



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:11 PM GMT

PDB ID : 1NVE  
Title : Crystal structure of 3-dehydroquinate synthase (DHQS) in complex with ZN2+ and NAD  
Authors : Nichols, C.E.; Ren, J.; Lamb, H.K.; Hawkins, A.R.; Stammers, D.K.  
Deposited on : 2003-02-03  
Resolution : 2.58 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

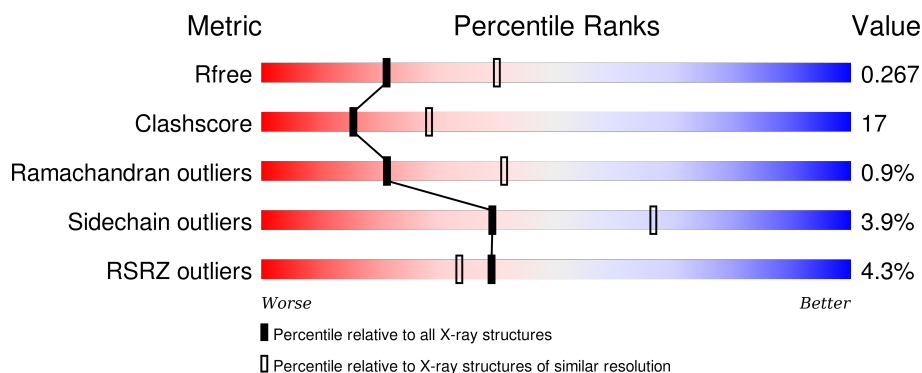
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.58 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))
$R_{free}$	91344	2636 (2.60-2.56)
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)
RSRZ outliers	91569	2642 (2.60-2.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	393	<div> <div>4%</div> <div>63%</div> <div>30%</div> <div>• •</div> </div>
1	B	393	<div> <div>4%</div> <div>68%</div> <div>27%</div> <div>• •</div> </div>
1	C	393	<div> <div>4%</div> <div>66%</div> <div>28%</div> <div>• •</div> </div>
1	D	393	<div> <div>4%</div> <div>62%</div> <div>31%</div> <div>• •</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	604	-	-	-	X
3	CL	C	1605	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12493 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-DEHYDROQUINATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	0	0
			2887	1834	499	542	12			
1	B	383	Total	C	N	O	S	0	0	0
			2933	1862	508	551	12			
1	C	377	Total	C	N	O	S	0	0	0
			2886	1831	499	544	12			
1	D	381	Total	C	N	O	S	0	0	0
			2915	1851	505	547	12			

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

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).

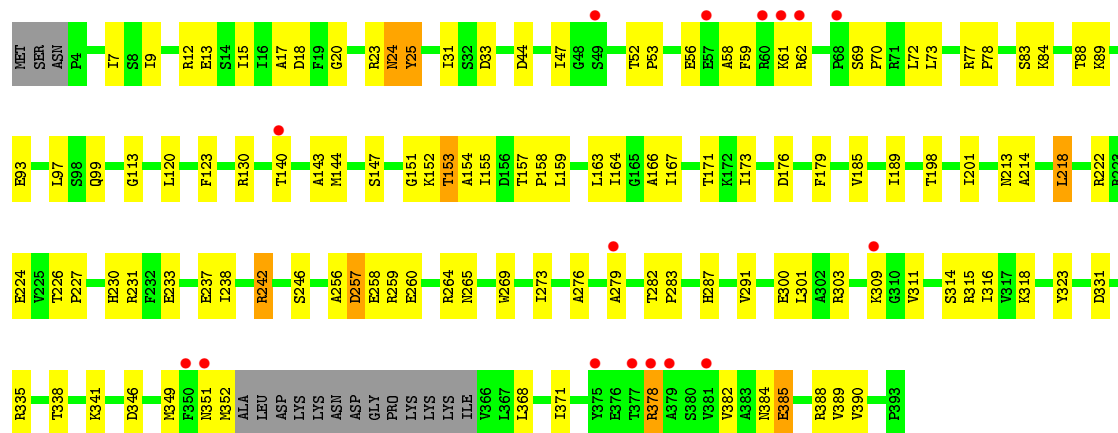


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

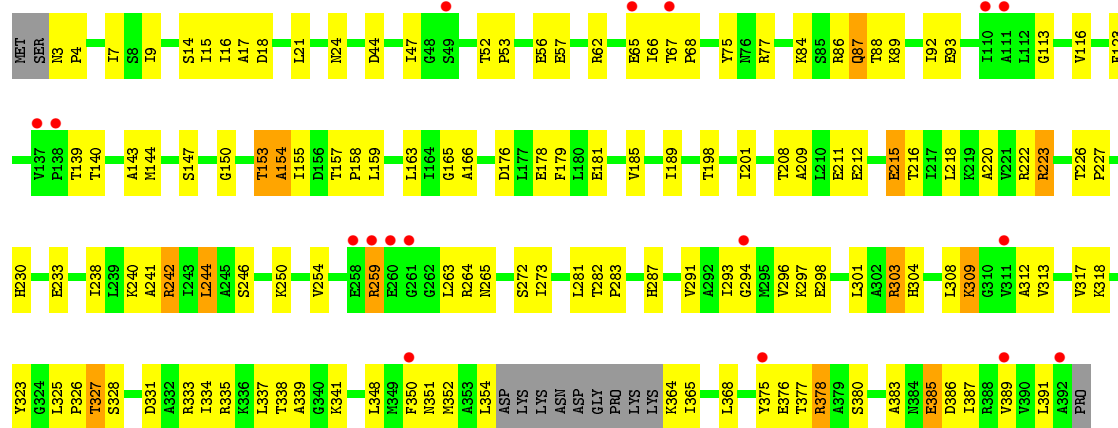
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	173	Total	O	0	0
			173	173		
5	B	162	Total	O	0	0
			162	162		
5	C	176	Total	O	0	0
			176	176		
5	D	179	Total	O	0	0
			179	179		





• Molecule 1: 3-DEHYDROQUINATE SYNTHASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.64Å 70.35Å 144.32Å 90.00° 90.78° 90.00°	Depositor
Resolution (Å)	25.57 – 2.58 25.56 – 2.58	Depositor EDS
% Data completeness (in resolution range)	98.4 (25.57-2.58) 98.5 (25.56-2.58)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.21 (at 2.57Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.208 , 0.268 0.207 , 0.267	Depositor DCC
$R_{free}$ test set	5121 reflections (9.82%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.8	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 61.6	EDS
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 52135 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12493	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.58 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.6086e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, NAD, CL

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	0/2935	0.58	0/3980
1	B	0.34	0/2982	0.59	0/4043
1	C	0.33	0/2935	0.59	0/3980
1	D	0.34	0/2963	0.59	0/4019
All	All	0.34	0/11815	0.59	0/16022

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	2887	0	2964	109	0
1	B	2933	0	3014	93	0
1	C	2886	0	2956	90	0
1	D	2915	0	2994	124	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
4	A	44	0	25	0	0
4	B	44	0	25	0	0
4	C	44	0	25	1	0
4	D	44	0	25	1	0
5	A	173	0	0	4	0
5	B	162	0	0	1	0
5	C	176	0	0	5	0
5	D	179	0	0	7	0
All	All	12493	0	12028	409	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 17.

