



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:25 AM UTC

PDB ID : 4CUK / pdb\_00004cuk  
Title : Structure of Salmonella D-Lactate Dehydrogenase in complex with NADH  
Authors : Attarataya, J.; Zaccai, N.R.; Brady, R.L.  
Deposited on : 2014-03-19  
Resolution : 2.18 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

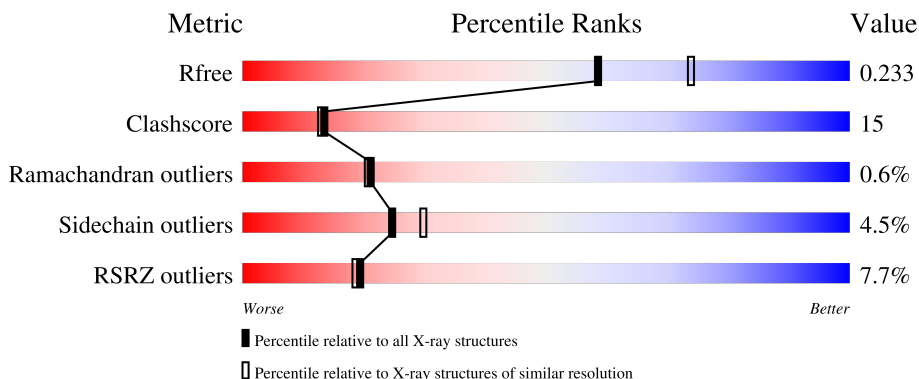
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.18 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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

Mol	Chain	Length	Quality of chain
1	A	338	
1	B	338	
1	C	338	
1	D	338	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10931 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 D-LACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	330	2565	1629	438	483	15	0	0	0
1	B	335	2615	1659	453	488	15	0	0	0
1	C	335	2615	1659	453	488	15	0	0	0
1	D	330	2565	1629	438	483	15	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

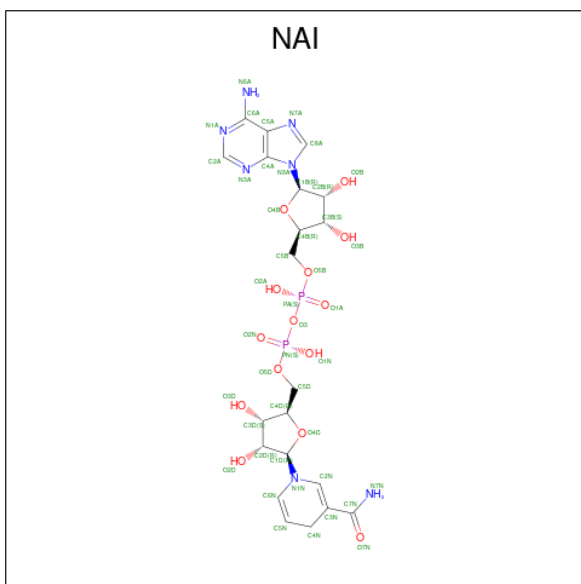
Chain	Residue	Modelled	Actual	Comment	Reference
A	330	LYS	-	expression tag	UNP Q8Z780
A	331	HIS	-	expression tag	UNP Q8Z780
A	332	HIS	-	expression tag	UNP Q8Z780
A	333	HIS	-	expression tag	UNP Q8Z780
A	334	HIS	-	expression tag	UNP Q8Z780
A	335	HIS	-	expression tag	UNP Q8Z780
A	336	HIS	-	expression tag	UNP Q8Z780
A	337	HIS	-	expression tag	UNP Q8Z780
A	338	HIS	-	expression tag	UNP Q8Z780
A	273	VAL	ASN	conflict	UNP Q8Z780
B	330	LYS	-	expression tag	UNP Q8Z780
B	331	HIS	-	expression tag	UNP Q8Z780
B	332	HIS	-	expression tag	UNP Q8Z780
B	333	HIS	-	expression tag	UNP Q8Z780
B	334	HIS	-	expression tag	UNP Q8Z780
B	335	HIS	-	expression tag	UNP Q8Z780
B	336	HIS	-	expression tag	UNP Q8Z780
B	337	HIS	-	expression tag	UNP Q8Z780
B	338	HIS	-	expression tag	UNP Q8Z780
B	273	VAL	ASN	conflict	UNP Q8Z780
C	330	LYS	-	expression tag	UNP Q8Z780

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	331	HIS	-	expression tag	UNP Q8Z780
C	332	HIS	-	expression tag	UNP Q8Z780
C	333	HIS	-	expression tag	UNP Q8Z780
C	334	HIS	-	expression tag	UNP Q8Z780
C	335	HIS	-	expression tag	UNP Q8Z780
C	336	HIS	-	expression tag	UNP Q8Z780
C	337	HIS	-	expression tag	UNP Q8Z780
C	338	HIS	-	expression tag	UNP Q8Z780
C	273	VAL	ASN	conflict	UNP Q8Z780
D	330	LYS	-	expression tag	UNP Q8Z780
D	331	HIS	-	expression tag	UNP Q8Z780
D	332	HIS	-	expression tag	UNP Q8Z780
D	333	HIS	-	expression tag	UNP Q8Z780
D	334	HIS	-	expression tag	UNP Q8Z780
D	335	HIS	-	expression tag	UNP Q8Z780
D	336	HIS	-	expression tag	UNP Q8Z780
D	337	HIS	-	expression tag	UNP Q8Z780
D	338	HIS	-	expression tag	UNP Q8Z780
D	273	VAL	ASN	conflict	UNP Q8Z780

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C<sub>21</sub>H<sub>29</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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

Continued on next page...

