



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:28 PM UTC

PDB ID : 5U0M / pdb_00005u0m
Title : Fatty aldehyde dehydrogenase from *Marinobacter aquaeolei* VT8 and cofactor complex
Authors : Shi, K.; Mulliner, K.; Barney, B.M.; Aihara, H.
Deposited on : 2016-11-24
Resolution : 3.08 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

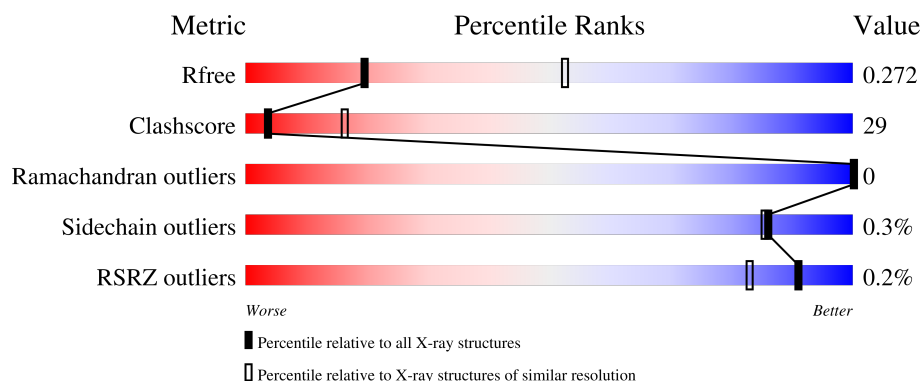
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.08 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	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

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	497	 55% 43% .
1	B	497	 55% 42% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7583 atoms, of which 74 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 N-succinylglutamate 5-semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	0	0
			3679	2328	646	694	11			
1	B	487	Total	C	N	O	S	0	0	0
			3671	2324	644	692	11			

There are 14 discrepancies between the modelled and reference sequences:

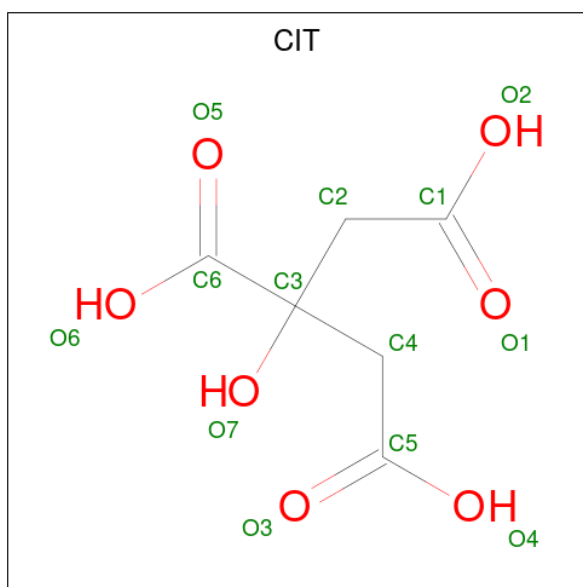
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP A1U5W8
A	-4	HIS	-	expression tag	UNP A1U5W8
A	-3	HIS	-	expression tag	UNP A1U5W8
A	-2	HIS	-	expression tag	UNP A1U5W8
A	-1	HIS	-	expression tag	UNP A1U5W8
A	0	HIS	-	expression tag	UNP A1U5W8
A	1	HIS	-	expression tag	UNP A1U5W8
B	-5	MET	-	initiating methionine	UNP A1U5W8
B	-4	HIS	-	expression tag	UNP A1U5W8
B	-3	HIS	-	expression tag	UNP A1U5W8
B	-2	HIS	-	expression tag	UNP A1U5W8
B	-1	HIS	-	expression tag	UNP A1U5W8
B	0	HIS	-	expression tag	UNP A1U5W8
B	1	HIS	-	expression tag	UNP A1U5W8

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O		0	0
			4	2	2			
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 3 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



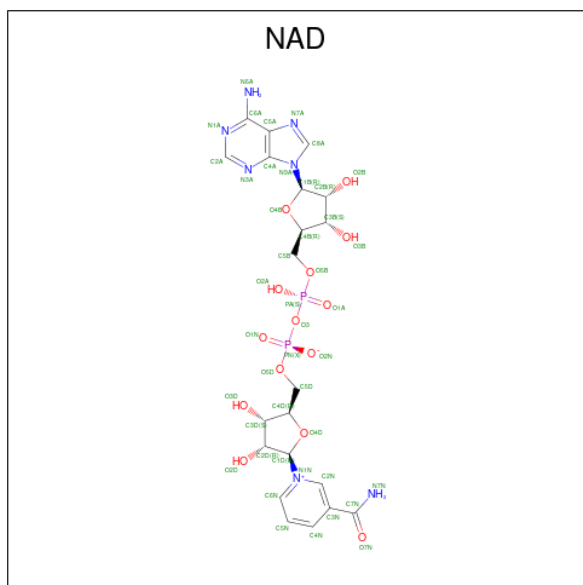
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			18	6	5	7		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			18	6	5	7		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 70	C 21	H 26	N 7	O 14	P 2	0	0
4	B	1	Total 70	C 21	H 26	N 7	O 14	P 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	20	Total O 20 20	0	0
5	B	13	Total O 13 13	0	0

P457	L375	R287
S458	E376	L288
A459	D377	L289
Y460	Q378	V290
Y461	E379	P291
A462	F380	
A463	F381	K294
D464	L384	K295
Y465	L385	G296
	T386	
M470	F387	F299
A471	Y388	L300
S472	R389	A301
L473	R390	R302
E474	Y390	L303
A475		V304
	F393	
		R309
L480	A396	
	L397	V312
P486		A313
L488	T403	E314
	R404	F315
A489	Y405	D316
F490		A317
ASP	S408	
	A409	P321
	G410	F322
	I411	M323
	L412	G324
		S325
	R416	V326
	Y419	I327
	N420	S328
	R421	
	L422	A332
	V423	
	E424	L335
	E425	
	V426	A338
	R427	
		A347
	I430	L350
	V431	L351
	W432	E352
	N434	M353
	R435	K354
	P436	
	L437	K357
	T438	G361
	G439	
		S364
	G447	
	G450	D369
	A451	A370
	S452	L373
		E373

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	99.35Å 99.35Å 254.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.79 – 3.08 34.79 – 3.08	Depositor EDS
% Data completeness (in resolution range)	95.2 (34.79-3.08) 95.2 (34.79-3.08)	Depositor EDS
R_{merge}	0.53	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 3.07Å)	Xtriage
Refinement program	PHENIX dev_2706	Depositor
R, R_{free}	0.219 , 0.273 0.225 , 0.272	Depositor DCC
R_{free} test set	1156 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	78.7	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 79.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7583	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% 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: EDO, NAD, CIT

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	0.15	0/3761	0.37	0/5110
1	B	0.14	0/3753	0.38	0/5099
All	All	0.14	0/7514	0.38	0/10209

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3679	0	3637	229	0
1	B	3671	0	3631	236	0
2	A	8	6	12	1	0
2	B	4	6	6	0	0
3	A	13	5	5	3	0
3	B	13	5	5	3	0
4	A	44	26	26	4	0
4	B	44	26	26	4	0
5	A	20	0	0	1	0
5	B	13	0	0	1	0
All	All	7509	74	7348	430	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 29.