All (409) 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:87:GLN:NE2	1:D:87:GLN:H	1.66	0.93
1:D:157:THR:HG22	1:D:159:LEU:H	1.34	0.93
1:D:341:LYS:HA	1:D:341:LYS:HE2	1.52	0.89
1:A:9:ILE:HD11	1:A:15:ILE:HD11	1.55	0.88
1:C:73:LEU:HD13	1:C:99:GLN:HG3	1.56	0.87
1:D:201:ILE:HG22	1:D:368:LEU:HD21	1.54	0.87
1:B:258:GLU:O	1:B:258:GLU:HG3	1.75	0.85
1:C:230:HIS:HB2	1:C:233:GLU:HG3	1.60	0.84
1:D:87:GLN:HE21	1:D:87:GLN:H	1.25	0.83
1:A:89:LYS:O	1:A:93:GLU:HG3	1.79	0.82
1:D:123:PHE:HB2	1:D:153:THR:HG23	1.60	0.82
1:D:84:LYS:HG3	1:D:116:VAL:HG13	1.61	0.81
1:D:226:THR:HG23	1:D:227:PRO:HD2	1.62	0.80
1:D:259:ARG:HA	1:D:259:ARG:HH11	1.47	0.80
1:A:253:VAL:HG13	1:A:263:LEU:HG	1.63	0.80
1:C:201:ILE:HG22	1:C:368:LEU:HD21	1.64	0.79
1:C:143:ALA:HA	1:C:147:SER:OG	1.84	0.78
1:C:84:LYS:HG2	1:C:155:ILE:HA	1.67	0.77
1:D:89:LYS:O	1:D:93:GLU:HG3	1.84	0.77
1:C:61:LYS:HG3	1:C:62:ARG:HD3	1.66	0.76
1:D:157:THR:HB	1:D:163:LEU:HD12	1.66	0.75
1:B:230:HIS:HB2	1:B:233:GLU:HG3	1.68	0.75
1:A:308:LEU:HD11	1:A:312:ALA:HB3	1.70	0.74
1:C:385:GLU:O	1:C:389:VAL:HG23	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:ALA:HB1	1:D:242:ARG:NH1	2.03	0.74
1:B:189:ILE:HD12	1:B:323:TYR:O	1.88	0.73
1:D:254:VAL:HG13	1:D:264:ARG:HH12	1.53	0.73
1:D:84:LYS:HD2	1:D:116:VAL:HA	1.70	0.73
1:C:157:THR:HG22	1:C:159:LEU:H	1.52	0.73
1:D:67:THR:HG23	5:D:1724:HOH:O	1.89	0.73
1:A:155:ILE:HD11	1:A:164:ILE:HB	1.69	0.72
1:C:47:ILE:HD13	1:C:113:GLY:HA2	1.70	0.72
1:C:301:LEU:HA	1:C:390:VAL:HG21	1.72	0.72
1:A:73:LEU:HD13	1:A:99:GLN:HG3	1.71	0.71
1:A:201:ILE:HG22	1:A:368:LEU:HD21	1.72	0.71
1:C:153:THR:HG22	1:C:166:ALA:O	1.90	0.71
1:A:238:ILE:H	1:A:238:ILE:HD12	1.56	0.70
1:D:150:GLY:HA2	1:D:254:VAL:HG11	1.73	0.70
1:A:7:ILE:HB	1:A:15:ILE:HB	1.72	0.69
1:A:225:VAL:HG13	1:A:229:GLU:HG3	1.74	0.69
1:A:226:THR:O	1:A:229:GLU:HG2	1.92	0.68
1:D:351:ASN:O	1:D:354:LEU:HB2	1.93	0.68
1:C:198:THR:HG21	1:C:246:SER:HA	1.75	0.68
1:D:387:ILE:O	1:D:391:LEU:HD13	1.94	0.68
1:B:262:GLY:O	1:B:265:ASN:HB2	1.92	0.68
1:D:303:ARG:HB3	1:D:303:ARG:HH11	1.58	0.68
1:B:47:ILE:HD13	1:B:113:GLY:HA2	1.75	0.68
1:B:264:ARG:H	1:B:264:ARG:HD2	1.59	0.67
1:D:348:LEU:O	1:D:352:MET:HG3	1.95	0.67
1:A:143:ALA:HA	1:A:147:SER:OG	1.94	0.67
1:C:273:ILE:HD13	1:C:352:MET:SD	2.35	0.66
1:A:57:GLU:HG2	1:A:60:ARG:HH11	1.60	0.66
1:B:73:LEU:HD13	1:B:99:GLN:HG3	1.76	0.66
1:A:257:ASP:OD2	1:A:264:ARG:HD2	1.96	0.66
1:A:189:ILE:HG22	1:A:325:LEU:HD23	1.78	0.66
1:D:62:ARG:O	1:D:65:GLU:HG2	1.96	0.65
1:D:242:ARG:HE	1:D:242:ARG:CA	2.10	0.65
1:A:238:ILE:HD12	1:A:238:ILE:N	2.11	0.65
1:B:84:LYS:HG2	1:B:155:ILE:HA	1.78	0.65
1:B:350:PHE:O	1:B:354:LEU:HD13	1.95	0.65
1:A:165:GLY:O	1:B:130:ARG:HA	1.96	0.65
1:D:385:GLU:H	1:D:385:GLU:CD	1.98	0.65
1:C:378:ARG:HD3	1:C:378:ARG:N	2.11	0.64
1:B:123:PHE:HB2	1:B:153:THR:HG23	1.79	0.64
1:C:12:ARG:HD2	1:C:13:GLU:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:HIS:HB2	1:A:233:GLU:HG3	1.79	0.64
1:B:189:ILE:HD11	1:B:218:LEU:HD11	1.78	0.63
1:A:383:ALA:HB1	1:A:385:GLU:OE1	1.98	0.63
1:B:226:THR:HG23	1:B:227:PRO:HD2	1.80	0.63
1:C:189:ILE:HD12	1:C:323:TYR:O	1.98	0.63
1:A:364:LYS:HG2	1:A:381:VAL:HG22	1.80	0.63
1:D:143:ALA:HA	1:D:147:SER:OG	1.98	0.63
1:B:155:ILE:HD11	1:B:164:ILE:HB	1.80	0.63
1:C:382:VAL:HA	5:C:1626:HOH:O	1.98	0.63
1:B:58:ALA:O	1:B:61:LYS:HG2	1.98	0.63
1:B:226:THR:CG2	1:B:227:PRO:HD2	2.29	0.62
1:D:189:ILE:HD12	1:D:323:TYR:O	1.99	0.62
1:D:293:ILE:O	1:D:297:LYS:HG2	1.99	0.62
1:B:52:THR:O	1:B:56:GLU:HG3	1.99	0.62
1:B:303:ARG:HG2	1:B:303:ARG:HH11	1.63	0.62
1:D:123:PHE:HA	1:D:153:THR:HG21	1.82	0.62
1:C:58:ALA:O	1:C:61:LYS:HG2	1.99	0.62
1:B:198:THR:HG21	1:B:246:SER:HA	1.81	0.62
1:A:157:THR:HG22	1:A:159:LEU:H	1.64	0.62
1:C:23:ARG:HB2	5:C:1613:HOH:O	2.00	0.62
1:C:157:THR:HG23	1:C:158:PRO:HD2	1.81	0.61
1:C:24:ASN:O	1:C:25:TYR:HB2	1.98	0.61
1:C:20:GLY:HA2	5:C:1613:HOH:O	1.99	0.61
1:B:15:ILE:O	1:B:16:ILE:HD13	2.00	0.61
1:C:349:MET:HE2	1:C:384:ASN:O	1.99	0.61
1:A:47:ILE:HD13	1:A:113:GLY:HA2	1.83	0.61
1:B:41:LEU:HB3	1:B:74:ILE:HD13	1.81	0.61
1:A:198:THR:HG21	1:A:246:SER:HA	1.81	0.61
1:D:313:VAL:O	1:D:317:VAL:HG23	1.99	0.60
1:B:237:GLU:H	1:B:237:GLU:CD	2.03	0.60
1:B:312:ALA:O	1:B:316:ILE:HG13	2.02	0.60
1:A:189:ILE:HG22	1:A:325:LEU:CD2	2.31	0.60
1:D:220:ALA:HA	1:D:223:ARG:HG2	1.82	0.60
1:B:335:ARG:CB	1:B:335:ARG:HH11	2.15	0.60
1:D:242:ARG:HE	1:D:242:ARG:N	2.00	0.59
1:D:153:THR:O	1:D:154:ALA:HB2	2.03	0.59
1:C:97:LEU:HD13	1:D:163:LEU:HD13	1.83	0.59
1:B:143:ALA:HA	1:B:147:SER:OG	2.02	0.59
