



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:46 PM UTC

PDB ID : 1EVJ / pdb_00001evj
Title : CRYSTAL STRUCTURE OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE (GFOR) DELTA1-22 S64D
Authors : Lott, J.S.; Halbig, D.; Baker, H.M.; Hardman, M.J.; Sprenger, G.A.; Baker, E.N.
Deposited on : 2000-04-20
Resolution : 2.70 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

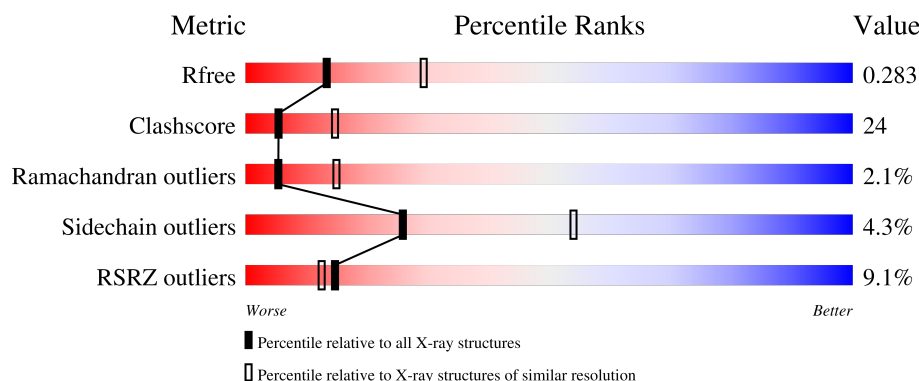
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	352	
1	B	352	
1	C	352	
1	D	352	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10609 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.

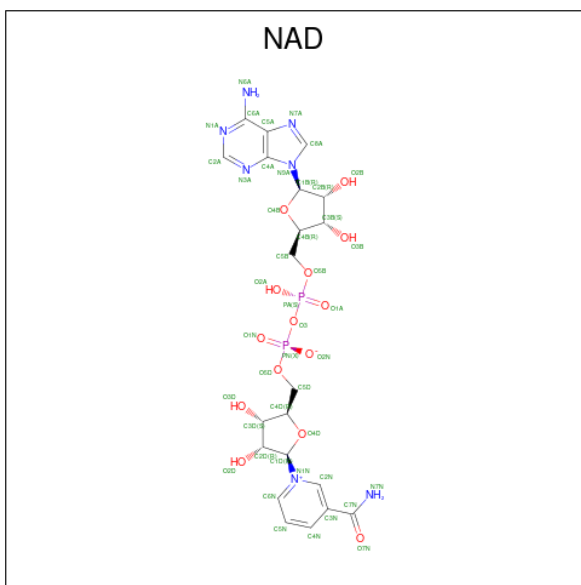
- Molecule 1 is a protein called GLUCOSE-FRUCTOSE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2583	1626	450	491	16			
1	B	338	Total	C	N	O	S	0	0	0
			2578	1618	455	490	15			
1	C	337	Total	C	N	O	S	0	0	0
			2579	1619	452	493	15			
1	D	338	Total	C	N	O	S	0	0	0
			2563	1611	446	491	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	ASP	SER	engineered mutation	UNP Q07982
B	64	ASP	SER	engineered mutation	UNP Q07982
C	64	ASP	SER	engineered mutation	UNP Q07982
D	64	ASP	SER	engineered mutation	UNP Q07982

- 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
2	C	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	D	1	Total 44	C 21	N 7	O 14	P 2	0	0

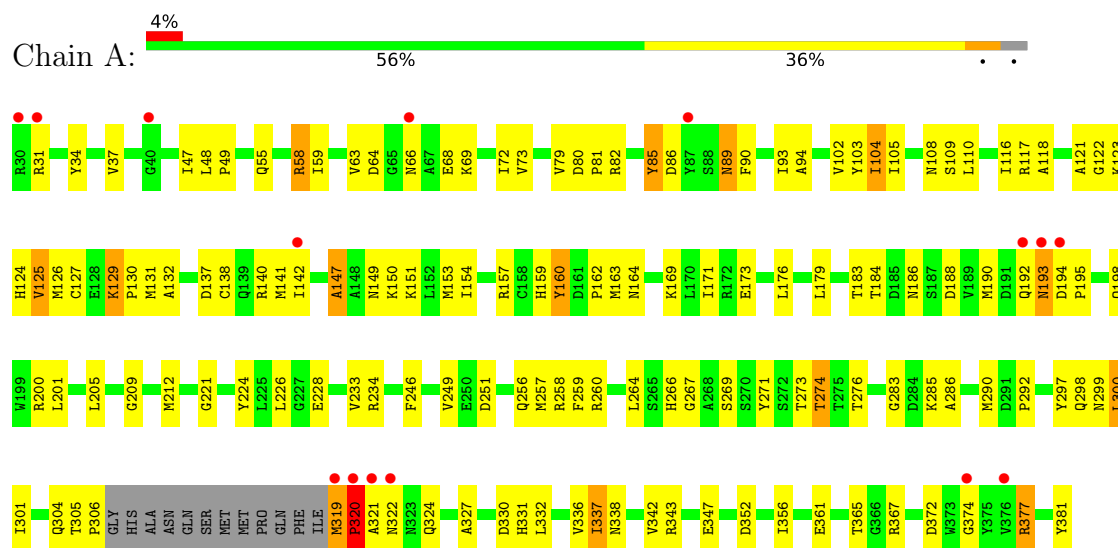
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	52	Total O 52 52	0	0
3	B	21	Total O 21 21	0	0
3	C	36	Total O 36 36	0	0
3	D	21	Total O 21 21	0	0

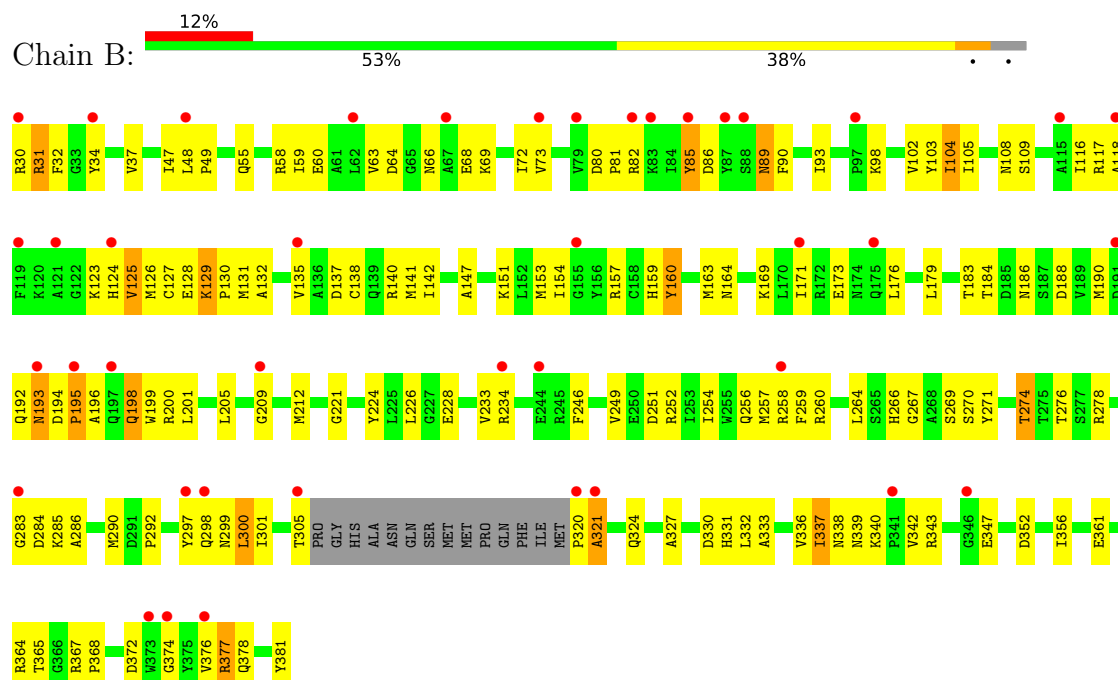
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

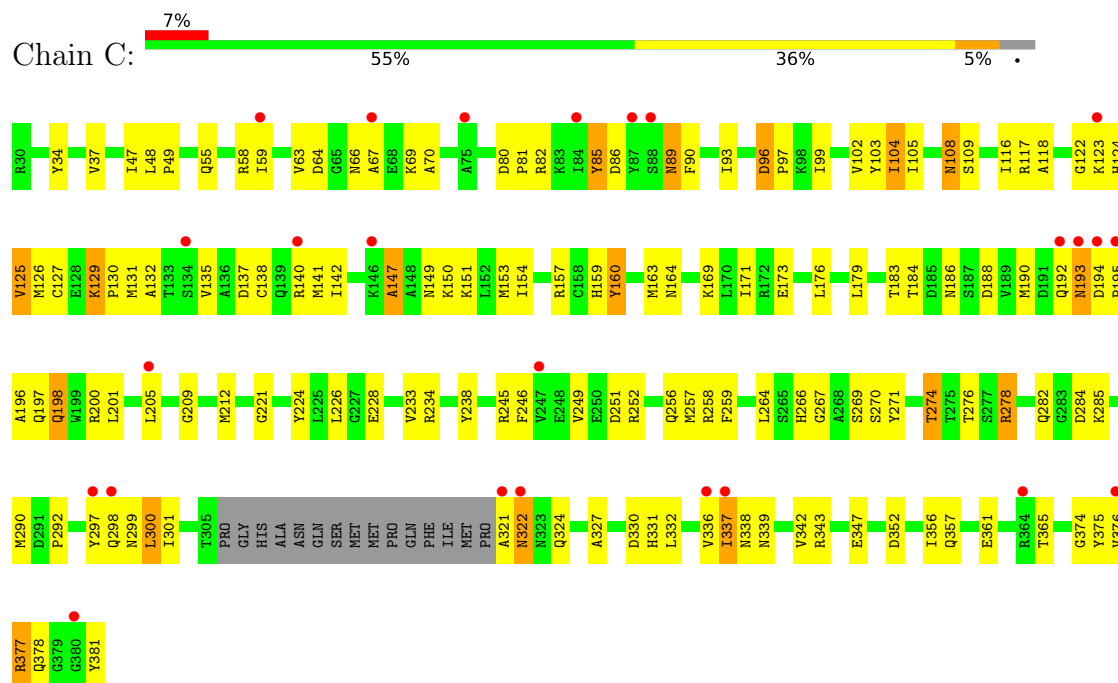
• Molecule 1: GLUCOSE-FRUCTOSE OXIDOREDUCTASE



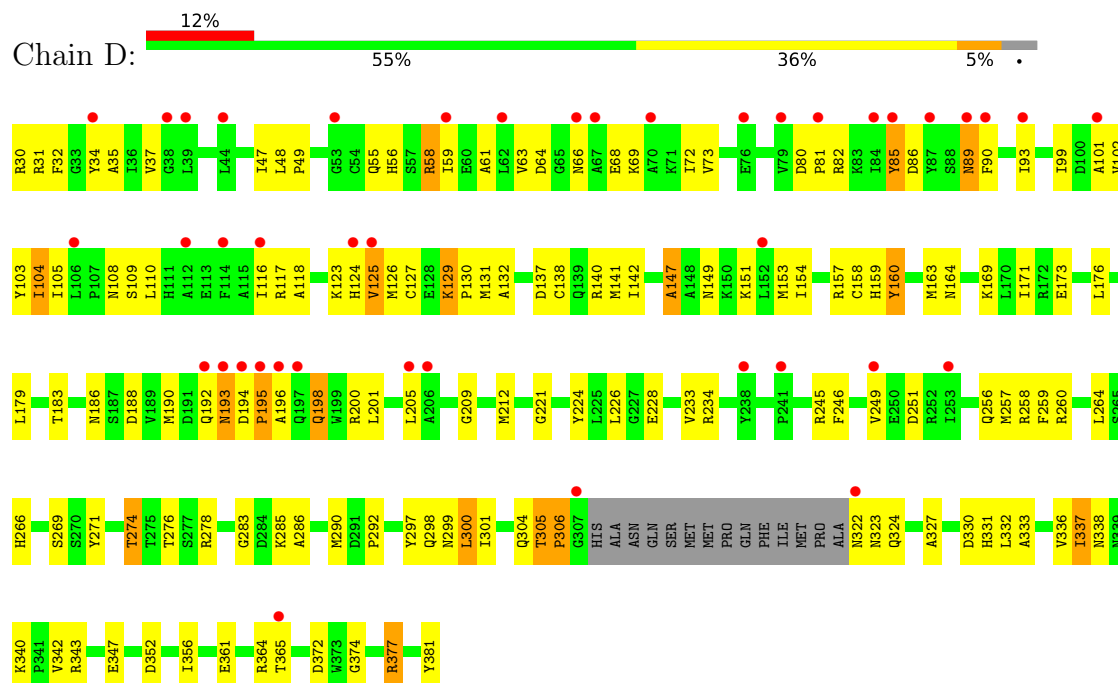
• Molecule 1: GLUCOSE-FRUCTOSE OXIDOREDUCTASE