All (430) 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:B:280:GLN:HE22	1:B:326:VAL:HA	1.16	1.06
1:B:409:ALA:O	1:B:431:VAL:HA	1.61	1.00
1:B:285:ALA:HB2	1:B:437:LEU:HD12	1.42	0.99
1:A:285:ALA:HB2	1:A:437:LEU:HD12	1.44	0.95
1:B:98:GLU:OE2	1:B:277:SER:OG	1.85	0.94
1:A:409:ALA:O	1:A:431:VAL:HA	1.68	0.92
1:A:120:ARG:HA	1:B:120:ARG:HH22	1.32	0.92
1:B:462:ALA:HA	1:B:465:TYR:CE1	2.04	0.91
1:B:256:ILE:HD13	1:B:289:LEU:HB2	1.52	0.90
1:B:353:MET:HE1	1:B:384:LEU:HB2	1.55	0.89
1:B:251:GLY:O	1:B:286:ARG:NH1	2.06	0.89
1:B:480:LEU:HD21	1:B:490:PHE:HE2	1.38	0.88
1:B:280:GLN:NE2	1:B:326:VAL:HA	1.90	0.86
1:A:435:ARG:HG2	1:B:475:ALA:HB2	1.60	0.84
1:A:26:GLN:OE1	1:A:29:THR:N	2.09	0.83
1:A:425:GLU:OE2	1:B:60:ARG:NH2	2.11	0.83
1:B:152:PRO:HB2	1:B:181:VAL:HG11	1.60	0.83
1:B:256:ILE:HD11	1:B:289:LEU:HD12	1.61	0.83
1:A:245:LEU:CD2	1:A:247:LEU:HG	2.09	0.82
1:A:419:TYR:CD1	1:A:433:TRP:HB2	2.15	0.82
1:A:447:GLY:HA3	1:A:457:PRO:HB3	1.59	0.82
1:A:306:VAL:HG11	1:B:490:PHE:HE1	1.44	0.81
1:B:201:LEU:HD21	1:B:203:GLN:HE21	1.46	0.80
1:A:353:MET:HE1	1:A:384:LEU:HB2	1.63	0.80
1:A:332:ALA:CB	1:A:363:LEU:HD21	2.12	0.80
1:A:332:ALA:HB1	1:A:363:LEU:HD21	1.63	0.79
1:B:125:GLU:HG3	1:B:134:VAL:HG22	1.62	0.79
1:A:201:LEU:HD21	1:A:203:GLN:HE21	1.49	0.78
1:A:294:LYS:HG2	1:A:295:LYS:HD3	1.66	0.77
1:A:260:VAL:HG11	1:A:266:ALA:HB2	1.67	0.77
1:A:336:LEU:HD21	1:A:363:LEU:HD11	1.65	0.77
1:A:125:GLU:HG2	1:A:134:VAL:HG22	1.68	0.76
1:B:375:LEU:HD13	1:B:376:GLU:N	1.99	0.76
1:A:39:ALA:CB	1:A:202:VAL:HG13	2.16	0.76
1:A:462:ALA:HA	1:A:465:TYR:CE1	2.22	0.75
1:B:419:TYR:CD1	1:B:433:TRP:HB2	2.22	0.75
1:B:294:LYS:HG2	1:B:295:LYS:HD2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:VAL:HG13	1:B:303:LEU:HD12	1.69	0.73
1:B:149:TYR:CE2	1:B:327:ILE:HB	2.24	0.73
1:A:317:ALA:HB3	1:A:321:PRO:HD3	1.70	0.73
1:B:128:VAL:HG22	1:B:129:ALA:H	1.54	0.73
1:A:470:MET:HE3	1:B:431:VAL:HB	1.70	0.72
1:B:290:VAL:HG21	1:B:300:LEU:HD21	1.69	0.72
1:A:251:GLY:HA2	1:A:405:TYR:HB3	1.71	0.72
1:A:350:LEU:HD11	1:A:369:ASP:HB2	1.70	0.72
1:A:226:SER:OG	1:A:229:VAL:HG12	1.90	0.72
1:A:237:PHE:CD2	1:A:245:LEU:HD12	2.26	0.71
1:A:8:VAL:HG13	1:A:201:LEU:O	1.89	0.71
1:A:245:LEU:HD21	1:A:247:LEU:HG	1.70	0.71
1:A:39:ALA:HB3	1:A:202:VAL:HG13	1.73	0.71
1:B:350:LEU:HD11	1:B:369:ASP:HB2	1.71	0.71
1:A:78:GLU:HB2	1:A:107:MET:HE3	1.73	0.70
1:A:157:ASN:OD1	1:A:161:VAL:HG23	1.92	0.70
1:A:78:GLU:OE1	1:A:107:MET:HE1	1.91	0.70
1:A:488:LEU:HD21	1:B:322:PHE:CD1	2.26	0.70
1:A:475:ALA:HB3	1:B:434:ASN:HB2	1.74	0.70
1:A:394:ASP:O	1:A:398:GLU:HG3	1.90	0.70
1:A:250:GLY:O	1:A:452:SER:OG	2.05	0.69
1:B:295:LYS:HD2	1:B:295:LYS:H	1.58	0.69
1:A:480:LEU:HD12	1:B:265:GLY:HA2	1.75	0.69
1:B:4:LEU:HD12	1:B:4:LEU:O	1.93	0.69
1:B:55:PHE:CE2	1:B:59:ARG:HD2	2.28	0.69
1:B:161:VAL:HB	1:B:162:PRO:HD3	1.73	0.69
1:B:4:LEU:HA	5:B:608:HOH:O	1.92	0.69
1:B:157:ASN:OD1	1:B:161:VAL:HG23	1.91	0.68
1:A:245:LEU:HD21	1:A:247:LEU:CD2	2.24	0.68
1:A:24:SER:HB3	1:A:34:TRP:HB3	1.75	0.68
1:B:285:ALA:HB2	1:B:437:LEU:CD1	2.19	0.68
1:A:489:ASN:HB3	1:B:309:ARG:HD3	1.76	0.67
1:B:250:GLY:O	1:B:452:SER:OG	2.10	0.67
1:A:404:ARG:NH2	2:A:501:EDO:H11	2.09	0.67
1:B:155:LEU:HD13	1:B:224:THR:HG21	1.77	0.67
1:A:257:VAL:HG11	1:A:299:PHE:CE2	2.30	0.66
1:A:280:GLN:HE22	1:A:326:VAL:HA	1.59	0.66
1:A:27:PRO:HB3	1:A:327:ILE:O	1.96	0.66
1:A:26:GLN:HE22	1:A:28:VAL:HG12	1.60	0.66
1:B:226:SER:OG	1:B:229:VAL:HG12	1.96	0.66
1:B:353:MET:CE	1:B:384:LEU:HB2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLU:HB2	1:A:107:MET:CE	2.26	0.65
1:B:375:LEU:HD22	1:B:376:GLU:H	1.60	0.65
1:B:425:GLU:O	1:B:427:ARG:NH1	2.30	0.65
1:B:420:ASN:O	1:B:424:GLU:HG3	1.97	0.64
1:B:152:PRO:HB2	1:B:181:VAL:CG1	2.28	0.64
1:B:393:PHE:HD2	1:B:421:ARG:HH21	1.44	0.64
1:A:214:ARG:HG3	1:A:236:GLN:NE2	2.12	0.64
1:A:434:ASN:HB2	1:B:475:ALA:HB3	1.79	0.64
1:A:470:MET:HE3	1:B:431:VAL:CG2	2.27	0.64
1:A:285:ALA:HB2	1:A:437:LEU:CD1	2.22	0.64
1:A:201:LEU:HD21	1:A:203:GLN:NE2	2.12	0.63
1:A:470:MET:HE3	1:B:431:VAL:CB	2.29	0.63
1:A:281:ARG:NH2	5:A:601:HOH:O	2.22	0.63
1:B:135:LEU:HD12	1:B:470:MET:O	1.99	0.63
1:A:161:VAL:HB	1:A:162:PRO:HD3	1.81	0.62
1:A:215:HIS:CE1	1:A:217:LEU:HB2	2.35	0.62
1:A:280:GLN:NE2	1:A:326:VAL:HA	2.13	0.62
1:B:121:THR:HA	1:B:137:HIS:CE1	2.33	0.62
1:A:155:LEU:HD13	1:A:224:THR:HG21	1.82	0.62
1:B:227:SER:HA	1:B:249:MET:SD	2.40	0.62
1:A:335:LEU:HD21	1:A:382:GLY:HA3	1.80	0.62
1:B:155:LEU:HB2	1:B:156:PRO:HD3	1.82	0.62
1:B:256:ILE:CD1	1:B:289:LEU:HB2	2.27	0.62
1:A:245:LEU:HD21	1:A:247:LEU:CG	2.29	0.62
1:B:290:VAL:HG11	1:B:300:LEU:CD2	2.30	0.62
1:A:98:GLU:O	1:A:101:THR:HB	2.00	0.61
1:A:284:CYS:HB3	1:A:286:ARG:HH21	1.64	0.61
1:A:419:TYR:CE1	1:A:433:TRP:HB2	2.36	0.61
1:B:256:ILE:CD1	1:B:289:LEU:HD12	2.29	0.61
1:B:480:LEU:HD21	1:B:490:PHE:CE2	2.29	0.61
1:A:294:LYS:HD3	1:A:295:LYS:NZ	2.16	0.61
1:B:90:LEU:HD23	1:B:315:PHE:CZ	2.35	0.61
1:B:119:GLU:OE1	1:B:460:TYR:OH	2.19	0.61
1:B:278:ALA:HA	1:B:323:MET:SD	2.40	0.61
1:B:152:PRO:CB	1:B:181:VAL:HG11	2.30	0.61
1:B:26:GLN:HE22	1:B:28:VAL:HG12	1.66	0.60
1:A:353:MET:CE	1:A:384:LEU:HB2	2.30	0.60
1:A:318:ASP:N	1:A:318:ASP:OD1	2.34	0.60
1:A:146:PHE:CE1	1:A:212:LEU:HD23	2.37	0.60
1:B:156:PRO:HB3	1:B:172:PHE:HE1	1.67	0.60
1:B:173:LYS:HE3	4:B:503:NAD:H1B	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:PHE:CZ	1:B:229:VAL:HG13	2.36	0.60
1:A:237:PHE:CE2	1:A:245:LEU:HD12	2.37	0.60
1:A:336:LEU:HD21	1:A:363:LEU:CD1	2.31	0.60
1:B:447:GLY:HA3	1:B:457:PRO:HB3	1.83	0.60
1:B:177:LEU:HD13	1:B:327:ILE:HG12	1.83	0.59
1:B:269:HIS:ND1	1:B:436:PRO:HD3	2.16	0.59
1:A:470:MET:HE1	1:B:423:VAL:HA	1.83	0.59
1:A:63:LEU:HD11	1:A:165:LEU:CD2	2.32	0.59
1:B:156:PRO:HB3	1:B:172:PHE:CE1	2.36	0.59
1:B:370:ALA:HB1	1:B:373:ILE:HB	1.83	0.59
1:B:347:ALA:HB2	1:B:370:ALA:HB2	1.85	0.59
1:B:120:ARG:HD2	1:B:461:TYR:CE1	2.37	0.59
1:A:420:ASN:O	1:A:424:GLU:HG3	2.03	0.59
1:B:462:ALA:HA	1:B:465:TYR:HE1	1.65	0.59
1:A:422:LEU:HD12	1:A:426:VAL:HB	1.84	0.58
1:B:70:ILE:O	1:B:73:PHE:HB3	2.02	0.58
1:A:475:ALA:HB3	1:B:434:ASN:CB	2.32	0.58
1:B:120:ARG:HD2	1:B:461:TYR:CD1	2.38	0.58
1:B:350:LEU:CD1	1:B:369:ASP:HB2	2.33	0.58
1:A:282:CYS:O	1:A:407:LEU:HD23	2.03	0.58
1:A:294:LYS:CG	1:A:295:LYS:HD3	2.33	0.58
1:A:194:LEU:HD23	1:A:199:ILE:HG22	1.85	0.58
1:B:251:GLY:HA2	1:B:405:TYR:HB3	1.84	0.58
1:A:173:LYS:NZ	1:A:204:GLY:O	2.37	0.58
1:B:370:ALA:HA	1:B:373:ILE:HD13	1.83	0.58
1:A:73:PHE:CE2	1:A:77:LEU:HD11	2.38	0.58
