



Full wwPDB X-ray Structure Validation Report

Feb 5, 2024 – 05:53 AM EST

PDB ID : 1XAL
Title : CRYSTAL STRUCTURE OF STAPHYLOCOCCUS AUREUS 3-DEHYDROQUINATE SYNTHASE (DHQS) IN COMPLEX WITH ZN²⁺, NAD⁺ AND CARBAPHOSPHONATE (SOAK)
Authors : Nichols, C.E.; Ren, J.; Leslie, K.; Dhaliwal, B.; Lockyer, M.; Charles, I.; Hawkins, A.R.; Stammers, D.K.
Deposited on : 2004-08-26
Resolution : 2.80 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

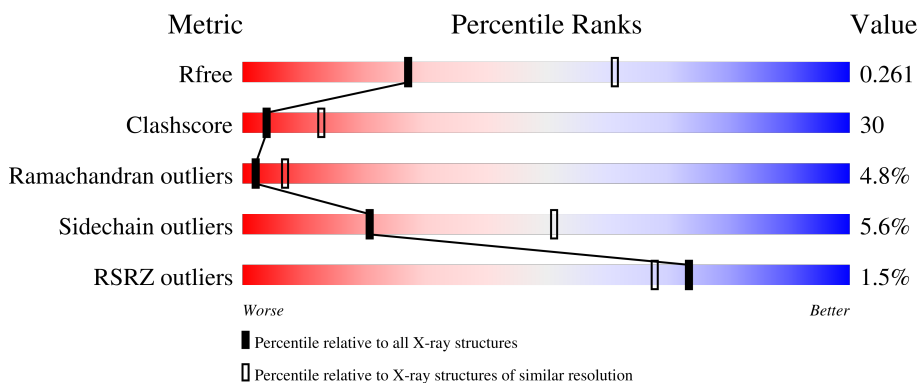
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	354	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 40%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 49%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 40% 49% 5% • 5%</p>
1	B	354	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 41%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 49%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">% 41% 49% 5% • 5%</p>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5640 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 3-dehydroquinase synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	336	2689	1737	449	495	8	0	0	0
1	B	336	2689	1737	449	495	8	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	LYS	ASP	see remark 999	UNP Q6GGU4
A	23	TYR	HIS	see remark 999	UNP Q6GGU4
A	25	GLY	SER	see remark 999	UNP Q6GGU4
A	28	LEU	ILE	see remark 999	UNP Q6GGU4
A	29	ASN	ASP	see remark 999	UNP Q6GGU4
A	36	LEU	ILE	see remark 999	UNP Q6GGU4
A	41	TYR	HIS	see remark 999	UNP Q6GGU4
A	48	ASN	ASP	see remark 999	UNP Q6GGU4
A	109	VAL	ILE	see remark 999	UNP Q6GGU4
A	170	LYS	GLU	see remark 999	UNP Q6GGU4
A	226	VAL	ILE	see remark 999	UNP Q6GGU4
A	282	SER	ASN	see remark 999	UNP Q6GGU4
A	326	MET	ILE	see remark 999	UNP Q6GGU4
B	22	LYS	ASP	see remark 999	UNP Q6GGU4
B	23	TYR	HIS	see remark 999	UNP Q6GGU4
B	25	GLY	SER	see remark 999	UNP Q6GGU4
B	28	LEU	ILE	see remark 999	UNP Q6GGU4
B	29	ASN	ASP	see remark 999	UNP Q6GGU4
B	36	LEU	ILE	see remark 999	UNP Q6GGU4
B	41	TYR	HIS	see remark 999	UNP Q6GGU4
B	48	ASN	ASP	see remark 999	UNP Q6GGU4
B	109	VAL	ILE	see remark 999	UNP Q6GGU4
B	170	LYS	GLU	see remark 999	UNP Q6GGU4
B	226	VAL	ILE	see remark 999	UNP Q6GGU4
B	282	SER	ASN	see remark 999	UNP Q6GGU4

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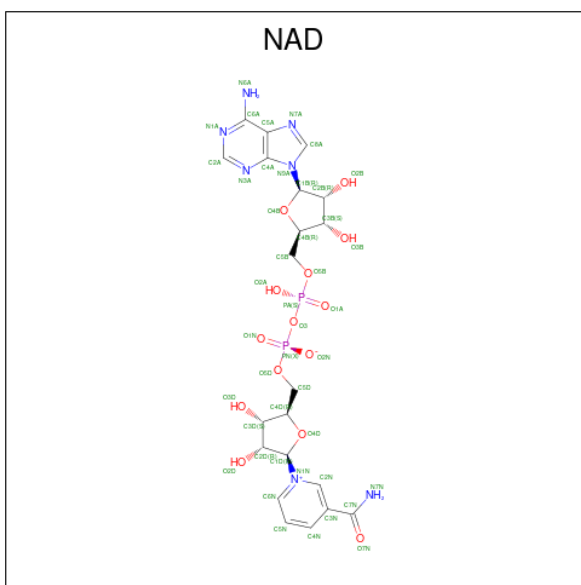
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Chain	Residue	Modelled	Actual	Comment	Reference
B	326	MET	ILE	see remark 999	UNP Q6GGU4

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

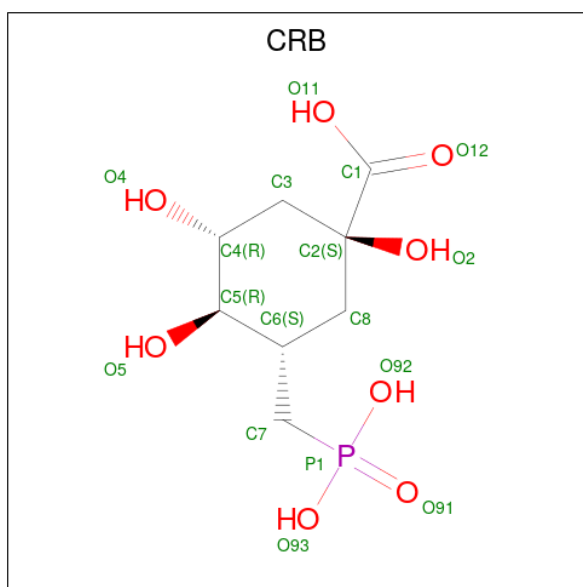
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 4 is [1R-(1ALPHA,3BETA,4ALPHA,5BETA)]-5-(PHOSPHONOMETHYL)-1,3,4-TRIHYDROXYCYCLOHEXANE-1-CARBOXYLIC ACID (three-letter code: CRB) (formula: C₈H₁₅O₈P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			17	8	8	1		
4	B	1	Total	C	O	P	0	0
			17	8	8	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	71	Total	O	0	0
			71	71		
5	B	67	Total	O	0	0
			67	67		

ASP	PHE	GLU	THR	LEU	TYR	GLN	TYR	R310	L311	S312	D313	K314	K315	N316	D317	K318	Q319	G320	V321	Q322	N323	R327	Q328	F329	G330	D331	I332	V333	V334	Q335	H336	V337	D338	Q339	L340	T341	L342	Q343	H344	A345	C346	E347	Q348	L349	K350	T351	Y352	PHE	LYS
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4 Data and refinement statistics i

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	55.10Å 55.10Å 232.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.86 – 2.80 29.85 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.7 (29.86-2.80) 97.8 (29.85-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.80Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.203 , 0.265 0.204 , 0.261	Depositor DCC
R_{free} test set	1663 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å ²)	60.4	Xtrriage
Anisotropy	0.295	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.477 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5640	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CRB, 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	0.34	0/2749	0.62	0/3717
1	B	0.35	0/2749	0.62	0/3717
All	All	0.34	0/5498	0.62	0/7434

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 [i](#)

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	2689	0	2668	168	0
1	B	2689	0	2668	178	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	44	0	26	2	0
3	B	44	0	26	2	0
4	A	17	0	12	1	0
4	B	17	0	12	1	0
5	A	71	0	0	4	0
5	B	67	0	0	4	0
All	All	5640	0	5412	332	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 30.

