



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 05:20 AM GMT

PDB ID : 3VDR  
Title : Crystal structure of D-3-hydroxybutyrate dehydrogenase, prepared in the presence of the substrate D-3-hydroxybutyrate and NAD(+)  
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Deposited on : 2012-01-06  
Resolution : 3.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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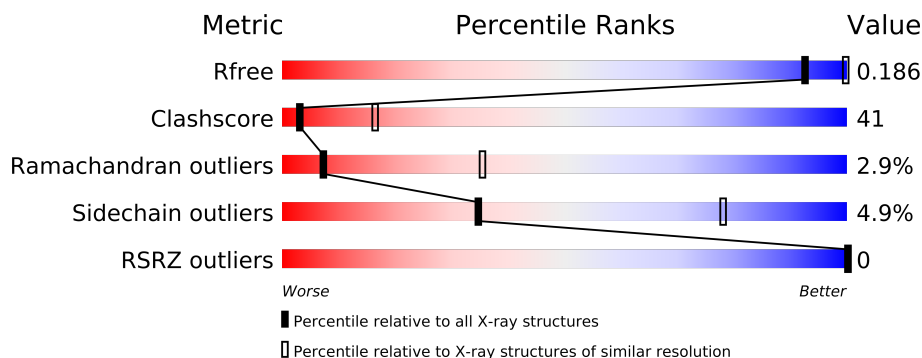
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.00 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))
$R_{free}$	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	260	
1	B	260	
1	C	260	
1	D	260	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CA	A	301	-	X
3	CL	A	302	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8281 atoms, of which 0 are hydrogen and 0 are deuterium.

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 D-3-hydroxybutyrate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			1906	1203	331	366	6			
1	B	260	Total	C	N	O	S	0	0	0
			1906	1203	331	366	6			
1	C	260	Total	C	N	O	S	0	0	0
			1906	1203	331	366	6			
1	D	260	Total	C	N	O	S	0	0	0
			1906	1203	331	366	6			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

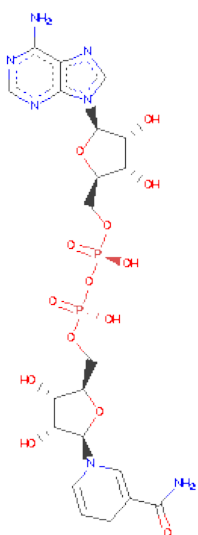
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		

- 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>).



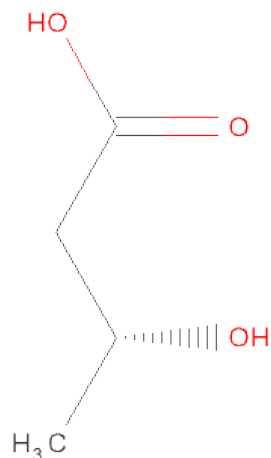
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	1
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	1
			44	21	7	14	2		
4	C	1	Total	C	N	O	P	0	1
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	0	1
			44	21	7	14	2		

- Molecule 5 is 1,4-DIHYDRONICOTINAMIDEADENINE DINUCLEOTIDE (three-letter code: NAI) (formula:  $C_{21}H_{29}N_7O_{14}P_2$ ).



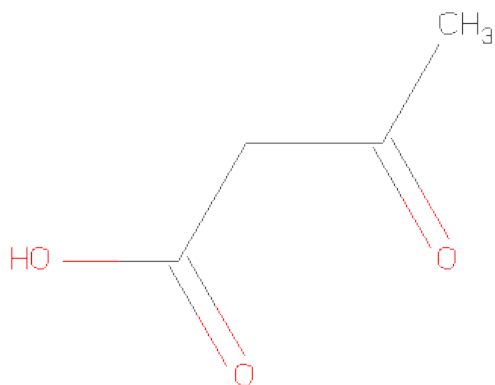
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	1
			44	21	7	14	2		
5	B	1	Total	C	N	O	P	0	1
			44	21	7	14	2		
5	C	1	Total	C	N	O	P	0	1
			44	21	7	14	2		
5	D	1	Total	C	N	O	P	0	1
			44	21	7	14	2		

- Molecule 6 is (3R)-3-HYDROXYBUTANOICACID (three-letter code: 3HR) (formula:  $C_4H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	1
			7	4	3		
6	B	1	Total	C	O	0	1
			7	4	3		
6	C	1	Total	C	O	0	1
			7	4	3		
6	D	1	Total	C	O	0	1
			7	4	3		

- Molecule 7 is ACETOACETIC ACID (three-letter code: AAE) (formula:  $C_4H_6O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	1
			7	4	3		
7	B	1	Total	C	O	0	1
			7	4	3		
7	C	1	Total	C	O	0	1
			7	4	3		
7	D	1	Total	C	O	0	1
			7	4	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	67	Total	O	0	0
			67	67		
8	B	51	Total	O	0	0
			51	51		
8	C	73	Total	O	0	0
			73	73		
8	D	53	Total	O	0	0
			53	53		



M1	L2	K3	K6	V9	T10	G11	S12	T13	S14	G15	T16	G17	L18	A19	M20	A21	T22	A25	G28	A29	D30	V31	V32	I33	N34	G35	F36	G37	P39	I42	E43	R44	E45	R46	K52	F53	G54	V55	Y58	Y59	L60	L64	S65	D66	A69	T70	R71	D72	F73
I74	A75	L81	L84	V88	N89	N90	A91	Q94	H95	T96	A97	P98	V99	F102	P103	V104	D105	K106	W107	N108	L113	S116	F119	H120	A124	A125	L126	P127	Q130	A141	S142	A143	H144	V147	N151	K152	V156	A157	A158	K159	V162	V163	G164	L165					
A170	N173	K176	I183	C184	P185	G186	W187	V188	R189	T190	P191	L192	V193	E194	K195	Q196	I197	E198	A199	I200	Q203	K204	G205	I206	D207	I208	K219	Q220	P221	S222	L223	Q224	T227	Q230	L231	G232	V236	M246	T247	T250	L251	S252	L253	D254	W257	R260			



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.10Å 91.10Å 262.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.00 – 3.00 43.02 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.0 (43.00-3.00) 91.2 (43.02-3.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.59 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.176 , 0.241 0.182 , 0.186	Depositor DCC
$R_{free}$ test set	2062 reflections (9.85%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.3	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 19.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 20937 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8281	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AAE, 3HR, NAD, CL, CA, NAI

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	0.32	0/1935	0.61	0/2623
1	B	0.30	0/1935	0.60	0/2623
1	C	0.32	0/1935	0.61	0/2623
1	D	0.30	0/1935	0.59	0/2623
All	All	0.31	0/7740	0.60	0/10492

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1906	0	1941	185	0
1	B	1906	0	1941	184	0
1	C	1906	0	1941	152	0
1	D	1906	0	1941	162	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	1	0
3	B	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
4	A	44	0	26	11	0
4	B	44	0	26	11	0
4	C	44	0	26	10	0
4	D	44	0	26	10	0
5	A	44	0	27	9	0
5	B	44	0	27	8	0
5	C	44	0	27	13	0
5	D	44	0	27	14	0
6	A	7	0	7	4	0
6	B	7	0	7	6	0
6	C	7	0	7	3	0
6	D	7	0	7	2	0
7	A	7	0	5	3	0
7	B	7	0	5	5	0
7	C	7	0	5	5	0
7	D	7	0	5	4	0
8	A	67	0	0	9	0
8	B	51	0	0	6	0
8	C	73	0	0	4	0
8	D	53	0	0	4	0
All	All	8281	0	8024	664	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 41.

All (664) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:74:ILE:HD12	1:D:75:ALA:N	1.41	1.33
1:B:56:LYS:HG3	8:B:402:HOH:O	1.14	1.26
1:C:74:ILE:HD12	1:C:75:ALA:N	1.56	1.19
1:D:64:LEU:HA	1:D:70:THR:HG22	1.31	1.11
1:C:246:MET:HB2	1:D:253:LEU:HD22	1.26	1.11
1:A:213:ARG:NH1	1:A:213:ARG:HB2	1.67	1.09
1:D:74:ILE:HG12	1:D:124:ALA:HB3	1.35	1.08
1:D:203:GLN:OE1	1:D:203:GLN:O	1.72	1.07
1:D:208:ILE:O	1:D:208:ILE:HD13	1.55	1.06
1:A:90:ASN:HB2	1:A:140:ILE:HD12	1.34	1.05
1:C:210:ALA:HA	1:C:213:ARG:HH12	1.15	1.05
1:A:208:ILE:O	1:A:208:ILE:HD13	1.55	1.05
1:A:213:ARG:HH11	1:A:213:ARG:CB	1.69	1.04
1:C:74:ILE:HD12	1:C:74:ILE:C	1.79	1.03