1:A:146:PHE:HE1	1:A:212:LEU:HD23	1.68	0.58
1:A:227:SER:O	1:A:231:HIS:ND1	2.28	0.58
1:B:78:GLU:OE1	1:B:107:MET:HE1	2.04	0.57
1:A:258:GLN:HB2	1:A:390:TYR:OH	2.04	0.57
1:A:223:PHE:CZ	1:A:229:VAL:HG13	2.39	0.57
1:A:356:LEU:HD11	1:A:364:SER:HB3	1.84	0.57
1:A:411:ILE:HG23	1:A:433:TRP:HD1	1.69	0.57
1:A:326:VAL:HG22	1:A:361:GLY:O	2.05	0.57
1:A:306:VAL:HG11	1:B:490:PHE:CE1	2.34	0.57
1:B:214:ARG:HD2	1:B:214:ARG:O	2.05	0.57
1:B:285:ALA:CB	1:B:437:LEU:HD12	2.27	0.57
1:B:294:LYS:HD2	1:B:294:LYS:N	2.20	0.57
1:A:138:ARG:NH2	1:B:423:VAL:HG12	2.20	0.57
1:A:435:ARG:CG	1:B:475:ALA:HB2	2.32	0.57
1:B:377:ASP:OD2	1:B:404:ARG:HD3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:ARG:HG2	1:B:420:ASN:ND2	2.20	0.57
1:A:278:ALA:HA	1:A:323:MET:SD	2.45	0.56
1:A:350:LEU:CD1	1:A:369:ASP:HB2	2.34	0.56
1:B:8:VAL:HG13	1:B:201:LEU:O	2.05	0.56
1:B:257:VAL:HG13	1:B:257:VAL:O	2.05	0.56
1:A:63:LEU:HD11	1:A:165:LEU:HD21	1.87	0.56
1:A:70:ILE:O	1:A:73:PHE:HB3	2.05	0.56
1:B:6:GLY:HA2	1:B:34:TRP:CZ2	2.40	0.56
1:B:61:LYS:HE2	1:B:65:GLU:OE1	2.06	0.56
1:B:294:LYS:HD2	1:B:294:LYS:H	1.69	0.56
1:B:480:LEU:CD2	1:B:490:PHE:HE2	2.14	0.56
1:B:26:GLN:OE1	1:B:28:VAL:HG12	2.06	0.56
1:B:215:HIS:CE1	1:B:217:LEU:HB2	2.41	0.56
1:A:90:LEU:HD23	1:A:315:PHE:CZ	2.41	0.56
1:B:294:LYS:CG	1:B:295:LYS:HD2	2.35	0.56
1:B:258:GLN:HG3	1:B:291:PRO:HG3	1.87	0.56
1:A:332:ALA:O	1:A:336:LEU:HD23	2.05	0.55
1:B:263:LEU:HD21	1:B:302:ARG:HB2	1.88	0.55
1:A:257:VAL:HG13	1:A:257:VAL:O	2.06	0.55
1:A:470:MET:CE	1:B:431:VAL:HB	2.37	0.55
1:B:312:VAL:HG22	1:B:323:MET:CG	2.37	0.55
1:B:173:LYS:NZ	1:B:204:GLY:O	2.40	0.55
1:A:245:LEU:HD23	1:A:245:LEU:C	2.31	0.55
1:A:26:GLN:HG2	1:A:90:LEU:O	2.07	0.54
1:B:96:LEU:HD23	1:B:316:ASP:HA	1.89	0.54
1:A:425:GLU:O	1:A:427:ARG:HD2	2.07	0.54
1:A:423:VAL:HG12	1:B:138:ARG:NH2	2.22	0.54
1:B:61:LYS:O	1:B:66:ARG:NH1	2.40	0.54
1:B:8:VAL:HG12	1:B:9:TYR:N	2.22	0.54
1:A:228:THR:O	1:A:232:LEU:HD23	2.08	0.54
1:B:97:TRP:HZ2	1:B:322:PHE:O	1.90	0.54
1:A:44:VAL:HG22	1:A:202:VAL:HG11	1.89	0.54
1:A:194:LEU:HD23	1:A:199:ILE:CG2	2.38	0.54
1:A:393:PHE:CE2	1:A:397:LEU:HD11	2.43	0.54
1:A:450:GLY:C	1:B:242:GLU:HG3	2.33	0.54
1:B:150:ASN:OD1	1:B:151:PHE:N	2.41	0.54
1:A:332:ALA:HB2	1:A:363:LEU:HD21	1.89	0.54
1:B:96:LEU:HB3	1:B:100:ARG:NH1	2.22	0.54
1:B:49:ARG:HE	1:B:217:LEU:CD1	2.21	0.54
1:B:174:PRO:HG3	1:B:182:ALA:CB	2.38	0.54
1:B:408:SER:HA	1:B:430:ILE:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:LEU:CD2	1:A:388:TYR:HB2	2.37	0.53
1:A:174:PRO:HG3	1:A:182:ALA:CB	2.38	0.53
1:B:63:LEU:HD11	1:B:165:LEU:HD21	1.89	0.53
1:A:318:ASP:CG	1:A:319:PRO:CD	2.82	0.53
1:B:63:LEU:HD11	1:B:165:LEU:CD2	2.39	0.53
1:B:294:LYS:HD3	1:B:295:LYS:CE	2.39	0.53
1:B:296:GLY:O	1:B:300:LEU:HD23	2.08	0.53
1:A:138:ARG:HH21	1:B:423:VAL:HG12	1.73	0.53
1:A:481:PRO:HD3	1:B:268:HIS:CE1	2.43	0.53
1:B:280:GLN:HE21	1:B:326:VAL:HG12	1.74	0.53
1:A:49:ARG:HE	1:A:217:LEU:CD1	2.22	0.53
1:A:318:ASP:OD1	1:A:319:PRO:HD2	2.09	0.53
1:A:294:LYS:HD2	1:A:294:LYS:N	2.24	0.52
1:A:242:GLU:HG3	1:B:450:GLY:C	2.34	0.52
1:B:128:VAL:HG22	1:B:129:ALA:N	2.22	0.52
1:B:375:LEU:HD13	1:B:376:GLU:H	1.73	0.52
1:A:121:THR:HA	1:A:137:HIS:CE1	2.44	0.52
1:B:294:LYS:CD	1:B:295:LYS:HD2	2.40	0.52
1:A:487:GLY:C	1:A:488:LEU:HD22	2.35	0.52
1:B:139:PRO:HB3	1:B:166:ALA:O	2.10	0.52
1:B:255:LEU:HD12	1:B:410:GLY:O	2.10	0.52
1:A:120:ARG:HA	1:B:120:ARG:NH2	2.14	0.52
1:A:351:LEU:HD12	1:A:365:PRO:O	2.10	0.52
1:B:26:GLN:NE2	1:B:28:VAL:HG12	2.25	0.51
1:B:228:THR:O	1:B:232:LEU:HD23	2.09	0.51
1:A:294:LYS:HG2	1:A:295:LYS:N	2.24	0.51
1:B:172:PHE:HE2	1:B:182:ALA:HB1	1.75	0.51
1:A:151:PHE:HE2	1:A:281:ARG:HG2	1.74	0.51
1:A:215:HIS:HE1	1:A:217:LEU:HD12	1.75	0.51
1:A:245:LEU:HD23	1:A:246:ALA:N	2.25	0.51
1:A:312:VAL:HG22	1:A:323:MET:HG3	1.93	0.51
1:A:318:ASP:CG	1:A:319:PRO:HD2	2.34	0.51
1:A:377:ASP:OD2	1:A:404:ARG:N	2.34	0.51
1:B:26:GLN:HG2	1:B:90:LEU:O	2.10	0.51
1:B:33:VAL:HG11	1:B:90:LEU:CD1	2.40	0.51
1:A:391:LYS:HB2	1:A:395:GLU:OE1	2.11	0.51
1:B:201:LEU:HD21	1:B:203:GLN:NE2	2.21	0.51
1:A:51:ALA:HB2	1:A:200:ASN:HD22	1.75	0.50
1:A:294:LYS:HD3	1:A:295:LYS:HZ3	1.75	0.50
1:A:434:ASN:CB	1:B:475:ALA:HB3	2.39	0.50
1:A:155:LEU:HB2	1:A:156:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:SER:OG	1:A:459:ALA:N	2.44	0.50
1:B:27:PRO:HB3	1:B:327:ILE:O	2.11	0.50
1:B:304:VAL:HG13	1:B:351:LEU:HD12	1.92	0.50
1:B:294:LYS:HD3	1:B:295:LYS:HE2	1.94	0.50
1:A:335:LEU:CD2	1:A:382:GLY:HA3	2.42	0.50
1:B:51:ALA:HB2	1:B:200:ASN:HD22	1.76	0.50
1:B:312:VAL:HG21	1:B:323:MET:HE3	1.93	0.50
1:A:294:LYS:CD	1:A:295:LYS:HD3	2.42	0.50
1:A:390:TYR:CD2	1:A:396:ALA:HB2	2.47	0.50
1:A:41:LEU:HD23	1:A:211:CYS:SG	2.51	0.50
1:A:97:TRP:HD1	1:A:320:GLN:HB3	1.77	0.50
1:A:439:GLY:N	3:A:503:CIT:O4	2.43	0.50
1:A:470:MET:HE3	1:B:431:VAL:HG21	1.93	0.49
1:B:9:TYR:OH	1:B:12:GLY:HA2	2.11	0.49
1:A:26:GLN:NE2	1:A:28:VAL:HG12	2.25	0.49
1:A:223:PHE:HZ	1:A:229:VAL:HG13	1.77	0.49
1:B:290:VAL:HG13	1:B:291:PRO:HD2	1.95	0.49
1:A:21:PRO:HG3	1:A:37:ASN:OD1	2.12	0.49
1:A:150:ASN:OD1	1:A:151:PHE:N	2.44	0.49
1:B:295:LYS:HD2	1:B:295:LYS:N	2.28	0.49
1:A:97:TRP:HA	1:A:100:ARG:HH11	1.77	0.49
1:A:173:LYS:HE3	4:A:504:NAD:H1B	1.95	0.49
1:A:41:LEU:HD13	1:A:41:LEU:C	2.38	0.49
1:B:226:SER:HG	1:B:229:VAL:HG12	1.78	0.49
1:A:312:VAL:HG22	1:A:323:MET:CG	2.43	0.49
1:A:336:LEU:CD2	1:A:363:LEU:HD11	2.39	0.49
1:B:84:LEU:HD12	1:B:184:LEU:HD23	1.94	0.48
1:B:260:VAL:HG11	1:B:266:ALA:HB2	1.94	0.48
1:B:289:LEU:CD2	1:B:388:TYR:HB2	2.43	0.48
1:A:322:PHE:CD1	1:B:488:LEU:HD11	2.48	0.48
1:A:24:SER:HB3	1:A:34:TRP:CB	2.40	0.48
1:A:312:VAL:HG21	1:A:323:MET:HE3	1.96	0.48
1:A:8:VAL:HG12	1:A:9:TYR:N	2.29	0.48
1:B:314:GLU:OE2	1:B:357:LYS:NZ	2.46	0.48
1:B:393:PHE:CE2	1:B:397:LEU:HD11	2.49	0.48
1:A:350:LEU:HD11	1:A:369:ASP:CB	2.42	0.48
1:B:149:TYR:HD2	1:B:327:ILE:HD13	1.79	0.48
1:B:250:GLY:HA3	1:B:379:GLU:OE1	2.14	0.48
1:A:245:LEU:HD21	1:A:247:LEU:HD21	1.95	0.48
1:B:33:VAL:HG11	1:B:90:LEU:HD12	1.96	0.48
1:B:202:VAL:HG23	1:B:202:VAL:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:LEU:HD11	1:B:299:PHE:HA	1.96	0.47
1:A:149:TYR:CE2	1:A:327:ILE:HB	2.49	0.47
1:B:312:VAL:HG22	1:B:323:MET:HG2	1.96	0.47
1:B:354:LYS:N	1:B:364:SER:OG	2.41	0.47
1:B:459:ALA:O	1:B:462:ALA:CB	2.63	0.47
1:A:280:GLN:HE22	1:A:326:VAL:CA	2.25	0.47
1:A:341:ALA:O	1:A:345:LYS:HB2	2.15	0.47
1:A:422:LEU:O	1:A:426:VAL:HG12	2.15	0.47
1:B:84:LEU:CD1	1:B:184:LEU:HD23	2.45	0.47