• Molecule 1: GLUCOSE-FRUCTOSE OXIDOREDUCTASE



• Molecule 1: GLUCOSE-FRUCTOSE OXIDOREDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	47.71Å 91.46Å 98.92Å 64.53° 84.45° 75.28°	Depositor
Resolution (Å)	39.14 – 2.70 39.14 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.8 (39.14-2.70) 96.9 (39.14-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.69Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.241 , 0.284 0.240 , 0.283	Depositor DCC
R_{free} test set	3897 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.670	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 75.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,-k+l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10609	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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

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	0.47	0/2635	1.02	10/3573 (0.3%)
1	B	0.43	0/2629	0.99	8/3564 (0.2%)
1	C	0.48	0/2629	0.99	12/3562 (0.3%)
1	D	0.43	0/2614	0.97	9/3546 (0.3%)
All	All	0.45	0/10507	0.99	39/14245 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	ARG	CD-NE-CZ	14.56	144.78	124.40
1	C	58	ARG	CD-NE-CZ	14.42	144.59	124.40
1	B	58	ARG	CD-NE-CZ	14.36	144.51	124.40
1	D	58	ARG	CD-NE-CZ	14.36	144.50	124.40
1	A	58	ARG	NE-CZ-NH2	12.86	130.77	119.20
1	B	58	ARG	NE-CZ-NH2	12.75	130.67	119.20
1	B	58	ARG	NE-CZ-NH1	-12.03	109.47	121.50
1	A	58	ARG	NE-CZ-NH1	-11.98	109.52	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	58	ARG	NE-CZ-NH2	-10.69	109.58	119.20
1	C	58	ARG	NE-CZ-NH2	-10.51	109.74	119.20
1	C	58	ARG	NE-CZ-NH1	9.16	130.66	121.50
1	C	47	ILE	N-CA-C	9.14	119.12	110.53
1	D	58	ARG	NE-CZ-NH1	9.12	130.62	121.50
1	B	47	ILE	N-CA-C	8.89	118.89	110.53
1	D	47	ILE	N-CA-C	8.87	118.87	110.53
1	A	47	ILE	N-CA-C	8.69	118.76	110.42
1	A	367	ARG	CA-C-N	-8.50	112.05	120.21
1	A	367	ARG	C-N-CA	-8.50	112.05	120.21
1	B	274	THR	N-CA-C	6.93	119.27	110.33
1	C	274	THR	N-CA-C	6.92	119.25	110.33
1	D	274	THR	N-CA-C	6.69	118.96	110.33
1	A	274	THR	N-CA-C	6.60	118.85	110.33
1	C	96	ASP	CA-C-N	6.58	126.21	119.56
1	C	96	ASP	C-N-CA	6.58	126.21	119.56
1	C	196	ALA	N-CA-C	-5.95	105.88	113.02
1	B	125	VAL	N-CA-C	5.68	116.77	108.53
1	C	125	VAL	N-CA-C	5.60	116.66	108.53
1	D	125	VAL	N-CA-C	5.55	116.47	108.48
1	B	108	ASN	N-CA-C	5.44	117.91	111.33
1	A	125	VAL	N-CA-C	5.43	116.40	108.53
1	C	108	ASN	N-CA-C	5.36	117.81	111.33
1	C	374	GLY	N-CA-C	5.34	122.56	114.61
1	D	108	ASN	N-CA-C	5.34	117.79	111.33
1	B	374	GLY	N-CA-C	5.31	122.53	114.61
1	A	108	ASN	N-CA-C	5.27	117.70	111.33
1	D	374	GLY	N-CA-C	5.25	122.43	114.61
1	A	374	GLY	N-CA-C	5.12	122.23	114.61
1	D	278	ARG	N-CA-C	5.11	116.72	108.34
1	C	278	ARG	N-CA-C	5.08	116.68	108.34

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	TYR	Sidechain
1	B	160	TYR	Sidechain
1	C	160	TYR	Sidechain
1	D	160	TYR	Sidechain

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	2583	0	2479	122	0
1	B	2578	0	2470	130	0
1	C	2579	0	2478	121	0
1	D	2563	0	2443	125	0
2	A	44	0	26	0	0
2	B	44	0	26	1	0
2	C	44	0	26	0	0
2	D	44	0	26	1	0
3	A	52	0	0	1	0
3	B	21	0	0	0	0
3	C	36	0	0	1	0
3	D	21	0	0	3	0
All	All	10609	0	9974	489	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 24.