1:C:269:TRP:HH2	1:C:316:ILE:HD13	1.68	0.59
1:C:385:GLU:CD	1:C:385:GLU:H	2.06	0.59
1:D:3:ASN:CG	1:D:4:PRO:HD2	2.23	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ARG:HD2	1:B:264:ARG:N	2.17	0.58
1:A:189:ILE:HD12	1:A:323:TYR:O	2.03	0.58
1:D:272:SER:HB2	1:D:298:GLU:OE2	2.02	0.58
1:A:123:PHE:HA	1:A:153:THR:HG21	1.85	0.58
1:A:157:THR:HB	1:A:163:LEU:HD12	1.85	0.58
1:A:348:LEU:O	1:A:352:MET:HG3	2.04	0.58
1:D:378:ARG:HG2	1:D:378:ARG:HH11	1.68	0.58
1:D:7:ILE:HB	1:D:15:ILE:HB	1.84	0.58
1:A:9:ILE:HG22	1:A:10:LEU:HD23	1.84	0.58
1:A:6:LYS:O	1:A:7:ILE:HD13	2.03	0.58
1:D:383:ALA:HB3	1:D:386:ASP:OD2	2.04	0.58
1:D:230:HIS:HB2	1:D:233:GLU:HG3	1.86	0.57
1:D:52:THR:O	1:D:56:GLU:HG3	2.03	0.57
1:A:185:VAL:O	1:A:189:ILE:HG12	2.04	0.57
1:A:238:ILE:H	1:A:238:ILE:CD1	2.17	0.57
1:A:298:GLU:HG2	1:A:365:ILE:HG21	1.86	0.57
1:C:231:ARG:HH11	1:C:231:ARG:HG3	1.69	0.57
1:B:331:ASP:HB3	1:B:334:ILE:HD12	1.85	0.57
1:A:365:ILE:HD12	1:A:365:ILE:N	2.19	0.57
1:B:150:GLY:HA2	1:B:254:VAL:HG11	1.87	0.57
1:B:201:ILE:HG22	1:B:368:LEU:HD21	1.85	0.57
1:C:238:ILE:N	1:C:238:ILE:HD12	2.20	0.57
1:B:257:ASP:O	1:B:258:GLU:C	2.43	0.56
1:B:153:THR:HG22	1:B:166:ALA:H	1.70	0.56
1:A:153:THR:O	1:A:154:ALA:HB2	2.05	0.56
1:D:157:THR:HG23	1:D:158:PRO:HD2	1.86	0.56
1:D:281:LEU:HD22	1:D:338:THR:HG21	1.87	0.56
1:D:189:ILE:HD11	1:D:218:LEU:HD21	1.88	0.55
1:A:303:ARG:HE	1:A:310:GLY:CA	2.18	0.55
1:A:308:LEU:HD11	1:A:312:ALA:CB	2.36	0.55
1:C:185:VAL:O	1:C:189:ILE:HG12	2.07	0.55
1:D:185:VAL:O	1:D:189:ILE:HG12	2.07	0.55
1:D:308:LEU:HD11	1:D:312:ALA:HB3	1.88	0.55
1:D:123:PHE:CB	1:D:153:THR:HG23	2.35	0.55
1:B:343:CYS:HB3	1:B:348:LEU:HD11	1.88	0.55
1:D:294:GLY:O	1:D:298:GLU:HG3	2.06	0.55
1:B:60:ARG:C	1:B:60:ARG:HD2	2.27	0.55
1:D:238:ILE:HD12	1:D:238:ILE:N	2.22	0.55
1:B:185:VAL:O	1:B:189:ILE:HG12	2.07	0.54
1:A:67:THR:HA	1:A:68:PRO:C	2.27	0.54
1:D:341:LYS:CE	1:D:341:LYS:HA	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:LEU:O	1:C:164:ILE:HD13	2.07	0.54
1:B:123:PHE:HA	1:B:153:THR:HG21	1.89	0.54
1:A:263:LEU:HD12	1:A:266:LEU:HD12	1.89	0.54
1:D:351:ASN:HA	1:D:354:LEU:HD13	1.90	0.54
1:B:335:ARG:HB3	1:B:335:ARG:NH1	2.22	0.54
1:A:66:ILE:HD12	1:A:66:ILE:N	2.23	0.54
1:A:3:ASN:N	5:A:678:HOH:O	2.40	0.53
1:A:73:LEU:CD1	1:A:99:GLN:HG3	2.38	0.53
1:C:89:LYS:HE3	1:C:123:PHE:CE2	2.43	0.53
1:A:279:ALA:HB3	1:A:351:ASN:HD22	1.73	0.53
1:B:364:LYS:HA	1:B:380:SER:O	2.08	0.53
1:D:68:PRO:HA	5:D:1724:HOH:O	2.08	0.53
1:B:58:ALA:HA	1:B:61:LYS:HD3	1.89	0.53
1:D:308:LEU:HD11	1:D:312:ALA:CB	2.38	0.53
1:B:265:ASN:ND2	1:B:378:ARG:NH1	2.56	0.53
1:B:198:THR:HG22	5:B:683:HOH:O	2.09	0.53
1:D:230:HIS:HB2	1:D:233:GLU:CG	2.38	0.53
1:D:215:GLU:HG3	1:D:216:THR:N	2.24	0.53
1:A:287:HIS:O	1:A:291:VAL:HG23	2.09	0.53
1:C:257:ASP:OD2	1:C:264:ARG:HG3	2.08	0.53
1:D:47:ILE:HD13	1:D:113:GLY:HA2	1.91	0.53
1:A:44:ASP:HA	1:A:77:ARG:O	2.09	0.52
1:D:364:LYS:C	1:D:365:ILE:HD12	2.30	0.52
1:A:52:THR:O	1:A:56:GLU:HG3	2.09	0.52
1:B:230:HIS:HB2	1:B:233:GLU:CG	2.39	0.52
1:A:364:LYS:HA	1:A:380:SER:O	2.10	0.52
1:D:189:ILE:HG23	1:D:323:TYR:O	2.09	0.52
1:D:350:PHE:O	1:D:354:LEU:HD13	2.10	0.52
1:C:237:GLU:CD	1:C:237:GLU:H	2.13	0.52
1:C:9:ILE:HD11	1:C:15:ILE:HD11	1.91	0.51
1:A:213:ASN:OD1	1:A:238:ILE:HG23	2.10	0.51
1:B:387:ILE:O	1:B:391:LEU:HD23	2.10	0.51
1:A:9:ILE:HG22	1:A:10:LEU:CD2	2.40	0.51
1:A:88:THR:O	1:A:92:ILE:HG13	2.11	0.51
1:D:287:HIS:O	1:D:291:VAL:HG23	2.11	0.51
1:D:87:GLN:N	1:D:87:GLN:NE2	2.47	0.51
1:B:303:ARG:NH1	1:B:303:ARG:HG2	2.26	0.51
1:B:73:LEU:CD1	1:B:99:GLN:HG3	2.40	0.51
1:C:287:HIS:O	1:C:291:VAL:HG23	2.11	0.51
1:B:155:ILE:C	1:B:155:ILE:HD12	2.32	0.50
1:B:153:THR:O	1:B:154:ALA:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:LEU:HD12	1:C:222:ARG:CZ	2.41	0.50
1:D:242:ARG:HE	1:D:242:ARG:HA	1.76	0.50
1:A:57:GLU:HG2	1:A:60:ARG:NH1	2.25	0.50
1:C:349:MET:HE2	1:C:388:ARG:HG3	1.92	0.50
1:B:41:LEU:HD11	1:B:112:LEU:HB3	1.93	0.50
1:B:385:GLU:H	1:B:385:GLU:CD	2.15	0.50
1:B:64:ALA:C	1:B:66:ILE:H	2.14	0.50
1:D:65:GLU:O	1:D:66:ILE:HD13	2.11	0.49
1:A:9:ILE:CD1	1:A:15:ILE:HD11	2.35	0.49
1:A:386:ASP:O	1:A:389:VAL:HG22	2.12	0.49
1:D:52:THR:N	1:D:53:PRO:CD	2.74	0.49
1:B:44:ASP:HA	1:B:77:ARG:O	2.12	0.49
1:C:303:ARG:HH11	1:C:303:ARG:HG2	1.77	0.49
1:B:140:THR:O	1:B:144:MET:HG3	2.11	0.49
1:A:240:LYS:O	1:A:244:LEU:HB2	2.12	0.49
1:C:230:HIS:HB2	1:C:233:GLU:CG	2.39	0.49
1:D:335:ARG:HD2	5:D:1629:HOH:O	2.12	0.49
1:C:231:ARG:NH1	1:C:231:ARG:HG3	2.28	0.49
1:C:44:ASP:HA	1:C:77:ARG:O	2.12	0.49