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:74:ILE:HD13	1:A:74:ILE:N	1.74	1.00
1:D:227:THR:OG1	1:D:230:GLN:HG3	1.63	0.99
1:A:71:ARG:HA	1:A:74:ILE:HD11	1.44	0.98
1:A:40:GLU:HG2	8:A:444:HOH:O	1.63	0.98
1:C:253:LEU:HD22	1:D:246:MET:HB2	1.45	0.98
1:D:90:ASN:OD1	4:D:302[A]:NAD:H4D	1.62	0.98
1:B:99:ILE:HG13	1:C:172:GLU:OE1	1.62	0.98
1:C:253:LEU:CD2	1:D:246:MET:HG3	1.95	0.97
1:D:90:ASN:OD1	5:D:303[B]:NAI:H4D	1.61	0.97
1:A:187:TRP:HZ3	7:A:306[B]:AAE:H41	1.29	0.96
1:B:227:THR:OG1	1:B:230:GLN:HG3	1.63	0.96
1:B:251:LEU:HD13	1:B:253:LEU:HD21	1.48	0.94
5:C:302[B]:NAI:H4N	7:C:304[B]:AAE:C5	1.98	0.93
1:D:74:ILE:C	1:D:74:ILE:HD12	1.88	0.93
1:A:70:THR:O	1:A:74:ILE:CD1	2.17	0.92
1:C:253:LEU:HD23	1:D:246:MET:HG3	1.52	0.92
1:A:187:TRP:CZ3	7:A:306[B]:AAE:H41	2.03	0.92
1:B:188:VAL:O	1:B:193:VAL:HG21	1.69	0.92
1:C:210:ALA:HA	1:C:213:ARG:NH1	1.86	0.91
1:B:20:MET:CE	1:B:232:GLY:HA2	2.01	0.91
1:B:66:ASP:O	1:B:70:THR:HG22	1.69	0.91
1:D:64:LEU:HA	1:D:70:THR:CG2	2.01	0.90
1:A:74:ILE:HD13	1:A:74:ILE:H	1.35	0.90
1:B:142:SER:O	1:B:184:CYS:HB3	1.71	0.90
1:D:74:ILE:HG12	1:D:124:ALA:CB	2.02	0.90
1:A:1:MET:HG3	8:A:454:HOH:O	1.72	0.89
1:B:187:TRP:CZ3	7:B:306[B]:AAE:H41	2.08	0.88
1:A:61:ASN:HD22	1:A:62:ALA:N	1.72	0.88
1:B:207:ASP:HB3	1:B:210:ALA:CB	2.02	0.88
4:C:301[A]:NAD:C4N	6:C:303[A]:3HR:H3	2.04	0.88
1:B:1:MET:CE	1:B:236:VAL:HG12	2.01	0.88
1:A:71:ARG:CA	1:A:74:ILE:HD11	2.04	0.87
1:A:187:TRP:HZ3	6:A:305[A]:3HR:H2	1.38	0.87
1:A:16:ILE:O	1:A:20:MET:HG3	1.74	0.86
1:C:208:ILE:HD13	1:C:208:ILE:O	1.75	0.86
1:A:213:ARG:NH1	1:A:213:ARG:CB	2.34	0.86
1:A:252:SER:O	1:A:253:LEU:HD23	1.77	0.85
1:B:87:LEU:HG	1:B:89:ASN:ND2	1.92	0.84
1:B:237:PHE:HE2	1:B:246:MET:HE1	1.40	0.83
1:C:246:MET:HB2	1:D:253:LEU:CD2	2.09	0.83
5:C:302[B]:NAI:H4N	7:C:304[B]:AAE:C9	2.09	0.82
1:B:90:ASN:OD1	5:B:304[B]:NAI:H4D	1.77	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:99:ILE:O	1:A:101:GLU:N	2.12	0.82
1:B:251:LEU:CD1	1:B:253:LEU:HD21	2.10	0.81
1:B:87:LEU:HG	1:B:89:ASN:HD21	1.43	0.81
1:D:72:ASP:OD1	8:D:404:HOH:O	1.98	0.81
1:C:44:ARG:HD3	8:C:449:HOH:O	1.81	0.81
1:C:100:GLU:N	1:C:100:GLU:OE1	2.12	0.81
1:B:90:ASN:OD1	4:B:303[A]:NAD:H4D	1.79	0.80
1:A:192:LEU:HD23	1:A:192:LEU:O	1.80	0.80
1:B:9:VAL:HG22	1:B:88:VAL:HB	1.63	0.80
1:B:207:ASP:HB3	1:B:210:ALA:HB3	1.63	0.80
1:A:74:ILE:CD1	1:A:74:ILE:H	1.95	0.79
1:B:1:MET:HE2	1:B:236:VAL:HG12	1.64	0.79
1:A:213:ARG:HH11	1:A:213:ARG:HB3	1.47	0.78
1:A:64:LEU:HD22	1:A:70:THR:HG23	1.64	0.78
1:C:74:ILE:CD1	1:C:75:ALA:N	2.43	0.78
1:B:87:LEU:CG	1:B:89:ASN:HD21	1.96	0.78
1:A:74:ILE:HG13	1:A:124:ALA:HB3	1.64	0.77
1:A:61:ASN:HD22	1:A:62:ALA:H	1.29	0.77
1:C:64:LEU:HD12	4:C:301[A]:NAD:H2A	1.65	0.77
1:B:204:LYS:O	1:B:206:ILE:HG23	1.85	0.77
1:A:198:GLU:O	1:A:202:GLN:HG3	1.84	0.77
1:C:227:THR:O	1:C:230:GLN:HB2	1.85	0.77
1:D:74:ILE:CD1	1:D:75:ALA:N	2.36	0.77
1:A:91:ALA:HB1	5:A:304[B]:NAI:C2A	2.15	0.77
1:D:205:GLY:O	1:D:206:ILE:HG23	1.84	0.77
1:A:104:VAL:HG23	1:D:120:HIS:HE1	1.49	0.76
1:D:74:ILE:HD11	1:D:124:ALA:HB1	1.66	0.76
1:C:74:ILE:HD12	1:C:75:ALA:CA	2.14	0.76
1:D:9:VAL:HG22	1:D:88:VAL:HB	1.67	0.76
1:C:253:LEU:HD22	1:D:246:MET:CB	2.15	0.76
1:A:122:THR:HG23	1:A:137:ILE:HD13	1.66	0.76
1:D:36:PHE:CD1	4:D:302[A]:NAD:N7A	2.54	0.76
1:C:64:LEU:HD12	5:C:302[B]:NAI:H2A	1.66	0.76
1:B:183:ILE:O	1:B:185:PRO:HD3	1.85	0.76
1:B:232:GLY:O	1:B:236:VAL:HG23	1.86	0.76
1:B:190:THR:HB	1:B:191:PRO:CD	2.15	0.75
1:C:34:ASN:HB2	1:C:60:LEU:O	1.84	0.75
1:A:213:ARG:O	8:A:462:HOH:O	2.03	0.75
1:C:96:THR:O	1:C:97:ALA:HB2	1.87	0.75
1:A:44:ARG:O	1:A:48:THR:HG22	1.87	0.75
1:C:224:GLN:HG2	8:C:447:HOH:O	1.87	0.75
1:A:91:ALA:HB1	4:A:303[A]:NAD:C2A	2.16	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:187:TRP:CZ3	6:A:305[A]:3HR:H2	2.22	0.74
5:B:304[B]:NAI:H4N	7:B:306[B]:AAE:C5	2.16	0.74
1:C:38:GLN:HA	1:C:38:GLN:OE1	1.86	0.74
1:D:20:MET:HG2	1:D:88:VAL:HG11	1.69	0.74
1:D:74:ILE:CD1	1:D:74:ILE:C	2.55	0.74
1:D:222:SER:O	1:D:224:GLN:HG3	1.87	0.74
1:B:64:LEU:HD12	5:B:304[B]:NAI:H2A	1.69	0.74
1:C:74:ILE:C	1:C:74:ILE:CD1	2.54	0.73
1:B:122:THR:HG22	1:B:126:LEU:CD1	2.18	0.73
1:B:120:HIS:HE1	1:C:104:VAL:HG12	1.53	0.73
1:D:196:GLN:NE2	7:D:305[B]:AAE:O3	2.22	0.73
1:A:70:THR:O	1:A:73:PHE:HB3	1.89	0.73
1:A:91:ALA:CB	4:A:303[A]:NAD:C2A	2.66	0.73
1:A:91:ALA:CB	5:A:304[B]:NAI:C2A	2.66	0.72
1:D:74:ILE:HD12	1:D:75:ALA:CA	2.17	0.72
1:B:251:LEU:HD13	1:B:253:LEU:CD2	2.18	0.72
1:B:64:LEU:HD12	4:B:303[A]:NAD:H2A	1.69	0.72
1:B:40:GLU:N	1:B:40:GLU:OE1	2.22	0.72
1:A:218:GLU:OE2	1:A:219:LYS:HE2	1.90	0.72
1:A:90:ASN:CB	1:A:140:ILE:HD12	2.18	0.71
1:B:219:LYS:O	1:B:221:PRO:HD3	1.88	0.71
1:D:36:PHE:CD1	5:D:303[B]:NAI:N7A	2.58	0.71
1:C:187:TRP:CZ2	1:C:215:LEU:HD11	2.25	0.71
1:D:91:ALA:HB1	5:D:303[B]:NAI:C2A	2.20	0.71
1:D:43:GLU:OE2	1:D:46:ARG:NE	2.18	0.71
1:A:64:LEU:HD12	4:A:303[A]:NAD:H2A	1.73	0.71
1:A:252:SER:C	1:A:253:LEU:HD23	2.12	0.70
1:D:74:ILE:CG1	1:D:124:ALA:HB3	2.19	0.70
1:A:20:MET:HE1	1:A:235:ALA:HB2	1.72	0.70
1:D:32:VAL:HG23	1:D:81:LEU:HD21	1.72	0.70
1:A:253:LEU:CD2	1:B:246:MET:HG3	2.21	0.70
1:A:150:VAL:HG23	3:A:302:CL:CL	2.28	0.70
1:B:237:PHE:HE2	1:B:246:MET:CE	2.05	0.70
1:B:257:TRP:O	1:B:257:TRP:HD1	1.75	0.70
1:B:20:MET:HE3	1:B:232:GLY:HA2	1.72	0.70
1:D:197:ILE:CG2	1:D:208:ILE:HD13	2.21	0.69
1:D:91:ALA:HB1	4:D:302[A]:NAD:C2A	2.22	0.69
1:D:142:SER:HA	1:D:185:PRO:HD2	1.73	0.69
1:A:253:LEU:HD22	1:B:246:MET:HB2	1.73	0.69
1:A:189:ARG:NH2	1:A:194:GLU:OE2	2.25	0.69
1:A:64:LEU:HD12	5:A:304[B]:NAI:H2A	1.74	0.69
1:C:59:TYR:O	1:C:60:LEU:HD23	1.91	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:103:PRO:HB2	1:B:106:LYS:HG2	1.75	0.69
1:D:10:THR:HB	1:D:64:LEU:HD11	1.74	0.69
1:C:9:VAL:HG22	1:C:88:VAL:HB	1.75	0.69
1:B:20:MET:HE1	1:B:231:LEU:O	1.93	0.68
1:B:237:PHE:CE2	1:B:246:MET:CE	2.76	0.68
1:C:126:LEU:HB2	1:C:127:PRO:HD3	1.75	0.68
1:D:74:ILE:CG1	1:D:124:ALA:CB	2.71	0.68
1:C:204:LYS:HE2	1:C:214:GLU:OE1	1.92	0.68
1:D:60:LEU:HB2	1:D:73:PHE:HE1	1.58	0.68
1:D:74:ILE:CD1	1:D:124:ALA:HB1	2.24	0.68
1:B:66:ASP:OD1	1:B:69:ALA:HB2	1.93	0.68
1:D:208:ILE:CD1	1:D:208:ILE:O	2.39	0.68
1:A:206:ILE:O	1:A:207:ASP:O	2.13	0.67
1:D:197:ILE:CG2	1:D:208:ILE:CD1	2.72	0.67
1:B:164:GLY:HA2	1:B:167:LYS:HD2	1.76	0.67
1:C:243:ALA:O	1:C:246:MET:N	2.24	0.67
1:A:20:MET:CE	1:A:235:ALA:HB2	2.24	0.67
1:B:160:HIS:O	1:C:160:HIS:HB3	1.95	0.67
1:A:87:LEU:HD12	1:A:88:VAL:N	2.10	0.67
1:B:225:PHE:HB3	8:B:416:HOH:O	1.95	0.66
1:C:221:PRO:HG2	1:C:255:GLY:O	1.94	0.66
1:C:20:MET:HE1	1:C:232:GLY:HA2	1.76	0.66
1:C:32:VAL:HG23	1:C:81:LEU:HD21	1.78	0.66
1:B:193:VAL:CG2	4:B:303[A]:NAD:H72N	2.07	0.66
1:D:197:ILE:HG21	1:D:208:ILE:CD1	2.25	0.66
1:C:253:LEU:CD2	1:D:246:MET:CG	2.72	0.66
1:B:193:VAL:HG23	4:B:303[A]:NAD:H72N	1.61	0.66
1:C:165:LEU:O	1:C:165:LEU:HD23	1.96	0.65
1:C:213:ARG:HH11	1:C:213:ARG:HB2	1.60	0.65
1:D:72:ASP:O	1:D:75:ALA:HB3	1.97	0.65
1:D:197:ILE:HG21	1:D:208:ILE:HD13	1.78	0.65
1:C:251:LEU:HD21	1:D:246:MET:HE1	1.79	0.65
1:B:213:ARG:NH1	1:B:213:ARG:HB2	2.13	0.64
1:B:165:LEU:O	1:B:165:LEU:HD23	1.96	0.64
1:B:23:GLU:HG3	8:B:406:HOH:O	1.96	0.64
1:D:10:THR:HB	1:D:64:LEU:CD1	2.26	0.64
1:D:194:GLU:O	1:D:198:GLU:HG3	1.97	0.64
1:C:192:LEU:HD23	1:C:192:LEU:C	2.17	0.64
1:A:246:MET:HE3	1:B:251:LEU:HD22	1.79	0.64
1:A:71:ARG:C	1:A:74:ILE:HD11	2.18	0.64
1:A:212:ALA:C	1:A:214:GLU:H	1.99	0.64
1:C:136:ARG:HE	1:C:239:SER:HA	1.62	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:45:GLU:HA	1:A:48:THR:CG2	2.27	0.64
1:C:91:ALA:HB1	5:C:302[B]:NAI:N3A	2.13	0.63
1:C:66:ASP:O	1:C:70:THR:HG22	1.98	0.63
1:B:207:ASP:HB3	1:B:210:ALA:HB2	1.80	0.63
1:D:32:VAL:HG23	1:D:81:LEU:CD2	2.28	0.63
1:A:122:THR:HG23	1:A:137:ILE:CD1	2.29	0.63
1:B:56:LYS:HD2	1:B:56:LYS:N	2.14	0.62
1:B:3:LYS:H	1:B:3:LYS:HD3	1.64	0.62
1:D:1:MET:O	1:D:2:LEU:HD23	1.99	0.62
1:B:192:LEU:HD23	1:B:192:LEU:O	1.99	0.62
1:A:91:ALA:HB1	5:A:304[B]:NAI:N3A	2.14	0.62
1:D:32:VAL:HG23	1:D:81:LEU:CG	2.29	0.62
1:A:208:ILE:C	1:A:208:ILE:HD13	2.20	0.62
1:A:32:VAL:HG23	1:A:81:LEU:HD11	1.81	0.62
1:A:70:THR:O	1:A:74:ILE:HD12	2.00	0.62
1:B:85:ASP:O	1:B:129:MET:HE2	2.00	0.61
1:C:3:LYS:HA	1:C:28:GLY:O	2.00	0.61
1:A:216:LEU:O	1:A:218:GLU:N	2.33	0.61
1:A:91:ALA:CB	5:A:304[B]:NAI:H2A	2.30	0.61
1:A:45:GLU:O	1:A:48:THR:HG23	2.00	0.61
1:A:201:SER:HB2	1:A:211:ALA:CB	2.30	0.61
1:B:40:GLU:H	1:B:40:GLU:CD	2.03	0.61
1:C:136:ARG:NE	1:C:239:SER:HA	2.15	0.61
1:B:122:THR:HG22	1:B:126:LEU:HD11	1.83	0.61
1:C:208:ILE:HD13	1:C:208:ILE:C	2.20	0.61
1:A:91:ALA:HB1	4:A:303[A]:NAD:N3A	2.15	0.61
1:C:144:HIS:HA	1:C:147:VAL:O	2.01	0.61
1:A:45:GLU:O	1:A:48:THR:CG2	2.49	0.61
1:B:190:THR:HB	1:B:191:PRO:HD2	1.83	0.60
1:B:194:GLU:O	1:B:198:GLU:HG3	2.01	0.60
1:B:90:ASN:O	1:B:90:ASN:CG	2.39	0.60
1:A:91:ALA:CB	4:A:303[A]:NAD:H2A	2.30	0.60
1:C:208:ILE:HG23	1:C:209:GLU:N	2.15	0.60
1:B:189:ARG:HD2	1:B:225:PHE:CE1	2.36	0.60
1:D:116:SER:O	1:D:119:PHE:HB3	2.02	0.60
1:B:237:PHE:CE2	1:B:246:MET:HE1	2.29	0.59
1:C:251:LEU:HD21	1:D:246:MET:CE	2.31	0.59
1:C:91:ALA:HB1	4:C:301[A]:NAD:N3A	2.16	0.59
1:C:9:VAL:HG12	1:C:12:SER:HB3	1.83	0.59
1:B:196:GLN:NE2	7:B:306[B]:AAE:O3	2.29	0.59
1:B:36:PHE:CE1	4:B:303[A]:NAD:N7A	2.70	0.59
1:D:64:LEU:CA	1:D:70:THR:HG22	2.21	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:100:GLU:HG2	1:A:101:GLU:HG3	1.84	0.59
1:A:26:LYS:HA	1:A:53:PHE:CD1	2.38	0.59
1:D:91:ALA:CB	5:D:303[B]:NAI:H2A	2.33	0.59
1:B:63:ASP:O	1:B:65:SER:N	2.36	0.59
1:D:91:ALA:HB1	5:D:303[B]:NAI:H2A	1.83	0.59
6:A:305[A]:3HR:H4A	6:A:305[A]:3HR:O1	2.02	0.59
1:B:43:GLU:OE2	1:B:46:ARG:NE	2.26	0.59