All (332) 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:64:ILE:HD11	1:B:102:THR:HG23	1.50	0.93
1:B:6:THR:HB	1:B:226:VAL:HG11	1.49	0.92
1:A:64:ILE:HD11	1:A:102:THR:HG23	1.50	0.92
1:A:6:THR:HB	1:A:226:VAL:HG11	1.49	0.90
1:A:85:SER:HA	1:B:143:GLN:HE21	1.43	0.84
1:A:143:GLN:HE21	1:B:85:SER:HA	1.44	0.82
1:A:268:PHE:CD2	1:A:279:HIS:ND1	2.48	0.82
1:B:268:PHE:CD2	1:B:279:HIS:ND1	2.48	0.81
1:B:28:LEU:HD11	1:B:53:ILE:HD12	1.63	0.80
1:A:314:LYS:HE3	1:B:115:ARG:HH12	1.46	0.80
1:A:28:LEU:HD11	1:A:53:ILE:HD12	1.63	0.79
1:A:115:ARG:HH12	1:B:314:LYS:HE3	1.48	0.79
1:A:268:PHE:CD2	1:A:279:HIS:CE1	2.73	0.77
1:B:191:THR:O	1:B:194:ILE:HG22	1.85	0.77
1:B:268:PHE:CD2	1:B:279:HIS:CE1	2.72	0.76
1:A:191:THR:O	1:A:194:ILE:HG22	1.85	0.76
1:B:231:GLU:HA	1:B:235:ARG:HB3	1.68	0.76
1:A:243:THR:HG21	1:A:323:MET:HG2	1.67	0.76
1:B:243:THR:HG21	1:B:323:MET:HG2	1.68	0.76
1:A:231:GLU:HA	1:A:235:ARG:HB3	1.68	0.74
1:B:139:ILE:O	1:B:146:ASN:HA	1.90	0.72
1:A:321:VAL:HG21	1:A:342:LEU:HD11	1.71	0.71
1:A:139:ILE:O	1:A:146:ASN:HA	1.90	0.71
1:B:321:VAL:HG21	1:B:342:LEU:HD11	1.71	0.71
1:A:85:SER:HA	1:B:143:GLN:NE2	2.05	0.71
1:A:143:GLN:NE2	1:B:85:SER:HA	2.06	0.70
1:A:313:ASP:HB3	1:A:316:ASN:OD1	1.94	0.69
1:B:39:ASP:HB3	1:B:42:VAL:HB	1.75	0.68
1:B:313:ASP:HB3	1:B:316:ASN:OD1	1.94	0.67
1:B:320:GLY:HA3	1:B:336:HIS:CE1	2.31	0.66
1:B:21:ILE:HG21	1:B:49:LYS:HE2	1.78	0.66
1:A:21:ILE:HG21	1:A:49:LYS:HE2	1.78	0.66
1:A:39:ASP:HB3	1:A:42:VAL:HB	1.77	0.64
1:A:38:ILE:CD1	1:A:43:ASN:HA	2.29	0.63
1:B:275:PHE:CD2	1:B:327:ARG:HG3	2.33	0.63
1:A:275:PHE:CD2	1:A:327:ARG:HG3	2.34	0.63
1:A:222:LEU:O	1:A:226:VAL:HG23	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:VAL:O	1:B:336:HIS:HA	1.98	0.62
1:B:222:LEU:O	1:B:226:VAL:HG23	1.99	0.62
1:B:327:ARG:NH1	1:B:331:ASP:OD1	2.33	0.62
1:A:39:ASP:OD1	1:A:66:ALA:HA	2.00	0.62
1:A:321:VAL:O	1:A:336:HIS:HA	2.00	0.62
1:B:187:GLY:HA2	1:B:329:PHE:HB3	1.82	0.62
1:B:38:ILE:CD1	1:B:43:ASN:HA	2.29	0.62
1:A:128:ALA:HA	1:A:131:SER:OG	2.00	0.61
1:A:187:GLY:HA2	1:A:329:PHE:HB3	1.82	0.61
1:B:228:ASP:CG	1:B:233:GLY:H	2.03	0.61
1:A:51:ASP:C	1:A:53:ILE:H	2.04	0.61
1:A:327:ARG:NH1	1:A:331:ASP:OD1	2.34	0.61
1:B:39:ASP:OD1	1:B:66:ALA:HA	2.01	0.61
1:B:32:ASP:OD2	1:B:91:ASN:HB3	2.01	0.61
1:A:129:HIS:O	1:A:218:ILE:HG12	2.02	0.60
1:A:228:ASP:CG	1:A:233:GLY:H	2.04	0.60
1:B:128:ALA:HA	1:B:131:SER:OG	2.00	0.60
1:B:51:ASP:C	1:B:53:ILE:H	2.04	0.60
1:A:289:ILE:HG12	1:A:295:LEU:CD1	2.32	0.60
1:B:69:LYS:HE2	5:B:602:HOH:O	2.01	0.60
1:B:289:ILE:HG12	1:B:295:LEU:CD1	2.32	0.59
1:B:129:HIS:O	1:B:218:ILE:HG12	2.02	0.59
1:B:127:LEU:HD23	1:B:127:LEU:O	2.02	0.59
1:A:148:ILE:HD12	1:A:148:ILE:N	2.19	0.58
1:A:127:LEU:O	1:A:127:LEU:HD23	2.03	0.58
1:B:68:GLU:OE1	1:B:145:LYS:HE3	2.04	0.58
1:B:320:GLY:HA3	1:B:336:HIS:HE1	1.66	0.58
1:A:323:MET:O	1:A:334:VAL:HA	2.04	0.58
1:A:32:ASP:OD2	1:A:91:ASN:HB3	2.03	0.58
1:B:338:ASP:OD1	1:B:340:LEU:HB3	2.04	0.58
1:B:323:MET:O	1:B:334:VAL:HA	2.04	0.58
1:B:43:ASN:O	1:B:47:ALA:HB2	2.03	0.57
1:B:228:ASP:OD2	1:B:231:GLU:HA	2.04	0.57
1:A:68:GLU:OE1	1:A:145:LYS:HE3	2.04	0.57
1:B:39:ASP:HB3	1:B:42:VAL:CB	2.34	0.57
1:B:28:LEU:CD1	1:B:53:ILE:HD12	2.32	0.57
1:B:199:LYS:HE3	5:B:621:HOH:O	2.05	0.57
1:B:148:ILE:N	1:B:148:ILE:HD12	2.19	0.57
1:B:269:ILE:HD11	1:B:349:LEU:HD13	1.86	0.57
1:A:43:ASN:O	1:A:47:ALA:HB2	2.04	0.57
1:A:228:ASP:OD2	1:A:231:GLU:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:LEU:HB3	1:B:61:LYS:HA	1.87	0.57
1:B:38:ILE:HD11	1:B:43:ASN:HA	1.86	0.56
1:B:123:PRO:HD2	1:B:158:ILE:O	2.05	0.56
1:A:28:LEU:CD1	1:A:53:ILE:HD12	2.32	0.56
1:A:39:ASP:HB3	1:A:42:VAL:CB	2.35	0.56
1:A:338:ASP:OD1	1:A:340:LEU:HB3	2.05	0.56
1:A:104:ASP:OD1	3:A:400:NAD:H2N	2.05	0.56
1:A:338:ASP:CG	1:A:340:LEU:HB3	2.25	0.56
1:B:104:ASP:OD1	3:B:401:NAD:H2N	2.05	0.56
1:A:38:ILE:HD11	1:A:43:ASN:HA	1.85	0.56
1:A:269:ILE:HD11	1:A:349:LEU:HD13	1.87	0.56
1:B:241:GLY:HA2	5:B:666:HOH:O	2.06	0.56
1:A:123:PRO:HD2	1:A:158:ILE:O	2.06	0.56
1:B:289:ILE:HG12	1:B:295:LEU:HD13	1.88	0.56
1:B:338:ASP:CG	1:B:340:LEU:HB3	2.25	0.56
1:A:269:ILE:HG21	1:A:345:ALA:HA	1.88	0.56
1:A:36:LEU:HB3	1:A:61:LYS:HA	1.88	0.55
1:A:84:LEU:C	1:A:86:HIS:H	2.10	0.55
1:B:160:ASP:HB3	1:B:163:PHE:CE2	2.41	0.55
1:B:269:ILE:HG21	1:B:345:ALA:HA	1.89	0.55
1:A:160:ASP:HB3	1:A:163:PHE:CE2	2.41	0.55
1:A:289:ILE:HG12	1:A:295:LEU:HD13	1.87	0.55
1:A:71:LYS:HD2	1:A:101:ALA:HA	1.89	0.55
1:B:71:LYS:HD2	1:B:101:ALA:HA	1.88	0.54
1:B:84:LEU:C	1:B:86:HIS:H	2.11	0.54
1:A:311:LEU:O	1:A:312:SER:HB2	2.08	0.54
1:A:58:ASN:ND2	1:A:59:VAL:HG23	2.23	0.54
1:B:311:LEU:O	1:B:312:SER:HB2	2.08	0.54
1:B:76:TYR:OH	1:B:112:THR:HG21	2.09	0.53
1:A:7:TYR:HB2	1:A:11:ASN:OD1	2.09	0.53
1:A:76:TYR:OH	1:A:112:THR:HG21	2.09	0.53
1:B:94:ILE:HG13	1:B:110:ALA:HB2	1.90	0.53
1:B:58:ASN:ND2	1:B:59:VAL:HG23	2.24	0.53