All (489) 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:D:292:PRO:HD2	1:D:300:LEU:HD23	1.48	0.95
1:A:292:PRO:HD2	1:A:300:LEU:HD23	1.48	0.94
1:C:292:PRO:HD2	1:C:300:LEU:HD23	1.50	0.93
1:B:198:GLN:NE2	1:B:200:ARG:H	1.67	0.93
1:B:292:PRO:HD2	1:B:300:LEU:HD23	1.50	0.91
1:A:162:PRO:HG3	1:A:319:MET:HB3	1.53	0.90
1:B:331:HIS:HE1	1:B:343:ARG:H	1.22	0.86
1:C:331:HIS:HE1	1:C:343:ARG:H	1.23	0.85
1:B:124:HIS:HD2	1:B:151:LYS:H	1.24	0.85
1:B:86:ASP:H	1:B:89:ASN:HD21	1.22	0.84
1:C:86:ASP:H	1:C:89:ASN:HD21	1.22	0.84
1:A:331:HIS:HE1	1:A:343:ARG:H	1.22	0.84
1:A:86:ASP:H	1:A:89:ASN:HD21	1.23	0.84
1:D:331:HIS:HE1	1:D:343:ARG:H	1.24	0.84
1:C:290:MET:HG2	1:C:301:ILE:HG22	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:PRO:CG	1:A:319:MET:HB3	2.09	0.83
1:B:124:HIS:CD2	1:B:151:LYS:H	1.97	0.82
1:D:86:ASP:H	1:D:89:ASN:HD21	1.22	0.82
1:B:290:MET:HG2	1:B:301:ILE:HG22	1.60	0.81
1:A:290:MET:HG2	1:A:301:ILE:HG22	1.61	0.80
1:D:290:MET:HG2	1:D:301:ILE:HG22	1.59	0.80
1:A:163:MET:HA	1:A:163:MET:HE2	1.64	0.80
1:D:163:MET:HA	1:D:163:MET:HE2	1.63	0.79
1:A:124:HIS:HD2	1:A:151:LYS:H	1.31	0.78
1:B:163:MET:HE2	1:B:163:MET:HA	1.65	0.78
1:C:163:MET:HE2	1:C:163:MET:HA	1.65	0.76
1:D:124:HIS:HD2	1:D:151:LYS:H	1.32	0.76
1:D:286:ALA:HB2	1:D:305:THR:HG23	1.68	0.76
1:A:124:HIS:CD2	1:A:151:LYS:H	2.07	0.70
1:B:331:HIS:CE1	1:B:343:ARG:H	2.09	0.69
1:A:162:PRO:HG3	1:A:319:MET:CB	2.23	0.69
1:C:86:ASP:H	1:C:89:ASN:ND2	1.90	0.69
1:A:169:LYS:O	1:A:173:GLU:HG3	1.93	0.69
1:C:86:ASP:N	1:C:89:ASN:HD21	1.91	0.69
1:C:169:LYS:O	1:C:173:GLU:HG3	1.93	0.68
1:D:124:HIS:CD2	1:D:151:LYS:H	2.11	0.68
1:D:86:ASP:H	1:D:89:ASN:ND2	1.90	0.68
1:D:86:ASP:N	1:D:89:ASN:HD21	1.92	0.68
1:B:169:LYS:O	1:B:173:GLU:HG3	1.93	0.68
1:B:86:ASP:N	1:B:89:ASN:HD21	1.92	0.68
1:D:138:CYS:HA	1:D:141:MET:HE3	1.76	0.68
1:B:138:CYS:HA	1:B:141:MET:HE3	1.76	0.67
1:D:93:ILE:HD12	1:D:123:LYS:HD2	1.77	0.67
1:A:102:VAL:HG11	1:A:118:ALA:HB1	1.78	0.66
1:B:102:VAL:HG11	1:B:118:ALA:HB1	1.77	0.66
1:D:169:LYS:O	1:D:173:GLU:HG3	1.95	0.66
1:B:86:ASP:H	1:B:89:ASN:ND2	1.90	0.66
1:B:198:GLN:HE21	1:B:198:GLN:C	2.02	0.66
1:D:102:VAL:HG11	1:D:118:ALA:HB1	1.78	0.66
1:B:93:ILE:HD12	1:B:123:LYS:HD2	1.77	0.66
1:C:331:HIS:CE1	1:C:343:ARG:H	2.10	0.66
1:A:93:ILE:HD12	1:A:123:LYS:HD2	1.77	0.66
1:A:377:ARG:HG3	1:A:381:TYR:CE2	2.31	0.66
1:C:93:ILE:HD12	1:C:123:LYS:HD2	1.77	0.66
1:C:124:HIS:HD2	1:C:151:LYS:H	1.44	0.65
1:C:102:VAL:HG11	1:C:118:ALA:HB1	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:ILE:HD12	1:D:104:ILE:N	2.12	0.65
1:A:138:CYS:HA	1:A:141:MET:HE3	1.77	0.65
1:B:377:ARG:HG3	1:B:381:TYR:CE2	2.31	0.65
1:A:331:HIS:CE1	1:A:343:ARG:H	2.09	0.65
1:C:124:HIS:CD2	1:C:151:LYS:H	2.15	0.65
1:A:86:ASP:N	1:A:89:ASN:HD21	1.92	0.65
1:D:331:HIS:CE1	1:D:343:ARG:H	2.10	0.65
1:B:104:ILE:N	1:B:104:ILE:HD12	2.12	0.64
1:C:194:ASP:CB	1:C:197:GLN:HE21	2.09	0.64
1:C:138:CYS:HA	1:C:141:MET:HE3	1.77	0.64
1:A:86:ASP:H	1:A:89:ASN:ND2	1.91	0.64
1:B:376:VAL:HG13	1:B:378:GLN:HE21	1.63	0.63
1:A:157:ARG:HH11	1:A:324:GLN:HE22	1.47	0.63
1:C:104:ILE:HD12	1:C:104:ILE:N	2.12	0.63
1:B:284:ASP:O	1:D:274:THR:HG23	1.98	0.63
1:A:306:PRO:HG2	1:C:274:THR:CG2	2.29	0.63
1:A:104:ILE:HD12	1:A:104:ILE:N	2.13	0.62
1:B:337:ILE:HG22	1:B:337:ILE:O	1.99	0.62
1:A:132:ALA:HB2	1:A:141:MET:HE1	1.81	0.62
1:A:164:ASN:ND2	1:A:224:TYR:OH	2.32	0.62
1:B:164:ASN:ND2	1:B:224:TYR:OH	2.32	0.62
1:D:201:LEU:HD22	1:D:245:ARG:O	1.98	0.62
1:D:377:ARG:HG3	1:D:381:TYR:CE2	2.35	0.62
1:A:286:ALA:CB	1:A:305:THR:HG22	2.29	0.62
1:D:132:ALA:HB2	1:D:141:MET:HE1	1.82	0.62
1:C:337:ILE:O	1:C:337:ILE:HG22	2.01	0.61
1:B:198:GLN:HE21	1:B:199:TRP:N	1.97	0.61
1:C:132:ALA:HB2	1:C:141:MET:HE1	1.80	0.61
1:C:164:ASN:ND2	1:C:224:TYR:OH	2.32	0.61
1:B:55:GLN:N	1:B:330:ASP:OD2	2.32	0.61
1:B:132:ALA:HB2	1:B:141:MET:HE1	1.83	0.61
1:D:337:ILE:HG22	1:D:337:ILE:O	2.00	0.61
1:B:198:GLN:HE21	1:B:200:ARG:H	1.46	0.61
1:B:104:ILE:HD12	1:B:104:ILE:H	1.66	0.61
1:C:157:ARG:HH11	1:C:324:GLN:HE22	1.49	0.61
1:C:104:ILE:HD12	1:C:104:ILE:H	1.66	0.60
1:A:337:ILE:O	1:A:337:ILE:HG22	2.00	0.60
1:D:164:ASN:ND2	1:D:224:TYR:OH	2.35	0.60
1:D:179:LEU:HG	3:D:699:HOH:O	2.00	0.60
1:D:104:ILE:HD12	1:D:104:ILE:H	1.66	0.60
1:D:129:LYS:HE2	1:D:129:LYS:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:THR:HG23	1:C:284:ASP:O	2.02	0.59
1:C:129:LYS:O	1:C:129:LYS:HE2	2.02	0.59
1:C:201:LEU:HD22	1:C:245:ARG:O	2.03	0.59
1:D:69:LYS:O	1:D:73:VAL:HG23	2.04	0.58
1:A:286:ALA:HB2	1:A:305:THR:HG22	1.84	0.58
1:B:194:ASP:C	1:B:196:ALA:H	2.11	0.58
1:C:153:MET:SD	1:C:342:VAL:HG21	2.43	0.58
1:B:129:LYS:HE2	1:B:129:LYS:O	2.04	0.58
1:D:352:ASP:O	1:D:356:ILE:HG13	2.03	0.58
1:A:129:LYS:O	1:A:129:LYS:HE2	2.04	0.57
1:B:48:LEU:HD22	1:B:59:ILE:HD13	1.85	0.57
1:C:85:TYR:N	1:C:85:TYR:CD2	2.72	0.57
1:C:321:ALA:O	1:C:322:ASN:HB2	2.01	0.57
1:A:48:LEU:HD22	1:A:59:ILE:HD13	1.86	0.57
1:C:48:LEU:HD22	1:C:59:ILE:HD13	1.85	0.57
1:B:48:LEU:HB2	1:B:49:PRO:HD3	1.86	0.57
1:D:157:ARG:HH11	1:D:324:GLN:HE22	1.50	0.57
1:C:132:ALA:HB2	1:C:141:MET:CE	2.35	0.56
1:A:48:LEU:HB2	1:A:49:PRO:HD3	1.87	0.56
1:A:85:TYR:CD2	1:A:85:TYR:N	2.73	0.56
1:A:352:ASP:O	1:A:356:ILE:HG13	2.04	0.56
1:B:299:ASN:C	1:B:300:LEU:HD22	2.30	0.56
1:D:48:LEU:HD22	1:D:59:ILE:HD13	1.86	0.56
1:A:104:ILE:HD12	1:A:104:ILE:H	1.68	0.56
1:C:299:ASN:C	1:C:300:LEU:HD22	2.31	0.56
1:B:286:ALA:HB2	1:B:305:THR:HG22	1.86	0.56
1:D:85:TYR:N	1:D:85:TYR:CD2	2.73	0.56
1:A:299:ASN:C	1:A:300:LEU:HD22	2.31	0.56
1:D:48:LEU:HB2	1:D:49:PRO:HD3	1.87	0.56
1:B:85:TYR:N	1:B:85:TYR:CD2	2.73	0.55
1:D:299:ASN:C	1:D:300:LEU:HD22	2.31	0.55
1:C:160:TYR:OH	1:C:343:ARG:HB3	2.06	0.55
1:D:209:GLY:HA2	1:D:249:VAL:HB	1.88	0.55
1:C:48:LEU:HB2	1:C:49:PRO:HD3	1.87	0.55
1:D:132:ALA:HB2	1:D:141:MET:CE	2.36	0.55
1:C:66:ASN:HB2	3:C:646:HOH:O	2.06	0.55
1:A:209:GLY:HA2	1:A:249:VAL:HB	1.89	0.55
1:C:159:HIS:O	1:C:343:ARG:NH1	2.39	0.55
1:C:209:GLY:HA2	1:C:249:VAL:HB	1.89	0.55
1:D:260:ARG:HH22	1:D:372:ASP:CG	2.15	0.55
1:C:80:ASP:C	1:C:82:ARG:H	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ARG:HH11	1:B:324:GLN:HE22	1.56	0.54
1:D:153:MET:SD	1:D:342:VAL:HG21	2.47	0.54
1:A:105:ILE:HG22	1:A:105:ILE:O	2.06	0.54
1:A:132:ALA:HB2	1:A:141:MET:CE	2.37	0.54
1:C:105:ILE:O	1:C:105:ILE:HG22	2.07	0.54
1:A:153:MET:SD	1:A:342:VAL:HG21	2.48	0.54
1:B:85:TYR:N	1:B:85:TYR:HD2	2.06	0.54
1:A:80:ASP:C	1:A:82:ARG:H	2.16	0.53
1:B:80:ASP:C	1:B:82:ARG:H	2.16	0.53
1:B:68:GLU:O	1:B:72:ILE:HG13	2.09	0.53
1:B:132:ALA:HB2	1:B:141:MET:CE	2.37	0.53
1:B:160:TYR:OH	1:B:343:ARG:HB3	2.08	0.53
1:C:99:ILE:HG22	1:C:123:LYS:HD3	1.91	0.53
1:D:80:ASP:C	1:D:82:ARG:H	2.16	0.53
1:C:198:GLN:HE21	1:C:200:ARG:H	1.56	0.53
1:A:85:TYR:N	1:A:85:TYR:HD2	2.06	0.53
1:C:85:TYR:N	1:C:85:TYR:HD2	2.05	0.53
1:A:264:LEU:HD11	1:C:238:TYR:HB3	1.91	0.53
1:B:209:GLY:HA2	1:B:249:VAL:HB	1.89	0.53
1:B:60:GLU:HG2	1:B:98:LYS:O	2.09	0.53
1:B:153:MET:SD	1:B:342:VAL:HG21	2.49	0.53
1:D:55:GLN:N	1:D:330:ASP:OD2	2.34	0.53
1:D:85:TYR:N	1:D:85:TYR:HD2	2.06	0.53
1:D:194:ASP:C	1:D:196:ALA:H	2.16	0.53
1:A:159:HIS:O	1:A:343:ARG:NH1	2.41	0.53
1:B:367:ARG:HB3	1:B:368:PRO:HD2	1.91	0.52
1:D:160:TYR:OH	1:D:343:ARG:HB3	2.07	0.52
1:C:171:ILE:HG12	1:C:176:LEU:HD22	1.92	0.52
1:D:105:ILE:HG22	1:D:105:ILE:O	2.09	0.52
1:A:157:ARG:HH11	1:A:324:GLN:NE2	2.07	0.52
1:A:160:TYR:OH	1:A:343:ARG:HB3	2.09	0.52
1:A:306:PRO:HG2	1:C:274:THR:HG22	1.92	0.51
1:A:55:GLN:N	1:A:330:ASP:OD2	2.40	0.51
1:A:79:VAL:HG13	3:A:687:HOH:O	2.10	0.51
1:B:30:ARG:CB	1:B:31:ARG:HH11	2.24	0.51
1:A:69:LYS:O	1:A:73:VAL:HG23	2.11	0.51
1:A:171:ILE:HG12	1:A:176:LEU:HD22	1.92	0.51
1:B:105:ILE:HG22	1:B:105:ILE:O	2.11	0.51
1:B:198:GLN:HE22	1:B:200:ARG:H	1.55	0.51
1:C:375:TYR:OH	1:C:377:ARG:HG2	2.11	0.51
1:A:163:MET:HE2	1:A:163:MET:CA	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:MET:HA	1:B:163:MET:CE	2.38	0.51
1:C:55:GLN:N	1:C:330:ASP:OD2	2.39	0.51
1:B:171:ILE:HG12	1:B:176:LEU:HD22	1.93	0.51
1:A:292:PRO:HG2	1:A:299:ASN:HA	1.93	0.50
1:B:128:GLU:OE1	2:B:501:NAD:H2N	2.11	0.50
1:C:198:GLN:HE21	1:C:198:GLN:C	2.19	0.50
1:D:34:TYR:OH	1:D:332:LEU:HB3	2.12	0.50
1:D:90:PHE:O	1:D:93:ILE:HG23	2.12	0.50
1:A:37:VAL:HG23	1:A:102:VAL:HG23	1.94	0.50
1:B:194:ASP:O	1:B:196:ALA:N	2.44	0.50
1:C:179:LEU:HD13	1:C:226:LEU:HD23	1.94	0.50
1:A:122:GLY:O	1:A:150:LYS:HE3	2.12	0.50
1:B:37:VAL:HG23	1:B:102:VAL:HG23	1.94	0.50
1:B:90:PHE:O	1:B:93:ILE:HG23	2.12	0.50
1:C:157:ARG:HH11	1:C:324:GLN:NE2	2.09	0.50
1:D:171:ILE:HG12	1:D:176:LEU:HD22	1.93	0.50
1:A:138:CYS:O	1:A:142:ILE:HG13	2.12	0.49
1:A:68:GLU:O	1:A:72:ILE:HG13	2.13	0.49
1:A:90:PHE:O	1:A:93:ILE:HG23	2.12	0.49
1:A:260:ARG:HH22	1:A:372:ASP:CG	2.19	0.49
1:B:163:MET:HE2	1:B:163:MET:CA	2.40	0.49
1:A:179:LEU:HD13	1:A:226:LEU:HD23	1.95	0.49
1:B:209:GLY:CA	1:B:249:VAL:HB	2.43	0.49
1:C:37:VAL:HG23	1:C:102:VAL:HG23	1.94	0.49
1:C:209:GLY:CA	1:C:249:VAL:HB	2.43	0.49
1:C:90:PHE:O	1:C:93:ILE:HG23	2.13	0.48
1:C:246:PHE:CG	1:C:251:ASP:HB2	2.48	0.48
1:D:37:VAL:HG23	1:D:102:VAL:HG23	1.94	0.48
1:B:138:CYS:O	1:B:142:ILE:HG13	2.13	0.48
1:B:194:ASP:C	1:B:196:ALA:N	2.72	0.48
1:D:64:ASP:C	1:D:66:ASN:H	2.22	0.48
1:D:163:MET:HE2	1:D:163:MET:CA	2.38	0.48
1:D:179:LEU:HD13	1:D:226:LEU:HD23	1.95	0.48
1:D:209:GLY:CA	1:D:249:VAL:HB	2.42	0.48
1:D:292:PRO:HG2	1:D:299:ASN:HA	1.95	0.48
1:C:138:CYS:O	1:C:142:ILE:HG13	2.13	0.48
1:A:209:GLY:CA	1:A:249:VAL:HB	2.43	0.48
1:B:37:VAL:HA	1:B:63:VAL:HB	1.95	0.48
1:C:103:TYR:CD2	1:C:126:MET:HG2	2.49	0.48
1:C:198:GLN:NE2	1:C:200:ARG:H	2.11	0.48
1:D:322:ASN:O	1:D:323:ASN:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ASN:N	1:A:89:ASN:HD22	2.11	0.48
1:B:190:MET:HG2	1:B:201:LEU:HD21	1.94	0.48
1:C:37:VAL:HA	1:C:63:VAL:HB	1.96	0.48
1:D:159:HIS:O	1:D:343:ARG:NH1	2.47	0.48
1:D:198:GLN:HA	1:D:198:GLN:NE2	2.28	0.48
1:B:34:TYR:OH	1:B:332:LEU:HB3	2.14	0.48
1:C:69:LYS:O	1:C:70:ALA:C	2.56	0.48
1:B:179:LEU:HD13	1:B:226:LEU:HD23	1.94	0.48
1:B:198:GLN:NE2	1:B:199:TRP:N	2.61	0.48
1:D:138:CYS:O	1:D:142:ILE:HG13	2.13	0.48
1:A:246:PHE:CG	1:A:251:ASP:HB2	2.49	0.47
1:B:64:ASP:C	1:B:66:ASN:H	2.21	0.47
1:B:190:MET:HE1	1:B:200:ARG:HD2	1.96	0.47
1:C:89:ASN:ND2	1:C:89:ASN:H	2.12	0.47
1:D:103:TYR:CD2	1:D:126:MET:HG2	2.49	0.47
1:B:159:HIS:O	1:B:343:ARG:NH1	2.45	0.47
1:A:64:ASP:C	1:A:66:ASN:H	2.22	0.47
1:B:246:PHE:CG	1:B:251:ASP:HB2	2.49	0.47
1:D:99:ILE:O	1:D:99:ILE:HG22	2.14	0.47
1:A:31:ARG:C	1:A:58:ARG:HH21	2.21	0.47
1:A:37:VAL:HA	1:A:63:VAL:HB	1.96	0.47
1:C:290:MET:HG2	1:C:301:ILE:CG2	2.38	0.47
1:B:89:ASN:N	1:B:89:ASN:HD22	2.12	0.47
1:A:147:ALA:C	1:A:149:ASN:H	2.22	0.47
1:B:292:PRO:HG2	1:B:299:ASN:HA	1.97	0.47
1:A:89:ASN:ND2	1:A:89:ASN:H	2.12	0.47
1:A:93:ILE:CD1	1:A:123:LYS:HD2	2.45	0.47