1:C:36:PHE:CD1	4:C:301[A]:NAD:N7A	2.71	0.59
1:A:61:ASN:ND2	1:A:62:ALA:N	2.47	0.59
1:A:71:ARG:O	1:A:74:ILE:HD11	2.03	0.58
1:D:158:ALA:O	1:D:162:VAL:HG23	2.03	0.58
1:C:10:THR:HB	1:C:64:LEU:CD1	2.33	0.58
1:B:158:ALA:O	1:B:162:VAL:HG23	2.02	0.58
1:B:150:VAL:HG13	3:B:302:CL:CL	2.41	0.58
5:B:304[B]:NAI:H4N	7:B:306[B]:AAE:O8	2.03	0.58
1:B:183:ILE:C	1:B:185:PRO:HD3	2.22	0.58
1:D:142:SER:O	1:D:184:CYS:HB3	2.03	0.58
1:D:69:ALA:HA	8:D:430:HOH:O	2.02	0.58
1:C:187:TRP:CH2	1:C:215:LEU:HD11	2.39	0.58
1:D:91:ALA:HB1	4:D:302[A]:NAD:H2A	1.84	0.58
6:B:305[A]:3HR:H4A	6:B:305[A]:3HR:O1	2.01	0.58
1:B:257:TRP:CD1	1:B:257:TRP:O	2.55	0.58
1:A:139:ASN:O	1:A:182:ALA:HA	2.04	0.58
1:A:165:LEU:O	1:A:165:LEU:HD23	2.02	0.58
1:D:22:THR:HG23	1:D:53:PHE:CE2	2.39	0.58
1:A:167:LYS:HE2	8:A:404:HOH:O	2.04	0.58
1:A:190:THR:HB	1:A:191:PRO:CD	2.33	0.58
1:B:192:LEU:HD23	1:B:192:LEU:C	2.24	0.58
1:A:207:ASP:HB3	1:A:210:ALA:CB	2.34	0.58
1:B:67:ALA:O	1:B:70:THR:HG23	2.04	0.58
1:D:64:LEU:O	1:D:70:THR:HG21	2.03	0.58
1:C:36:PHE:CE1	4:C:301[A]:NAD:N7A	2.72	0.58
1:B:159:LYS:NZ	5:B:304[B]:NAI:O2D	2.28	0.58
1:B:101:GLU:OE2	8:B:437:HOH:O	2.17	0.57
1:D:64:LEU:HD23	1:D:70:THR:HG22	1.84	0.57
1:B:1:MET:CE	1:B:236:VAL:CG1	2.80	0.57
1:C:91:ALA:HB1	5:C:302[B]:NAI:C2A	2.35	0.57
1:B:167:LYS:HB3	1:C:148:ALA:HB3	1.85	0.57
1:C:168:VAL:O	1:C:172:GLU:HG3	2.04	0.57
1:A:206:ILE:O	1:A:207:ASP:C	2.42	0.57
1:A:20:MET:SD	1:A:140:ILE:HD11	2.45	0.57
1:A:71:ARG:O	1:A:74:ILE:CD1	2.52	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:74:ILE:HG13	1:A:124:ALA:CB	2.33	0.57
1:B:70:THR:O	1:B:73:PHE:HB3	2.05	0.57
1:D:190:THR:HB	1:D:191:PRO:HD2	1.87	0.57
1:D:17:GLY:HA3	1:D:90:ASN:ND2	2.19	0.57
1:A:32:VAL:HG23	1:A:81:LEU:CD1	2.35	0.57
1:A:166:THR:HG23	1:A:180:CYS:SG	2.44	0.57
1:D:17:GLY:CA	1:D:90:ASN:ND2	2.68	0.57
1:D:205:GLY:O	1:D:206:ILE:CG2	2.52	0.57
1:D:64:LEU:HD12	5:D:303[B]:NAI:H2A	1.87	0.56
1:A:207:ASP:HB3	1:A:210:ALA:HB2	1.87	0.56
1:C:10:THR:HB	1:C:64:LEU:HD11	1.87	0.56
1:B:36:PHE:CE1	5:B:304[B]:NAI:N7A	2.73	0.56
1:A:10:THR:O	1:A:11:GLY:C	2.43	0.56
1:A:212:ALA:C	1:A:214:GLU:N	2.58	0.56
1:B:89:ASN:HD22	1:B:89:ASN:N	2.03	0.56
1:D:91:ALA:CB	4:D:302[A]:NAD:H2A	2.34	0.56
1:D:197:ILE:HG22	1:D:208:ILE:CD1	2.35	0.56
1:B:159:LYS:NZ	4:B:303[A]:NAD:O2D	2.30	0.56
1:A:232:GLY:O	1:A:236:VAL:HG23	2.05	0.56
1:A:88:VAL:HG22	1:A:138:ILE:HB	1.86	0.56
1:D:9:VAL:HG12	1:D:12:SER:HB3	1.87	0.56
1:D:52:LYS:HE3	1:D:53:PHE:CZ	2.41	0.56
1:A:153:SER:HB3	8:A:445:HOH:O	2.04	0.56
1:C:36:PHE:CE1	5:C:302[B]:NAI:N7A	2.74	0.56
1:B:155:TYR:CZ	1:B:159:LYS:HE3	2.41	0.56
1:C:94:GLN:OE1	1:C:94:GLN:HA	2.06	0.56
1:B:144:HIS:O	1:B:159:LYS:HB2	2.06	0.56
1:C:208:ILE:C	1:C:208:ILE:CD1	2.75	0.56
1:D:32:VAL:HG23	1:D:81:LEU:HG	1.88	0.56
1:C:74:ILE:HG12	1:C:124:ALA:CB	2.36	0.55
1:C:90:ASN:OD1	4:C:301[A]:NAD:H4D	2.06	0.55
1:B:122:THR:CG2	1:B:126:LEU:HD11	2.35	0.55
1:C:39:PRO:HG2	1:C:40:GLU:OE2	2.06	0.55
1:C:36:PHE:CD1	5:C:302[B]:NAI:N7A	2.75	0.55
1:C:97:ALA:H	1:C:151:ASN:HB3	1.71	0.55
1:B:260:ARG:OXT	1:D:147:VAL:HG11	2.06	0.55
1:D:64:LEU:HD12	4:D:302[A]:NAD:H2A	1.89	0.55
1:B:18:LEU:HD11	1:B:45:GLU:HG3	1.88	0.55
1:D:36:PHE:CE1	4:D:302[A]:NAD:N7A	2.74	0.55
1:B:16:ILE:HD11	1:B:188:VAL:HG21	1.87	0.55
1:C:185:PRO:HG3	1:C:231:LEU:HD22	1.89	0.55
1:D:59:TYR:O	1:D:60:LEU:HD23	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:303[A]:NAD:C4N	6:B:305[A]:3HR:H3	2.37	0.55
1:A:96:THR:O	1:A:97:ALA:HB2	2.07	0.55
1:D:200:ILE:O	1:D:204:LYS:HB2	2.07	0.55
1:D:190:THR:HB	1:D:191:PRO:CD	2.37	0.55
5:C:302[B]:NAI:C4N	7:C:304[B]:AAE:C9	2.83	0.55
1:A:104:VAL:HG23	1:D:120:HIS:CE1	2.35	0.55
1:A:189:ARG:CZ	1:A:194:GLU:OE1	2.55	0.55
1:B:167:LYS:HB2	1:C:148:ALA:HB2	1.89	0.55
1:D:64:LEU:CA	1:D:70:THR:CG2	2.82	0.54
1:D:60:LEU:HB2	1:D:73:PHE:CE1	2.40	0.54
1:D:199:ALA:O	1:D:203:GLN:CB	2.55	0.54
1:B:10:THR:HB	1:B:64:LEU:CD1	2.38	0.54
1:D:103:PRO:HB2	1:D:106:LYS:HB2	1.90	0.54
1:A:45:GLU:CA	1:A:48:THR:HG22	2.37	0.54
1:D:64:LEU:CD2	1:D:70:THR:HG22	2.37	0.54
1:B:94:GLN:HE22	1:B:152:LYS:HD3	1.73	0.54
1:A:104:VAL:CG1	8:A:464:HOH:O	2.55	0.54
1:B:120:HIS:CE1	1:C:104:VAL:HG12	2.39	0.54
1:A:93:ILE:HG23	1:A:113:LEU:CD2	2.36	0.54
1:A:45:GLU:HA	1:A:48:THR:HG22	1.90	0.54
1:D:141:ALA:O	1:D:142:SER:HB2	2.07	0.54
1:B:167:LYS:HB3	1:C:148:ALA:CB	2.37	0.54
1:A:254:ASP:HB2	1:A:257:TRP:CB	2.37	0.54
1:A:91:ALA:CB	5:A:304[B]:NAI:N3A	2.71	0.54
1:C:90:ASN:OD1	5:C:302[B]:NAI:H4D	2.07	0.54
1:B:190:THR:CB	1:B:191:PRO:CD	2.86	0.54
6:D:304[A]:3HR:H4A	6:D:304[A]:3HR:O1	2.08	0.54
1:C:129:MET:HE1	1:C:136:ARG:H	1.71	0.54
5:C:302[B]:NAI:H4N	7:C:304[B]:AAE:H93	1.87	0.53
1:B:87:LEU:CD2	1:B:89:ASN:HD21	2.21	0.53
1:B:87:LEU:CG	1:B:89:ASN:ND2	2.64	0.53
1:A:32:VAL:HG23	1:A:81:LEU:CG	2.38	0.53
1:B:253:LEU:HD23	1:B:253:LEU:N	2.22	0.53
1:B:96:THR:O	1:B:97:ALA:HB2	2.08	0.53
1:A:70:THR:O	1:A:74:ILE:HD13	2.03	0.53
1:C:91:ALA:HB1	4:C:301[A]:NAD:C2A	2.38	0.53
1:A:136:ARG:NE	1:A:238:LEU:O	2.39	0.53
1:B:1:MET:HE2	1:B:236:VAL:CG1	2.38	0.53
1:C:20:MET:CE	1:C:232:GLY:HA2	2.37	0.53
1:D:141:ALA:O	1:D:142:SER:CB	2.57	0.53
1:D:152:LYS:O	1:D:156:VAL:HG23	2.07	0.53
1:C:74:ILE:CG1	1:C:124:ALA:HB1	2.39	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:194:GLU:HB2	8:A:402:HOH:O	2.09	0.53
1:C:165:LEU:HD23	1:C:165:LEU:C	2.28	0.53
1:C:208:ILE:CG2	1:C:209:GLU:N	2.72	0.53
1:B:122:THR:HG22	1:B:126:LEU:HD12	1.90	0.53
1:C:257:TRP:CD1	1:C:257:TRP:C	2.83	0.53
1:D:203:GLN:O	1:D:203:GLN:CD	2.44	0.53
1:A:32:VAL:CG2	1:A:81:LEU:HG	2.39	0.53
1:B:66:ASP:CG	1:B:69:ALA:HB2	2.30	0.52
1:A:93:ILE:HG12	1:A:113:LEU:HD23	1.91	0.52
1:D:18:LEU:HD21	1:D:45:GLU:HG2	1.91	0.52
1:A:253:LEU:HD22	1:B:246:MET:CB	2.39	0.52
1:D:32:VAL:CG2	1:D:81:LEU:HG	2.39	0.52
1:D:113:LEU:HD11	4:D:302[A]:NAD:C2A	2.38	0.52
1:D:36:PHE:CE1	5:D:303[B]:NAI:N7A	2.77	0.52
1:A:246:MET:HE3	1:B:251:LEU:CD2	2.38	0.52
1:A:45:GLU:C	1:A:48:THR:HG22	2.30	0.52
1:A:251:LEU:C	1:A:251:LEU:CD2	2.77	0.52
1:A:193:VAL:HG23	4:A:303[A]:NAD:H72N	1.75	0.52
1:B:43:GLU:OE1	1:B:43:GLU:O	2.27	0.52
1:C:150:VAL:CG1	1:C:151:ASN:N	2.71	0.52
1:B:94:GLN:HG2	1:B:155:TYR:CD2	2.45	0.52
1:C:43:GLU:O	1:C:47:SER:HB2	2.10	0.52
1:B:6:LYS:HE3	1:B:82:GLY:O	2.09	0.52
1:B:213:ARG:HH11	1:B:213:ARG:CB	2.23	0.52
1:A:91:ALA:CB	4:A:303[A]:NAD:N3A	2.72	0.52
1:A:246:MET:CE	1:B:251:LEU:HD22	2.39	0.52
1:D:113:LEU:HD11	5:D:303[B]:NAI:C2A	2.39	0.52
1:B:227:THR:HG1	1:B:230:GLN:HG3	1.74	0.51
1:C:94:GLN:NE2	1:C:152:LYS:HD3	2.25	0.51
1:A:210:ALA:O	1:A:214:GLU:HB2	2.10	0.51
1:C:194:GLU:O	1:C:198:GLU:HG3	2.10	0.51
1:D:38:GLN:OE1	1:D:38:GLN:HA	2.08	0.51
1:D:74:ILE:HD12	1:D:75:ALA:H	1.59	0.51
1:C:96:THR:O	1:C:97:ALA:CB	2.53	0.51
1:A:254:ASP:O	1:A:256:GLY:N	2.43	0.51
1:A:90:ASN:OD1	4:A:303[A]:NAD:H4D	2.10	0.51
1:D:104:VAL:HG23	1:D:105:ASP:N	2.24	0.51
1:B:5:LYS:CE	8:B:411:HOH:O	2.58	0.51
1:C:99:ILE:C	1:C:101:GLU:H	2.14	0.51
1:A:32:VAL:HG23	1:A:81:LEU:HG	1.92	0.51
1:A:94:GLN:OE1	1:A:95:HIS:N	2.44	0.51
6:C:303[A]:3HR:O1	6:C:303[A]:3HR:H4A	2.09	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:142:SER:O	1:B:184:CYS:CB	2.53	0.51
1:C:20:MET:CE	1:C:231:LEU:C	2.80	0.51
1:C:70:THR:O	1:C:73:PHE:HB3	2.11	0.51
1:C:74:ILE:HG12	1:C:124:ALA:HB1	1.93	0.50
1:B:90:ASN:HB2	1:B:140:ILE:HG13	1.91	0.50
1:A:99:ILE:C	1:A:101:GLU:N	2.64	0.50
1:D:58:TYR:CD1	1:D:58:TYR:N	2.79	0.50
1:B:16:ILE:O	1:B:20:MET:HG2	2.11	0.50
1:C:38:GLN:OE1	1:C:38:GLN:CA	2.58	0.50
1:D:95:HIS:O	1:D:102:PHE:HE1	1.94	0.50
1:B:167:LYS:CB	1:C:148:ALA:HB2	2.42	0.50
1:B:204:LYS:O	1:B:205:GLY:C	2.50	0.50
1:A:254:ASP:HB2	1:A:257:TRP:HB2	1.92	0.50
1:C:122:THR:HG23	1:C:137:ILE:HD13	1.93	0.50
1:A:104:VAL:HG12	8:A:464:HOH:O	2.12	0.50
1:D:97:ALA:HB3	1:D:102:PHE:CD1	2.47	0.50
1:C:76:LYS:HD2	8:C:415:HOH:O	2.10	0.50
1:D:197:ILE:CG2	1:D:208:ILE:HD11	2.40	0.50
1:B:20:MET:HE3	1:B:232:GLY:CA	2.42	0.50
1:B:187:TRP:CZ3	6:B:305[A]:3HR:H2	2.47	0.50
1:A:97:ALA:C	1:A:151:ASN:HB3	2.33	0.49
1:A:254:ASP:O	1:A:255:GLY:C	2.50	0.49
1:B:32:VAL:HG23	1:B:81:LEU:HD11	1.93	0.49
1:C:50:GLU:HG3	1:C:55:VAL:O	2.12	0.49
1:C:66:ASP:O	1:C:70:THR:CG2	2.61	0.49
1:A:141:ALA:O	1:A:142:SER:CB	2.59	0.49
1:A:192:LEU:HD23	1:A:192:LEU:C	2.31	0.49
1:A:200:ILE:O	1:A:200:ILE:HG22	2.11	0.49
1:A:153:SER:CB	8:A:445:HOH:O	2.58	0.49
1:B:112:ALA:O	1:B:116:SER:HB2	2.11	0.49
1:C:106:LYS:O	1:C:110:ILE:HG13	2.13	0.49
1:A:212:ALA:O	1:A:214:GLU:N	2.46	0.49
5:C:302[B]:NAI:C4N	7:C:304[B]:AAE:H93	2.41	0.49
1:A:253:LEU:HD23	1:B:246:MET:HG3	1.92	0.49
1:C:76:LYS:CD	8:C:415:HOH:O	2.61	0.49
1:A:127:PRO:HA	1:A:130:GLN:NE2	2.27	0.49
1:A:187:TRP:CE3	1:A:187:TRP:HA	2.48	0.49
1:A:252:SER:O	1:B:246:MET:HG3	2.13	0.49
1:D:185:PRO:HB3	1:D:231:LEU:HD21	1.95	0.49
1:A:193:VAL:HG21	5:A:304[B]:NAI:O7N	2.12	0.49
1:C:213:ARG:HB2	1:C:213:ARG:NH1	2.28	0.49
1:A:246:MET:CE	1:B:251:LEU:CD2	2.91	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:237:PHE:CE2	1:B:246:MET:HE3	2.48	0.48
1:D:104:VAL:CG2	1:D:105:ASP:N	2.75	0.48
1:D:199:ALA:O	1:D:203:GLN:HB2	2.13	0.48
1:A:90:ASN:OD1	5:A:304[B]:NAI:H4D	2.13	0.48
1:B:67:ALA:O	1:B:70:THR:CG2	2.61	0.48
1:B:129:MET:CE	1:B:136:ARG:H	2.26	0.48
1:D:199:ALA:O	1:D:203:GLN:HB3	2.14	0.48
1:A:186:GLY:O	4:A:303[A]:NAD:H4N	2.13	0.48
1:B:187:TRP:HZ3	7:B:306[B]:AAE:H41	1.73	0.48
1:B:207:ASP:CB	1:B:210:ALA:HB3	2.40	0.48
1:C:113:LEU:O	1:C:117:ALA:HB3	2.14	0.48
1:D:11:GLY:O	1:D:90:ASN:ND2	2.46	0.48
1:B:257:TRP:C	1:B:257:TRP:CD1	2.86	0.48
1:C:67:ALA:O	1:C:70:THR:HG23	2.14	0.48
1:A:251:LEU:C	1:A:251:LEU:HD23	2.34	0.48
1:D:173:ASN:HA	1:D:176:LYS:HD2	1.96	0.48