1:B:248:VAL:O	1:B:252:HIS:HB2	2.09	0.53
1:A:39:ASP:HB3	1:A:42:VAL:CG2	2.39	0.53
1:A:192:GLN:O	1:A:196:GLN:HG3	2.09	0.53
1:A:94:ILE:HG13	1:A:110:ALA:HB2	1.91	0.52
1:B:225:VAL:HG23	1:B:226:VAL:N	2.25	0.52
1:B:39:ASP:HB3	1:B:42:VAL:CG2	2.39	0.52
1:B:256:HIS:O	1:B:260:VAL:HG23	2.10	0.52
1:A:332:ILE:HD12	1:A:332:ILE:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:670:HOH:O	1:B:87:HIS:HA	2.10	0.52
1:B:192:GLN:O	1:B:196:GLN:HG3	2.08	0.52
1:A:256:HIS:O	1:A:260:VAL:HG23	2.10	0.52
1:A:286:GLN:O	1:A:290:GLN:HG3	2.09	0.52
1:B:286:GLN:O	1:B:290:GLN:HG3	2.10	0.52
1:B:7:TYR:HB2	1:B:11:ASN:OD1	2.10	0.51
1:B:332:ILE:N	1:B:332:ILE:HD12	2.25	0.51
1:A:207:LEU:HD12	5:A:615:HOH:O	2.10	0.51
1:A:37:LEU:HD13	1:A:94:ILE:HG23	1.92	0.51
1:B:239:ASN:CB	1:B:315:LYS:HD3	2.39	0.51
1:A:225:VAL:HG23	1:A:226:VAL:N	2.24	0.51
1:B:119:PHE:O	1:B:155:THR:N	2.42	0.51
1:B:265:ILE:HD13	1:B:285:ILE:HD13	1.92	0.51
1:A:239:ASN:CB	1:A:315:LYS:HD3	2.40	0.51
1:B:22:LYS:HG3	1:B:23:TYR:N	2.25	0.51
1:B:337:VAL:HG12	1:B:342:LEU:HG	1.92	0.51
1:B:345:ALA:C	1:B:347:GLU:H	2.13	0.51
1:A:265:ILE:HD13	1:A:285:ILE:HD13	1.92	0.51
1:A:345:ALA:C	1:A:347:GLU:H	2.13	0.51
1:A:228:ASP:O	1:A:235:ARG:HB2	2.11	0.50
1:A:337:VAL:HG12	1:A:342:LEU:HG	1.91	0.50
1:A:115:ARG:NE	1:B:136:LYS:HG2	2.25	0.50
1:B:268:PHE:CE2	1:B:279:HIS:CE1	3.00	0.50
1:A:251:TYR:O	1:A:252:HIS:HD2	1.94	0.50
1:A:22:LYS:HG3	1:A:23:TYR:N	2.26	0.50
1:A:136:LYS:HG2	1:B:115:ARG:NE	2.27	0.50
1:A:294:PRO:O	1:A:295:LEU:HB2	2.12	0.50
1:B:228:ASP:O	1:B:235:ARG:HB2	2.12	0.50
1:A:51:ASP:C	1:A:53:ILE:N	2.65	0.49
1:B:51:ASP:C	1:B:53:ILE:N	2.65	0.49
1:A:51:ASP:O	1:A:53:ILE:N	2.46	0.49
1:A:334:VAL:O	1:A:335:GLN:HB3	2.13	0.49
1:B:37:LEU:HD13	1:B:94:ILE:HG23	1.93	0.49
1:B:228:ASP:CG	1:B:232:GLN:H	2.16	0.49
1:B:294:PRO:O	1:B:295:LEU:HB2	2.13	0.49
1:B:19:GLY:N	1:B:160:ASP:OD2	2.35	0.49
1:B:334:VAL:O	1:B:335:GLN:HB3	2.12	0.49
1:A:268:PHE:CE2	1:A:279:HIS:CE1	3.01	0.49
1:A:188:GLU:O	1:A:189:SER:C	2.51	0.48
1:A:244:PHE:O	1:A:248:VAL:HG23	2.13	0.48
1:B:244:PHE:O	1:B:248:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:TYR:O	1:B:252:HIS:HD2	1.96	0.48
1:B:268:PHE:HD2	1:B:279:HIS:CE1	2.30	0.48
1:A:258:HIS:O	1:A:262:VAL:HG23	2.13	0.48
1:A:344:HIS:O	1:A:348:GLN:N	2.46	0.48
1:B:169:PHE:CZ	1:B:201:ARG:HG3	2.49	0.48
1:B:45:TYR:HB3	1:B:46:PHE:CE1	2.48	0.48
1:A:119:PHE:O	1:A:155:THR:N	2.43	0.48
1:A:248:VAL:O	1:A:252:HIS:HB2	2.13	0.48
1:B:94:ILE:HB	1:B:110:ALA:HB2	1.94	0.48
1:B:147:LEU:C	1:B:148:ILE:HD12	2.34	0.48
1:A:228:ASP:CG	1:A:232:GLN:H	2.17	0.48
1:B:258:HIS:O	1:B:262:VAL:HG23	2.14	0.48
1:A:45:TYR:HB3	1:A:46:PHE:CE1	2.49	0.47
1:A:249:GLU:O	1:A:253:LYS:N	2.46	0.47
1:B:51:ASP:O	1:B:53:ILE:N	2.47	0.47
1:A:19:GLY:N	1:A:160:ASP:OD2	2.35	0.47
1:A:115:ARG:CZ	1:B:136:LYS:HG2	2.44	0.47
1:A:169:PHE:CZ	1:A:201:ARG:HG3	2.50	0.47
1:B:269:ILE:CG2	1:B:345:ALA:HA	2.44	0.47
1:A:147:LEU:C	1:A:148:ILE:HD12	2.34	0.47
1:A:258:HIS:HD2	1:A:294:PRO:HG2	1.80	0.47
1:A:314:LYS:HE3	1:B:115:ARG:NH1	2.24	0.47
1:A:39:ASP:HB3	1:A:42:VAL:HG23	1.97	0.47
1:A:158:ILE:O	1:A:158:ILE:HG22	2.13	0.47
1:A:336:HIS:CD2	1:A:337:VAL:H	2.32	0.47
1:A:147:LEU:HD22	1:A:147:LEU:N	2.29	0.47
1:A:94:ILE:HB	1:A:110:ALA:HB2	1.96	0.47
1:A:327:ARG:HH11	1:A:327:ARG:HB3	1.80	0.47
1:B:14:ILE:HD13	1:B:133:VAL:HG22	1.97	0.47
1:B:31:PHE:HA	1:B:91:ASN:ND2	2.30	0.47
1:B:258:HIS:HD2	1:B:294:PRO:HG2	1.80	0.47
1:A:37:LEU:HA	1:A:62:VAL:O	2.15	0.46
1:A:187:GLY:HA3	5:A:612:HOH:O	2.14	0.46
1:B:41:TYR:O	1:B:44:GLN:HB2	2.15	0.46
1:B:158:ILE:O	1:B:158:ILE:HG22	2.14	0.46
1:B:188:GLU:O	1:B:189:SER:C	2.53	0.46
1:B:39:ASP:HB3	1:B:42:VAL:HG23	1.98	0.46
1:B:174:SER:O	1:B:257:GLY:HA3	2.15	0.46
1:A:238:LEU:HB3	4:A:500:CRB:H32	1.96	0.46
1:A:225:VAL:HG23	1:A:226:VAL:H	1.79	0.46
1:A:269:ILE:HG23	1:A:348:GLN:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:LEU:HA	1:B:62:VAL:O	2.16	0.46
1:B:30:GLN:O	1:B:30:GLN:HG3	2.16	0.46
1:B:147:LEU:N	1:B:147:LEU:HD22	2.30	0.46
1:B:180:TYR:CE2	1:B:287:TYR:HE1	2.34	0.46
1:A:269:ILE:CG2	1:A:345:ALA:HA	2.45	0.46
1:A:6:THR:HG22	1:A:6:THR:O	2.16	0.46
1:B:9:SER:O	1:B:10:ASN:HB2	2.15	0.46
1:B:340:LEU:C	1:B:340:LEU:HD13	2.36	0.46
1:A:120:ILE:HD13	1:A:120:ILE:HA	1.84	0.45
1:A:136:LYS:HG2	1:B:115:ARG:CZ	2.46	0.45
1:B:117:VAL:O	1:B:152:TYR:OH	2.29	0.45
1:A:41:TYR:O	1:A:44:GLN:HB2	2.16	0.45
1:A:129:HIS:HD2	1:A:218:ILE:HG13	1.82	0.45
1:A:268:PHE:HD2	1:A:279:HIS:CE1	2.30	0.45
1:A:340:LEU:HD13	1:A:340:LEU:C	2.37	0.45
1:A:174:SER:O	1:A:257:GLY:HA3	2.16	0.45
1:B:129:HIS:HD2	1:B:218:ILE:HG13	1.81	0.45
1:A:115:ARG:NH1	1:B:314:LYS:HE3	2.25	0.45
1:A:272:ASN:HA	1:A:277:SER:H	1.80	0.45
1:A:315:LYS:HE3	1:A:315:LYS:HB2	1.79	0.45
1:A:31:PHE:HA	1:A:91:ASN:ND2	2.31	0.45
1:A:130:ASP:O	1:A:221:LYS:NZ	2.49	0.45
1:B:238:LEU:HB3	4:B:501:CRB:H32	1.97	0.45
