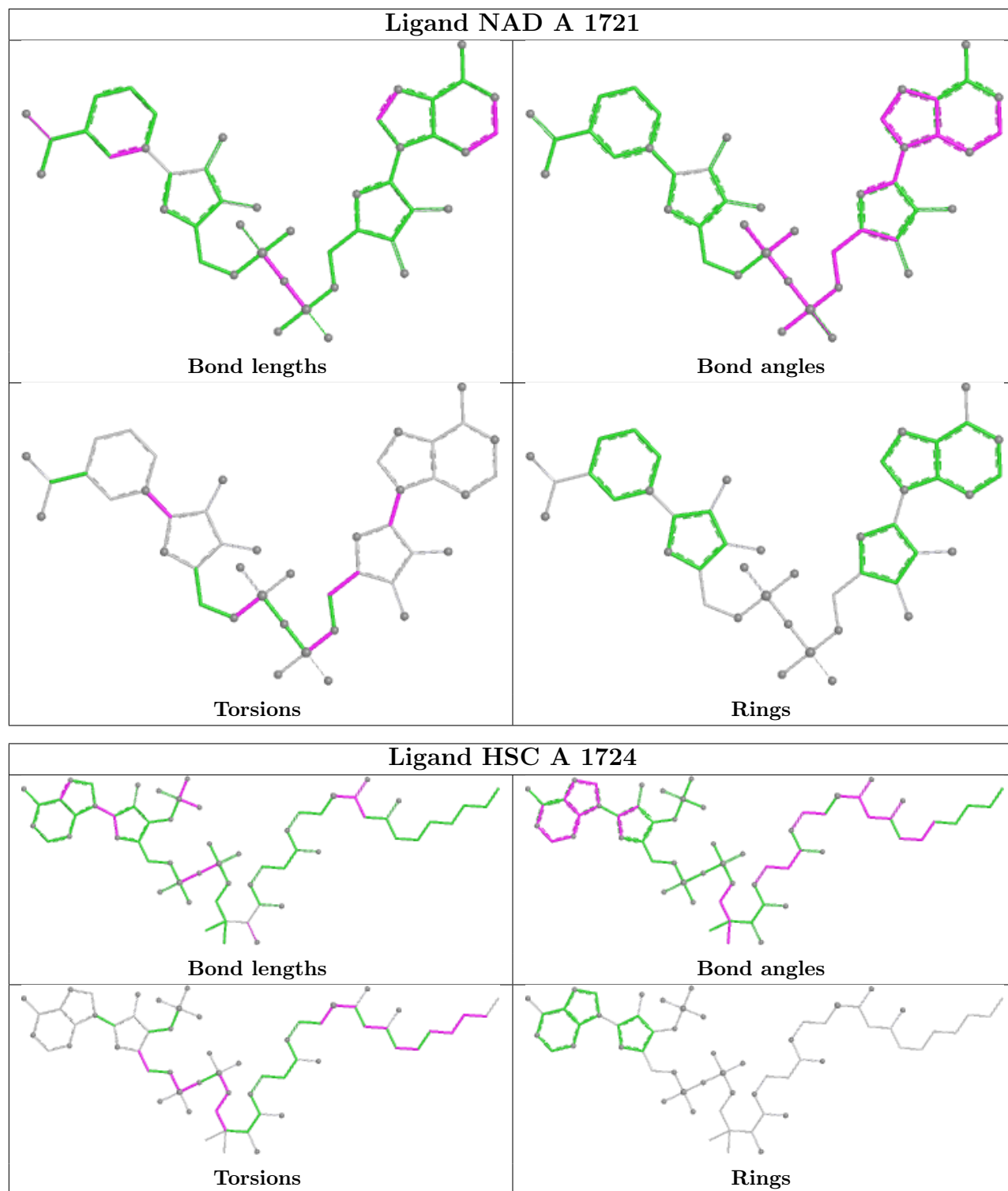
5 monomers are involved in 26 short contacts:

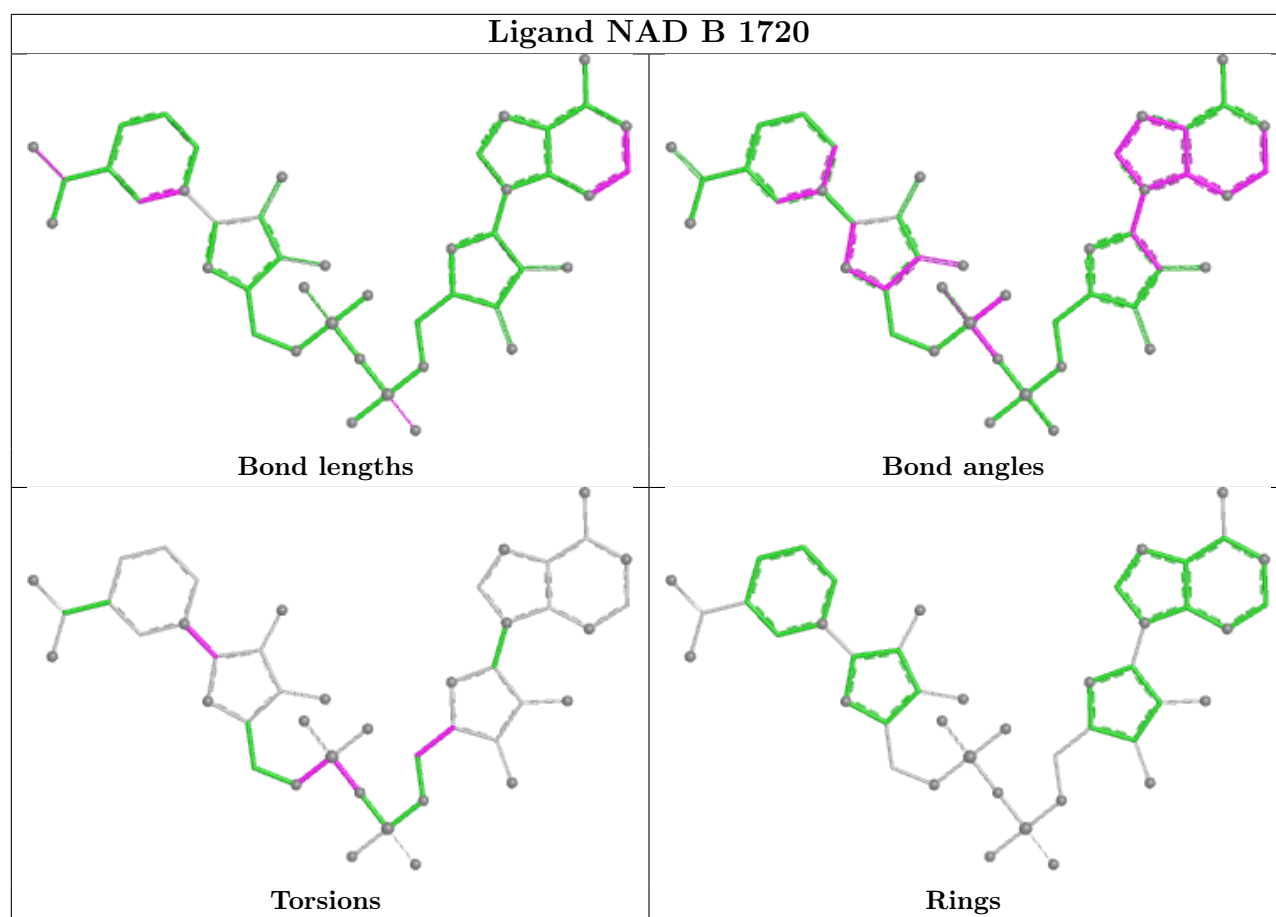
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1722	HSC	8	0
2	A	1721	NAD	4	0
5	B	1719	GOL	4	0
4	A	1724	HSC	9	0
3	B	1721	SO4	1	0