1:A:187:TRP:CZ3	6:A:305[A]:3HR:H4B	2.48	0.48
1:B:213:ARG:NH1	1:B:213:ARG:CB	2.77	0.48
1:A:44:ARG:O	1:A:48:THR:CG2	2.61	0.48
1:A:172:GLU:OE2	1:D:151:ASN:N	2.47	0.48
1:D:232:GLY:O	1:D:236:VAL:HG23	2.14	0.48
1:B:142:SER:OG	1:B:143:ALA:N	2.47	0.48
1:D:9:VAL:CG1	1:D:12:SER:HB3	2.43	0.48
1:B:142:SER:HA	1:B:185:PRO:HD2	1.96	0.48
1:A:99:ILE:C	1:A:101:GLU:H	2.17	0.48
1:D:22:THR:HG23	1:D:53:PHE:CZ	2.49	0.48
1:D:103:PRO:HB2	1:D:106:LYS:CG	2.43	0.48
1:A:26:LYS:HB2	1:A:53:PHE:CE1	2.49	0.47
1:A:187:TRP:HB2	1:A:220:GLN:OE1	2.14	0.47
1:B:20:MET:HE2	1:B:232:GLY:HA2	1.94	0.47
1:B:94:GLN:HE22	1:B:152:LYS:CD	2.27	0.47
1:D:39:PRO:O	1:D:43:GLU:HB2	2.14	0.47
1:B:252:SER:C	1:B:253:LEU:HD23	2.34	0.47
1:B:66:ASP:CG	1:B:69:ALA:CB	2.82	0.47
1:A:99:ILE:O	1:A:102:PHE:N	2.47	0.47
1:A:150:VAL:HG12	1:A:151:ASN:CG	2.35	0.47
1:B:36:PHE:CD1	4:B:303[A]:NAD:N7A	2.82	0.47
1:C:204:LYS:CE	1:C:214:GLU:OE1	2.60	0.47
1:B:58:TYR:CE1	1:B:81:LEU:HD23	2.50	0.47
1:D:107:TRP:CD1	1:D:107:TRP:C	2.88	0.47
1:B:187:TRP:CD2	1:B:215:LEU:HD21	2.50	0.47
1:B:191:PRO:HA	1:B:194:GLU:HB2	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:19:ALA:O	1:A:22:THR:HB	2.15	0.47
1:A:219:LYS:O	1:A:221:PRO:HD3	2.14	0.47
1:B:130:GLN:OE1	1:C:100:GLU:OE2	2.33	0.47
1:A:187:TRP:CD1	1:A:216:LEU:HD23	2.50	0.47
1:B:89:ASN:N	1:B:89:ASN:ND2	2.63	0.47
1:B:113:LEU:O	1:B:117:ALA:HB3	2.13	0.47
1:A:99:ILE:O	1:A:100:GLU:C	2.52	0.47
1:D:42:ILE:HG21	1:D:59:TYR:CZ	2.50	0.47
1:B:91:ALA:HB1	5:B:304[B]:NAI:C2A	2.45	0.47
1:B:129:MET:HE1	1:B:136:ARG:O	2.15	0.47
1:D:18:LEU:HD21	1:D:45:GLU:CG	2.45	0.47
1:D:91:ALA:CB	5:D:303[B]:NAI:C2A	2.91	0.46
1:A:193:VAL:O	1:A:197:ILE:HG13	2.15	0.46
1:B:12:SER:OG	1:B:33:ILE:HA	2.15	0.46
1:D:126:LEU:HB2	1:D:127:PRO:HD3	1.96	0.46
1:A:244:ASP:HB2	1:B:230:GLN:NE2	2.31	0.46
1:A:95:HIS:CD2	1:A:106:LYS:HG3	2.50	0.46
1:D:219:LYS:O	1:D:221:PRO:HD3	2.16	0.46
1:D:220:GLN:HG3	1:D:254:ASP:O	2.15	0.46
1:C:136:ARG:NE	1:C:238:LEU:O	2.48	0.46
1:A:183:ILE:O	1:A:185:PRO:HD3	2.16	0.46
4:B:303[A]:NAD:H4N	6:B:305[A]:3HR:H3	1.96	0.46
1:C:9:VAL:HG22	1:C:88:VAL:CB	2.45	0.46
1:B:56:LYS:CD	1:B:56:LYS:N	2.78	0.46
1:C:91:ALA:CB	5:C:302[B]:NAI:C2A	2.94	0.46
1:B:3:LYS:N	1:B:3:LYS:HD3	2.31	0.46
1:A:201:SER:HB2	1:A:211:ALA:HB3	1.96	0.46
1:C:253:LEU:HD22	1:D:246:MET:CG	2.43	0.46
1:A:190:THR:HB	1:A:191:PRO:HD2	1.96	0.46
1:B:84:LEU:HD23	1:B:84:LEU:C	2.36	0.46
1:C:44:ARG:O	1:C:48:THR:HG23	2.15	0.46
1:B:196:GLN:NE2	6:B:305[A]:3HR:O3	2.42	0.46
1:C:20:MET:HE3	1:C:231:LEU:C	2.36	0.45
1:B:6:LYS:HB3	1:B:81:LEU:HD13	1.97	0.45
1:D:187:TRP:CZ3	7:D:305[B]:AAE:H41	2.50	0.45
1:C:91:ALA:CB	5:C:302[B]:NAI:N3A	2.78	0.45
1:D:127:PRO:HA	1:D:130:GLN:HE21	1.81	0.45
1:C:243:ALA:O	1:C:245:GLN:N	2.50	0.45
1:D:1:MET:N	8:D:407:HOH:O	2.49	0.45
5:D:303[B]:NAI:H4N	7:D:305[B]:AAE:C5	2.46	0.45
1:C:207:ASP:O	1:C:210:ALA:HB3	2.16	0.45
1:A:190:THR:O	1:A:194:GLU:HB2	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:74:ILE:HD12	1:C:75:ALA:HA	1.94	0.45
1:A:213:ARG:CZ	1:A:213:ARG:HB2	2.41	0.45
1:C:20:MET:O	1:C:24:LEU:HG	2.16	0.45
1:A:113:LEU:O	1:A:117:ALA:HB3	2.16	0.45
1:D:227:THR:HG1	1:D:230:GLN:HG3	1.78	0.45
1:B:38:GLN:O	1:B:40:GLU:N	2.50	0.45
1:D:91:ALA:CB	4:D:302[A]:NAD:C2A	2.93	0.45
1:B:183:ILE:HG22	1:B:185:PRO:HG3	1.98	0.45
1:B:32:VAL:HG23	1:B:81:LEU:HD21	1.98	0.45
1:D:195:LYS:HA	8:D:405:HOH:O	2.16	0.45
5:D:303[B]:NAI:H4N	7:D:305[B]:AAE:O8	2.17	0.45
1:D:3:LYS:HA	1:D:28:GLY:O	2.17	0.45
1:B:91:ALA:HB1	4:B:303[A]:NAD:C2A	2.46	0.45
1:D:74:ILE:CG1	1:D:124:ALA:HB1	2.42	0.44
1:B:167:LYS:CB	1:C:148:ALA:CB	2.95	0.44
1:A:106:LYS:HA	1:A:106:LYS:HD3	1.78	0.44
1:D:6:LYS:NZ	1:D:30:ASP:OD2	2.48	0.44
1:B:221:PRO:HG3	1:B:260:ARG:CZ	2.47	0.44
1:A:208:ILE:CD1	1:A:208:ILE:C	2.86	0.44
4:C:301[A]:NAD:H4N	6:C:303[A]:3HR:H3	1.95	0.44
1:B:98:PRO:HG3	1:B:151:ASN:OD1	2.18	0.44
1:C:99:ILE:C	1:C:101:GLU:N	2.70	0.44
1:D:257:TRP:CD1	1:D:257:TRP:C	2.91	0.44
1:B:14:SER:HB2	8:B:410:HOH:O	2.17	0.44
1:D:91:ALA:HB1	5:D:303[B]:NAI:N3A	2.32	0.44
1:D:66:ASP:O	1:D:70:THR:HG23	2.18	0.44
1:C:32:VAL:HG23	1:C:81:LEU:CD2	2.47	0.44
1:A:188:VAL:HG12	1:A:190:THR:HG23	1.98	0.44
1:B:13:THR:HG23	1:B:35:GLY:HA3	1.99	0.44
1:C:220:GLN:HA	1:C:221:PRO:HD2	1.81	0.44
1:D:144:HIS:O	1:D:159:LYS:HB2	2.18	0.44
1:D:9:VAL:HG22	1:D:88:VAL:CB	2.43	0.43
1:B:141:ALA:O	1:B:142:SER:HB2	2.17	0.43
1:A:45:GLU:HA	1:A:48:THR:HG21	2.00	0.43
1:D:162:VAL:O	1:D:163:VAL:C	2.54	0.43
1:C:219:LYS:HB3	1:C:257:TRP:CE2	2.53	0.43
1:C:257:TRP:HD1	1:C:257:TRP:O	2.01	0.43
1:A:193:VAL:HG23	4:A:303[A]:NAD:N7N	2.33	0.43
1:A:73:PHE:O	1:A:74:ILE:C	2.56	0.43
1:A:187:TRP:HA	1:A:187:TRP:HE3	1.82	0.43
1:B:234:ALA:HB2	1:B:253:LEU:HD11	2.01	0.43
1:B:36:PHE:CD1	5:B:304[B]:NAI:N7A	2.86	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:243:ALA:O	1:C:244:ASP:C	2.57	0.43
1:D:191:PRO:O	1:D:192:LEU:C	2.57	0.43
1:C:94:GLN:HE22	1:C:152:LYS:HD3	1.83	0.43
1:A:254:ASP:HB2	1:A:257:TRP:HB3	1.99	0.43
1:D:95:HIS:O	1:D:102:PHE:CE1	2.71	0.43
1:D:107:TRP:CD1	1:D:108:ASN:N	2.87	0.43
1:C:91:ALA:CB	4:C:301[A]:NAD:C2A	2.97	0.43
1:C:91:ALA:CB	4:C:301[A]:NAD:N3A	2.80	0.43
1:C:218:GLU:HG2	1:C:219:LYS:HG2	2.00	0.43
1:C:254:ASP:HB2	1:C:257:TRP:HB3	2.01	0.43
1:D:91:ALA:HB1	4:D:302[A]:NAD:N3A	2.33	0.43
1:D:196:GLN:NE2	6:D:304[A]:3HR:O3	2.50	0.43
1:C:97:ALA:N	1:C:151:ASN:HB3	2.34	0.43
1:C:141:ALA:O	1:C:142:SER:HB2	2.18	0.43
1:A:104:VAL:CG1	1:A:105:ASP:N	2.81	0.43
1:C:228:PRO:O	1:C:229:GLU:C	2.56	0.43
1:B:9:VAL:CG1	1:B:12:SER:HB3	2.49	0.43
1:C:94:GLN:OE1	1:C:94:GLN:CA	2.66	0.43
1:D:103:PRO:HB2	1:D:106:LYS:CB	2.49	0.43
1:D:197:ILE:HG21	1:D:208:ILE:HD11	1.99	0.43
1:D:205:GLY:C	1:D:206:ILE:HG23	2.38	0.43
1:C:66:ASP:C	1:C:66:ASP:OD2	2.58	0.43
1:C:76:LYS:HB2	1:C:76:LYS:HE3	1.83	0.43
1:B:102:PHE:CE2	1:B:154:ALA:HB2	2.54	0.43
1:C:245:GLN:HA	1:C:245:GLN:OE1	2.18	0.42
1:A:32:VAL:CG2	1:A:81:LEU:CD1	2.97	0.42
1:A:165:LEU:O	1:A:165:LEU:CD2	2.67	0.42
1:D:197:ILE:HG22	1:D:208:ILE:HD13	1.97	0.42
1:D:13:THR:O	1:D:14:SER:HB3	2.19	0.42
1:D:188:VAL:HB	5:D:303[B]:NAI:C7N	2.49	0.42
1:B:155:TYR:O	1:B:159:LYS:HG2	2.18	0.42
1:D:254:ASP:OD1	1:D:257:TRP:N	2.52	0.42
1:C:222:SER:O	1:C:223:LEU:HB2	2.19	0.42
1:B:188:VAL:O	1:B:193:VAL:CG2	2.55	0.42
1:B:33:ILE:HD11	1:B:46:ARG:HB2	2.00	0.42
1:B:50:GLU:HG2	1:B:55:VAL:O	2.19	0.42
1:B:46:ARG:HH11	1:B:46:ARG:HG2	1.83	0.42
1:D:116:SER:O	1:D:119:PHE:N	2.53	0.42
1:B:63:ASP:C	1:B:65:SER:H	2.23	0.42
1:C:99:ILE:O	1:C:101:GLU:N	2.53	0.42
1:A:85:ASP:HB3	1:A:134:TRP:HZ3	1.84	0.42
1:A:78:ALA:O	1:A:82:GLY:N	2.50	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:193:VAL:HG21	4:A:303[A]:NAD:O7N	2.19	0.42
1:C:36:PHE:N	1:C:36:PHE:CD2	2.88	0.42
1:C:227:THR:OG1	1:C:230:GLN:HG3	2.20	0.42
1:B:219:LYS:HB3	1:B:257:TRP:CD2	2.54	0.42
1:B:216:LEU:C	1:B:218:GLU:H	2.23	0.42
1:A:152:LYS:O	1:A:156:VAL:HG23	2.19	0.42
1:A:187:TRP:CE3	7:A:306[B]:AAE:H93	2.55	0.42
1:A:216:LEU:O	1:A:219:LYS:N	2.45	0.42
1:D:184:CYS:SG	1:D:250:THR:HB	2.59	0.42
1:C:165:LEU:CD2	1:C:165:LEU:C	2.87	0.42
1:A:60:LEU:CD1	1:A:77:ALA:HA	2.50	0.42
1:B:38:GLN:HB2	1:B:41:ASP:OD2	2.19	0.42
1:A:138:ILE:HG22	1:A:138:ILE:O	2.19	0.42
1:A:112:ALA:HA	1:A:116:SER:HB2	2.02	0.42
1:B:193:VAL:CG2	4:B:303[A]:NAD:N7N	2.79	0.41
1:C:38:GLN:HB2	1:C:41:ASP:OD2	2.19	0.41
1:B:153:SER:O	1:B:154:ALA:C	2.58	0.41
1:D:71:ARG:HG3	1:D:120:HIS:HB3	2.02	0.41
1:C:144:HIS:HB3	1:C:156:VAL:HG22	2.02	0.41
1:B:66:ASP:C	1:B:66:ASP:OD2	2.59	0.41
1:C:9:VAL:CG1	1:C:12:SER:HB3	2.48	0.41
1:A:165:LEU:CD2	1:A:165:LEU:C	2.89	0.41
1:D:18:LEU:CD2	1:D:45:GLU:HG2	2.51	0.41
1:C:72:ASP:O	1:C:76:LYS:HB2	2.20	0.41
1:D:25:ALA:HB1	1:D:55:VAL:HG21	2.02	0.41
1:A:70:THR:O	1:A:74:ILE:HD11	2.16	0.41
1:A:227:THR:O	1:A:230:GLN:HB2	2.21	0.41
1:B:9:VAL:HG22	1:B:88:VAL:CB	2.42	0.41
1:C:9:VAL:HG22	1:C:88:VAL:CG2	2.50	0.41
1:D:34:ASN:HB2	1:D:73:PHE:CZ	2.55	0.41
1:A:185:PRO:HB2	5:A:304[B]:NAI:C5N	2.51	0.41
1:B:188:VAL:HG13	1:B:226:VAL:O	2.20	0.41
1:C:20:MET:HE1	1:C:231:LEU:O	2.21	0.41
1:B:187:TRP:HZ3	6:B:305[A]:3HR:H2	1.86	0.41
1:D:14:SER:HA	1:D:18:LEU:HD22	2.03	0.41
1:A:143:ALA:C	1:A:145:GLY:H	2.24	0.41
1:A:197:ILE:HG23	1:A:212:ALA:HB2	2.03	0.41
1:A:197:ILE:O	1:A:197:ILE:HG22	2.21	0.41
1:A:104:VAL:HG13	1:A:105:ASP:N	2.35	0.41
1:D:183:ILE:O	1:D:185:PRO:HD3	2.21	0.41
1:C:88:VAL:HA	1:C:138:ILE:O	2.21	0.41
1:A:32:VAL:CG2	1:A:81:LEU:HD11	2.50	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:93:ILE:HG13	1:C:110:ILE:HG12	2.03	0.41
1:A:6:LYS:N	1:A:6:LYS:HD2	2.36	0.41
1:C:58:TYR:N	1:C:58:TYR:CD1	2.89	0.41
1:A:242:ALA:O	1:B:230:GLN:HB3	2.21	0.41
1:B:160:HIS:CG	1:C:164:GLY:HA3	2.56	0.41
1:D:11:GLY:O	1:D:17:GLY:HA3	2.22	0.40
1:D:16:ILE:HD12	5:D:303[B]:NAI:C2N	2.50	0.40
1:B:50:GLU:HA	1:B:55:VAL:O	2.21	0.40
1:D:170:ALA:HB1	1:D:247:THR:OG1	2.21	0.40
1:B:210:ALA:HA	1:B:213:ARG:NH2	2.36	0.40
1:D:162:VAL:C	1:D:164:GLY:N	2.73	0.40
1:B:76:LYS:HB2	1:B:76:LYS:HE3	1.78	0.40
1:C:252:SER:O	1:C:253:LEU:HD23	2.21	0.40
1:C:38:GLN:O	1:C:40:GLU:N	2.54	0.40
1:A:87:LEU:HD12	1:A:88:VAL:H	1.80	0.40
1:C:192:LEU:HD23	1:C:192:LEU:O	2.21	0.40
1:C:158:ALA:O	1:C:162:VAL:HG23	2.22	0.40
1:C:107:TRP:O	1:C:111:ILE:HG12	2.22	0.40
1:B:66:ASP:HB3	1:B:69:ALA:HB3	2.03	0.40
1:C:106:LYS:HA	1:C:106:LYS:HD3	1.88	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	258/260 (99%)	221 (86%)	24 (9%)	13 (5%)	3 19
1	B	258/260 (99%)	230 (89%)	23 (9%)	5 (2%)	12 51
1	C	258/260 (99%)	225 (87%)	25 (10%)	8 (3%)	7 34
1	D	258/260 (99%)	222 (86%)	32 (12%)	4 (2%)	14 56
All	All	1032/1040 (99%)	898 (87%)	104 (10%)	30 (3%)	7 35