1:B:129:HIS:HB2	1:B:218:ILE:HD11	1.99	0.45
1:B:188:GLU:O	1:B:191:THR:N	2.50	0.45
1:A:106:ALA:O	1:A:109:VAL:HB	2.16	0.45
1:A:180:TYR:CE2	1:A:287:TYR:HE1	2.34	0.45
1:B:225:VAL:HG23	1:B:226:VAL:H	1.79	0.45
1:B:249:GLU:O	1:B:253:LYS:N	2.46	0.45
1:B:6:THR:O	1:B:6:THR:HG22	2.16	0.45
1:B:194:ILE:HG13	1:B:213:TYR:CD2	2.52	0.45
1:A:129:HIS:HB2	1:A:218:ILE:HD11	1.99	0.45
1:B:106:ALA:O	1:B:109:VAL:HB	2.16	0.45
1:B:233:GLY:O	1:B:236:LYS:HB2	2.17	0.45
1:A:336:HIS:O	1:A:337:VAL:HG23	2.17	0.45
1:B:267:GLN:HE21	1:B:267:GLN:HB3	1.57	0.45
1:B:127:LEU:HB2	1:B:175:GLY:HA2	1.98	0.44
1:A:14:ILE:HD13	1:A:133:VAL:HG22	1.98	0.44
1:A:194:ILE:HG13	1:A:213:TYR:CD2	2.52	0.44
1:A:233:GLY:O	1:A:236:LYS:HB2	2.16	0.44
1:B:277:SER:CB	1:B:279:HIS:CD2	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:LYS:HE3	1:B:315:LYS:HB2	1.78	0.44
1:B:327:ARG:HH11	1:B:327:ARG:HB3	1.81	0.44
1:A:30:GLN:HG3	1:A:30:GLN:O	2.16	0.44
1:B:340:LEU:HD13	1:B:341:THR:N	2.32	0.44
1:B:38:ILE:HD13	1:B:43:ASN:HA	1.99	0.44
1:B:66:ALA:O	1:B:69:LYS:HB2	2.18	0.44
1:B:287:TYR:O	1:B:291:LEU:HG	2.18	0.44
1:B:344:HIS:O	1:B:348:GLN:N	2.46	0.44
1:A:188:GLU:O	1:A:191:THR:N	2.50	0.44
1:B:195:GLU:HG2	1:B:287:TYR:CE1	2.53	0.44
1:B:94:ILE:CB	1:B:110:ALA:HB2	2.47	0.44
1:B:254:ILE:HG22	1:B:255:PRO:CD	2.48	0.44
1:B:336:HIS:O	1:B:337:VAL:HG23	2.18	0.44
1:A:6:THR:HB	1:A:226:VAL:CG1	2.35	0.43
1:A:287:TYR:O	1:A:291:LEU:HG	2.18	0.43
1:B:277:SER:HB3	1:B:279:HIS:CD2	2.53	0.43
1:B:269:ILE:HG23	1:B:348:GLN:OE1	2.18	0.43
1:A:200:ASP:OD1	1:A:203:ILE:HG13	2.18	0.43
1:A:272:ASN:O	1:A:276:ASP:HA	2.18	0.43
1:A:293:TYR:O	1:A:295:LEU:HG	2.18	0.43
1:A:340:LEU:HD13	1:A:341:THR:N	2.32	0.43
1:B:272:ASN:HA	1:B:277:SER:H	1.81	0.43
1:B:296:ASP:OD2	1:B:296:ASP:N	2.51	0.43
1:A:241:GLY:HA2	5:A:667:HOH:O	2.17	0.43
1:B:130:ASP:O	1:B:221:LYS:NZ	2.50	0.43
1:B:313:ASP:CG	1:B:314:LYS:H	2.22	0.43
1:A:5:THR:OG1	1:A:11:ASN:HB3	2.19	0.43
1:A:254:ILE:HG22	1:A:255:PRO:CD	2.49	0.43
1:B:293:TYR:O	1:B:295:LEU:HG	2.18	0.43
1:B:258:HIS:CD2	1:B:294:PRO:HG2	2.54	0.43
1:A:84:LEU:HD11	1:B:148:ILE:HD11	2.01	0.43
1:B:86:HIS:O	1:B:87:HIS:C	2.57	0.43
1:B:219:GLU:O	1:B:222:LEU:HB3	2.19	0.43
1:B:272:ASN:O	1:B:276:ASP:HA	2.19	0.43
1:B:347:GLU:O	1:B:350:LYS:HB2	2.19	0.43
1:A:94:ILE:CB	1:A:110:ALA:HB2	2.48	0.42
1:B:5:THR:OG1	1:B:11:ASN:HB3	2.19	0.42
1:A:9:SER:O	1:A:10:ASN:HB2	2.20	0.42
1:A:195:GLU:HG2	1:A:287:TYR:CE1	2.53	0.42
1:A:313:ASP:CG	1:A:314:LYS:H	2.22	0.42
1:A:113:LEU:O	1:A:117:VAL:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:HIS:CD2	1:A:294:PRO:HG2	2.54	0.42
1:B:232:GLN:HA	1:B:232:GLN:NE2	2.34	0.42
1:B:239:ASN:HB2	1:B:315:LYS:HD3	2.01	0.42
1:B:200:ASP:OD1	1:B:203:ILE:HG13	2.19	0.42
1:B:285:ILE:O	1:B:289:ILE:HG13	2.20	0.42
1:B:333:VAL:HA	5:B:643:HOH:O	2.20	0.42
1:A:127:LEU:HB2	1:A:175:GLY:HA2	2.01	0.42
1:A:232:GLN:HA	1:A:232:GLN:NE2	2.34	0.42
1:A:239:ASN:HB2	1:A:315:LYS:HD3	2.02	0.42
1:B:181:LYS:O	1:B:184:LEU:HB2	2.19	0.42
1:B:243:THR:OG1	1:B:315:LYS:NZ	2.51	0.42
1:A:104:ASP:OD1	3:A:400:NAD:H1D	2.20	0.42
1:B:113:LEU:O	1:B:117:VAL:HG13	2.20	0.42
1:B:171:GLN:HA	1:B:171:GLN:NE2	2.35	0.42
1:A:135:GLY:O	1:A:151:PHE:HA	2.20	0.42
1:A:243:THR:OG1	1:A:315:LYS:NZ	2.51	0.42
1:B:31:PHE:HA	1:B:91:ASN:HD21	1.85	0.42
1:B:264:ILE:O	1:B:267:GLN:NE2	2.53	0.41
1:A:280:ASP:O	1:A:283:HIS:HB3	2.21	0.41
1:B:189:SER:O	1:B:193:ASP:HB2	2.20	0.41
1:A:38:ILE:HD13	1:A:43:ASN:HA	1.99	0.41
1:A:171:GLN:HA	1:A:171:GLN:NE2	2.36	0.41
1:A:219:GLU:O	1:A:222:LEU:HB3	2.19	0.41
1:A:148:ILE:HD11	1:B:84:LEU:HD11	2.02	0.41
1:B:6:THR:HB	1:B:226:VAL:CG1	2.34	0.41
1:B:104:ASP:OD1	3:B:401:NAD:H1D	2.20	0.41
1:A:347:GLU:O	1:A:350:LYS:HB2	2.20	0.41
1:A:267:GLN:HE21	1:A:267:GLN:HB3	1.58	0.41
1:B:338:ASP:C	1:B:340:LEU:N	2.73	0.41
1:A:181:LYS:O	1:A:184:LEU:HB2	2.21	0.41
1:A:189:SER:O	1:A:193:ASP:HB2	2.20	0.41
1:A:221:LYS:O	1:A:224:ILE:N	2.54	0.41
1:A:296:ASP:N	1:A:296:ASP:OD2	2.51	0.41
1:B:30:GLN:O	1:B:30:GLN:CG	2.68	0.41
1:B:168:PRO:O	1:B:172:ILE:HG13	2.20	0.41
1:A:31:PHE:HA	1:A:91:ASN:HD21	1.86	0.41
1:A:117:VAL:O	1:A:152:TYR:OH	2.30	0.40
1:A:86:HIS:O	1:A:87:HIS:C	2.58	0.40
1:A:261:MET:O	1:A:264:ILE:HB	2.21	0.40
1:A:346:CYS:SG	1:A:346:CYS:O	2.80	0.40
1:B:222:LEU:O	1:B:226:VAL:CG2	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:GLY:O	1:A:247:ALA:N	2.55	0.40
1:B:135:GLY:O	1:B:151:PHE:HA	2.22	0.40
1:A:264:ILE:O	1:A:267:GLN:NE2	2.54	0.40
1:B:221:LYS:O	1:B:224:ILE:N	2.54	0.40
1:B:346:CYS:SG	1:B:346:CYS:O	2.79	0.40
1:B:84:LEU:C	1:B:86:HIS:N	2.74	0.40
1:B:94:ILE:CG1	1:B:110:ALA:HB2	2.51	0.40
1:B:261:MET:O	1:B:264:ILE:HB	2.21	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	330/354 (93%)	251 (76%)	62 (19%)	17 (5%)	2	6
1	B	330/354 (93%)	252 (76%)	63 (19%)	15 (4%)	2	8
All	All	660/708 (93%)	503 (76%)	125 (19%)	32 (5%)	2	7