1:B:151:PHE:CE2	1:B:281:ARG:HG2	2.50	0.47
1:A:281:ARG:HD3	3:A:503:CIT:H42	1.95	0.47
1:B:125:GLU:HG2	1:B:132:HIS:CE1	2.50	0.47
1:A:244:ILE:HG13	1:A:456:ARG:NH1	2.30	0.46
1:A:39:ALA:HB3	1:A:202:VAL:CG1	2.43	0.46
1:A:150:ASN:HD21	4:A:504:NAD:H5N	1.79	0.46
1:A:201:LEU:CD2	1:A:203:GLN:HE21	2.25	0.46
1:A:253:ASN:HB2	1:A:284:CYS:O	2.16	0.46
1:A:234:HIS:HB2	1:A:247:LEU:HD11	1.97	0.46
1:A:251:GLY:HA2	1:A:405:TYR:CB	2.42	0.46
1:A:294:LYS:HD2	1:A:294:LYS:H	1.81	0.46
1:B:277:SER:HB2	1:B:281:ARG:HG3	1.98	0.46
1:A:290:VAL:HG13	1:A:291:PRO:HD2	1.96	0.46
1:B:98:GLU:O	1:B:101:THR:HB	2.15	0.46
1:A:432:ASN:OD1	1:B:473:LEU:HB2	2.16	0.46
1:B:9:TYR:CZ	1:B:12:GLY:HA2	2.51	0.46
1:B:201:LEU:HD11	1:B:203:GLN:NE2	2.31	0.46
1:A:151:PHE:CE2	1:A:281:ARG:HG2	2.50	0.46
1:A:227:SER:HA	1:A:249:MET:SD	2.55	0.46
1:B:267:VAL:HG13	1:B:303:LEU:CD1	2.41	0.46
1:A:76:LEU:HD12	1:A:192:ALA:HB2	1.98	0.45
1:A:269:HIS:HE1	1:A:435:ARG:NH1	2.14	0.45
1:B:150:ASN:HD21	4:B:503:NAD:C5N	2.28	0.45
1:B:458:SER:OG	1:B:459:ALA:N	2.44	0.45
1:A:250:GLY:HA3	1:A:379:GLU:OE1	2.16	0.45
1:A:265:GLY:O	1:A:268:HIS:HB3	2.17	0.45
1:B:151:PHE:HE2	1:B:281:ARG:HG2	1.80	0.45
1:B:256:ILE:HB	1:B:411:ILE:HG13	1.98	0.45
1:B:223:PHE:HZ	1:B:229:VAL:HG13	1.81	0.45
1:A:422:LEU:CD1	1:A:426:VAL:HB	2.47	0.45
1:A:221:LEU:C	1:A:221:LEU:HD23	2.41	0.45
1:B:277:SER:O	1:B:280:GLN:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:ALA:O	1:B:462:ALA:HB3	2.17	0.45
1:B:290:VAL:HG11	1:B:300:LEU:HD21	1.98	0.45
1:B:317:ALA:HB3	1:B:321:PRO:HD3	1.97	0.45
1:B:335:LEU:O	1:B:338:ALA:HB3	2.17	0.45
1:A:23:GLU:HB2	1:A:34:TRP:O	2.17	0.44
1:B:90:LEU:HD13	1:B:90:LEU:C	2.43	0.44
1:A:264:ASP:OD1	1:A:302:ARG:NE	2.48	0.44
1:A:322:PHE:HB2	1:B:486:PRO:O	2.17	0.44
1:A:423:VAL:HG12	1:B:138:ARG:HH21	1.82	0.44
1:A:475:ALA:HB2	1:B:435:ARG:HG2	1.99	0.44
1:B:287:ARG:HA	1:B:386:THR:O	2.17	0.44
1:B:312:VAL:HG22	1:B:323:MET:HG3	1.99	0.44
1:A:249:MET:HE3	1:A:453:GLY:N	2.32	0.44
1:B:381:PHE:CE2	4:B:503:NAD:H3D	2.52	0.44
1:B:156:PRO:O	1:B:160:ILE:HG13	2.17	0.44
1:A:377:ASP:OD2	1:A:403:THR:HA	2.18	0.43
1:B:120:ARG:HD3	1:B:464:ASP:OD1	2.18	0.43
1:A:284:CYS:CB	1:A:286:ARG:HH21	2.31	0.43
1:A:355:GLN:NE2	1:A:358:PRO:O	2.51	0.43
1:B:9:TYR:HB3	1:B:201:LEU:HB3	2.01	0.43
1:B:438:THR:HA	3:B:502:CIT:O4	2.18	0.43
1:A:281:ARG:HD3	3:A:503:CIT:C4	2.48	0.43
1:B:281:ARG:HD3	3:B:502:CIT:C4	2.48	0.43
1:A:393:PHE:CD1	1:A:418:LEU:HD22	2.53	0.43
1:B:106:MET:HB3	1:B:157:ASN:HD22	1.83	0.43
1:B:377:ASP:OD2	1:B:403:THR:HA	2.19	0.43
1:A:63:LEU:HD11	1:A:165:LEU:HD23	1.99	0.43
1:B:277:SER:CB	1:B:281:ARG:HG3	2.48	0.43
1:A:94:LYS:O	1:A:315:PHE:HB2	2.19	0.43
1:A:172:PHE:CE2	1:A:174:PRO:HB3	2.54	0.43
1:A:373:ILE:HG22	1:A:374:GLU:N	2.32	0.43
1:B:94:LYS:O	1:B:315:PHE:HB2	2.19	0.43
1:A:244:ILE:HG13	1:A:456:ARG:HH12	1.83	0.43
1:B:96:LEU:HD21	1:B:316:ASP:HB3	2.00	0.43
1:A:289:LEU:HD23	1:A:388:TYR:HB2	2.00	0.43
1:B:422:LEU:O	1:B:426:VAL:HG12	2.18	0.43
1:B:480:LEU:HD11	1:B:490:PHE:CD2	2.54	0.43
1:A:55:PHE:CE2	1:A:59:ARG:HD2	2.53	0.42
1:A:225:GLY:O	1:A:249:MET:HA	2.19	0.42
1:B:26:GLN:HB3	1:B:29:THR:OG1	2.19	0.42
1:A:186:VAL:HG21	1:A:201:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:VAL:HA	1:A:323:MET:O	2.19	0.42
1:A:381:PHE:CE2	4:A:504:NAD:H2D	2.55	0.42
1:B:8:VAL:CG1	1:B:9:TYR:N	2.82	0.42
1:B:215:HIS:HE1	1:B:217:LEU:HB2	1.82	0.42
1:A:282:CYS:HB3	4:A:504:NAD:C3N	2.49	0.42
1:B:295:LYS:H	1:B:295:LYS:CD	2.29	0.42
1:A:6:GLY:HA2	1:A:34:TRP:CZ2	2.53	0.42
1:A:119:GLU:OE1	1:A:460:TYR:OH	2.31	0.42
1:A:259:ASN:C	1:A:259:ASN:HD22	2.26	0.42
1:B:76:LEU:HD12	1:B:192:ALA:HB2	2.01	0.42
1:B:93:GLY:O	1:B:324:GLY:HA3	2.19	0.42
1:B:439:GLY:H	3:B:502:CIT:C5	2.32	0.42
1:A:61:LYS:HE2	1:A:65:GLU:OE1	2.20	0.42
1:A:172:PHE:HE2	1:A:182:ALA:HB1	1.84	0.42
1:A:419:TYR:HB2	1:A:433:TRP:CD1	2.54	0.42
1:B:26:GLN:CD	1:B:28:VAL:HG12	2.45	0.42
1:B:256:ILE:O	1:B:411:ILE:HA	2.19	0.42
1:B:390:TYR:CE2	1:B:396:ALA:HB2	2.54	0.42
1:B:24:SER:HB3	1:B:34:TRP:HB3	2.01	0.42
1:B:136:ARG:HH12	1:B:472:SER:HB2	1.85	0.42
1:A:106:MET:HB3	1:A:157:ASN:HD22	1.84	0.42
1:A:294:LYS:HD3	1:A:295:LYS:HD3	2.02	0.42
1:B:251:GLY:HA2	1:B:405:TYR:CB	2.50	0.42
1:A:148:PRO:HG3	1:A:155:LEU:HD12	2.02	0.42
1:A:450:GLY:O	1:B:242:GLU:HG3	2.20	0.42
1:B:41:LEU:HD23	1:B:41:LEU:C	2.45	0.42
1:B:91:GLU:OE2	1:B:179:PRO:HD2	2.20	0.42
1:A:143:VAL:O	1:A:143:VAL:HG23	2.19	0.42
1:A:295:LYS:HD3	1:A:295:LYS:H	1.85	0.42
1:B:326:VAL:HG21	1:B:332:ALA:HB2	2.02	0.42
1:B:173:LYS:O	1:B:173:LYS:HD3	2.20	0.41
1:B:218:ILE:O	1:B:243:LYS:HE3	2.20	0.41
1:B:326:VAL:HG22	1:B:361:GLY:O	2.19	0.41
1:A:120:ARG:HD2	1:B:120:ARG:NH2	2.35	0.41
1:A:269:HIS:ND1	1:A:436:PRO:HD3	2.34	0.41
1:B:150:ASN:HD21	4:B:503:NAD:H5N	1.85	0.41
1:A:61:LYS:O	1:A:66:ARG:NH1	2.54	0.41
1:A:489:ASN:OD1	1:A:490:PHE:N	2.53	0.41
1:B:164:LEU:CD2	1:B:170:VAL:HG23	2.50	0.41
1:B:257:VAL:HG11	1:B:299:PHE:CE2	2.56	0.41
1:A:139:PRO:HB2	1:A:168:ASN:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:GLY:O	1:A:373:ILE:HD11	2.20	0.41
1:B:177:LEU:HD13	1:B:327:ILE:CG1	2.48	0.41
1:B:267:VAL:HG13	1:B:303:LEU:HA	2.02	0.41
1:A:139:PRO:HB3	1:A:166:ALA:O	2.21	0.41
1:A:478:SER:OG	1:B:412:LEU:HD22	2.20	0.41
1:A:114:VAL:HG22	1:A:165:LEU:HD11	2.02	0.41
1:A:393:PHE:CE1	1:A:418:LEU:HD22	2.56	0.41
1:B:55:PHE:CE1	1:B:141:GLY:HA2	2.56	0.41
1:B:458:SER:HA	1:B:465:TYR:HE1	1.86	0.41
1:A:268:HIS:HB2	1:B:480:LEU:CD2	2.51	0.41
1:B:312:VAL:HG21	1:B:323:MET:CE	2.50	0.41
1:B:416:ARG:HG2	1:B:420:ASN:HD21	1.85	0.41
1:A:215:HIS:HE1	1:A:217:LEU:HB2	1.81	0.40
1:A:330:GLU:O	1:A:333:ASN:HB3	2.21	0.40
1:B:223:PHE:HZ	1:B:229:VAL:CG1	2.33	0.40
1:B:287:ARG:HG2	1:B:386:THR:OG1	2.21	0.40
1:B:88:ILE:HG12	1:B:181:VAL:HG21	2.03	0.40
1:B:254:PRO:HA	1:B:287:ARG:O	2.22	0.40
1:A:327:ILE:HG23	1:A:328:SER:N	2.36	0.40
1:A:392:GLY:O	1:A:395:GLU:HB3	2.22	0.40
1:A:38:ALA:CB	1:A:204:GLY:HA2	2.52	0.40
1:A:135:LEU:HD12	1:A:470:MET:O	2.22	0.40
1:B:326:VAL:HG23	1:B:328:SER:O	2.21	0.40
1:B:375:LEU:CD2	1:B:376:GLU:H	2.31	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	486/497 (98%)	452 (93%)	34 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	485/497 (98%)	450 (93%)	35 (7%)	0	100	100
All	All	971/994 (98%)	902 (93%)	69 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	378/386 (98%)	377 (100%)	1 (0%)	86	85
1	B	377/386 (98%)	376 (100%)	1 (0%)	86	85
All	All	755/772 (98%)	753 (100%)	2 (0%)	86	85