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	725/742 (97%)	0.53	91 (12%)	8 9	9, 31, 62, 99	0
1	B	719/742 (96%)	0.65	78 (10%)	11 12	10, 32, 62, 96	0
All	All	1444/1484 (97%)	0.59	169 (11%)	9 10	9, 32, 62, 99	0

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	PHE	6.1
1	A	356	ALA	5.9
1	B	541	PRO	5.4
1	B	354	GLY	5.2
1	A	-3	ARG	4.8
1	B	449	TYR	4.6
1	A	449	TYR	4.5
1	A	425	GLN	4.3
1	B	356	ALA	4.3
1	A	70	THR	4.2
1	A	68	ALA	4.2
1	A	398	LEU	4.2
1	B	545	PRO	4.1
1	B	43	HIS	4.0
1	A	71	PRO	3.9
1	B	0	HIS	3.9
1	B	368	THR	3.8
1	A	364	PHE	3.8
1	A	397	ALA	3.8
1	A	5	LEU	3.7
1	B	330	LYS	3.7
1	A	368	THR	3.6
1	B	358	ALA	3.6
1	B	718	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	358	ALA	3.5
1	B	535	GLY	3.5
1	B	8	PRO	3.4
1	A	354	GLY	3.4
1	A	350	ALA	3.4
1	A	393	ALA	3.4
1	A	718	HIS	3.4
1	A	422	ASP	3.4
1	A	65	GLY	3.3
1	A	540	GLY	3.3
1	B	185	GLN	3.3
1	A	351	HIS	3.2
1	A	72	GLY	3.2
1	A	67	SER	3.2
1	A	-2	GLY	3.2
1	A	-4	PRO	3.2
1	B	373	THR	3.2
1	A	411	ALA	3.1
1	B	180	ALA	3.1
1	A	535	GLY	3.1
1	A	365	SER	3.1
1	B	363	ARG	3.0
1	A	345	LYS	3.0
1	A	66	PHE	3.0
1	A	241	LYS	3.0
1	B	372	SER	2.9
1	A	554	ASN	2.9
1	B	12	ALA	2.9
1	B	351	HIS	2.9
1	B	608	ILE	2.9
1	B	178	GLU	2.9
1	A	363	ARG	2.9
1	A	355	GLN	2.9
1	A	382	PHE	2.9
1	B	5	LEU	2.9
1	B	362	LEU	2.9
1	B	66	PHE	2.8
1	A	532	ILE	2.8
1	A	386	ASN	2.8
1	A	352	GLN	2.7
1	A	366	SER	2.7
1	B	347	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	7	LEU	2.7
1	A	372	SER	2.7
1	B	295	PRO	2.7
1	B	395	LEU	2.7
1	B	531	LYS	2.7
1	B	45	VAL	2.6
1	B	207	ASN	2.6
1	B	537	GLY	2.6
1	B	176	PRO	2.6
1	A	324	ALA	2.6
1	A	347	ALA	2.6
1	B	422	ASP	2.6
1	B	47	ALA	2.6
1	A	341	PHE	2.6
1	A	322	VAL	2.6
1	A	402	GLY	2.5
1	A	337	LYS	2.5
1	B	349	ARG	2.5
1	A	416	ASP	2.5
1	A	348	SER	2.5
1	A	536	GLN	2.5
1	A	370	GLU	2.5
1	A	541	PRO	2.5
1	A	336	LYS	2.5
1	A	242	HIS	2.5
1	B	9	HIS	2.5
1	A	329	PRO	2.5
1	B	401	PRO	2.5
1	A	6	ARG	2.4
1	B	10	SER	2.4
1	B	371	LEU	2.4
1	A	0	HIS	2.4
1	B	536	GLN	2.4
1	A	357	SER	2.4
1	B	189	ASP	2.4
1	B	553	GLY	2.4
1	A	369	LYS	2.4
1	A	301	VAL	2.4
1	A	543	LEU	2.4
1	B	554	ASN	2.4
1	A	371	LEU	2.4
1	B	336	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	367	SER	2.3
1	A	608	ILE	2.3
1	B	360	PRO	2.3
1	B	361	LYS	2.3
1	B	40	GLY	2.3
1	A	2	ALA	2.3
1	B	338	ILE	2.3
1	B	177	VAL	2.3
1	A	330	LYS	2.3
1	B	704	GLY	2.3
1	A	334	ALA	2.3
1	B	44	THR	2.3
1	B	425	GLN	2.3
1	B	339	ILE	2.3
1	B	7	LEU	2.3
1	A	399	CYS	2.3
1	B	546	GLY	2.3
1	A	4	TYR	2.3
1	A	30	ARG	2.3
1	B	64	HIS	2.3
1	B	186	LYS	2.3
1	A	362	LEU	2.2
1	A	528	VAL	2.3
1	B	11	LEU	2.2
1	B	332	LEU	2.2
1	A	353	ASN	2.2
1	A	-1	SER	2.2
1	A	537	GLY	2.2
1	A	293	ALA	2.2
1	B	335	ALA	2.2
1	B	359	LYS	2.2
1	B	713	SER	2.2
1	A	395	LEU	2.2
1	A	390	LYS	2.2
1	B	91	ALA	2.2
1	B	281	SER	2.2
1	B	171	VAL	2.2
1	B	370	GLU	2.2
1	B	402	GLY	2.2
1	A	720	SER	2.2
1	B	350	ALA	2.2
1	B	600	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	188	ILE	2.1
1	B	355	GLN	2.1
1	B	291	ALA	2.1
1	A	359	LYS	2.1
1	A	421	THR	2.1
1	A	180	ALA	2.1
1	A	3	GLU	2.1
1	A	609	GLU	2.1
1	B	357	SER	2.1
1	B	369	LYS	2.1
1	A	178	GLU	2.1
1	A	8	PRO	2.1
1	A	300	GLY	2.1
1	B	41	SER	2.0
1	A	403	ALA	2.0
1	A	43	HIS	2.0
1	A	63	ILE	2.0
1	B	345	LYS	2.0
1	B	590	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	B	1721	5/5	0.77	0.16	69,70,74,75	0
4	HSC	A	1724	60/60	0.79	0.16	24,62,79,81	0
3	SO4	A	1723	5/5	0.82	0.15	79,82,82,84	0
4	HSC	B	1722	60/60	0.83	0.15	56,76,83,83	0