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	GLU
1	A	207	ASP
1	A	217	ALA
1	B	141	ALA
1	C	150	VAL
1	D	99	ILE
1	A	73	PHE
1	A	99	ILE
1	A	142	SER
1	A	255	GLY
1	B	64	LEU
1	B	217	ALA
1	C	97	ALA
1	C	151	ASN
1	C	244	ASP
1	D	141	ALA
1	D	142	SER
1	B	67	ALA
1	B	142	SER
1	C	141	ALA
1	C	62	ALA
1	C	100	GLU
1	A	141	ALA
1	A	213	ARG
1	A	144	HIS
1	D	207	ASP
1	A	74	ILE
1	A	97	ALA
1	C	98	PRO
1	A	11	GLY

### 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	192/192 (100%)	183 (95%)	9 (5%)	36	80
1	B	192/192 (100%)	184 (96%)	8 (4%)	40	83
1	C	192/192 (100%)	183 (95%)	9 (5%)	36	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	192/192 (100%)	180 (94%)	12 (6%)	25	66
All	All	768/768 (100%)	730 (95%)	38 (5%)	35	78

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	61	ASN
1	A	74	ILE
1	A	84	LEU
1	A	165	LEU
1	A	187	TRP
1	A	208	ILE
1	A	220	GLN
1	A	251	LEU
1	B	20	MET
1	B	23	GLU
1	B	34	ASN
1	B	40	GLU
1	B	43	GLU
1	B	70	THR
1	B	220	GLN
1	B	253	LEU
1	C	34	ASN
1	C	38	GLN
1	C	70	THR
1	C	74	ILE
1	C	84	LEU
1	C	94	GLN
1	C	105	ASP
1	C	208	ILE
1	C	213	ARG
1	D	34	ASN
1	D	45	GLU
1	D	58	TYR
1	D	74	ILE
1	D	84	LEU
1	D	94	GLN
1	D	130	GLN
1	D	165	LEU
1	D	203	GLN
1	D	208	ILE