1:B:103:TYR:CD2	1:B:126:MET:HG2	2.49	0.47
1:C:99:ILE:HG22	1:C:99:ILE:O	2.14	0.47
1:D:246:PHE:CG	1:D:251:ASP:HB2	2.49	0.47
1:D:337:ILE:O	1:D:337:ILE:CG2	2.63	0.47
1:A:109:SER:OG	1:A:205:LEU:HA	2.15	0.47
1:A:195:PRO:CB	1:A:201:LEU:HD12	2.45	0.47
1:B:337:ILE:O	1:B:337:ILE:CG2	2.63	0.47
1:D:109:SER:OG	1:D:205:LEU:HA	2.15	0.47
1:B:260:ARG:HH22	1:B:372:ASP:CG	2.22	0.47
1:C:64:ASP:C	1:C:66:ASN:H	2.22	0.47
1:A:102:VAL:HG11	1:A:118:ALA:CB	2.44	0.47
1:C:221:GLY:HA2	1:C:224:TYR:CE2	2.50	0.47
1:B:221:GLY:HA2	1:B:224:TYR:CE2	2.50	0.46
1:B:89:ASN:ND2	1:B:89:ASN:H	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ASP:O	1:B:141:MET:HG3	2.16	0.46
1:C:80:ASP:C	1:C:82:ARG:N	2.73	0.46
1:C:137:ASP:O	1:C:141:MET:HG3	2.15	0.46
1:D:31:ARG:C	1:D:58:ARG:HH21	2.23	0.46
1:C:361:GLU:O	1:C:365:THR:HG23	2.15	0.46
1:C:376:VAL:HG13	1:C:378:GLN:HE21	1.80	0.46
1:D:290:MET:HG2	1:D:301:ILE:CG2	2.38	0.46
1:A:103:TYR:CD2	1:A:126:MET:HG2	2.49	0.46
1:A:319:MET:O	1:A:320:PRO:C	2.58	0.46
1:B:109:SER:OG	1:B:205:LEU:HA	2.16	0.46
1:C:89:ASN:HD22	1:C:89:ASN:N	2.12	0.46
1:D:37:VAL:HA	1:D:63:VAL:HB	1.96	0.46
1:D:93:ILE:CD1	1:D:123:LYS:HD2	2.45	0.46
2:D:503:NAD:H2D	3:D:652:HOH:O	2.16	0.46
1:A:337:ILE:O	1:A:337:ILE:CG2	2.63	0.46
1:B:320:PRO:O	1:B:321:ALA:HB2	2.15	0.46
1:C:190:MET:HE1	1:C:200:ARG:HD2	1.97	0.46
1:C:337:ILE:O	1:C:337:ILE:CG2	2.64	0.46
1:C:352:ASP:O	1:C:356:ILE:HD12	2.15	0.46
1:B:338:ASN:C	1:B:340:LYS:N	2.73	0.46
1:D:68:GLU:O	1:D:72:ILE:HG13	2.14	0.46
1:D:89:ASN:N	1:D:89:ASN:HD22	2.12	0.46
1:D:190:MET:HE1	1:D:200:ARG:HD2	1.98	0.46
1:C:292:PRO:HG2	1:C:299:ASN:HA	1.98	0.46
1:D:157:ARG:HH11	1:D:324:GLN:NE2	2.13	0.46
1:D:89:ASN:ND2	1:D:89:ASN:H	2.12	0.46
1:D:99:ILE:HG22	1:D:123:LYS:HD3	1.98	0.46
1:A:258:ARG:HG3	1:A:264:LEU:CD2	2.46	0.46
1:B:290:MET:HG2	1:B:301:ILE:CG2	2.38	0.46
1:C:109:SER:OG	1:C:205:LEU:HA	2.16	0.46
1:C:224:TYR:HB2	1:C:381:TYR:HB3	1.98	0.46
1:B:254:ILE:HD13	1:D:266:HIS:HB3	1.98	0.45
1:C:34:TYR:OH	1:C:332:LEU:HB3	2.16	0.45
1:C:163:MET:HE2	1:C:163:MET:CA	2.40	0.45
1:C:186:ASN:O	1:C:269:SER:HA	2.16	0.45
1:D:32:PHE:CD1	1:D:333:ALA:HA	2.51	0.45
1:A:190:MET:HE1	1:A:200:ARG:HD2	1.98	0.45
1:A:221:GLY:HA2	1:A:224:TYR:CE2	2.51	0.45
1:B:69:LYS:O	1:B:73:VAL:HG23	2.15	0.45
1:C:163:MET:HA	1:C:163:MET:CE	2.39	0.45
1:B:80:ASP:C	1:B:82:ARG:N	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ASN:HD22	1:B:89:ASN:C	2.23	0.45
1:B:193:ASN:O	1:B:193:ASN:CG	2.59	0.45
1:D:160:TYR:HH	1:D:343:ARG:HB3	1.81	0.45
1:D:193:ASN:O	1:D:193:ASN:CG	2.60	0.45
1:D:137:ASP:O	1:D:141:MET:HG3	2.15	0.45
1:D:194:ASP:O	1:D:196:ALA:N	2.49	0.45
1:B:131:MET:HG2	1:B:141:MET:HE1	1.98	0.45
1:C:193:ASN:CG	1:C:193:ASN:O	2.59	0.45
1:A:137:ASP:O	1:A:141:MET:HG3	2.16	0.45
1:A:193:ASN:CG	1:A:193:ASN:O	2.59	0.45
1:A:233:VAL:HG22	1:A:257:MET:HG2	1.98	0.45
1:D:102:VAL:HG11	1:D:118:ALA:CB	2.44	0.45
1:D:198:GLN:NE2	1:D:198:GLN:CA	2.79	0.45
1:D:221:GLY:HA2	1:D:224:TYR:CE2	2.51	0.45
1:D:258:ARG:HG3	1:D:264:LEU:CD2	2.47	0.45
1:B:361:GLU:O	1:B:365:THR:HG23	2.17	0.45
1:D:361:GLU:O	1:D:365:THR:HG23	2.17	0.45
1:B:186:ASN:O	1:B:269:SER:HA	2.17	0.45
1:B:352:ASP:O	1:B:356:ILE:HG13	2.17	0.45
1:C:258:ARG:HG3	1:C:264:LEU:CD2	2.46	0.45
1:D:31:ARG:O	1:D:58:ARG:NH2	2.49	0.45
1:D:147:ALA:C	1:D:149:ASN:H	2.24	0.45
1:C:89:ASN:HD22	1:C:89:ASN:C	2.24	0.45
1:C:147:ALA:C	1:C:149:ASN:H	2.24	0.45
1:D:80:ASP:C	1:D:82:ARG:N	2.74	0.45
1:A:80:ASP:C	1:A:82:ARG:N	2.74	0.44
1:A:89:ASN:HD22	1:A:89:ASN:C	2.24	0.44
1:B:90:PHE:HB3	1:B:117:ARG:NH2	2.33	0.44
1:B:224:TYR:HB2	1:B:381:TYR:HB3	1.99	0.44
1:B:376:VAL:HG13	1:B:378:GLN:NE2	2.32	0.44
1:C:93:ILE:O	1:C:123:LYS:HE3	2.17	0.44
1:D:61:ALA:CB	1:D:99:ILE:HD11	2.48	0.44
1:A:122:GLY:C	1:A:150:LYS:HE3	2.43	0.44
1:A:186:ASN:HA	1:A:276:THR:O	2.17	0.44
1:A:290:MET:HG2	1:A:301:ILE:CG2	2.38	0.44
1:A:361:GLU:O	1:A:365:THR:HG23	2.17	0.44
1:D:89:ASN:HD22	1:D:89:ASN:C	2.24	0.44
1:A:34:TYR:OH	1:A:332:LEU:HB3	2.16	0.44
1:B:233:VAL:HG22	1:B:257:MET:HG2	1.99	0.44
1:D:30:ARG:HA	1:D:56:HIS:O	2.17	0.44
1:B:102:VAL:HG11	1:B:118:ALA:CB	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ILE:CD1	1:B:125:VAL:HG13	2.48	0.44
1:C:102:VAL:HG11	1:C:118:ALA:CB	2.45	0.44
1:C:186:ASN:HA	1:C:276:THR:O	2.18	0.44
1:D:104:ILE:CD1	1:D:125:VAL:HG13	2.48	0.44
1:D:194:ASP:C	1:D:196:ALA:N	2.75	0.44
1:B:32:PHE:CD1	1:B:333:ALA:HA	2.53	0.44
1:B:258:ARG:HG3	1:B:264:LEU:CD2	2.46	0.44
1:C:233:VAL:HG22	1:C:257:MET:HG2	1.99	0.44
1:D:61:ALA:HB2	1:D:99:ILE:HD11	1.98	0.44
1:A:304:GLN:OE1	1:C:278:ARG:NH2	2.50	0.44
1:B:93:ILE:O	1:B:123:LYS:HE3	2.18	0.44
1:C:80:ASP:O	1:C:82:ARG:N	2.51	0.44
1:C:192:GLN:NE2	1:C:195:PRO:HD3	2.33	0.44
1:D:131:MET:HG2	1:D:141:MET:HE1	2.00	0.44
1:D:193:ASN:O	1:D:194:ASP:C	2.61	0.44
1:D:336:VAL:C	1:D:338:ASN:H	2.26	0.44
1:A:90:PHE:HB3	1:A:117:ARG:NH2	2.33	0.44
1:C:104:ILE:CD1	1:C:125:VAL:HG13	2.48	0.44
1:A:130:PRO:HG3	1:A:212:MET:O	2.18	0.44
1:B:195:PRO:CB	1:B:201:LEU:HD12	2.47	0.44
1:B:246:PHE:CD1	1:B:251:ASP:HB2	2.53	0.44
1:C:338:ASN:O	1:C:339:ASN:C	2.61	0.44
1:D:186:ASN:HA	1:D:276:THR:O	2.18	0.44
1:D:228:GLU:HG3	1:D:259:PHE:CD2	2.53	0.43
1:D:234:ARG:HB2	1:D:256:GLN:HE21	1.83	0.43
1:A:104:ILE:CD1	1:A:125:VAL:HG13	2.48	0.43
1:A:129:LYS:H	1:A:129:LYS:HG3	1.54	0.43
1:A:336:VAL:C	1:A:338:ASN:H	2.26	0.43
1:B:192:GLN:NE2	1:B:195:PRO:HD3	2.34	0.43
1:B:234:ARG:HB2	1:B:256:GLN:HE21	1.84	0.43
1:C:63:VAL:O	1:C:64:ASP:HB2	2.18	0.43
1:C:67:ALA:HA	1:C:70:ALA:HB3	2.00	0.43
1:D:90:PHE:HB3	1:D:117:ARG:NH2	2.33	0.43
1:B:278:ARG:NH2	1:D:304:GLN:OE1	2.51	0.43
1:C:93:ILE:CD1	1:C:123:LYS:HD2	2.45	0.43
1:D:327:ALA:O	1:D:331:HIS:HB2	2.18	0.43
1:A:234:ARG:HB2	1:A:256:GLN:HE21	1.84	0.43
1:A:246:PHE:CD1	1:A:251:ASP:HB2	2.54	0.43
1:D:93:ILE:O	1:D:123:LYS:HE3	2.18	0.43
1:A:183:THR:HG23	1:A:266:HIS:CE1	2.53	0.43
1:B:80:ASP:O	1:B:82:ARG:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ASN:ND2	1:B:89:ASN:N	2.67	0.43
1:B:93:ILE:CD1	1:B:123:LYS:HD2	2.45	0.43
1:B:336:VAL:C	1:B:338:ASN:H	2.27	0.43
1:C:327:ALA:O	1:C:331:HIS:HB2	2.19	0.43
1:A:93:ILE:O	1:A:123:LYS:HE3	2.18	0.43
1:A:228:GLU:HG3	1:A:259:PHE:CD2	2.54	0.43
1:A:273:THR:HB	1:C:282:GLN:HB3	2.00	0.43
1:B:116:ILE:HD11	1:B:140:ARG:HG2	2.00	0.43
1:C:193:ASN:O	1:C:194:ASP:C	2.62	0.43
1:D:186:ASN:O	1:D:269:SER:HA	2.19	0.43
1:D:233:VAL:HG22	1:D:257:MET:HG2	2.01	0.43
1:A:186:ASN:O	1:A:269:SER:HA	2.19	0.43
1:B:104:ILE:H	1:B:104:ILE:CD1	2.32	0.43
1:D:63:VAL:O	1:D:64:ASP:HB2	2.19	0.43
1:B:186:ASN:HA	1:B:276:THR:O	2.19	0.43
1:B:228:GLU:HG3	1:B:259:PHE:CD2	2.54	0.43
1:C:90:PHE:HB3	1:C:117:ARG:NH2	2.33	0.43
1:C:104:ILE:N	1:C:104:ILE:CD1	2.82	0.43
1:C:116:ILE:HD11	1:C:140:ARG:HG2	2.00	0.43
1:C:234:ARG:HB2	1:C:256:GLN:HE21	1.84	0.43
1:D:338:ASN:C	1:D:340:LYS:H	2.27	0.43
1:C:127:CYS:O	1:C:154:ILE:HA	2.19	0.43
1:C:131:MET:HG2	1:C:141:MET:HE1	2.00	0.43
1:D:198:GLN:CA	1:D:198:GLN:HE21	2.32	0.43
1:B:300:LEU:HD22	1:B:300:LEU:N	2.34	0.42
1:C:129:LYS:H	1:C:129:LYS:HG3	1.53	0.42
1:C:336:VAL:C	1:C:338:ASN:H	2.26	0.42
1:D:80:ASP:O	1:D:82:ARG:N	2.52	0.42
1:A:147:ALA:C	1:A:149:ASN:N	2.77	0.42
1:A:327:ALA:O	1:A:331:HIS:HB2	2.19	0.42
1:D:300:LEU:HD22	1:D:300:LEU:N	2.34	0.42
1:A:131:MET:HG2	1:A:141:MET:HE1	2.00	0.42
1:B:184:THR:O	1:B:267:GLY:HA2	2.20	0.42
1:B:193:ASN:O	1:B:194:ASP:C	2.62	0.42
1:D:89:ASN:ND2	1:D:89:ASN:N	2.66	0.42
1:D:192:GLN:NE2	1:D:195:PRO:HD3	2.34	0.42
1:A:193:ASN:O	1:A:194:ASP:C	2.62	0.42
1:B:127:CYS:O	1:B:154:ILE:HA	2.20	0.42
1:B:130:PRO:HG3	1:B:212:MET:O	2.19	0.42
1:C:130:PRO:HG3	1:C:212:MET:O	2.19	0.42
1:C:147:ALA:C	1:C:149:ASN:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:THR:O	1:C:267:GLY:HA2	2.20	0.42
1:D:130:PRO:HG3	1:D:212:MET:O	2.18	0.42
1:A:116:ILE:HD11	1:A:140:ARG:HG2	2.01	0.42
1:A:80:ASP:O	1:A:82:ARG:N	2.53	0.42
1:A:127:CYS:O	1:A:154:ILE:HA	2.20	0.42
1:B:327:ALA:O	1:B:331:HIS:HB2	2.19	0.42
1:D:116:ILE:HD11	1:D:140:ARG:HG2	2.01	0.42
1:D:183:THR:HG23	1:D:266:HIS:CE1	2.55	0.42
1:D:246:PHE:CD1	1:D:251:ASP:HB2	2.55	0.42
1:A:163:MET:HA	1:A:163:MET:CE	2.38	0.42
1:A:192:GLN:NE2	1:A:195:PRO:HD3	2.34	0.42
1:B:135:VAL:O	1:B:138:CYS:HB2	2.20	0.42
1:D:147:ALA:C	1:D:149:ASN:N	2.78	0.42
1:B:63:VAL:O	1:B:64:ASP:HB2	2.20	0.42
1:B:176:LEU:C	1:B:285:LYS:HB2	2.45	0.42
1:B:338:ASN:C	1:B:340:LYS:H	2.27	0.42
1:D:129:LYS:H	1:D:129:LYS:HG3	1.54	0.42
1:D:176:LEU:C	1:D:285:LYS:HB2	2.45	0.42
1:A:63:VAL:O	1:A:64:ASP:HB2	2.19	0.41
1:A:162:PRO:HG2	1:A:319:MET:HB3	1.97	0.41
1:A:322:ASN:OD1	1:A:327:ALA:HB2	2.19	0.41
1:B:176:LEU:O	1:B:283:GLY:HA3	2.20	0.41
1:C:228:GLU:HG3	1:C:259:PHE:CD2	2.55	0.41
1:C:347:GLU:OE1	1:C:347:GLU:N	2.53	0.41
1:B:104:ILE:N	1:B:104:ILE:CD1	2.81	0.41
1:C:130:PRO:HG2	1:C:212:MET:HE3	2.02	0.41
1:B:347:GLU:N	1:B:347:GLU:OE1	2.53	0.41
1:D:104:ILE:H	1:D:104:ILE:CD1	2.32	0.41
1:D:347:GLU:N	1:D:347:GLU:OE1	2.53	0.41
1:D:127:CYS:O	1:D:154:ILE:HA	2.19	0.41
1:A:176:LEU:C	1:A:285:LYS:HB2	2.45	0.41
1:A:184:THR:O	1:A:267:GLY:HA2	2.21	0.41
1:C:252:ARG:HG2	1:C:270:SER:HB2	2.02	0.41
1:B:124:HIS:HD2	1:B:151:LYS:N	2.05	0.41
1:A:94:ALA:HB2	1:A:121:ALA:HB1	2.03	0.41
1:A:104:ILE:H	1:A:104:ILE:CD1	2.33	0.41
1:B:130:PRO:HG2	1:B:212:MET:HE3	2.03	0.41
1:B:183:THR:HG23	1:B:266:HIS:CE1	2.55	0.41
1:B:195:PRO:HB3	1:B:201:LEU:HD12	2.03	0.41
1:B:252:ARG:HG2	1:B:270:SER:HB2	2.03	0.41
1:B:361:GLU:HA	1:B:364:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:ILE:H	1:C:104:ILE:CD1	2.32	0.41
1:C:122:GLY:O	1:C:150:LYS:HE3	2.21	0.41
1:C:135:VAL:HG21	1:C:357:GLN:NE2	2.36	0.41
1:C:176:LEU:C	1:C:285:LYS:HB2	2.45	0.41
1:D:158:CYS:HB2	3:D:684:HOH:O	2.20	0.41
1:A:110:LEU:N	1:A:110:LEU:HD22	2.36	0.41
1:C:96:ASP:HA	1:C:97:PRO:HD2	1.93	0.41
1:C:195:PRO:C	1:C:197:GLN:H	2.28	0.41
1:D:361:GLU:HA	1:D:364:ARG:NH2	2.36	0.41
1:A:347:GLU:N	1:A:347:GLU:OE1	2.54	0.40
1:A:377:ARG:HG3	1:A:381:TYR:CD2	2.56	0.40
1:D:35:ALA:N	1:D:101:ALA:O	2.53	0.40
1:D:176:LEU:O	1:D:283:GLY:HA3	2.21	0.40
1:A:176:LEU:O	1:A:283:GLY:HA3	2.21	0.40
1:A:300:LEU:HD22	1:A:300:LEU:N	2.35	0.40
1:C:183:THR:HG23	1:C:266:HIS:CE1	2.57	0.40
1:C:246:PHE:CD1	1:C:251:ASP:HB2	2.55	0.40
1:B:198:GLN:HE21	1:B:198:GLN:CA	2.32	0.40
1:D:110:LEU:N	1:D:110:LEU:HD22	2.36	0.40
1:A:258:ARG:HG3	1:A:264:LEU:HD21	2.04	0.40
1:B:274:THR:CG2	1:D:306:PRO:HG2	2.51	0.40
1:C:108:ASN:OD1	1:C:130:PRO:HD2	2.21	0.40
1:A:130:PRO:HG2	1:A:212:MET:HE3	2.04	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	336/352 (96%)	302 (90%)	27 (8%)	7 (2%)	5	15
1	B	334/352 (95%)	300 (90%)	26 (8%)	8 (2%)	4	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	333/352 (95%)	300 (90%)	27 (8%)	6 (2%)	6	18
1	D	334/352 (95%)	300 (90%)	27 (8%)	7 (2%)	5	15
All	All	1337/1408 (95%)	1202 (90%)	107 (8%)	28 (2%)	5	15