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	88	VAL
1	A	312	SER
1	A	313	ASP
1	A	319	GLN
1	B	28	LEU
1	B	88	VAL
1	B	312	SER
1	B	313	ASP
1	B	319	GLN

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Mol	Chain	Res	Type
1	A	52	ASP
1	A	318	LYS
1	B	52	ASP
1	B	318	LYS
1	A	26	THR
1	A	189	SER
1	A	246	HIS
1	A	294	PRO
1	B	26	THR
1	B	189	SER
1	B	246	HIS
1	B	294	PRO
1	A	295	LEU
1	B	295	LEU
1	A	85	SER
1	A	146	ASN
1	B	85	SER
1	B	87	HIS
1	B	146	ASN
1	A	87	HIS
1	A	165	LYS
1	A	205	GLN

5.3.2 Protein sidechains [i](#)

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	288/306 (94%)	272 (94%)	16 (6%)	21	51
1	B	288/306 (94%)	272 (94%)	16 (6%)	21	51
All	All	576/612 (94%)	544 (94%)	32 (6%)	21	51

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLN

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Mol	Chain	Res	Type
1	A	36	LEU
1	A	51	ASP
1	A	58	ASN
1	A	146	ASN
1	A	159	TYR
1	A	202	GLU
1	A	204	LEU
1	A	216	LYS
1	A	243	THR
1	A	254	ILE
1	A	267	GLN
1	A	275	PHE
1	A	294	PRO
1	A	297	MET
1	A	321	VAL
1	B	30	GLN
1	B	36	LEU
1	B	51	ASP
1	B	58	ASN
1	B	146	ASN
1	B	159	TYR
1	B	202	GLU
1	B	204	LEU
1	B	216	LYS
1	B	243	THR
1	B	254	ILE
1	B	267	GLN
1	B	275	PHE
1	B	294	PRO
1	B	297	MET
1	B	321	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	30	GLN
1	A	58	ASN
1	A	91	ASN
1	A	171	GLN
1	A	205	GLN
1	A	232	GLN

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Mol	Chain	Res	Type
1	A	239	ASN
1	A	252	HIS
1	A	286	GLN
1	A	290	GLN
1	A	336	HIS
1	A	344	HIS
1	B	10	ASN
1	B	30	GLN
1	B	58	ASN
1	B	77	GLN
1	B	91	ASN
1	B	171	GLN
1	B	205	GLN
1	B	232	GLN
1	B	239	ASN
1	B	252	HIS
1	B	286	GLN
1	B	290	GLN
1	B	336	HIS
1	B	344	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	NAD	A	400	-	42,48,48	1.92	10 (23%)	50,73,73	1.65	7 (14%)
4	CRB	A	500	2	16,17,17	2.00	5 (31%)	22,27,27	1.50	3 (13%)
4	CRB	B	501	2	16,17,17	1.99	4 (25%)	22,27,27	1.51	4 (18%)
3	NAD	B	401	-	42,48,48	1.90	10 (23%)	50,73,73	1.67	7 (14%)

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	NAD	A	400	-	-	3/26/62/62	0/5/5/5
4	CRB	A	500	2	-	1/11/29/29	0/1/1/1
4	CRB	B	501	2	-	1/11/29/29	0/1/1/1
3	NAD	B	401	-	-	3/26/62/62	0/5/5/5

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	500	CRB	P1-C7	4.57	1.83	1.78
4	B	501	CRB	P1-C7	4.57	1.83	1.78
3	A	400	NAD	O4D-C1D	4.54	1.47	1.41
3	B	401	NAD	O4D-C1D	4.45	1.47	1.41
3	A	400	NAD	C4A-N3A	4.10	1.41	1.35
3	B	401	NAD	C4A-N3A	4.07	1.41	1.35
3	A	400	NAD	C6N-N1N	3.94	1.45	1.35
3	A	400	NAD	C3N-C7N	3.90	1.56	1.50
3	B	401	NAD	C3N-C7N	3.85	1.56	1.50
3	B	401	NAD	C6N-N1N	3.82	1.44	1.35
3	A	400	NAD	C4N-C3N	3.68	1.45	1.39
3	B	401	NAD	C4N-C3N	3.67	1.45	1.39
3	B	401	NAD	C2N-N1N	3.59	1.39	1.35
3	A	400	NAD	C2B-C1B	-3.59	1.48	1.53
3	B	401	NAD	C2B-C1B	-3.58	1.48	1.53
3	A	400	NAD	C2N-N1N	3.47	1.39	1.35
4	A	500	CRB	C4-C5	3.36	1.57	1.52
4	B	501	CRB	C4-C5	3.25	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	400	NAD	O4B-C1B	3.19	1.45	1.41
4	B	501	CRB	C8-C6	-3.09	1.47	1.53
3	B	401	NAD	O4B-C1B	3.05	1.45	1.41
4	A	500	CRB	C8-C6	-2.99	1.47	1.53
3	B	401	NAD	C2A-N1A	2.39	1.38	1.33
3	A	400	NAD	C5N-C4N	2.38	1.43	1.38
3	B	401	NAD	C5N-C4N	2.32	1.43	1.38
3	A	400	NAD	C2A-N1A	2.32	1.38	1.33
4	B	501	CRB	C6-C5	2.19	1.56	1.53
4	A	500	CRB	C6-C5	2.13	1.55	1.53
4	A	500	CRB	C2-C1	2.04	1.55	1.53

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	NAD	C5N-C4N-C3N	-5.90	113.36	120.34
3	A	400	NAD	C5N-C4N-C3N	-5.78	113.50	120.34
3	B	401	NAD	C6N-C5N-C4N	4.87	126.52	119.44
3	A	400	NAD	C6N-C5N-C4N	4.80	126.41	119.44
3	A	400	NAD	C5N-C6N-N1N	-3.97	114.71	120.40
3	B	401	NAD	C5N-C6N-N1N	-3.96	114.72	120.40
3	B	401	NAD	C2N-C3N-C4N	3.75	122.51	118.26
3	A	400	NAD	C2N-C3N-C4N	3.67	122.42	118.26
4	B	501	CRB	C8-C2-C3	3.44	112.92	110.72
4	A	500	CRB	C8-C2-C3	3.32	112.85	110.72
3	B	401	NAD	C5A-C6A-N6A	3.05	124.99	120.35
3	A	400	NAD	C5A-C6A-N6A	2.99	124.89	120.35
3	A	400	NAD	C2N-N1N-C1D	-2.93	112.62	119.14
3	B	401	NAD	C2N-N1N-C1D	-2.93	112.62	119.14
4	A	500	CRB	C8-C2-C1	-2.87	103.65	109.96
4	B	501	CRB	C8-C2-C1	-2.83	103.75	109.96
3	B	401	NAD	C4N-C3N-C7N	-2.25	115.02	121.04
3	A	400	NAD	C4N-C3N-C7N	-2.24	115.05	121.04
4	B	501	CRB	O92-P1-C7	-2.05	101.73	106.74
4	A	500	CRB	O92-P1-C7	-2.04	101.74	106.74
4	B	501	CRB	O93-P1-O92	2.02	113.99	108.08