1:C:153:THR:O	1:C:154:ALA:HB2	2.12	0.48
1:D:226:THR:CG2	1:D:227:PRO:HD2	2.40	0.48
1:C:58:ALA:HA	1:C:61:LYS:HE2	1.96	0.48
1:C:18:ASP:O	1:C:176:ASP:HA	2.13	0.48
1:A:7:ILE:HG22	1:A:8:SER:N	2.28	0.48
1:C:269:TRP:CH2	1:C:316:ILE:HD13	2.49	0.48
1:A:153:THR:HG22	1:A:166:ALA:O	2.12	0.48
1:A:130:ARG:HD3	1:B:167:ILE:HD12	1.94	0.48
1:D:3:ASN:N	5:D:1639:HOH:O	2.45	0.48
1:D:88:THR:O	1:D:92:ILE:HG13	2.14	0.48
1:A:7:ILE:O	1:A:13:GLU:HA	2.13	0.48
1:A:189:ILE:O	1:A:325:LEU:HD21	2.14	0.48
1:D:17:ALA:O	1:D:18:ASP:HB2	2.14	0.48
1:C:140:THR:O	1:C:144:MET:HG3	2.14	0.48
1:B:338:THR:HB	1:B:341:LYS:HB2	1.95	0.48
1:A:59:PHE:CE2	1:A:72:LEU:HB2	2.49	0.48
1:D:44:ASP:HA	1:D:77:ARG:O	2.14	0.48
1:A:9:ILE:HD11	1:A:15:ILE:CD1	2.35	0.47
1:D:230:HIS:H	1:D:233:GLU:CD	2.17	0.47
1:B:287:HIS:O	1:B:291:VAL:HG23	2.13	0.47
1:B:156:ASP:OD1	1:B:161:LYS:HA	2.14	0.47
1:B:258:GLU:O	1:B:258:GLU:CG	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:LYS:HE3	1:C:123:PHE:CD2	2.49	0.47
1:C:130:ARG:HA	1:D:165:GLY:O	2.14	0.47
1:C:300:GLU:HB3	1:C:390:VAL:HG13	1.95	0.47
1:A:225:VAL:CG1	1:A:229:GLU:HG3	2.42	0.47
1:B:12:ARG:HH22	1:B:171:THR:HA	1.79	0.47
1:B:12:ARG:NH2	1:B:171:THR:HA	2.29	0.47
1:B:314:SER:O	1:B:318:LYS:HG2	2.14	0.47
1:D:3:ASN:OD1	1:D:4:PRO:HD2	2.13	0.47
1:D:87:GLN:N	1:D:87:GLN:HE21	2.04	0.47
1:B:258:GLU:O	1:B:259:ARG:HB3	2.15	0.47
1:A:123:PHE:N	1:A:153:THR:OG1	2.47	0.47
1:A:21:LEU:HD22	1:A:25:TYR:CD1	2.49	0.47
1:B:300:GLU:OE1	1:B:300:GLU:HA	2.15	0.47
1:A:326:PRO:HG3	1:A:334:ILE:HD11	1.96	0.47
1:A:230:HIS:HB2	1:A:233:GLU:CG	2.45	0.47
1:A:378:ARG:HH11	1:A:378:ARG:HG2	1.80	0.47
1:D:208:THR:HA	1:D:211:GLU:OE1	2.14	0.47
1:A:130:ARG:HA	1:B:165:GLY:O	2.15	0.47
1:B:265:ASN:ND2	1:B:378:ARG:HH12	2.13	0.47
1:C:314:SER:O	1:C:318:LYS:HG2	2.15	0.47
1:B:41:LEU:HD23	1:B:74:ILE:CD1	2.45	0.46
1:A:84:LYS:HG2	1:A:155:ILE:HA	1.97	0.46
1:D:140:THR:O	1:D:144:MET:HG3	2.16	0.46
1:C:279:ALA:HB3	1:C:351:ASN:HD22	1.81	0.46
1:D:338:THR:O	1:D:339:ALA:C	2.53	0.46
1:C:9:ILE:HG21	5:C:1640:HOH:O	2.15	0.46
1:A:388:ARG:HD3	5:A:715:HOH:O	2.14	0.46
1:A:130:ARG:CD	1:B:167:ILE:HD12	2.45	0.46
1:C:311:VAL:O	1:C:315:ARG:HG3	2.15	0.46
1:A:155:ILE:HD12	1:A:155:ILE:C	2.35	0.46
1:D:375:TYR:CD2	1:D:376:GLU:HG3	2.51	0.46
1:C:52:THR:N	1:C:53:PRO:CD	2.79	0.46
1:A:301:LEU:O	1:A:304:HIS:HB3	2.16	0.46
1:D:241:ALA:HB1	1:D:242:ARG:HH21	1.80	0.45
1:D:254:VAL:HG13	1:D:264:ARG:NH1	2.27	0.45
1:D:272:SER:CB	1:D:365:ILE:HG13	2.46	0.45
1:A:303:ARG:HE	1:A:310:GLY:HA3	1.81	0.45
1:A:252:TYR:HE2	1:A:263:LEU:HD21	1.81	0.45
1:C:238:ILE:N	1:C:238:ILE:CD1	2.79	0.45
1:C:12:ARG:NH1	1:C:171:THR:O	2.50	0.45
1:D:17:ALA:CB	1:D:244:LEU:HD11	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:THR:HB	1:B:163:LEU:HD12	1.99	0.45
1:C:7:ILE:HB	1:C:15:ILE:HB	1.97	0.45
1:A:314:SER:O	1:A:318:LYS:HG2	2.16	0.45
1:D:155:ILE:C	1:D:155:ILE:HD12	2.36	0.45
1:A:252:TYR:CE2	1:A:263:LEU:HD21	2.51	0.45
1:D:263:LEU:HD13	1:D:377:THR:O	2.16	0.45
1:D:296:VAL:HG21	1:D:327:THR:HG22	1.98	0.45
1:D:208:THR:O	1:D:212:GLU:HG2	2.17	0.45
1:B:385:GLU:O	1:B:389:VAL:HG23	2.16	0.45
1:A:28:LYS:HB2	1:A:62:ARG:NE	2.31	0.45
1:C:58:ALA:C	1:C:61:LYS:HG2	2.37	0.45
1:B:226:THR:HB	1:B:229:GLU:CD	2.37	0.45
1:B:15:ILE:C	1:B:16:ILE:HD13	2.37	0.44
1:C:226:THR:CG2	1:C:227:PRO:HD2	2.47	0.44
1:D:157:THR:HG23	1:D:158:PRO:CD	2.47	0.44
1:B:61:LYS:NZ	1:B:62:ARG:CZ	2.80	0.44
1:B:335:ARG:CB	1:B:335:ARG:NH1	2.78	0.44
1:C:276:ALA:HB2	1:C:352:MET:HG3	1.99	0.44
1:D:176:ASP:HB3	1:D:179:PHE:CD2	2.53	0.44
1:B:123:PHE:CB	1:B:153:THR:HG23	2.45	0.44
1:B:41:LEU:HD12	1:B:42:VAL:N	2.31	0.44
1:D:17:ALA:HB3	1:D:244:LEU:HD21	1.99	0.44
1:D:240:LYS:O	1:D:244:LEU:HB2	2.17	0.44
1:A:388:ARG:C	1:A:390:VAL:H	2.19	0.44
1:A:22:TRP:CZ2	1:A:55:PHE:HB2	2.52	0.44
1:C:78:PRO:HG2	1:C:83:SER:OG	2.18	0.44
1:A:232:PHE:CD1	1:A:239:LEU:HD22	2.52	0.44
1:D:326:PRO:HD3	5:D:1641:HOH:O	2.17	0.44
1:D:333:ARG:HD2	1:D:337:LEU:HD11	1.99	0.44
1:C:151:GLY:O	1:C:167:ILE:HA	2.18	0.44
1:C:338:THR:HB	1:C:341:LYS:HB2	1.99	0.44
1:D:259:ARG:CA	1:D:259:ARG:HH11	2.25	0.44
1:B:89:LYS:O	1:B:93:GLU:HG3	2.18	0.44
1:C:214:ALA:HA	1:C:323:TYR:CZ	2.53	0.44
1:D:7:ILE:HG22	1:D:9:ILE:CD1	2.47	0.44
1:D:198:THR:HG21	1:D:246:SER:HA	1.99	0.44
1:D:242:ARG:CA	1:D:242:ARG:NE	2.80	0.43
1:B:89:LYS:HE3	1:B:123:PHE:CE2	2.53	0.43
1:A:17:ALA:O	1:A:18:ASP:HB2	2.16	0.43
1:D:293:ILE:HD11	1:D:334:ILE:CD1	2.48	0.43
1:A:364:LYS:C	1:A:365:ILE:HD12	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:386:ASP:O	1:D:389:VAL:HG22	2.18	0.43