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	321	ALA
1	B	321	ALA
1	A	193	ASN
1	A	298	GLN
1	A	320	PRO
1	B	193	ASN
1	B	298	GLN
1	C	193	ASN
1	C	298	GLN
1	C	322	ASN
1	D	193	ASN
1	D	298	GLN
1	B	195	PRO
1	A	147	ALA
1	B	147	ALA
1	B	339	ASN
1	C	147	ALA
1	D	147	ALA
1	D	195	PRO
1	D	306	PRO
1	A	337	ILE
1	B	81	PRO
1	B	337	ILE
1	D	337	ILE
1	A	81	PRO
1	C	81	PRO
1	C	337	ILE
1	D	81	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	259/286 (91%)	247 (95%)	12 (5%)	24	51
1	B	258/286 (90%)	247 (96%)	11 (4%)	26	54
1	C	260/286 (91%)	250 (96%)	10 (4%)	29	58
1	D	256/286 (90%)	245 (96%)	11 (4%)	26	54
All	All	1033/1144 (90%)	989 (96%)	44 (4%)	26	54

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	TYR
1	A	89	ASN
1	A	104	ILE
1	A	129	LYS
1	A	188	ASP
1	A	198	GLN
1	A	271	TYR
1	A	297	TYR
1	A	300	LEU
1	A	319	MET
1	A	320	PRO
1	A	377	ARG
1	B	31	ARG
1	B	85	TYR
1	B	89	ASN
1	B	104	ILE
1	B	129	LYS
1	B	188	ASP
1	B	198	GLN
1	B	271	TYR
1	B	297	TYR
1	B	300	LEU
1	B	377	ARG
1	C	85	TYR
1	C	89	ASN
1	C	104	ILE
1	C	129	LYS
1	C	188	ASP
1	C	198	GLN
1	C	271	TYR

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Mol	Chain	Res	Type
1	C	297	TYR
1	C	300	LEU
1	C	377	ARG
1	D	85	TYR
1	D	89	ASN
1	D	104	ILE
1	D	129	LYS
1	D	188	ASP
1	D	198	GLN
1	D	271	TYR
1	D	297	TYR
1	D	300	LEU
1	D	305	THR
1	D	377	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	89	ASN
1	A	124	HIS
1	A	164	ASN
1	A	174	ASN
1	A	192	GLN
1	A	198	GLN
1	A	256	GLN
1	A	324	GLN
1	A	331	HIS
1	B	45	ASN
1	B	89	ASN
1	B	124	HIS
1	B	164	ASN
1	B	174	ASN
1	B	192	GLN
1	B	198	GLN
1	B	220	ASN
1	B	256	GLN
1	B	324	GLN
1	B	331	HIS
1	B	378	GLN
1	C	45	ASN
1	C	89	ASN

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Mol	Chain	Res	Type
1	C	124	HIS
1	C	164	ASN
1	C	174	ASN
1	C	192	GLN
1	C	197	GLN
1	C	198	GLN
1	C	220	ASN
1	C	256	GLN
1	C	324	GLN
1	C	331	HIS
1	C	357	GLN
1	C	378	GLN
1	D	45	ASN
1	D	89	ASN
1	D	124	HIS
1	D	164	ASN
1	D	174	ASN
1	D	192	GLN
1	D	198	GLN
1	D	220	ASN
1	D	256	GLN
1	D	324	GLN

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](#)

4 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	500	-	46,48,48	1.76	8 (17%)	64,73,73	1.84	11 (17%)
2	NAD	D	503	-	46,48,48	1.74	7 (15%)	64,73,73	1.85	12 (18%)
2	NAD	C	502	-	46,48,48	1.79	8 (17%)	64,73,73	1.85	12 (18%)
2	NAD	B	501	-	46,48,48	1.78	8 (17%)	64,73,73	1.83	12 (18%)

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	500	-	-	5/30/62/62	0/5/5/5
2	NAD	D	503	-	-	5/30/62/62	0/5/5/5
2	NAD	C	502	-	-	5/30/62/62	0/5/5/5
2	NAD	B	501	-	-	5/30/62/62	0/5/5/5