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	400	NAD	PN-O3-PA-O5B

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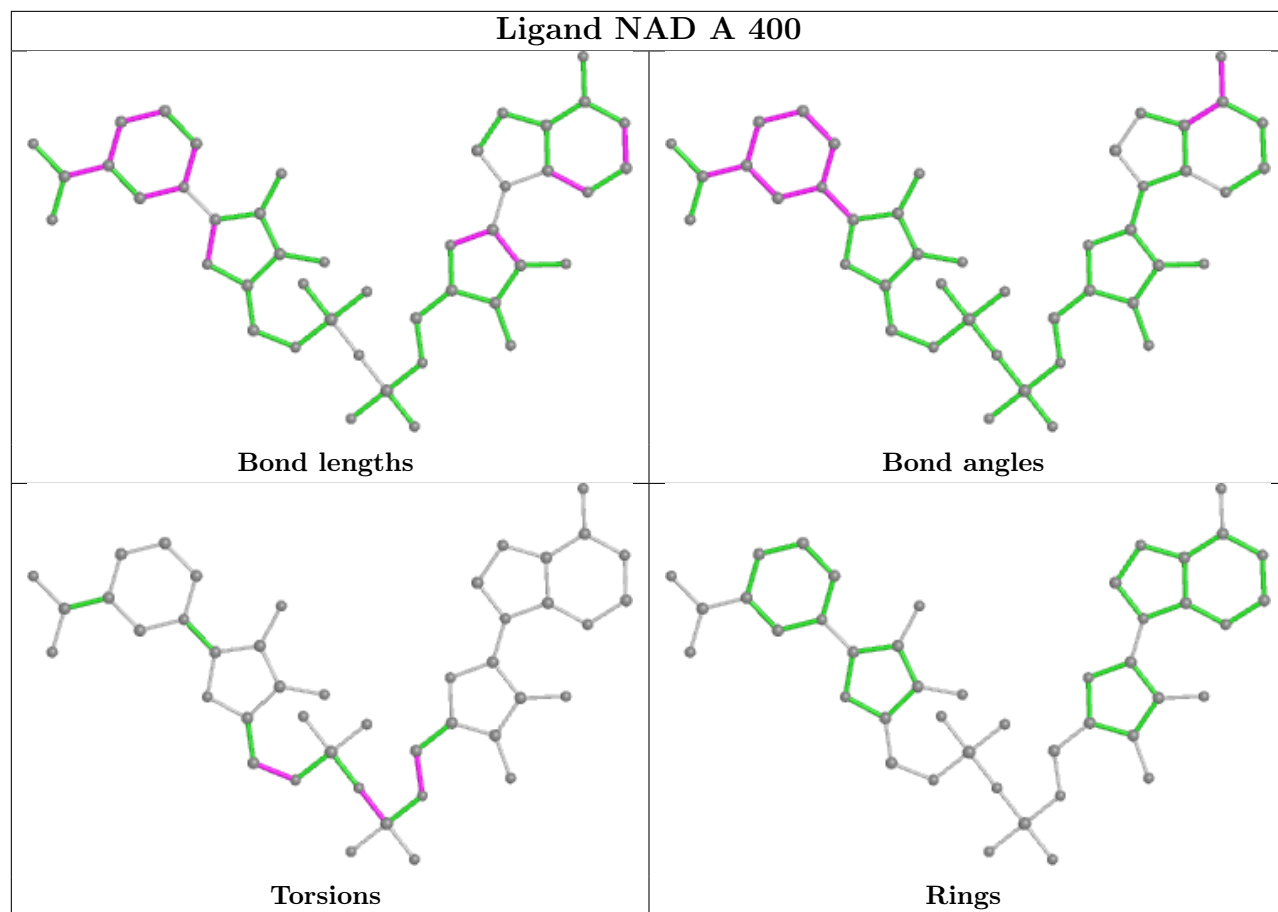
Mol	Chain	Res	Type	Atoms
3	B	401	NAD	PN-O3-PA-O5B
4	A	500	CRB	C6-C7-P1-O92
3	A	400	NAD	C4D-C5D-O5D-PN
3	B	401	NAD	C4D-C5D-O5D-PN
4	B	501	CRB	C6-C7-P1-O92
3	A	400	NAD	C4B-C5B-O5B-PA
3	B	401	NAD	C4B-C5B-O5B-PA

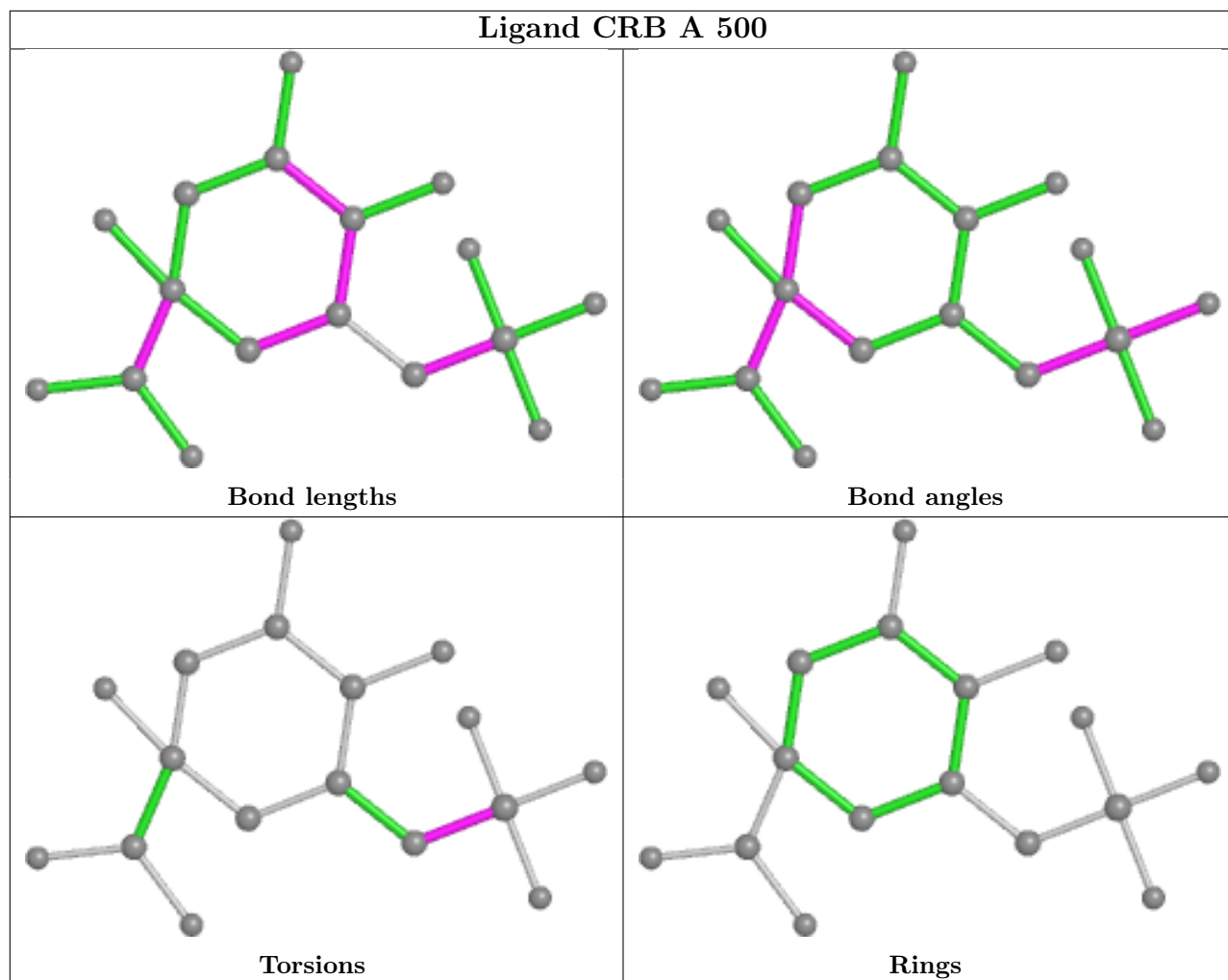
There are no ring outliers.