1:B:17:ALA:O	1:B:18:ASP:HB2	2.18	0.43
1:C:256:ALA:O	1:C:258:GLU:N	2.52	0.43
1:D:364:LYS:HA	1:D:380:SER:O	2.18	0.43
1:C:226:THR:HG23	1:C:227:PRO:HD2	2.00	0.43
1:A:218:LEU:HD22	1:A:222:ARG:HD2	2.00	0.43
1:C:157:THR:HB	1:C:163:LEU:HD12	1.99	0.43
1:D:318:LYS:NZ	5:D:1717:HOH:O	2.51	0.43
1:D:16:ILE:HG22	1:D:21:LEU:HD11	2.00	0.43
1:C:331:ASP:O	1:C:335:ARG:HG3	2.19	0.43
1:C:93:GLU:OE1	1:D:86:ARG:NH2	2.44	0.43
1:B:9:ILE:HD11	1:B:15:ILE:HD11	1.99	0.43
1:A:18:ASP:O	1:A:176:ASP:HA	2.19	0.43
1:C:258:GLU:HG3	1:C:259:ARG:N	2.32	0.43
1:C:59:PHE:CE2	1:C:72:LEU:HB2	2.54	0.43
1:C:309:LYS:HB2	5:C:1704:HOH:O	2.19	0.43
1:B:153:THR:HG22	1:B:166:ALA:N	2.34	0.43
1:B:335:ARG:HB2	1:B:335:ARG:HH11	1.82	0.43
1:B:18:ASP:O	1:B:176:ASP:HA	2.18	0.43
1:A:123:PHE:HB2	1:A:153:THR:HG23	2.01	0.42
1:B:58:ALA:O	1:B:62:ARG:HG2	2.19	0.42
1:C:316:ILE:HG13	1:C:371:ILE:HD11	2.01	0.42
1:B:298:GLU:HG2	1:B:365:ILE:HG21	1.99	0.42
1:B:30:LEU:O	1:B:34:CYS:N	2.49	0.42
1:C:15:ILE:HG12	1:C:173:ILE:HB	2.02	0.42
1:A:240:LYS:HD2	5:A:758:HOH:O	2.20	0.42
1:A:268:ASN:HD22	1:A:268:ASN:HA	1.59	0.42
1:B:95:TRP:CE3	1:B:96:MET:HG3	2.55	0.42
1:B:60:ARG:O	1:B:60:ARG:HD2	2.19	0.42
1:D:212:GLU:HG2	1:D:212:GLU:H	1.67	0.42
1:A:155:ILE:CD1	1:A:164:ILE:HB	2.44	0.42
1:C:282:THR:OG1	1:C:283:PRO:HA	2.19	0.42
1:A:262:GLY:O	1:A:265:ASN:HB2	2.20	0.42
1:D:218:LEU:HD13	1:D:222:ARG:CZ	2.50	0.42
1:D:282:THR:OG1	1:D:283:PRO:HA	2.20	0.42
1:B:232:PHE:CD1	1:B:239:LEU:HD22	2.55	0.42
1:B:216:THR:CG2	1:B:235:THR:HG21	2.48	0.42
1:D:123:PHE:HA	1:D:153:THR:CG2	2.49	0.42
1:D:123:PHE:CA	1:D:153:THR:CG2	2.98	0.42
1:D:241:ALA:HB1	1:D:242:ARG:NH2	2.35	0.42
1:A:44:ASP:C	1:A:44:ASP:OD1	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ASP:HB3	1:B:179:PHE:CD2	2.55	0.42
1:D:301:LEU:O	1:D:304:HIS:HB3	2.20	0.42
1:A:253:VAL:HG13	1:A:263:LEU:CG	2.41	0.42
1:B:157:THR:CG2	1:B:158:PRO:HD2	2.49	0.42
1:C:213:ASN:HD22	1:C:242:ARG:HD3	1.84	0.42
1:B:264:ARG:H	1:B:264:ARG:CD	2.29	0.42
1:A:176:ASP:HB3	1:A:179:PHE:CD2	2.54	0.42
1:D:309:LYS:HE3	1:D:309:LYS:HA	2.02	0.42
1:D:153:THR:O	1:D:154:ALA:CB	2.68	0.42
1:A:385:GLU:O	1:A:389:VAL:HG13	2.20	0.42
1:C:152:LYS:HB2	4:C:402:NAD:H72N	1.84	0.42
1:A:157:THR:HG23	1:A:158:PRO:HD2	2.02	0.41
1:C:84:LYS:CG	1:C:155:ILE:HA	2.42	0.41
1:B:282:THR:OG1	1:B:283:PRO:HA	2.20	0.41
1:B:41:LEU:HD11	1:B:112:LEU:CB	2.50	0.41
1:C:176:ASP:HB3	1:C:179:PHE:CD2	2.55	0.41
1:A:54:SER:OG	1:A:55:PHE:N	2.53	0.41
1:A:242:ARG:HE	1:A:242:ARG:HA	1.85	0.41
1:C:61:LYS:HG3	1:C:62:ARG:CD	2.45	0.41
1:A:303:ARG:HE	1:A:310:GLY:HA2	1.84	0.41
1:D:238:ILE:CD1	1:D:238:ILE:N	2.84	0.41
1:C:31:ILE:HD12	1:C:62:ARG:HB3	2.01	0.41
1:A:281:LEU:HD22	1:A:338:THR:HG21	2.02	0.41
1:D:328:SER:O	1:D:331:ASP:HB2	2.21	0.41
1:A:23:ARG:HH11	1:A:23:ARG:HG2	1.84	0.41
1:C:143:ALA:HA	1:C:147:SER:HG	1.81	0.41
1:D:218:LEU:HD23	1:D:218:LEU:HA	1.85	0.41
1:A:40:VAL:HG13	1:A:95:TRP:HZ3	1.85	0.41
1:B:210:LEU:HD23	1:B:242:ARG:CG	2.51	0.41
1:A:7:ILE:HD12	1:A:248:ARG:HE	1.85	0.41
1:C:301:LEU:CA	1:C:390:VAL:HG21	2.47	0.41
1:D:139:THR:HB	4:D:1403:NAD:H61A	1.86	0.41
1:C:88:THR:HG22	1:C:120:LEU:HD11	2.03	0.41
1:A:155:ILE:O	1:A:155:ILE:HD12	2.21	0.41
1:A:364:LYS:HE3	1:A:381:VAL:HG23	2.02	0.41
1:C:52:THR:O	1:C:56:GLU:HG3	2.20	0.41
1:D:325:LEU:HA	5:D:1641:HOH:O	2.20	0.41
1:A:140:THR:O	1:A:144:MET:HG3	2.21	0.41
1:C:157:THR:CG2	1:C:158:PRO:HD2	2.50	0.40
1:D:385:GLU:CD	1:D:385:GLU:N	2.70	0.40
1:C:58:ALA:HA	1:C:61:LYS:HG2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:273:ILE:HD12	1:D:391:LEU:HD11	2.03	0.40
1:C:17:ALA:O	1:C:18:ASP:HB2	2.21	0.40
1:A:69:SER:HA	1:A:70:PRO:HD3	1.89	0.40
1:D:351:ASN:HA	1:D:354:LEU:HD22	2.04	0.40
1:D:378:ARG:CG	1:D:378:ARG:HH11	2.34	0.40
1:D:75:TYR:CD1	1:D:75:TYR:C	2.95	0.40
1:A:8:SER:HB3	1:A:13:GLU:N	2.37	0.40
1:C:69:SER:HA	1:C:70:PRO:HD3	1.88	0.40
1:D:153:THR:HB	1:D:166:ALA:O	2.20	0.40
1:D:352:MET:C	1:D:354:LEU:H	2.25	0.40
1:A:264:ARG:HD3	5:A:635:HOH:O	2.21	0.40
1:A:270:GLY:N	1:A:298:GLU:OE1	2.39	0.40
1:D:189:ILE:CD1	1:D:218:LEU:HD21	2.50	0.40
1:C:24:ASN:ND2	1:C:24:ASN:O	2.48	0.40
1:D:365:ILE:N	1:D:365:ILE:HD12	2.36	0.40
1:D:178:GLU:O	1:D:181:GLU:HG3	2.22	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	372/393 (95%)	351 (94%)	16 (4%)	5 (1%)	15	29
1	B	379/393 (96%)	355 (94%)	20 (5%)	4 (1%)	17	35
1	C	373/393 (95%)	353 (95%)	17 (5%)	3 (1%)	24	45
1	D	377/393 (96%)	361 (96%)	15 (4%)	1 (0%)	46	70
All	All	1501/1572 (96%)	1420 (95%)	68 (4%)	13 (1%)	21	41