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	318	ASP
1	B	294	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	140	HIS
1	A	236	GLN
1	A	259	ASN
1	A	280	GLN
1	B	7	ASN
1	B	118	ASN
1	B	123	HIS
1	B	203	GLN
1	B	259	ASN
1	B	280	GLN

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Mol	Chain	Res	Type
1	B	320	GLN
1	B	378	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
3	CIT	B	502	-	12,12,12	1.08	0	17,17,17	1.44	1 (5%)
2	EDO	A	502	-	3,3,3	0.45	0	2,2,2	0.29	0
2	EDO	A	501	-	3,3,3	0.42	0	2,2,2	0.42	0
4	NAD	A	504	-	46,48,48	2.19	12 (26%)	64,73,73	1.84	15 (23%)
4	NAD	B	503	-	46,48,48	2.20	13 (28%)	64,73,73	1.93	17 (26%)
2	EDO	B	501	-	3,3,3	0.45	0	2,2,2	0.30	0
3	CIT	A	503	-	12,12,12	1.09	0	17,17,17	1.51	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CIT	B	502	-	-	5/16/16/16	-
2	EDO	A	502	-	-	1/1/1/1	-
2	EDO	A	501	-	-	0/1/1/1	-
4	NAD	A	504	-	-	13/30/62/62	0/5/5/5
4	NAD	B	503	-	-	9/30/62/62	0/5/5/5
2	EDO	B	501	-	-	0/1/1/1	-
3	CIT	A	503	-	-	9/16/16/16	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	504	NAD	C3N-C7N	-7.23	1.39	1.50
4	B	503	NAD	C3N-C7N	-7.17	1.39	1.50
4	A	504	NAD	C2N-N1N	6.03	1.41	1.35
4	B	503	NAD	O4D-C1D	5.78	1.48	1.40
4	A	504	NAD	O4D-C1D	5.63	1.48	1.40
4	B	503	NAD	C2N-N1N	5.53	1.41	1.35
4	A	504	NAD	C2A-N3A	3.59	1.40	1.33
4	B	503	NAD	C2A-N3A	3.54	1.40	1.33
4	A	504	NAD	C2A-N1A	3.33	1.39	1.33
4	B	503	NAD	PN-O3	3.28	1.63	1.59
4	B	503	NAD	C2A-N1A	3.26	1.39	1.33
4	A	504	NAD	C5A-N7A	-3.09	1.33	1.39
4	A	504	NAD	O4B-C1B	3.05	1.49	1.42
4	B	503	NAD	C5A-N7A	-3.03	1.33	1.39
4	B	503	NAD	O4B-C1B	3.00	1.48	1.42
4	B	503	NAD	C5A-C4A	-2.95	1.33	1.39
4	A	504	NAD	C5A-C4A	-2.84	1.34	1.39
4	B	503	NAD	PA-O3	2.81	1.62	1.59
4	B	503	NAD	C5A-C6A	-2.51	1.34	1.41
4	A	504	NAD	C5A-C6A	-2.48	1.34	1.41
4	B	503	NAD	C6N-N1N	2.47	1.41	1.35
4	B	503	NAD	C8A-N9A	-2.37	1.33	1.37
4	A	504	NAD	C6N-N1N	2.28	1.40	1.35
4	A	504	NAD	C8A-N9A	-2.28	1.33	1.37
4	A	504	NAD	PN-O3	2.22	1.61	1.59