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Mol	Chain	Res	Type
1	D	220	GLN
1	D	252	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	89	ASN
1	A	130	GLN
1	A	132	GLN
1	A	139	ASN
1	A	173	ASN
1	A	202	GLN
1	B	89	ASN
1	B	108	ASN
1	B	130	GLN
1	B	139	ASN
1	B	173	ASN
1	C	89	ASN
1	C	130	GLN
1	C	139	ASN
1	C	173	ASN
1	D	130	GLN
1	D	132	GLN
1	D	139	ASN
1	D	173	ASN
1	D	202	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 5 are monoatomic - leaving 16 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	303[A]	-	48,48,48	1.57	10 (20%)	73,73,73	2.22	19 (26%)
5	NAI	A	304[B]	-	48,48,48	1.58	7 (14%)	73,73,73	2.12	17 (23%)
6	3HR	A	305[A]	-	6,6,6	0.88	0	7,7,7	1.15	0
7	AAE	A	306[B]	-	6,6,6	1.90	2 (33%)	7,7,7	1.07	0
4	NAD	B	303[A]	-	48,48,48	1.60	8 (16%)	73,73,73	2.23	17 (23%)
5	NAI	B	304[B]	-	48,48,48	1.62	7 (14%)	73,73,73	2.15	16 (21%)
6	3HR	B	305[A]	-	6,6,6	0.87	0	7,7,7	1.15	0
7	AAE	B	306[B]	-	6,6,6	1.89	2 (33%)	7,7,7	1.07	0
4	NAD	C	301[A]	-	48,48,48	1.64	10 (20%)	73,73,73	2.24	17 (23%)
5	NAI	C	302[B]	-	48,48,48	1.63	8 (16%)	73,73,73	2.15	17 (23%)
6	3HR	C	303[A]	-	6,6,6	0.88	0	7,7,7	1.15	0
7	AAE	C	304[B]	-	6,6,6	1.92	2 (33%)	7,7,7	1.19	0
4	NAD	D	302[A]	-	48,48,48	1.61	8 (16%)	73,73,73	2.20	18 (24%)
5	NAI	D	303[B]	-	48,48,48	1.63	7 (14%)	73,73,73	2.14	16 (21%)
6	3HR	D	304[A]	-	6,6,6	0.87	0	7,7,7	1.11	0
7	AAE	D	305[B]	-	6,6,6	1.88	2 (33%)	7,7,7	1.11	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAD	A	303[A]	-	-	0/30/62/62	0/3/5/5
5	NAI	A	304[B]	-	-	0/30/72/72	0/3/5/5
6	3HR	A	305[A]	-	-	0/4/4/4	0/0/0/0
7	AAE	A	306[B]	-	-	0/4/4/4	0/0/0/0
4	NAD	B	303[A]	-	-	0/30/62/62	0/3/5/5
5	NAI	B	304[B]	-	-	0/30/72/72	0/3/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	3HR	B	305[A]	-	-	0/4/4/4	0/0/0/0
7	AAE	B	306[B]	-	-	0/4/4/4	0/0/0/0
4	NAD	C	301[A]	-	-	0/30/62/62	0/3/5/5
5	NAI	C	302[B]	-	-	0/30/72/72	0/3/5/5
6	3HR	C	303[A]	-	-	0/4/4/4	0/0/0/0
7	AAE	C	304[B]	-	-	0/4/4/4	0/0/0/0
4	NAD	D	302[A]	-	-	0/30/62/62	0/3/5/5
5	NAI	D	303[B]	-	-	0/30/72/72	0/3/5/5
6	3HR	D	304[A]	-	-	0/4/4/4	0/0/0/0
7	AAE	D	305[B]	-	-	0/4/4/4	0/0/0/0