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	502	NAD	C2N-N1N	7.28	1.43	1.35
2	A	500	NAD	C2N-N1N	7.11	1.42	1.35
2	B	501	NAD	C2N-N1N	7.10	1.42	1.35
2	D	503	NAD	C2N-N1N	6.93	1.42	1.35
2	B	501	NAD	C5A-N7A	-4.41	1.31	1.39
2	C	502	NAD	C5A-N7A	-4.40	1.31	1.39
2	A	500	NAD	C5A-N7A	-4.29	1.31	1.39
2	D	503	NAD	C5A-N7A	-4.28	1.31	1.39
2	D	503	NAD	C6N-N1N	3.91	1.44	1.35
2	A	500	NAD	C6N-N1N	3.88	1.44	1.35
2	B	501	NAD	C6N-N1N	3.86	1.44	1.35
2	C	502	NAD	C6N-N1N	3.81	1.44	1.35
2	A	500	NAD	O4D-C1D	3.08	1.44	1.40
2	B	501	NAD	O4D-C1D	3.06	1.44	1.40
2	C	502	NAD	O4D-C1D	3.03	1.44	1.40
2	D	503	NAD	O4D-C1D	2.96	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	502	NAD	C3N-C7N	2.91	1.54	1.50
2	A	500	NAD	C3N-C7N	2.76	1.54	1.50
2	B	501	NAD	C3N-C7N	2.73	1.54	1.50
2	D	503	NAD	C3N-C7N	2.70	1.54	1.50
2	D	503	NAD	C2A-N1A	2.64	1.38	1.33
2	A	500	NAD	C2A-N1A	2.56	1.38	1.33
2	B	501	NAD	C2A-N1A	2.53	1.38	1.33
2	C	502	NAD	C2A-N1A	2.44	1.38	1.33
2	A	500	NAD	C2A-N3A	2.42	1.38	1.33
2	B	501	NAD	C2A-N3A	2.37	1.38	1.33
2	C	502	NAD	C2A-N3A	2.27	1.38	1.33
2	D	503	NAD	C2A-N3A	2.15	1.37	1.33
2	B	501	NAD	C4N-C3N	2.12	1.42	1.39
2	C	502	NAD	C4N-C3N	2.12	1.42	1.39
2	A	500	NAD	C4N-C3N	2.04	1.42	1.39

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	502	NAD	N3A-C4A-N9A	7.14	139.31	127.17
2	D	503	NAD	N3A-C4A-N9A	7.14	139.30	127.17
2	A	500	NAD	N3A-C4A-N9A	7.13	139.30	127.17
2	B	501	NAD	N3A-C4A-N9A	7.09	139.23	127.17
2	C	502	NAD	C5A-C4A-N3A	-6.23	118.14	126.72
2	A	500	NAD	C5A-C4A-N3A	-6.17	118.22	126.72
2	B	501	NAD	C5A-C4A-N3A	-6.17	118.22	126.72
2	D	503	NAD	C5A-C4A-N3A	-6.13	118.27	126.72
2	A	500	NAD	C6A-C5A-N7A	-4.62	123.18	132.09
2	D	503	NAD	C6A-C5A-N7A	-4.62	123.18	132.09
2	C	502	NAD	C6A-C5A-N7A	-4.60	123.22	132.09
2	B	501	NAD	C6A-C5A-N7A	-4.58	123.27	132.09
2	D	503	NAD	C6A-C5A-C4A	4.57	123.42	117.18
2	C	502	NAD	C6A-C5A-C4A	4.56	123.41	117.18
2	B	501	NAD	C6A-C5A-C4A	4.56	123.40	117.18
2	A	500	NAD	C6A-C5A-C4A	4.54	123.38	117.18
2	D	503	NAD	N9A-C8A-N7A	-3.69	108.71	113.94
2	C	502	NAD	N9A-C8A-N7A	-3.67	108.73	113.94
2	B	501	NAD	N9A-C8A-N7A	-3.65	108.76	113.94
2	A	500	NAD	N9A-C8A-N7A	-3.61	108.82	113.94
2	C	502	NAD	N3A-C2A-N1A	-3.45	123.36	128.58
2	B	501	NAD	N3A-C2A-N1A	-3.35	123.52	128.58
2	D	503	NAD	N3A-C2A-N1A	-3.34	123.53	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	NAD	N3A-C2A-N1A	-3.32	123.55	128.58
2	D	503	NAD	C5A-C4A-N9A	-3.11	102.42	105.81
2	A	500	NAD	C5A-C4A-N9A	-3.05	102.49	105.81
2	C	502	NAD	C5A-C4A-N9A	-2.99	102.55	105.81
2	B	501	NAD	C5A-C4A-N9A	-2.99	102.55	105.81
2	C	502	NAD	C6N-N1N-C2N	-2.58	119.68	121.88
2	D	503	NAD	C6N-N1N-C2N	-2.57	119.69	121.88
2	C	502	NAD	C2A-N3A-C4A	2.50	117.94	111.83
2	A	500	NAD	C4A-C5A-N7A	2.50	113.44	110.58
2	A	500	NAD	C6N-N1N-C2N	-2.49	119.76	121.88
2	D	503	NAD	C4A-C5A-N7A	2.46	113.39	110.58
2	A	500	NAD	C2A-N3A-C4A	2.44	117.80	111.83
2	B	501	NAD	C6N-N1N-C2N	-2.43	119.81	121.88
2	C	502	NAD	C4A-C5A-N7A	2.43	113.36	110.58
2	D	503	NAD	C2A-N3A-C4A	2.43	117.77	111.83
2	B	501	NAD	C2A-N3A-C4A	2.42	117.73	111.83
2	B	501	NAD	C4A-C5A-N7A	2.40	113.33	110.58
2	D	503	NAD	C4A-N9A-C8A	2.38	108.24	105.74
2	A	500	NAD	C4A-N9A-C8A	2.31	108.16	105.74
2	B	501	NAD	C4A-N9A-C8A	2.29	108.14	105.74
2	C	502	NAD	C4A-N9A-C8A	2.29	108.14	105.74
2	D	503	NAD	C5A-N7A-C8A	2.05	106.68	103.45
2	C	502	NAD	C5A-N7A-C8A	2.03	106.63	103.45
2	B	501	NAD	C5A-N7A-C8A	2.01	106.62	103.45

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	NAD	O4D-C1D-N1N-C2N
2	A	500	NAD	O4D-C1D-N1N-C6N
2	B	501	NAD	O4D-C1D-N1N-C2N
2	B	501	NAD	O4D-C1D-N1N-C6N
2	C	502	NAD	O4D-C1D-N1N-C2N
2	C	502	NAD	O4D-C1D-N1N-C6N
2	D	503	NAD	O4D-C1D-N1N-C2N
2	D	503	NAD	O4D-C1D-N1N-C6N
2	A	500	NAD	O4B-C1B-N9A-C8A
2	B	501	NAD	O4B-C1B-N9A-C8A
2	C	502	NAD	O4B-C1B-N9A-C8A
2	D	503	NAD	O4B-C1B-N9A-C8A
2	D	503	NAD	C2B-C1B-N9A-C8A

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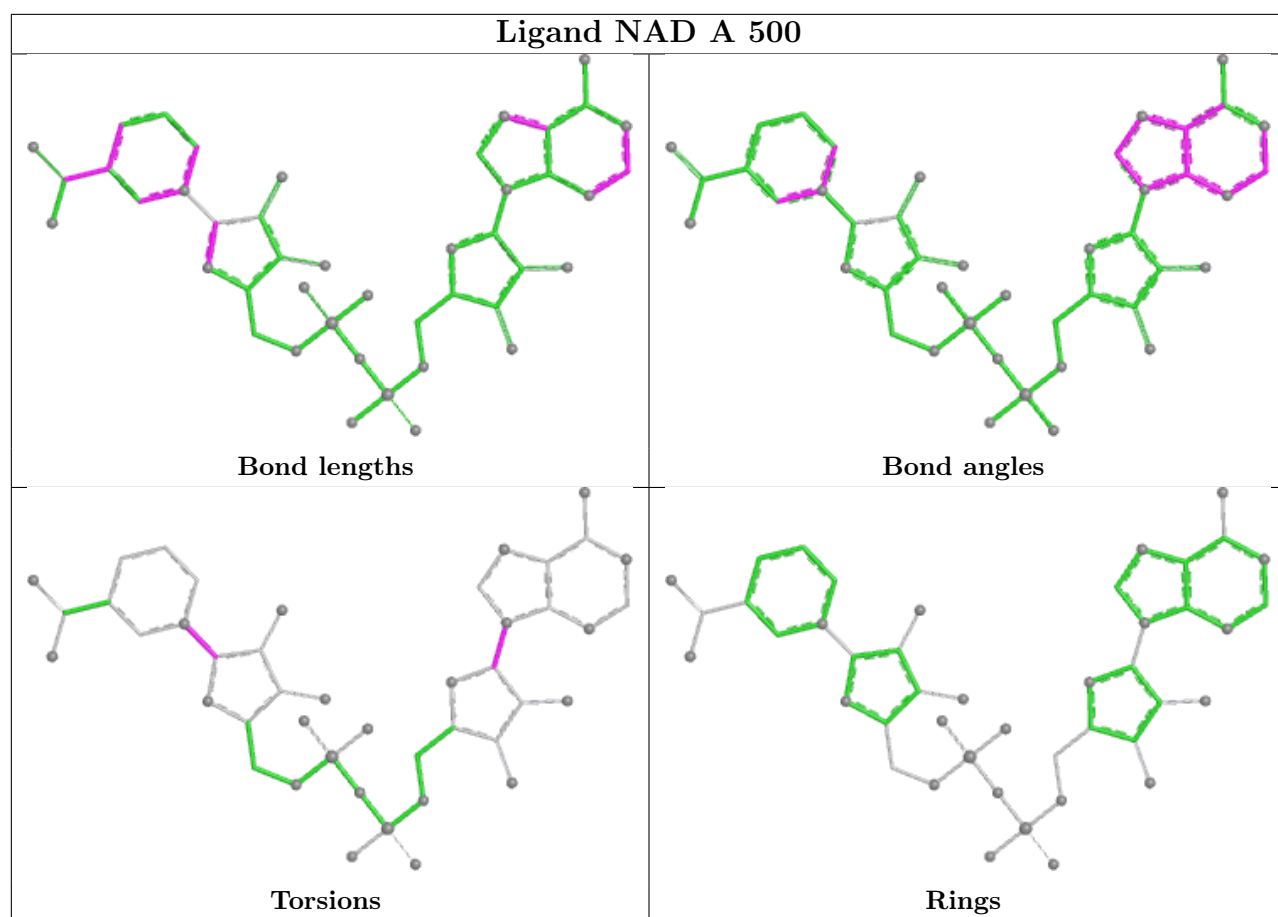
Mol	Chain	Res	Type	Atoms
2	A	500	NAD	C2B-C1B-N9A-C8A
2	B	501	NAD	C2B-C1B-N9A-C8A
2	C	502	NAD	C2B-C1B-N9A-C8A
2	A	500	NAD	C2B-C1B-N9A-C4A
2	B	501	NAD	C2B-C1B-N9A-C4A
2	C	502	NAD	C2B-C1B-N9A-C4A
2	D	503	NAD	C2B-C1B-N9A-C4A