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	NAD	N3A-C2A-N1A	-6.62	118.56	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	504	NAD	N3A-C2A-N1A	-6.50	118.74	128.58
4	A	504	NAD	C5A-C4A-N3A	-4.69	120.26	126.72
4	B	503	NAD	C5A-C4A-N3A	-4.56	120.43	126.72
4	B	503	NAD	N9A-C8A-N7A	-4.11	108.10	113.94
4	B	503	NAD	C6N-N1N-C2N	-4.01	118.47	121.88
4	A	504	NAD	N9A-C8A-N7A	-3.96	108.32	113.94
3	A	503	CIT	O6-C6-C3	3.94	120.70	113.14
4	B	503	NAD	C4D-O4D-C1D	-3.78	106.47	109.92
3	B	502	CIT	O6-C6-C3	3.78	120.39	113.14
4	A	504	NAD	C6N-N1N-C2N	-3.65	118.77	121.88
4	B	503	NAD	C2B-C3B-C4B	-3.51	95.83	102.61
4	A	504	NAD	C2B-C3B-C4B	-3.42	96.00	102.61
4	B	503	NAD	C2A-N3A-C4A	3.24	119.75	111.83
4	A	504	NAD	C2A-N3A-C4A	3.23	119.71	111.83
4	A	504	NAD	C5A-N7A-C8A	3.07	108.28	103.45
4	B	503	NAD	C5A-N7A-C8A	3.04	108.23	103.45
4	A	504	NAD	C6A-C5A-C4A	2.80	121.00	117.18
4	B	503	NAD	C5A-C6A-N6A	-2.76	116.46	123.29
4	A	504	NAD	C4A-C5A-N7A	-2.71	107.48	110.58
4	A	504	NAD	C5A-C6A-N6A	-2.68	116.66	123.29
4	B	503	NAD	C6A-C5A-C4A	2.66	120.81	117.18
4	B	503	NAD	C4A-C5A-N7A	-2.62	107.59	110.58
4	A	504	NAD	C5A-C4A-N9A	2.49	108.53	105.81
4	B	503	NAD	N3A-C4A-N9A	2.39	131.23	127.17
4	A	504	NAD	N3A-C4A-N9A	2.38	131.21	127.17
4	B	503	NAD	O4B-C4B-C3B	-2.36	100.48	105.15
4	A	504	NAD	C4D-O4D-C1D	-2.35	107.77	109.92
4	B	503	NAD	C5A-C4A-N9A	2.32	108.34	105.81
4	A	504	NAD	C2D-C3D-C4D	-2.14	98.46	102.61
4	A	504	NAD	O4B-C4B-C3B	-2.12	100.94	105.15
4	B	503	NAD	C4A-N9A-C1B	-2.08	121.77	126.63
4	B	503	NAD	C2D-C3D-C4D	-2.03	98.70	102.61
4	B	503	NAD	O4D-C4D-C3D	-2.02	101.14	105.15