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	ALA
1	C	257	ASP
1	A	13	GLU
1	B	25	TYR
1	C	25	TYR
1	A	14	SER
1	B	258	GLU
1	A	154	ALA
1	B	14	SER
1	C	260	GLU
1	D	154	ALA
1	B	262	GLY
1	A	227	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	311/326 (95%)	300 (96%)	11 (4%)	43	70
1	B	316/326 (97%)	305 (96%)	11 (4%)	43	70
1	C	311/326 (95%)	301 (97%)	10 (3%)	46	73
1	D	314/326 (96%)	297 (95%)	17 (5%)	27	51
All	All	1252/1304 (96%)	1203 (96%)	49 (4%)	39	66

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	24	ASN
1	A	57	GLU
1	A	100	ASN
1	A	153	THR
1	A	218	LEU
1	A	242	ARG
1	A	257	ASP
1	A	268	ASN

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Mol	Chain	Res	Type
1	A	369	SER
1	A	378	ARG
1	B	24	ASN
1	B	33	ASP
1	B	153	THR
1	B	218	LEU
1	B	242	ARG
1	B	257	ASP
1	B	265	ASN
1	B	300	GLU
1	B	328	SER
1	B	346	ASP
1	B	385	GLU
1	C	24	ASN
1	C	33	ASP
1	C	153	THR
1	C	218	LEU
1	C	224	GLU
1	C	242	ARG
1	C	265	ASN
1	C	346	ASP
1	C	378	ARG
1	C	385	GLU
1	D	14	SER
1	D	24	ASN
1	D	57	GLU
1	D	87	GLN
1	D	153	THR
1	D	215	GLU
1	D	223	ARG
1	D	242	ARG
1	D	244	LEU
1	D	250	LYS
1	D	259	ARG
1	D	265	ASN
1	D	303	ARG
1	D	309	LYS
1	D	327	THR
1	D	378	ARG
1	D	385	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	76	ASN
1	A	100	ASN
1	A	268	ASN
1	B	24	ASN
1	B	265	ASN
1	B	268	ASN
1	C	87	GLN
1	C	213	ASN
1	C	271	HIS
1	D	24	ASN
1	D	87	GLN
1	D	268	ASN
1	D	271	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 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	$\# Z  > 2$
4	NAD	A	400	-	38,48,48	2.31	9 (23%)	47,73,73	1.86	9 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAD	B	401	-	38,48,48	2.33	10 (26%)	47,73,73	1.81	10 (21%)
4	NAD	C	402	-	38,48,48	2.38	9 (23%)	47,73,73	1.81	10 (21%)
4	NAD	D	1403	-	38,48,48	2.45	9 (23%)	47,73,73	1.79	9 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAD	A	400	-	-	0/22/62/62	0/5/5/5
4	NAD	B	401	-	-	0/22/62/62	0/5/5/5
4	NAD	C	402	-	-	0/22/62/62	0/5/5/5
4	NAD	D	1403	-	-	0/22/62/62	0/5/5/5