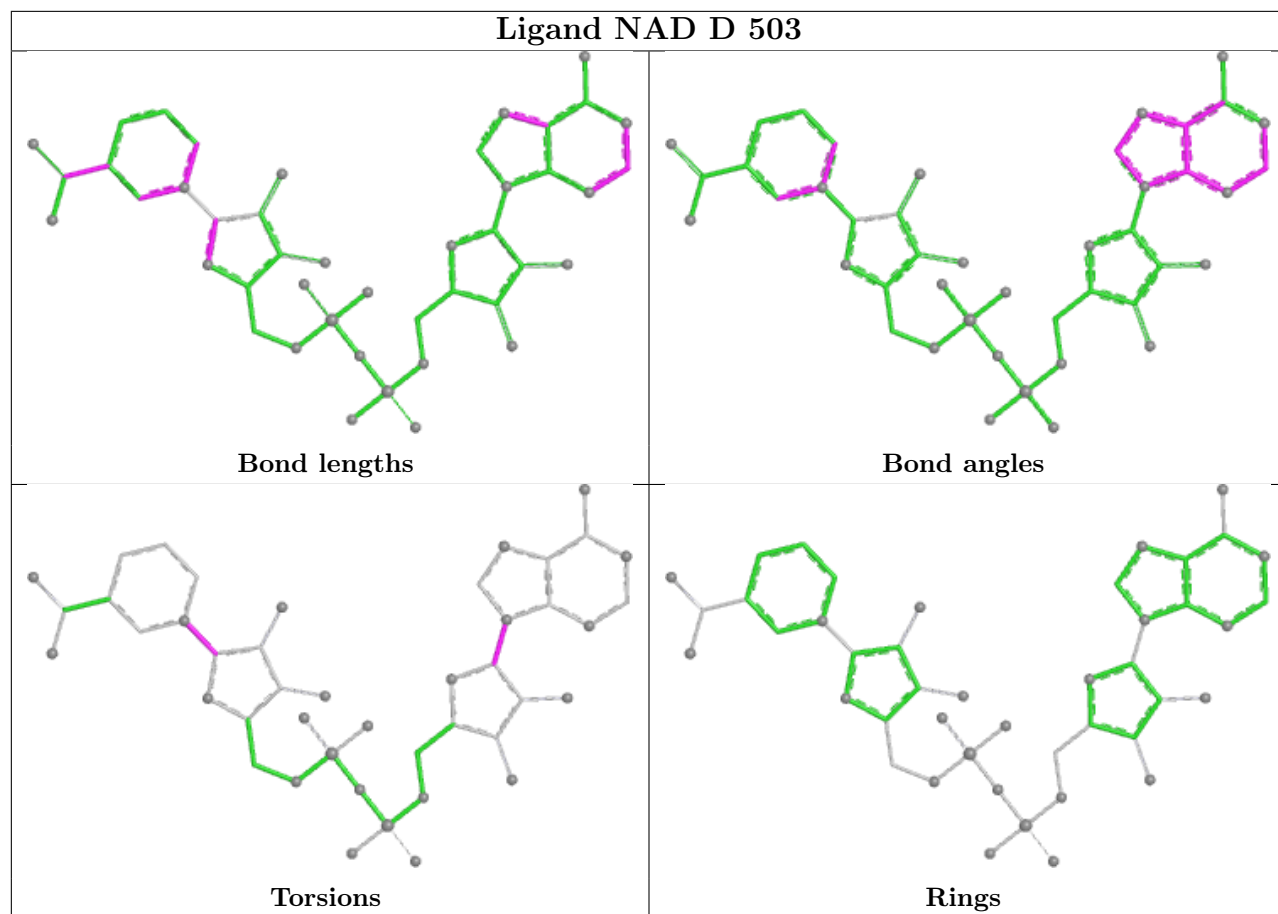
There are no ring outliers.

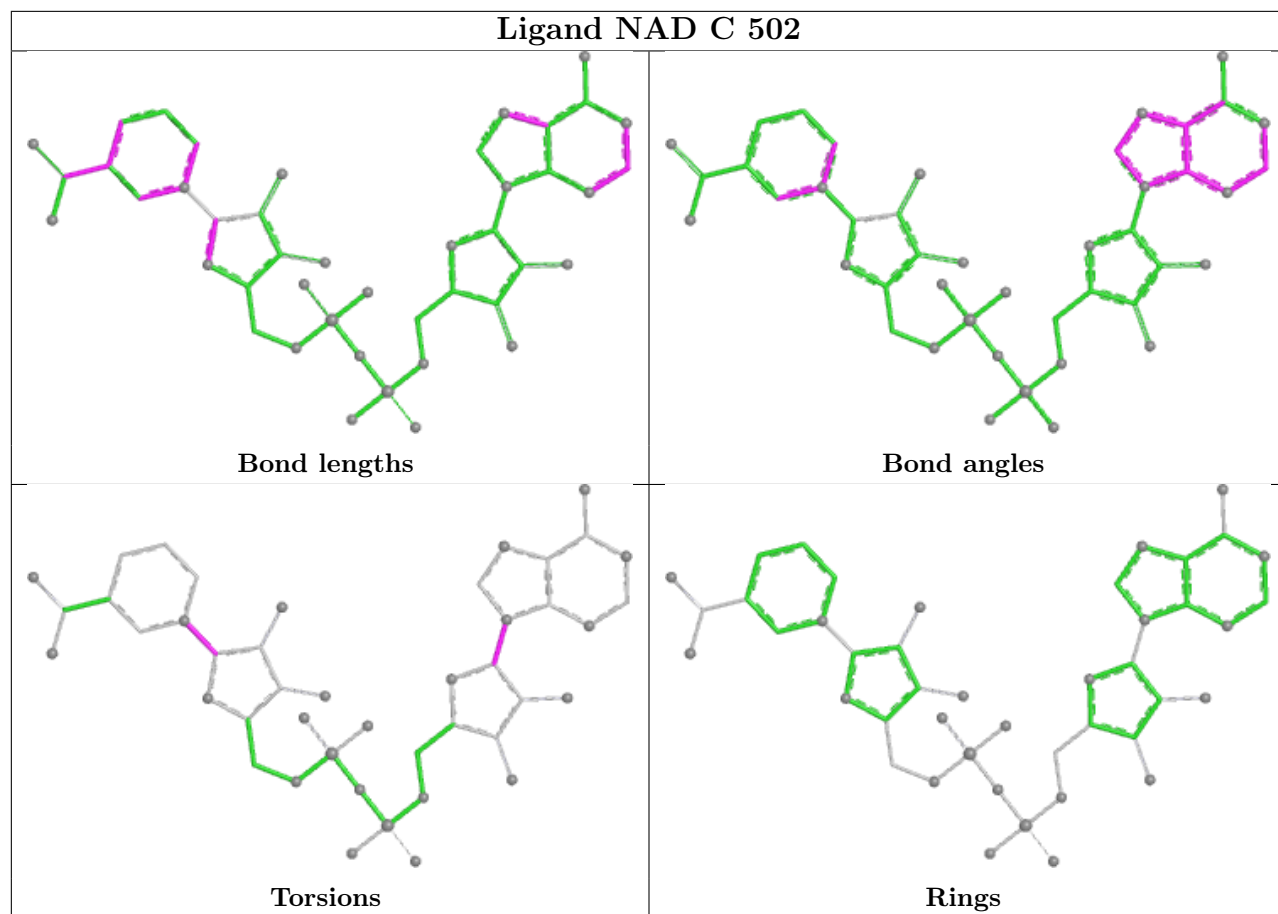
2 monomers are involved in 2 short contacts:

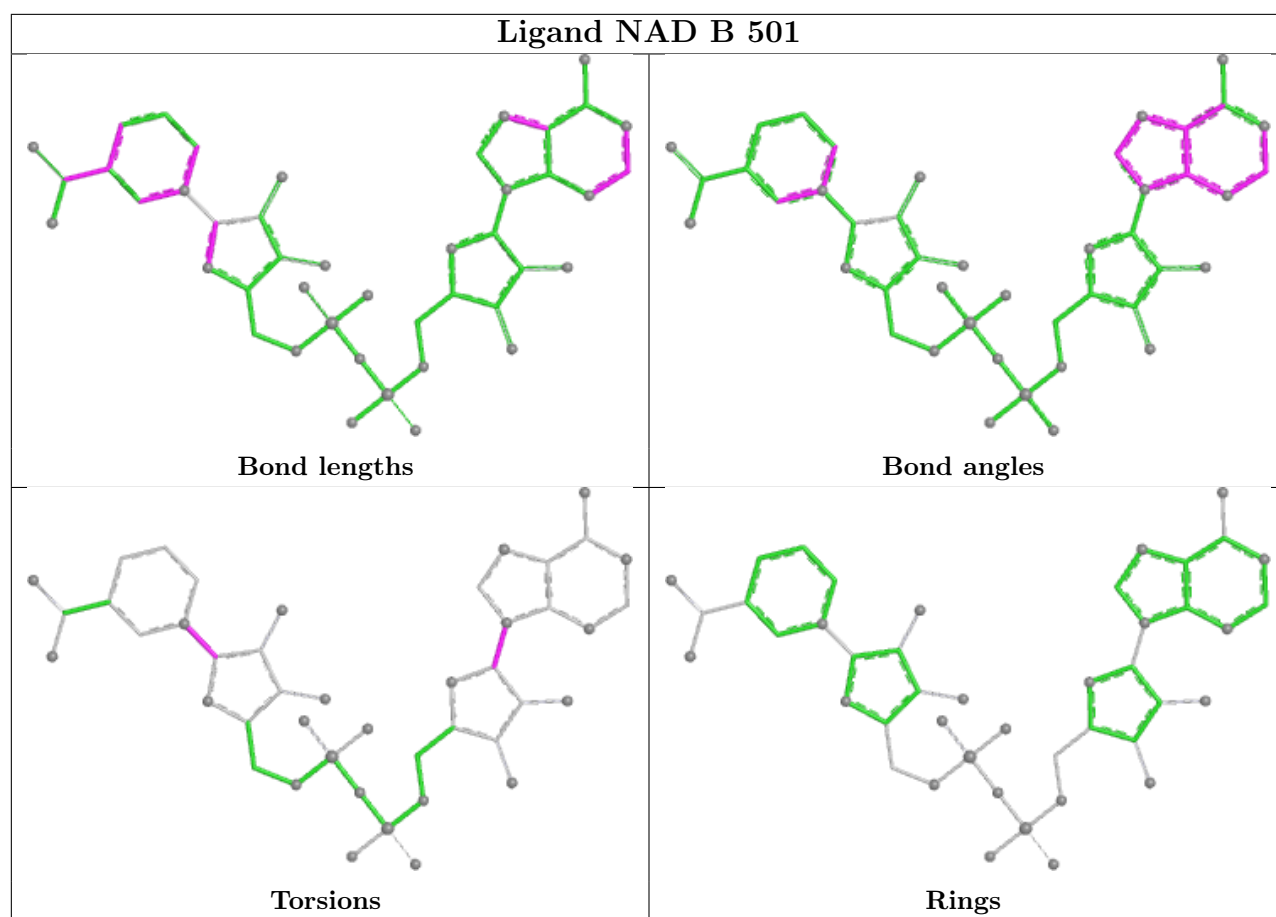
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	503	NAD	1	0
2	B	501	NAD	1	0

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	340/352 (96%)	0.50	15 (4%) 39 35	12, 47, 83, 100	0
1	B	338/352 (96%)	0.89	41 (12%) 8 7	27, 60, 96, 103	0
1	C	337/352 (95%)	0.57	25 (7%) 20 18	16, 46, 88, 103	0
1	D	338/352 (96%)	0.91	42 (12%) 8 7	25, 61, 98, 103	0
All	All	1353/1408 (96%)	0.71	123 (9%) 15 12	12, 54, 94, 103	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	321	ALA	7.9
1	C	297	TYR	5.1
1	C	321	ALA	5.0
1	A	322	ASN	4.4
1	D	84	ILE	4.0
1	D	192	GLN	3.9
1	D	87	TYR	3.8
1	B	297	TYR	3.7
1	D	62	LEU	3.5
1	B	118	ALA	3.4
1	A	319	MET	3.4
1	D	322	ASN	3.3
1	D	114	PHE	3.2
1	B	88	SER	3.2
1	D	90	PHE	3.2
1	D	44	LEU	3.2
1	D	67	ALA	3.1
1	A	320	PRO	3.1
1	D	89	ASN	3.1
1	B	62	LEU	3.1
1	A	40	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	85	TYR	3.1
1	A	87	TYR	3.0
1	B	195	PRO	3.0
1	C	336	VAL	3.0
1	A	31	ARG	3.0
1	B	67	ALA	3.0
1	B	305	THR	3.0
1	C	195	PRO	2.9
1	A	142	ILE	2.9
1	B	82	ARG	2.8
1	C	193	ASN	2.8
1	C	298	GLN	2.8
1	D	39	LEU	2.8
1	D	195	PRO	2.8
1	D	152	LEU	2.8
1	D	34	TYR	2.8
1	D	307	GLY	2.7
1	B	244	GLU	2.7
1	D	194	ASP	2.7
1	A	193	ASN	2.7
1	D	193	ASN	2.7
1	B	175	GLN	2.6
1	C	84	ILE	2.6
1	C	376	VAL	2.6
1	B	298	GLN	2.6
1	B	30	ARG	2.6
1	B	321	ALA	2.6
1	C	322	ASN	2.6
1	D	196	ALA	2.6
1	D	38	GLY	2.6
1	D	81	PRO	2.6
1	D	106	LEU	2.5
1	B	320	PRO	2.5
1	D	112	ALA	2.5
1	D	238	TYR	2.5
1	B	34	TYR	2.5
1	D	53	GLY	2.5
1	C	192	GLN	2.5
1	C	59	ILE	2.5
1	A	376	VAL	2.5
1	B	119	PHE	2.5
1	D	197	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	87	TYR	2.4
1	B	171	ILE	2.4
1	A	194	ASP	2.4
1	C	194	ASP	2.4
1	C	364	ARG	2.4
1	D	124	HIS	2.4
1	B	97	PRO	2.4
1	D	79	VAL	2.4
1	D	59	ILE	2.3
1	B	155	GLY	2.3
1	B	79	VAL	2.3
1	D	76	GLU	2.3
1	A	374	GLY	2.3
1	B	121	ALA	2.3
1	D	205	LEU	2.3
1	C	67	ALA	2.3
1	A	30	ARG	2.3
1	B	341	PRO	2.3
1	A	192	GLN	2.3
1	D	249	VAL	2.3
1	B	124	HIS	2.2
1	B	115	ALA	2.2
1	B	135	VAL	2.2
1	C	337	ILE	2.2
1	D	365	THR	2.2
1	B	197	GLN	2.2
1	B	209	GLY	2.2
1	D	70	ALA	2.2
1	D	241	PRO	2.1
1	C	87	TYR	2.1
1	C	123	LYS	2.1
1	B	48	LEU	2.1
1	B	374	GLY	2.1
1	D	93	ILE	2.1
1	D	253	ILE	2.1
1	B	373	TRP	2.1
1	D	85	TYR	2.1
1	D	116	ILE	2.1
1	C	75	ALA	2.1
1	C	380	GLY	2.1
1	C	247	VAL	2.1
1	D	125	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	258	ARG	2.1
1	D	101	ALA	2.1
1	C	205	LEU	2.1
1	B	193	ASN	2.1
1	B	346	GLY	2.1
1	B	191	ASP	2.0
1	C	140	ARG	2.0
1	C	88	SER	2.0
1	B	83	LYS	2.0
1	D	66	ASN	2.0
1	B	283	GLY	2.0
1	B	376	VAL	2.0
1	C	146	LYS	2.0
1	D	206	ALA	2.0
1	C	134	SER	2.0
1	A	66	ASN	2.0
1	B	73	VAL	2.0
1	B	234	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](#)