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	CIT	C1-C2-C3-O7
3	A	503	CIT	O7-C3-C6-O5
3	A	503	CIT	O7-C3-C6-O6
3	A	503	CIT	C4-C3-C6-O5

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Mol	Chain	Res	Type	Atoms
3	A	503	CIT	C4-C3-C6-O6
3	B	502	CIT	C2-C3-C6-O5
3	B	502	CIT	C2-C3-C6-O6
3	B	502	CIT	O7-C3-C6-O5
3	B	502	CIT	O7-C3-C6-O6
4	A	504	NAD	C5D-O5D-PN-O3
4	A	504	NAD	C5D-O5D-PN-O1N
4	A	504	NAD	C5D-O5D-PN-O2N
4	A	504	NAD	O4D-C1D-N1N-C2N
4	A	504	NAD	O4D-C1D-N1N-C6N
4	A	504	NAD	C2D-C1D-N1N-C2N
4	B	503	NAD	C5D-O5D-PN-O3
4	B	503	NAD	C5D-O5D-PN-O1N
4	B	503	NAD	C3D-C4D-C5D-O5D
3	A	503	CIT	C1-C2-C3-C4
3	A	503	CIT	C1-C2-C3-C6
3	A	503	CIT	C2-C3-C6-O6
4	B	503	NAD	O4D-C4D-C5D-O5D
4	A	504	NAD	C2B-C1B-N9A-C8A
4	B	503	NAD	C2B-C1B-N9A-C8A
4	A	504	NAD	C4B-C5B-O5B-PA
4	A	504	NAD	PN-O3-PA-O2A
4	A	504	NAD	C2B-C1B-N9A-C4A
4	B	503	NAD	C2B-C1B-N9A-C4A
3	A	503	CIT	C2-C3-C6-O5
4	B	503	NAD	C4B-C5B-O5B-PA
4	A	504	NAD	C2D-C1D-N1N-C6N
4	A	504	NAD	O4B-C1B-N9A-C8A
4	B	503	NAD	O4B-C1B-N9A-C8A
2	A	502	EDO	O1-C1-C2-O2
4	A	504	NAD	PN-O3-PA-O1A
4	B	503	NAD	C4D-C5D-O5D-PN
3	B	502	CIT	C2-C3-C4-C5

There are no ring outliers.

5 monomers are involved in 15 short contacts:

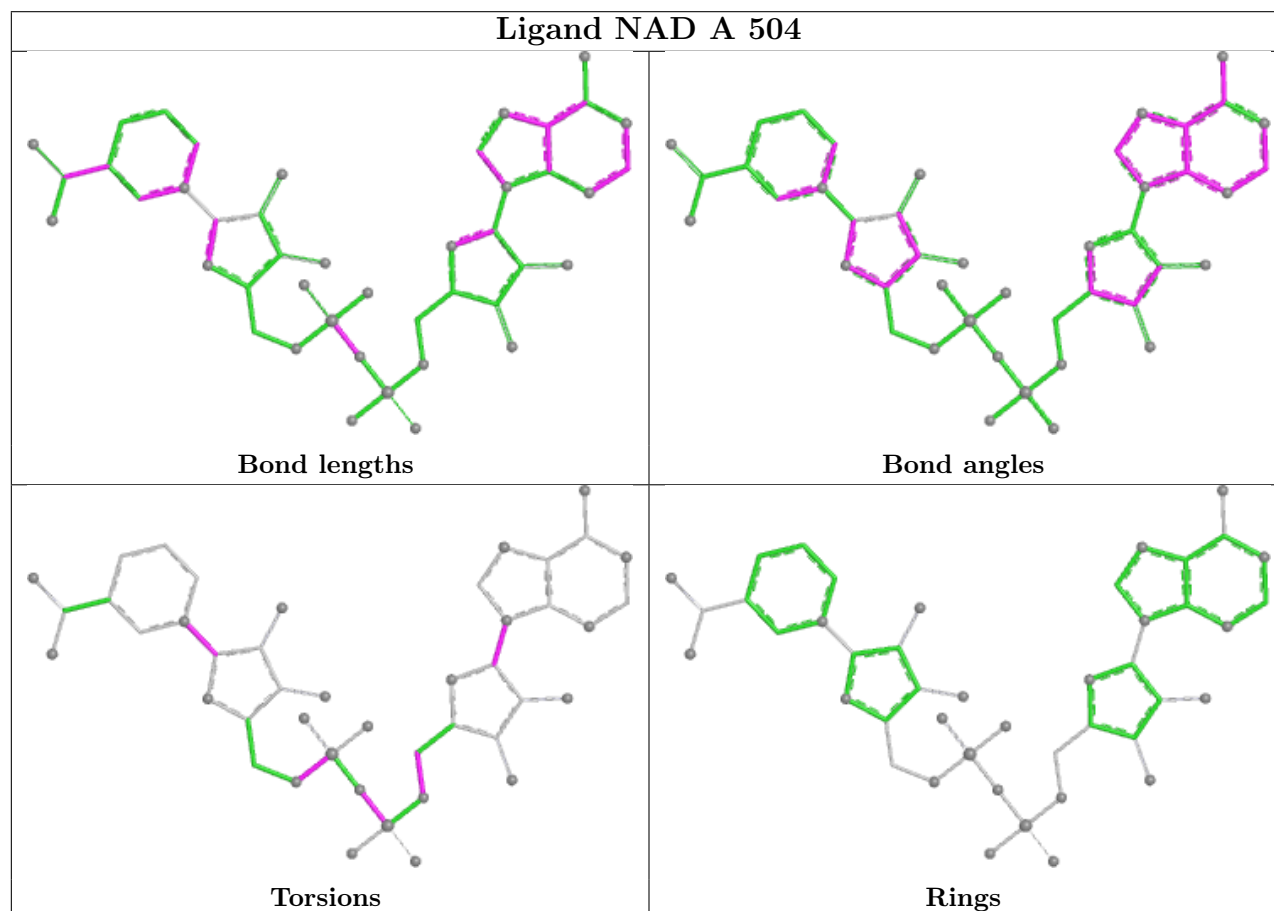
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	CIT	3	0
2	A	501	EDO	1	0
4	A	504	NAD	4	0
4	B	503	NAD	4	0