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	301[A]	NAD	C8A-N9A	4.45	1.43	1.36
5	C	302[B]	NAI	C8A-N9A	4.43	1.43	1.36
4	D	302[A]	NAD	C8A-N9A	4.33	1.43	1.36
5	D	303[B]	NAI	C8A-N9A	4.28	1.43	1.36
5	B	304[B]	NAI	O4B-C1B	4.27	1.47	1.41
4	B	303[A]	NAD	O4B-C1B	4.26	1.47	1.41
4	B	303[A]	NAD	C8A-N9A	4.25	1.42	1.36
4	C	301[A]	NAD	O4B-C1B	4.24	1.47	1.41
5	B	304[B]	NAI	C8A-N9A	4.24	1.42	1.36
5	C	302[B]	NAI	O4B-C1B	4.18	1.47	1.41
5	D	303[B]	NAI	O4B-C1B	4.07	1.47	1.41
4	D	302[A]	NAD	O4B-C1B	4.06	1.47	1.41
5	A	304[B]	NAI	C6N-C5N	4.05	1.41	1.33
5	D	303[B]	NAI	C6N-C5N	3.94	1.41	1.33
5	C	302[B]	NAI	C6N-C5N	3.89	1.41	1.33
5	B	304[B]	NAI	C6N-C5N	3.80	1.41	1.33
5	A	304[B]	NAI	O4B-C1B	3.78	1.47	1.41
4	A	303[A]	NAD	O4B-C1B	3.78	1.47	1.41
4	A	303[A]	NAD	C8A-N9A	3.75	1.42	1.36
5	A	304[B]	NAI	C8A-N9A	3.73	1.42	1.36
7	A	306[B]	AAE	O3-C2	3.71	1.35	1.22
7	B	306[B]	AAE	O3-C2	3.71	1.35	1.22
7	D	305[B]	AAE	O3-C2	3.67	1.35	1.22
5	C	302[B]	NAI	C4N-C3N	-3.62	1.43	1.50
7	C	304[B]	AAE	O3-C2	3.62	1.35	1.22
5	B	304[B]	NAI	C4N-C3N	-3.60	1.43	1.50
5	D	303[B]	NAI	C4N-C3N	-3.59	1.43	1.50
5	A	304[B]	NAI	C4N-C3N	-3.54	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	301[A]	NAD	C2D-C1D	-3.43	1.48	1.53
4	D	302[A]	NAD	C2D-C1D	-3.37	1.48	1.53
4	B	303[A]	NAD	C2D-C1D	-3.17	1.48	1.53
4	D	302[A]	NAD	C2N-N1N	3.17	1.39	1.35
4	B	303[A]	NAD	C2N-N1N	3.09	1.39	1.35
4	A	303[A]	NAD	C2D-C1D	-3.08	1.49	1.53
4	C	301[A]	NAD	C2N-N1N	2.98	1.39	1.35
4	A	303[A]	NAD	C2N-N1N	2.90	1.39	1.35
4	C	301[A]	NAD	C5N-C4N	2.65	1.45	1.39
7	B	306[B]	AAE	O1-C2	-2.61	1.21	1.30
7	C	304[B]	AAE	O1-C2	-2.59	1.21	1.30
4	B	303[A]	NAD	C5N-C4N	2.59	1.45	1.39
4	A	303[A]	NAD	C5N-C4N	2.58	1.45	1.39
7	D	305[B]	AAE	O1-C2	-2.56	1.21	1.30
4	D	302[A]	NAD	C5N-C4N	2.55	1.44	1.39
7	A	306[B]	AAE	O1-C2	-2.55	1.21	1.30
5	B	304[B]	NAI	O4D-C4D	2.43	1.50	1.45
4	A	303[A]	NAD	O4D-C4D	2.40	1.50	1.45
4	C	301[A]	NAD	C3N-C7N	-2.40	1.46	1.50
4	D	302[A]	NAD	C2A-N3A	2.40	1.36	1.32
4	B	303[A]	NAD	O4D-C4D	2.39	1.50	1.45
5	D	303[B]	NAI	C2A-N3A	2.38	1.36	1.32
5	A	304[B]	NAI	O4D-C4D	2.36	1.50	1.45
4	A	303[A]	NAD	C2A-N3A	2.36	1.36	1.32
4	C	301[A]	NAD	O3D-C3D	2.30	1.48	1.43
5	A	304[B]	NAI	C2A-N3A	2.29	1.36	1.32
5	C	302[B]	NAI	O3D-C3D	2.27	1.48	1.43
5	D	303[B]	NAI	O4D-C4D	2.27	1.50	1.45
4	D	302[A]	NAD	O4D-C4D	2.26	1.50	1.45
5	B	304[B]	NAI	C2A-N3A	2.26	1.36	1.32
4	A	303[A]	NAD	C3N-C7N	-2.25	1.46	1.50
5	D	303[B]	NAI	O3D-C3D	2.24	1.48	1.43
4	D	302[A]	NAD	O3D-C3D	2.24	1.48	1.43
4	B	303[A]	NAD	C2A-N3A	2.23	1.36	1.32
4	A	303[A]	NAD	O3D-C3D	2.22	1.48	1.43
4	C	301[A]	NAD	C2A-N3A	2.22	1.36	1.32
5	A	304[B]	NAI	O3D-C3D	2.20	1.48	1.43
5	C	302[B]	NAI	C2A-N3A	2.19	1.36	1.32
4	C	301[A]	NAD	C2B-C1B	-2.13	1.50	1.53
4	B	303[A]	NAD	O3D-C3D	2.10	1.48	1.43
4	C	301[A]	NAD	O4D-C4D	2.10	1.49	1.45
4	A	303[A]	NAD	O7N-C7N	2.09	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	302[B]	NAI	O4D-C4D	2.05	1.49	1.45
5	B	304[B]	NAI	O3D-C3D	2.04	1.47	1.43
5	C	302[B]	NAI	C2B-C1B	-2.00	1.50	1.53