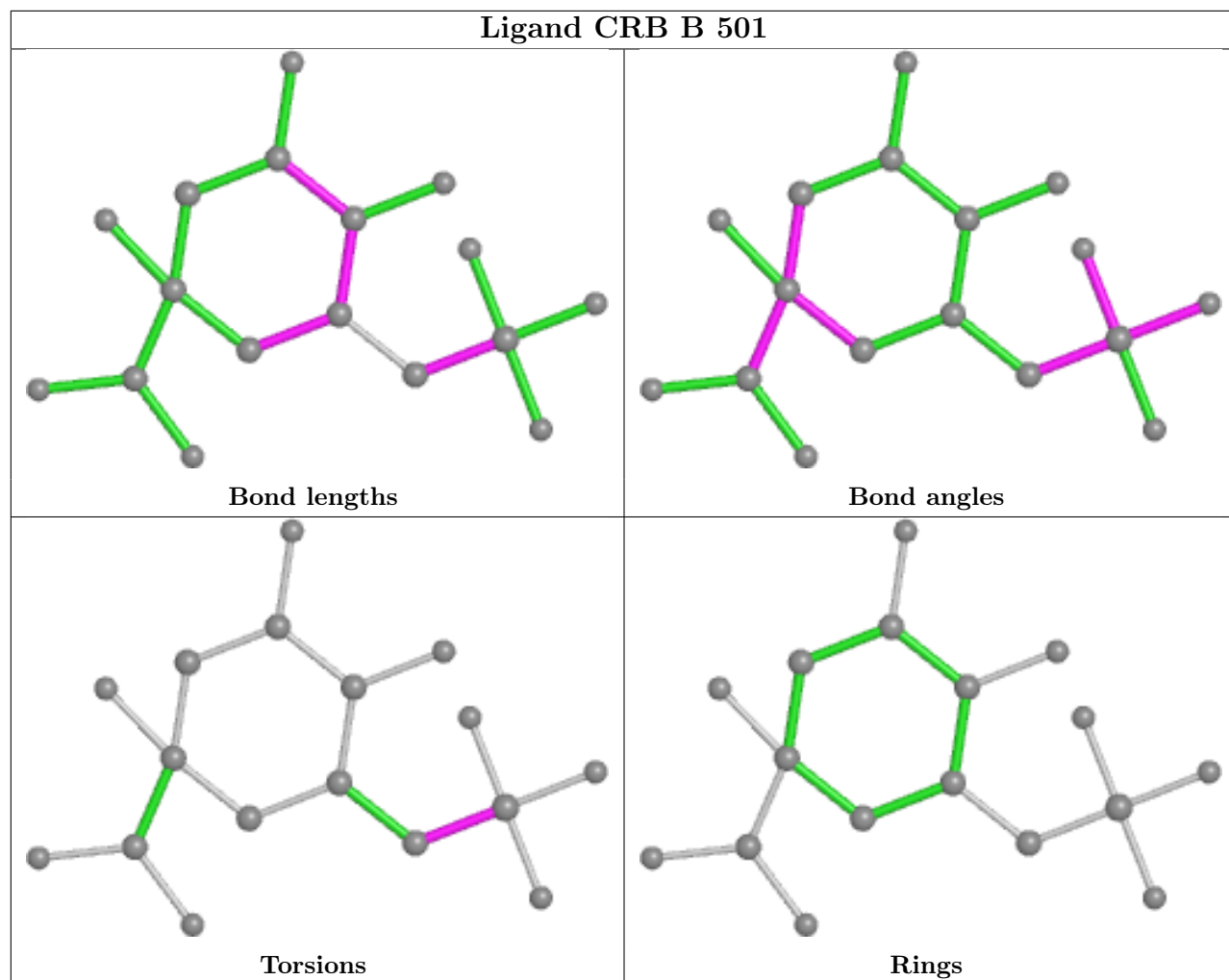
4 monomers are involved in 6 short contacts:

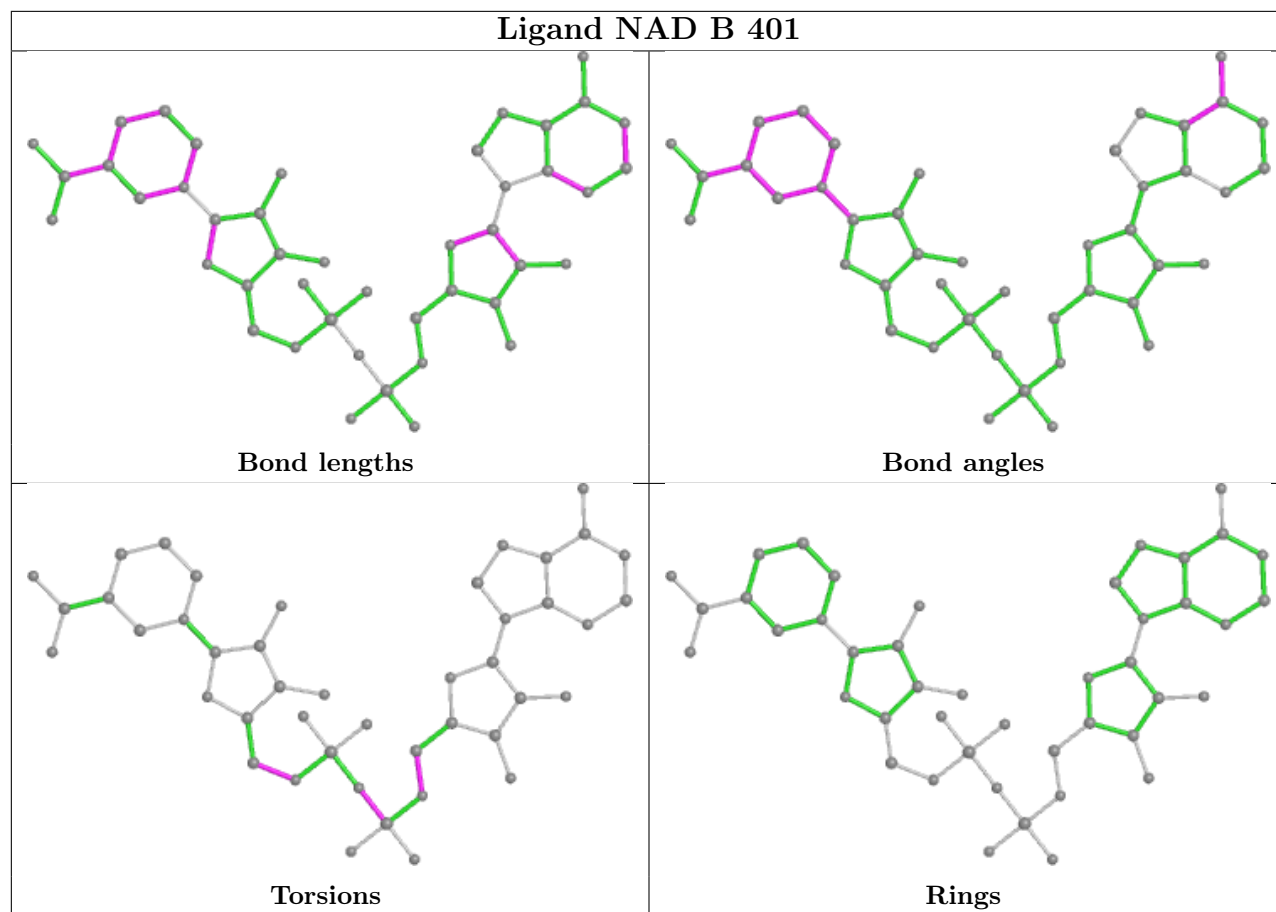
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	400	NAD	2	0
4	A	500	CRB	1	0
4	B	501	CRB	1	0
3	B	401	NAD	2	0

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	336/354 (94%)	-0.42	6 (1%) 68 61	28, 57, 106, 135	0
1	B	336/354 (94%)	-0.43	4 (1%) 79 73	28, 57, 104, 137	0
All	All	672/708 (94%)	-0.43	10 (1%) 73 68	28, 57, 105, 137	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	LEU	3.7
1	B	250	TYR	2.9
1	B	28	LEU	2.8
1	B	251	TYR	2.7
1	A	251	TYR	2.5
1	A	318	LYS	2.4
1	A	313	ASP	2.4
1	A	312	SER	2.2
1	B	318	LYS	2.2
1	A	250	TYR	2.1

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](#)