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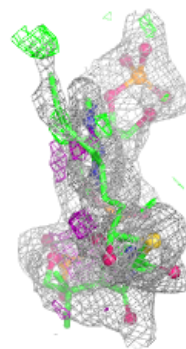
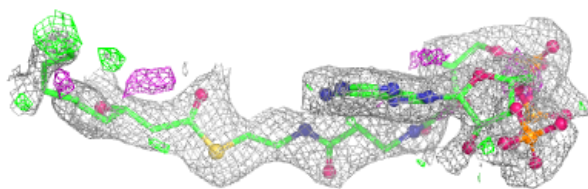
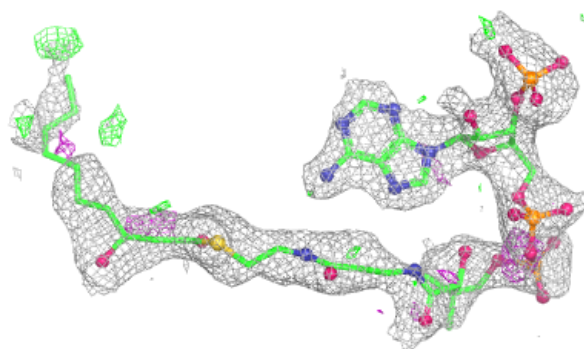
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	A	1721	44/44	0.89	0.11	33,42,49,52	0
5	GOL	B	1719	6/6	0.90	0.13	43,47,48,50	0
3	SO4	A	1722	5/5	0.97	0.09	27,31,32,35	0
2	NAD	B	1720	44/44	0.97	0.06	24,33,41,42	0

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.