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	400	NAD	O3B-C3B	-8.47	1.22	1.43
4	C	402	NAD	O3B-C3B	-8.42	1.22	1.43
4	D	1403	NAD	O3B-C3B	-8.35	1.23	1.43
4	B	401	NAD	O3B-C3B	-8.31	1.23	1.43
4	B	401	NAD	C7N-N7N	2.18	1.37	1.33
4	C	402	NAD	C5N-C4N	2.23	1.43	1.38
4	A	400	NAD	C5N-C4N	2.29	1.43	1.38
4	B	401	NAD	C5N-C4N	2.42	1.43	1.38
4	B	401	NAD	C2A-N1A	2.47	1.38	1.33
4	D	1403	NAD	C2A-N1A	2.51	1.38	1.33
4	A	400	NAD	C2A-N1A	2.52	1.38	1.33
4	D	1403	NAD	C5N-C4N	2.59	1.44	1.38
4	C	402	NAD	C2A-N1A	2.77	1.39	1.33
4	A	400	NAD	C3N-C7N	2.96	1.55	1.50
4	D	1403	NAD	C3N-C7N	3.26	1.55	1.50
4	B	401	NAD	C3N-C7N	3.37	1.55	1.50
4	A	400	NAD	C6N-N1N	3.43	1.44	1.35
4	A	400	NAD	C4N-C3N	3.45	1.45	1.39
4	C	402	NAD	C4A-N3A	3.47	1.40	1.35
4	C	402	NAD	C6N-N1N	3.55	1.45	1.35
4	D	1403	NAD	C4N-C3N	3.65	1.45	1.39
4	C	402	NAD	C4N-C3N	3.67	1.45	1.39
4	C	402	NAD	C3N-C7N	3.71	1.56	1.50
4	B	401	NAD	C4A-N3A	3.86	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	NAD	C6N-N1N	3.87	1.45	1.35
4	A	400	NAD	C4A-N3A	3.87	1.41	1.35
4	B	401	NAD	O4B-C1B	3.88	1.46	1.41
4	A	400	NAD	O4D-C1D	3.90	1.46	1.41
4	D	1403	NAD	C6N-N1N	3.95	1.46	1.35
4	D	1403	NAD	C4A-N3A	4.01	1.41	1.35
4	B	401	NAD	C4N-C3N	4.01	1.46	1.39
4	B	401	NAD	O4D-C1D	4.59	1.47	1.41
4	D	1403	NAD	O4D-C1D	4.82	1.47	1.41
4	C	402	NAD	O4D-C1D	4.92	1.47	1.41
4	C	402	NAD	O4B-C1B	5.34	1.47	1.41
4	A	400	NAD	O4B-C1B	5.66	1.48	1.41
4	D	1403	NAD	O4B-C1B	6.15	1.49	1.41