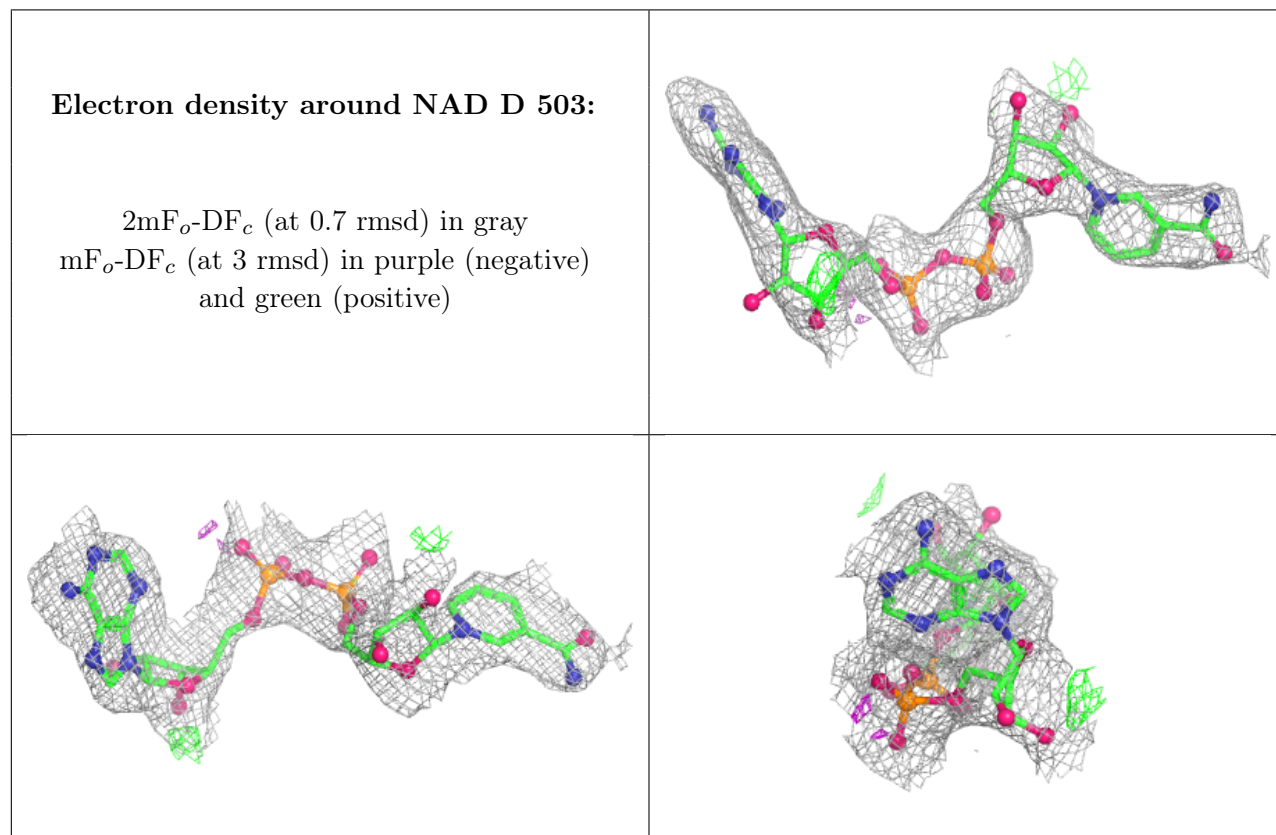
There are no oligosaccharides in this entry.

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.

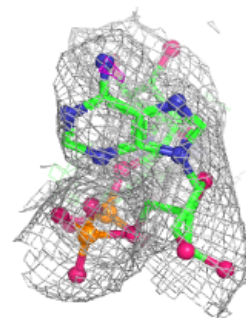
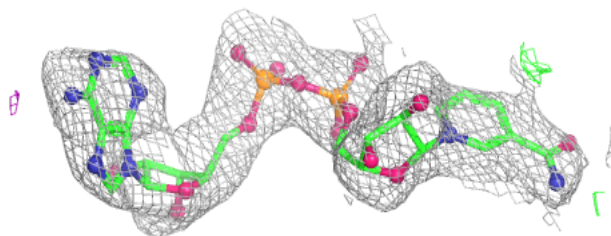
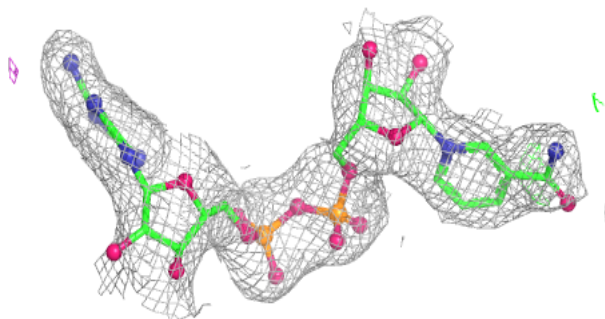
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	D	503	44/44	0.83	0.14	76,76,76,76	0
2	NAD	B	501	44/44	0.87	0.14	76,76,76,76	0
2	NAD	C	502	44/44	0.90	0.15	74,74,74,74	0
2	NAD	A	500	44/44	0.90	0.15	76,76,76,76	0

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.

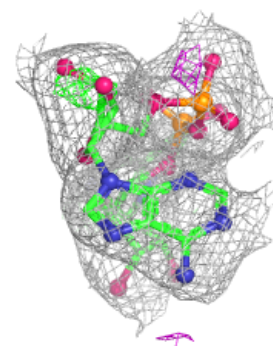
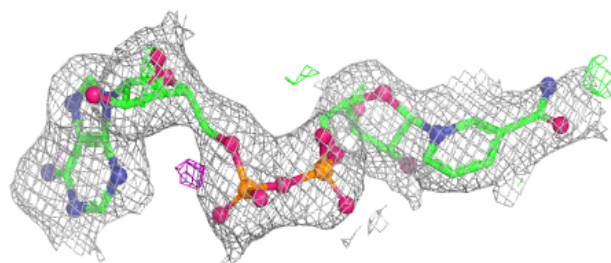
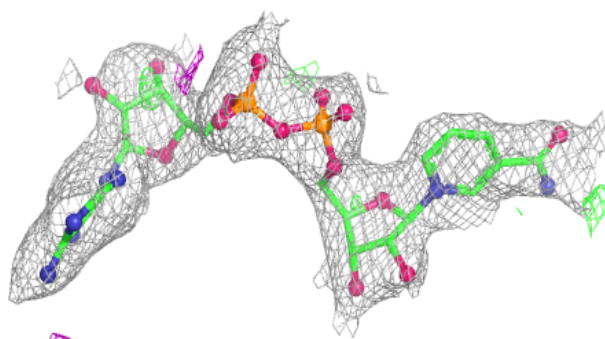


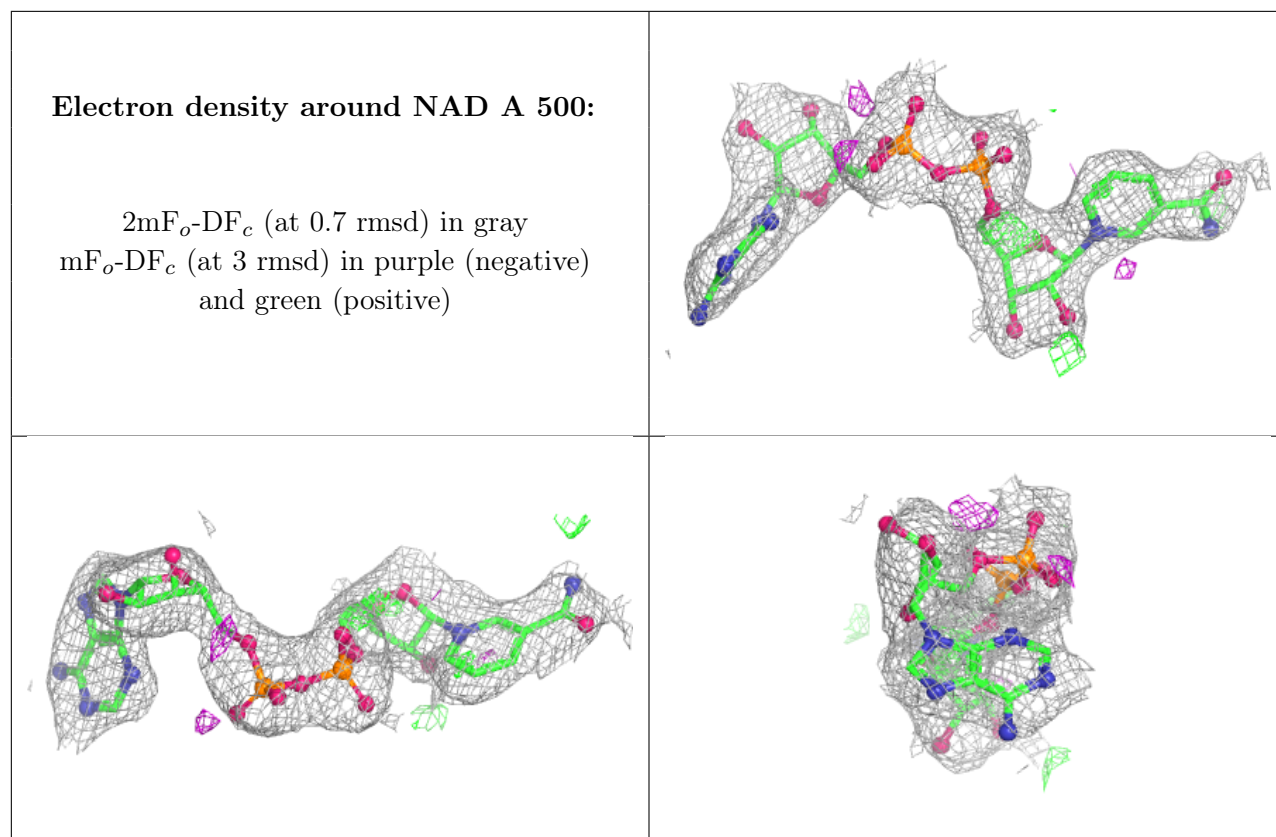
Electron density around NAD B 501:

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

**Electron density around NAD C 502:**

$2mF_o-DF_c$ (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.