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	301[A]	NAD	O3D-C3D-C4D	7.66	133.66	111.08
5	C	302[B]	NAI	O3D-C3D-C4D	7.65	133.61	111.08
4	D	302[A]	NAD	O3D-C3D-C4D	7.61	133.49	111.08
4	B	303[A]	NAD	O3D-C3D-C4D	7.57	133.37	111.08
4	A	303[A]	NAD	O3D-C3D-C4D	7.56	133.36	111.08
5	D	303[B]	NAI	O3D-C3D-C4D	7.54	133.30	111.08
5	A	304[B]	NAI	O3D-C3D-C4D	7.53	133.28	111.08
5	B	304[B]	NAI	O3D-C3D-C4D	7.53	133.25	111.08
4	A	303[A]	NAD	O2D-C2D-C1D	-7.03	89.95	111.23
4	D	302[A]	NAD	O2D-C2D-C1D	-7.01	90.02	111.23
4	C	301[A]	NAD	O2D-C2D-C1D	-6.98	90.11	111.23
4	B	303[A]	NAD	O2D-C2D-C1D	-6.95	90.20	111.23
5	D	303[B]	NAI	PN-O3-PA	-6.31	113.17	131.68
4	B	303[A]	NAD	C4D-O4D-C1D	-6.10	103.12	109.75
4	C	301[A]	NAD	C4D-O4D-C1D	-6.03	103.20	109.75
4	D	302[A]	NAD	C8A-N9A-C4A	-6.03	102.30	106.90
5	D	303[B]	NAI	C8A-N9A-C4A	-5.98	102.33	106.90
5	A	304[B]	NAI	O2D-C2D-C1D	-5.97	89.72	110.04
4	A	303[A]	NAD	C4D-O4D-C1D	-5.96	103.28	109.75
4	C	301[A]	NAD	C8A-N9A-C4A	-5.95	102.36	106.90
5	D	303[B]	NAI	O2D-C2D-C1D	-5.92	89.89	110.04
5	C	302[B]	NAI	O2D-C2D-C1D	-5.89	89.98	110.04
5	B	304[B]	NAI	O2D-C2D-C1D	-5.88	90.02	110.04
5	C	302[B]	NAI	C8A-N9A-C4A	-5.85	102.44	106.90
5	C	302[B]	NAI	N3A-C2A-N1A	-5.82	123.84	128.71
5	B	304[B]	NAI	N3A-C2A-N1A	-5.81	123.85	128.71
5	B	304[B]	NAI	C8A-N9A-C4A	-5.80	102.47	106.90
4	B	303[A]	NAD	C8A-N9A-C4A	-5.78	102.49	106.90
4	A	303[A]	NAD	N3A-C2A-N1A	-5.78	123.88	128.71
4	C	301[A]	NAD	N3A-C2A-N1A	-5.77	123.88	128.71
4	B	303[A]	NAD	N3A-C2A-N1A	-5.76	123.89	128.71
5	B	304[B]	NAI	PN-O3-PA	-5.72	114.90	131.68
5	A	304[B]	NAI	N3A-C2A-N1A	-5.68	123.96	128.71
4	A	303[A]	NAD	C8A-N9A-C4A	-5.66	102.58	106.90
4	D	302[A]	NAD	C4D-O4D-C1D	-5.64	103.63	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	304[B]	NAI	C8A-N9A-C4A	-5.60	102.62	106.90
5	C	302[B]	NAI	PN-O3-PA	-5.57	115.34	131.68
4	D	302[A]	NAD	N3A-C2A-N1A	-5.57	124.05	128.71
5	D	303[B]	NAI	N3A-C2A-N1A	-5.55	124.06	128.71
5	A	304[B]	NAI	PN-O3-PA	-5.55	115.39	131.68
4	D	302[A]	NAD	PN-O3-PA	-4.68	112.86	132.95
4	C	301[A]	NAD	O4B-C1B-C2B	-4.54	99.82	106.77
5	C	302[B]	NAI	O4B-C1B-C2B	-4.53	99.82	106.77
5	B	304[B]	NAI	O4B-C1B-C2B	-4.32	100.15	106.77
4	B	303[A]	NAD	PN-O3-PA	-4.31	114.45	132.95
5	A	304[B]	NAI	O4B-C1B-C2B	-4.28	100.20	106.77
4	B	303[A]	NAD	O4B-C1B-C2B	-4.27	100.22	106.77
4	A	303[A]	NAD	O4B-C1B-C2B	-4.25	100.26	106.77
4	A	303[A]	NAD	PN-O3-PA	-4.12	115.23	132.95
4	C	301[A]	NAD	PN-O3-PA	-4.13	115.23	132.95
5	D	303[B]	NAI	O4B-C1B-C2B	-4.00	100.64	106.77
4	D	302[A]	NAD	O4B-C1B-C2B	-3.98	100.68	106.77
5	B	304[B]	NAI	C6N-N1N-C2N	3.51	124.03	119.44
5	C	302[B]	NAI	C6N-N1N-C2N	3.41	123.90	119.44
5	B	304[B]	NAI	C4N-C3N-C2N	-3.28	117.68	121.68
5	D	303[B]	NAI	C6N-N1N-C2N	3.28	123.73	119.44
5	A	304[B]	NAI	C6N-N1N-C2N	3.25	123.69	119.44
5	D	303[B]	NAI	C4N-C3N-C2N	-3.21	117.77	121.68
5	A	304[B]	NAI	C4N-C3N-C2N	-3.10	117.90	121.68
5	C	302[B]	NAI	C4N-C3N-C2N	-3.09	117.92	121.68
5	C	302[B]	NAI	C5N-C6N-N1N	-2.96	116.98	123.03
5	A	304[B]	NAI	C5N-C6N-N1N	-2.96	116.99	123.03
5	B	304[B]	NAI	C5N-C6N-N1N	-2.93	117.06	123.03
5	D	303[B]	NAI	C5N-C6N-N1N	-2.90	117.11	123.03
5	B	304[B]	NAI	C4D-O4D-C1D	-2.88	102.95	109.51
5	C	302[B]	NAI	C4D-O4D-C1D	-2.80	103.13	109.51
4	D	302[A]	NAD	PN-O5D-C5D	-2.78	110.64	120.24
5	A	304[B]	NAI	C4D-O4D-C1D	-2.73	103.29	109.51
4	B	303[A]	NAD	PN-O5D-C5D	-2.71	110.87	120.24
4	A	303[A]	NAD	O4D-C1D-N1N	2.67	110.68	107.95
5	B	304[B]	NAI	C5N-C4N-C3N	2.67	119.83	112.60
4	A	303[A]	NAD	PN-O5D-C5D	-2.65	111.07	120.24
5	D	303[B]	NAI	C5N-C4N-C3N	2.63	119.73	112.60
5	D	303[B]	NAI	C4D-O4D-C1D	-2.62	103.53	109.51
4	D	302[A]	NAD	O2N-PN-O1N	-2.62	110.81	118.72
5	C	302[B]	NAI	C2A-N1A-C6A	2.62	123.50	118.77
4	C	301[A]	NAD	O2N-PN-O1N	-2.62	110.83	118.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	302[B]	NAI	C5N-C4N-C3N	2.61	119.66	112.60
4	C	301[A]	NAD	C2A-N1A-C6A	2.60	123.47	118.77
4	B	303[A]	NAD	O4D-C1D-N1N	2.60	110.61	107.95
4	A	303[A]	NAD	O2N-PN-O1N	-2.60	110.88	118.72
4	B	303[A]	NAD	C2A-N1A-C6A	2.58	123.44	118.77
4	B	303[A]	NAD	O2N-PN-O1N	-2.58	110.92	118.72
5	B	304[B]	NAI	C2A-N1A-C6A	2.57	123.41	118.77
4	A	303[A]	NAD	C2A-N1A-C6A	2.56	123.39	118.77
4	C	301[A]	NAD	C2D-C1D-N1N	2.55	118.18	113.86
5	D	303[B]	NAI	C2A-N1A-C6A	2.55	123.37	118.77
4	D	302[A]	NAD	C2A-N1A-C6A	2.54	123.36	118.77
5	A	304[B]	NAI	C5N-C4N-C3N	2.53	119.44	112.60
5	A	304[B]	NAI	C2A-N1A-C6A	2.52	123.32	118.77
4	C	301[A]	NAD	C2N-C3N-C4N	2.51	121.16	118.31
4	D	302[A]	NAD	O5B-C5B-C4B	-2.48	99.83	108.94
4	C	301[A]	NAD	O4D-C1D-C2D	2.47	110.56	106.77
5	B	304[B]	NAI	C1D-N1N-C6N	-2.46	115.35	120.79
4	C	301[A]	NAD	PN-O5D-C5D	-2.45	111.78	120.24
4	A	303[A]	NAD	C2N-C3N-C4N	2.44	121.08	118.31
5	D	303[B]	NAI	O5B-C5B-C4B	-2.44	99.98	108.94
4	A	303[A]	NAD	O5B-C5B-C4B	-2.42	100.05	108.94
5	C	302[B]	NAI	C4N-C5N-C6N	-2.40	118.20	122.61
4	B	303[A]	NAD	O4D-C1D-C2D	2.40	110.45	106.77
5	A	304[B]	NAI	O5B-C5B-C4B	-2.39	100.16	108.94
4	B	303[A]	NAD	O5B-C5B-C4B	-2.37	100.22	108.94
5	B	304[B]	NAI	C4N-C5N-C6N	-2.37	118.25	122.61
5	B	304[B]	NAI	O5B-C5B-C4B	-2.36	100.26	108.94
4	D	302[A]	NAD	C2N-C3N-C4N	2.36	120.99	118.31
4	B	303[A]	NAD	C2N-C3N-C4N	2.35	120.97	118.31
5	C	302[B]	NAI	C1D-N1N-C6N	-2.34	115.61	120.79
5	D	303[B]	NAI	C4N-C5N-C6N	-2.34	118.32	122.61
4	C	301[A]	NAD	C5N-C6N-N1N	-2.33	116.51	120.43
5	A	304[B]	NAI	C4N-C5N-C6N	-2.32	118.34	122.61
4	D	302[A]	NAD	O4D-C1D-C2D	2.30	110.30	106.77
4	D	302[A]	NAD	C2D-C1D-N1N	2.28	117.72	113.86
4	B	303[A]	NAD	C5N-C6N-N1N	-2.28	116.59	120.43
4	A	303[A]	NAD	C5N-C6N-N1N	-2.25	116.65	120.43
4	A	303[A]	NAD	O4D-C1D-C2D	2.24	110.21	106.77
4	D	302[A]	NAD	C5N-C6N-N1N	-2.24	116.66	120.43
5	C	302[B]	NAI	O2D-C2D-C3D	-2.23	104.59	111.83
4	B	303[A]	NAD	C4N-C3N-C7N	-2.20	115.26	121.10
4	C	301[A]	NAD	O2D-C2D-C3D	-2.18	104.75	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	301[A]	NAD	C4N-C3N-C7N	-2.18	115.32	121.10
4	C	301[A]	NAD	O5B-C5B-C4B	-2.17	100.95	108.94
4	D	302[A]	NAD	C4N-C3N-C7N	-2.17	115.32	121.10
4	D	302[A]	NAD	O4D-C1D-N1N	2.17	110.17	107.95
4	A	303[A]	NAD	C2D-C1D-N1N	2.16	117.52	113.86
4	A	303[A]	NAD	O2D-C2D-C3D	-2.16	104.81	111.83
4	D	302[A]	NAD	O2D-C2D-C3D	-2.16	104.81	111.83
5	A	304[B]	NAI	O2D-C2D-C3D	-2.16	104.81	111.83
5	C	302[B]	NAI	O5B-C5B-C4B	-2.16	101.02	108.94
5	B	304[B]	NAI	O2D-C2D-C3D	-2.15	104.83	111.83
5	D	303[B]	NAI	O2D-C2D-C3D	-2.14	104.86	111.83
4	B	303[A]	NAD	O2D-C2D-C3D	-2.13	104.90	111.83
5	A	304[B]	NAI	C1D-N1N-C6N	-2.12	116.10	120.79
5	D	303[B]	NAI	C1D-N1N-C6N	-2.08	116.19	120.79
5	A	304[B]	NAI	C5B-C4B-C3B	-2.08	106.89	115.21
4	A	303[A]	NAD	C5B-C4B-C3B	-2.05	107.02	115.21
4	A	303[A]	NAD	C4N-C3N-C7N	-2.01	115.75	121.10
5	C	302[B]	NAI	C2D-C1D-N1N	2.01	118.34	113.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	260/260 (100%)	-0.42	0 100 100	21, 35, 92, 108	0
1	B	260/260 (100%)	-0.43	0 100 100	20, 38, 63, 80	0
1	C	260/260 (100%)	-0.44	0 100 100	19, 35, 64, 77	0
1	D	260/260 (100%)	-0.33	0 100 100	26, 40, 82, 93	0
All	All	1040/1040 (100%)	-0.41	0 100 100	19, 37, 72, 108	0

There are no RSRZ outliers to report.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates 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. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	CL	A	302	1/1	0.23	3.75	81,81,81,81	0
2	CA	A	301	1/1	0.26	2.84	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	AAE	A	306[B]	7/7	0.28	1.41	69,70,71,72	7
6	3HR	A	305[A]	7/7	0.27	1.33	60,61,64,65	7
7	AAE	B	306[B]	7/7	0.21	1.33	47,48,50,51	7
4	NAD	A	303[A]	44/44	0.20	1.02	46,51,54,55	44
4	NAD	D	302[A]	44/44	0.20	1.00	48,53,57,59	44
5	NAI	A	304[B]	44/44	0.20	0.98	47,51,54,55	44
5	NAI	D	303[B]	44/44	0.20	0.97	48,53,58,59	44
4	NAD	B	303[A]	44/44	0.18	0.83	42,45,51,52	44
5	NAI	B	304[B]	44/44	0.18	0.83	41,45,51,52	44
6	3HR	B	305[A]	7/7	0.21	0.81	44,44,47,47	7
4	NAD	C	301[A]	44/44	0.17	0.62	35,40,52,53	44
5	NAI	C	302[B]	44/44	0.17	0.62	35,40,52,53	44
2	CA	B	301	1/1	0.18	0.50	43,43,43,43	0
3	CL	B	302	1/1	0.17	0.45	69,69,69,69	0
6	3HR	D	304[A]	7/7	0.18	0.44	48,49,51,52	7
7	AAE	D	305[B]	7/7	0.17	0.28	50,51,53,54	7
7	AAE	C	304[B]	7/7	0.15	-0.59	41,42,43,43	7
6	3HR	C	303[A]	7/7	0.14	-0.85	36,37,37,38	7
3	CL	D	301	1/1	0.10	-1.56	54,54,54,54	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.