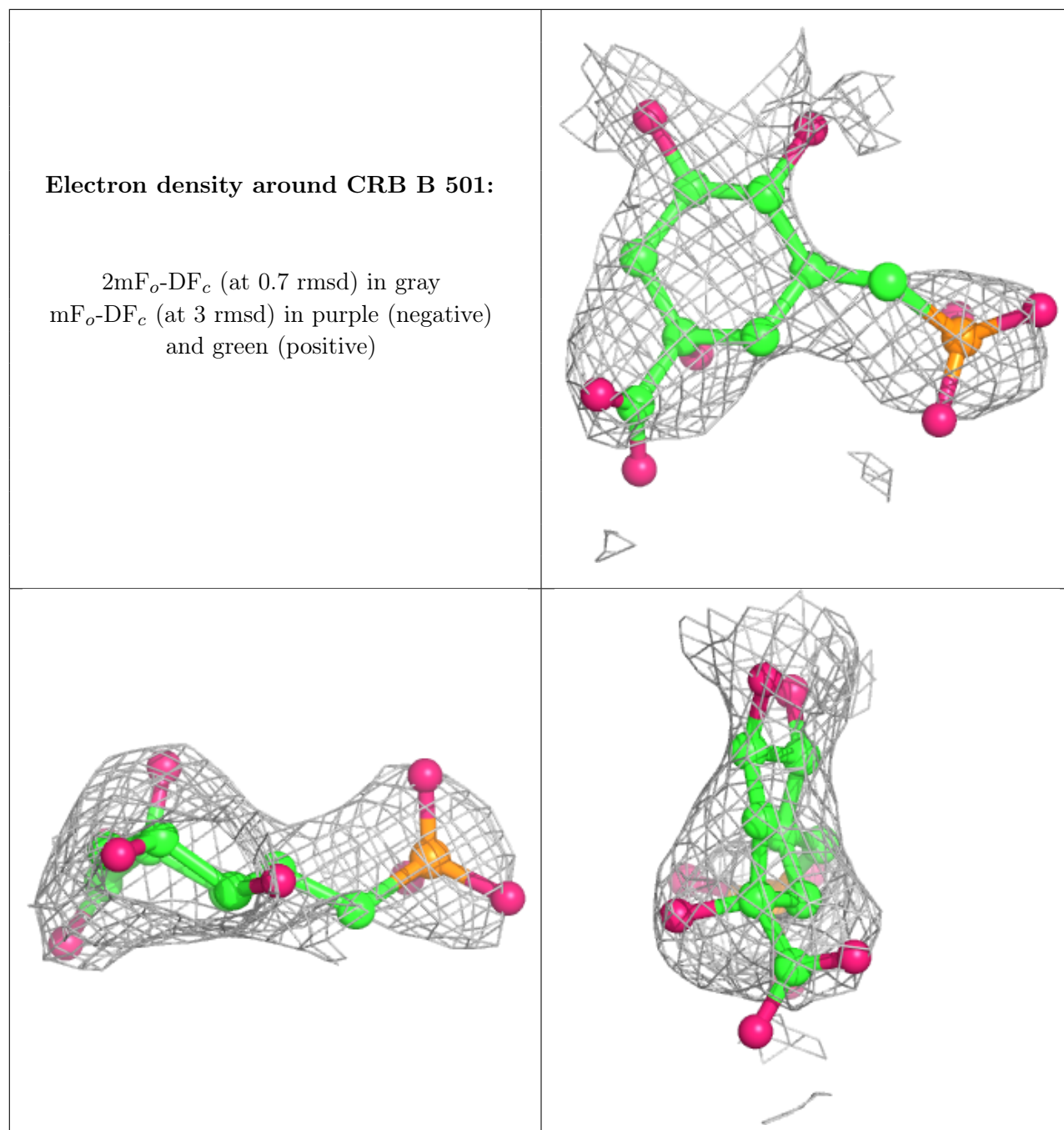
There are no monosaccharides in this entry.

6.4 Ligands

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.

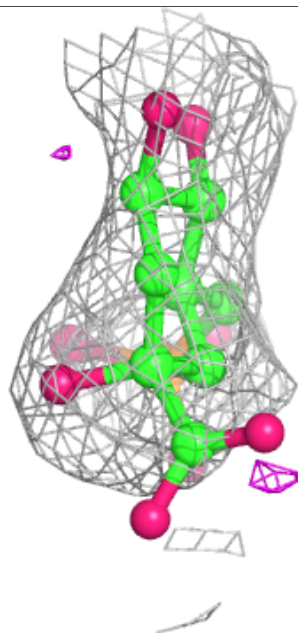
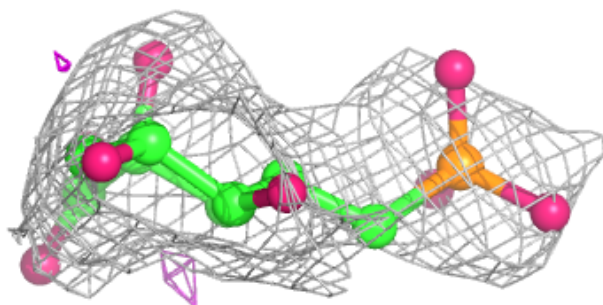
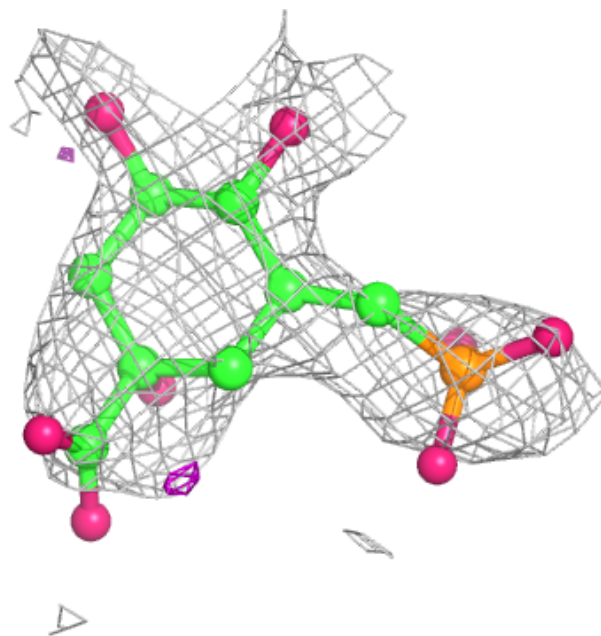
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CRB	B	501	17/17	0.89	0.31	84,108,127,127	0
4	CRB	A	500	17/17	0.90	0.28	77,109,125,129	0
2	ZN	B	601	1/1	0.94	0.08	124,124,124,124	0
2	ZN	A	600	1/1	0.95	0.07	130,130,130,130	0
3	NAD	B	401	44/44	0.96	0.14	27,49,63,72	0
3	NAD	A	400	44/44	0.97	0.14	29,49,63,72	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.



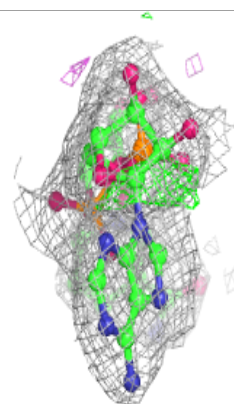
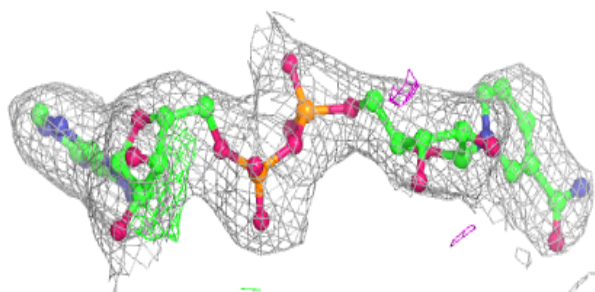
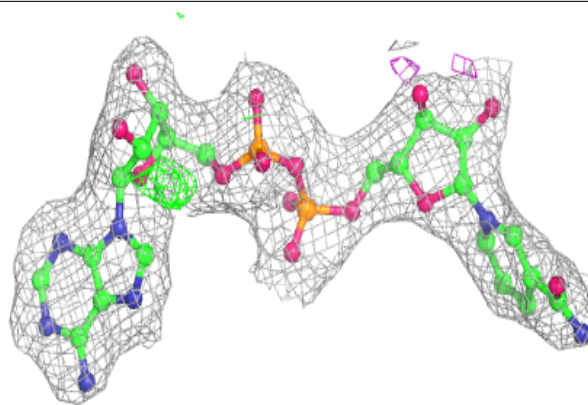
Electron density around CRB A 500:

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

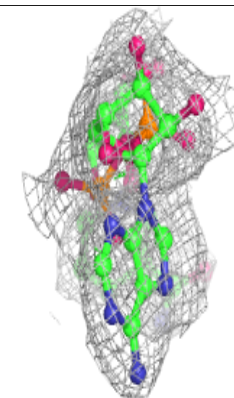
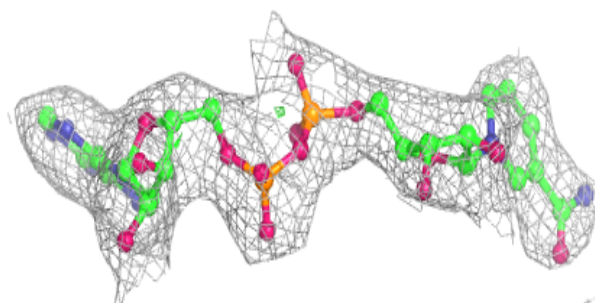
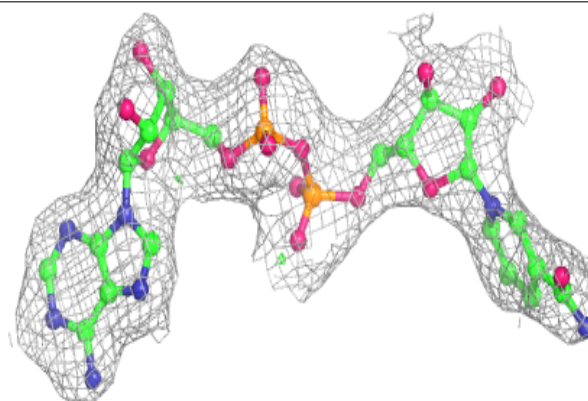


Electron density around NAD B 401:

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

**Electron density around NAD A 400:**

$2mF_o-DF_c$ (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.