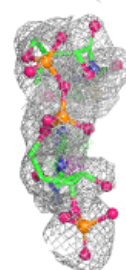
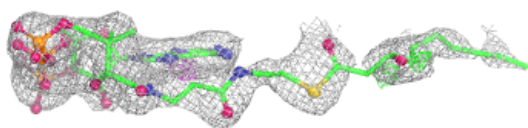
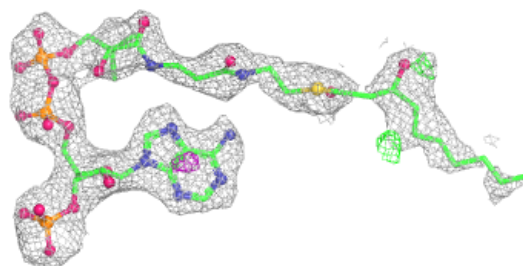
Electron density around HSC A 1724:

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

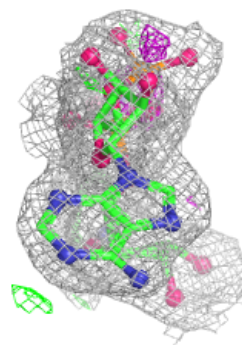
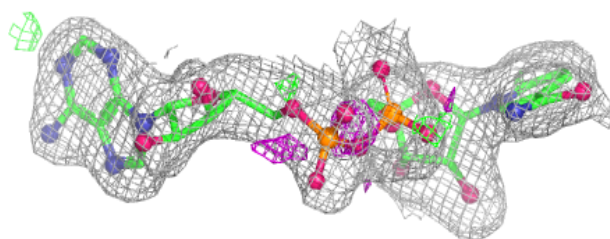
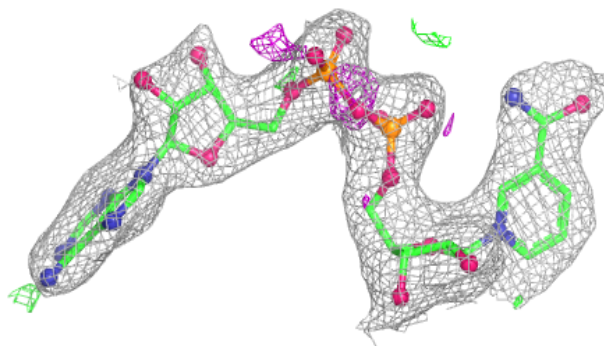


Electron density around HSC B 1722:

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

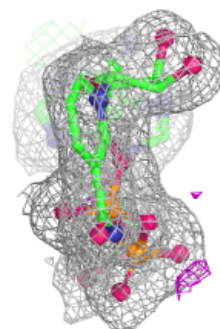
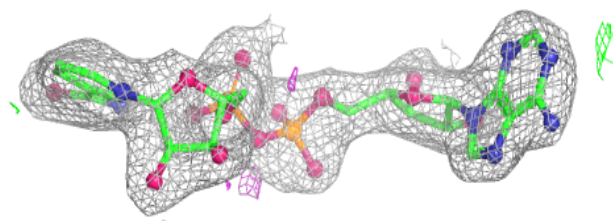
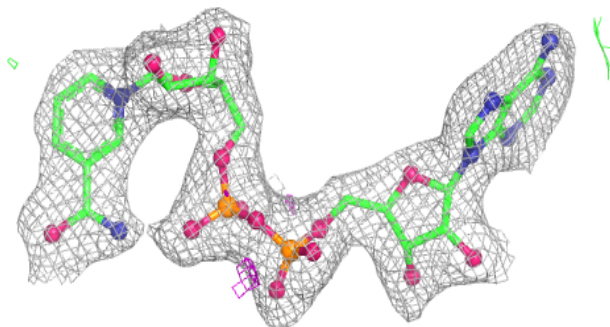
**Electron density around NAD A 1721:**

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



Electron density around NAD B 1720:

$2mF_o - DF_c$ (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.