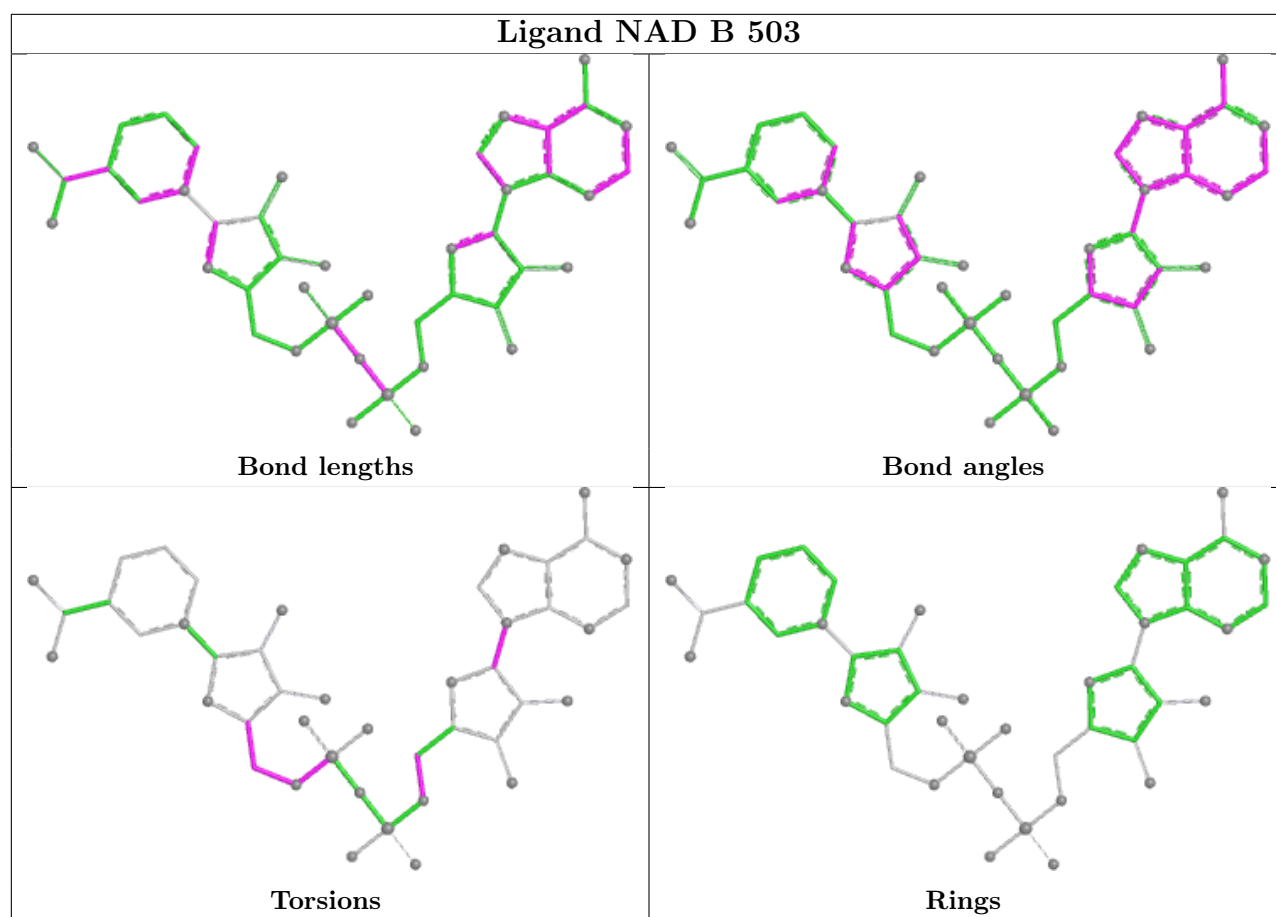
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	CIT	3	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	488/497 (98%)	-0.51	0	100 100	36, 68, 101, 126	0
1	B	487/497 (97%)	-0.40	2 (0%)	88 75	46, 80, 119, 162	0
All	All	975/994 (98%)	-0.45	2 (0%)	91 83	36, 73, 115, 162	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	251	GLY	2.8
1	B	4	LEU	2.3

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(Å ²)	Q<0.9
2	EDO	B	501	4/4	0.77	0.09	76,91,93,93	0
2	EDO	A	501	4/4	0.78	0.12	76,79,83,84	0
4	NAD	B	503	44/44	0.79	0.17	142,184,222,229	0

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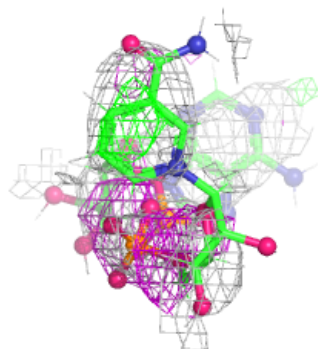
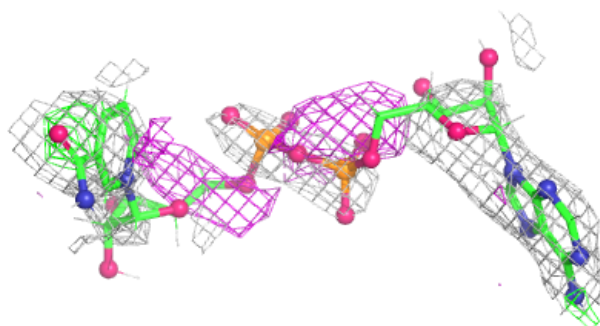
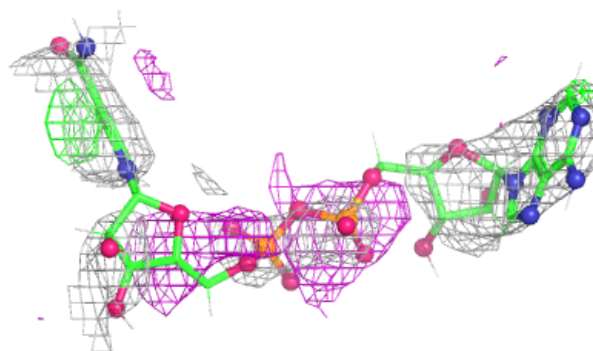
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAD	A	504	44/44	0.80	0.18	132,185,242,245	0
2	EDO	A	502	4/4	0.85	0.14	71,85,87,87	0
3	CIT	A	503	13/13	0.93	0.08	80,87,105,111	0
3	CIT	B	502	13/13	0.93	0.10	98,106,127,127	0

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.

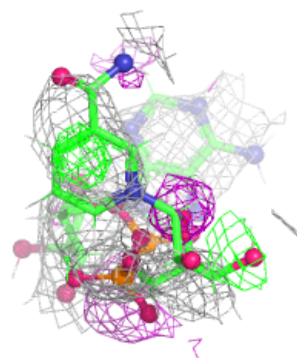
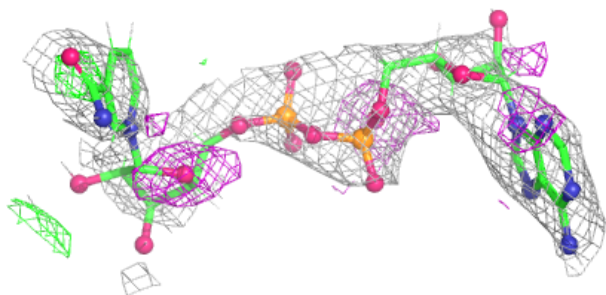
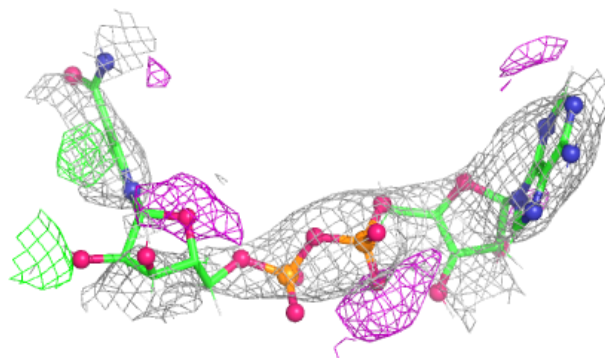
Electron density around NAD B 503:

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



Electron density around NAD A 504:

$2mF_o-DF_c$ (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.