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	NAD	C5N-C4N-C3N	-6.33	112.38	120.33
4	A	400	NAD	C5N-C4N-C3N	-5.75	113.11	120.33
4	C	402	NAD	C5N-C4N-C3N	-5.61	113.28	120.33
4	D	1403	NAD	C5N-C4N-C3N	-5.41	113.53	120.33
4	D	1403	NAD	O4D-C1D-N1N	-3.95	103.80	108.13
4	A	400	NAD	O4D-C1D-N1N	-3.83	103.92	108.13
4	A	400	NAD	O4B-C1B-N9A	-3.60	100.56	108.10
4	C	402	NAD	O4B-C1B-N9A	-3.29	101.21	108.10
4	A	400	NAD	C5N-C6N-N1N	-3.25	114.85	120.47
4	B	401	NAD	O4B-C1B-N9A	-3.04	101.73	108.10
4	D	1403	NAD	C5N-C6N-N1N	-3.04	115.22	120.47
4	B	401	NAD	C5N-C6N-N1N	-2.96	115.35	120.47
4	D	1403	NAD	O4B-C1B-N9A	-2.96	101.91	108.10
4	B	401	NAD	O4D-C1D-N1N	-2.83	105.02	108.13
4	C	402	NAD	C5N-C6N-N1N	-2.78	115.67	120.47
4	C	402	NAD	C4D-O4D-C1D	-2.77	106.68	109.72
4	C	402	NAD	O4D-C1D-N1N	-2.51	105.37	108.13
4	C	402	NAD	C4N-C3N-C7N	-2.35	114.88	121.09
4	B	401	NAD	C4D-O4D-C1D	-2.31	107.18	109.72
4	D	1403	NAD	C4N-C3N-C7N	-2.29	115.03	121.09
4	A	400	NAD	C4N-C3N-C7N	-2.24	115.16	121.09
4	B	401	NAD	C4N-C3N-C7N	-2.23	115.19	121.09
4	C	402	NAD	C4B-O4B-C1B	2.18	112.11	109.72
4	B	401	NAD	C4B-O4B-C1B	2.22	112.16	109.72
4	D	1403	NAD	C4B-O4B-C1B	2.36	112.31	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	400	NAD	C4B-O4B-C1B	2.39	112.35	109.72
4	B	401	NAD	C2N-C3N-C4N	3.61	122.31	118.29
4	D	1403	NAD	C2B-C1B-N9A	3.66	119.89	114.29
4	B	401	NAD	C2B-C1B-N9A	3.83	120.14	114.29
4	A	400	NAD	C2B-C1B-N9A	3.88	120.23	114.29
4	C	402	NAD	C2B-C1B-N9A	3.89	120.23	114.29
4	A	400	NAD	C2N-C3N-C4N	3.93	122.67	118.29
4	C	402	NAD	C2N-C3N-C4N	4.03	122.78	118.29
4	D	1403	NAD	C2N-C3N-C4N	4.10	122.85	118.29
4	B	401	NAD	C6N-C5N-C4N	4.46	126.19	119.44
4	D	1403	NAD	C6N-C5N-C4N	4.55	126.32	119.44
4	A	400	NAD	C6N-C5N-C4N	4.63	126.44	119.44
4	C	402	NAD	C6N-C5N-C4N	4.84	126.75	119.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	402	NAD	1	0
4	D	1403	NAD	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	378/393 (96%)	0.03	16 (4%) 40 35	32, 51, 89, 118	0
1	B	383/393 (97%)	-0.00	17 (4%) 38 33	31, 49, 89, 121	0
1	C	377/393 (95%)	0.08	16 (4%) 40 35	32, 53, 96, 120	0
1	D	381/393 (96%)	0.01	17 (4%) 37 32	29, 49, 85, 113	0
All	All	1519/1572 (96%)	0.03	66 (4%) 39 33	29, 51, 90, 121	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	259	ARG	6.2
1	C	377	THR	5.5
1	C	378	ARG	4.6
1	C	350	PHE	4.3
1	D	67	THR	4.1
1	B	377	THR	3.8
1	A	10	LEU	3.8
1	B	354	LEU	3.7
1	C	379	ALA	3.7
1	B	261	GLY	3.7
1	A	378	ARG	3.6
1	A	9	ILE	3.4
1	D	258	GLU	3.4
1	B	137	VAL	3.3
1	A	3	ASN	3.3
1	A	225	VAL	3.3
1	C	375	TYR	3.3
1	C	279	ALA	3.3
1	D	260	GLU	3.2
1	C	61	LYS	3.2
1	D	110	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	364	LYS	3.2
1	B	3	ASN	3.2
1	D	259	ARG	3.1
1	A	111	ALA	3.1
1	D	261	GLY	3.0
1	C	351	ASN	3.0
1	D	311	VAL	2.9
1	A	109	VAL	2.9
1	B	121	THR	2.8
1	A	66	ILE	2.8
1	A	12	ARG	2.8
1	B	350	PHE	2.7
1	A	110	ILE	2.7
1	D	392	ALA	2.7
1	B	294	GLY	2.7
1	B	378	ARG	2.7
1	D	375	TYR	2.6
1	C	68	PRO	2.5
1	D	138	PRO	2.5
1	B	340	GLY	2.5
1	C	381	VAL	2.5
1	D	49	SER	2.5
1	B	62	ARG	2.5
1	D	389	VAL	2.4
1	A	180	LEU	2.4
1	C	62	ARG	2.3
1	D	111	ALA	2.3
1	D	294	GLY	2.3
1	C	140	THR	2.3
1	C	309	LYS	2.3
1	B	260	GLU	2.2
1	A	142	LEU	2.2
1	C	60	ARG	2.2
1	D	350	PHE	2.2
1	C	57	GLU	2.2
1	B	124	VAL	2.1
1	A	393	PRO	2.1
1	D	65	GLU	2.1
1	A	264	ARG	2.1
1	A	67	THR	2.1
1	D	137	VAL	2.1
1	B	111	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	138	PRO	2.0
1	B	295	MET	2.0
1	C	49	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	CL	A	604	1/1	0.89	0.21	2.72	61,61,61,61	0
3	CL	C	1605	1/1	0.94	0.20	2.00	59,59,59,59	0
4	NAD	A	400	44/44	0.97	0.12	-0.81	28,44,56,62	0
4	NAD	B	401	44/44	0.98	0.11	-0.95	23,40,47,50	0
4	NAD	C	402	44/44	0.97	0.10	-0.96	31,45,52,54	0
4	NAD	D	1403	44/44	0.97	0.11	-1.15	25,39,49,56	0
2	ZN	D	1603	1/1	0.80	0.12	-1.46	102,102,102,102	0
2	ZN	C	602	1/1	0.96	0.09	-	117,117,117,117	0
2	ZN	A	600	1/1	0.75	0.10	-	116,116,116,116	0
2	ZN	B	601	1/1	0.95	0.04	-	100,100,100,100	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.