*Continued from previous page...*

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

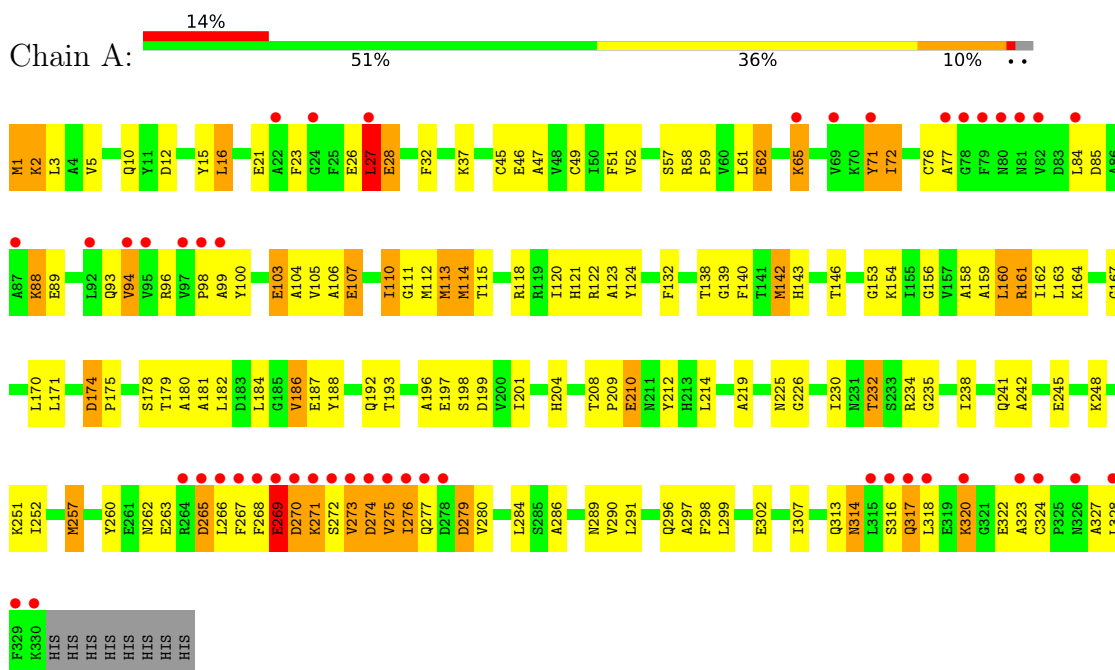
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	104	Total 104	O 104	0	0
3	B	125	Total 125	O 125	0	0
3	C	148	Total 148	O 148	0	0
3	D	106	Total 106	O 106	0	0

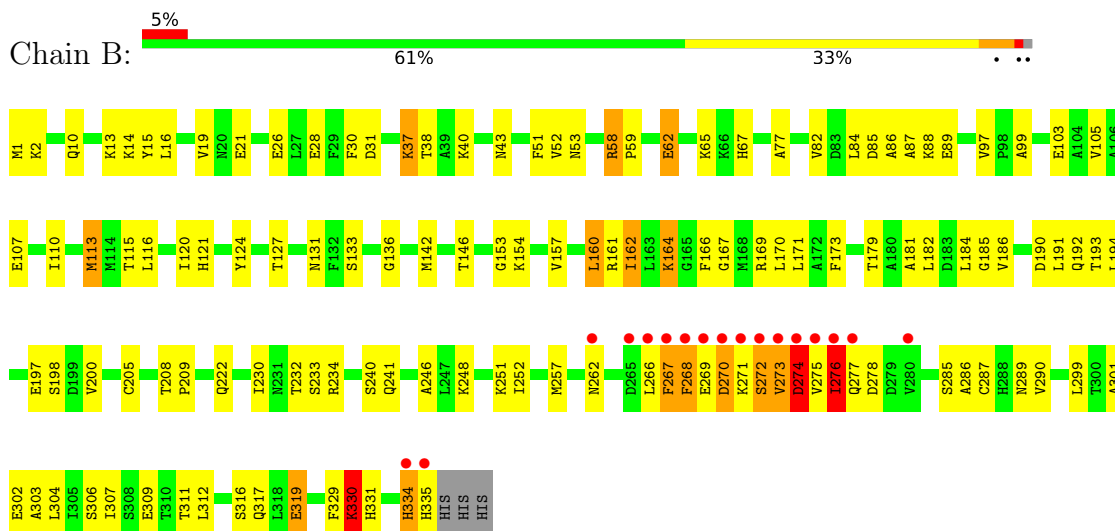
### 3 Residue-property plots i

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

#### • Molecule 1: D-LACTATE DEHYDROGENASE



#### • Molecule 1: D-LACTATE DEHYDROGENASE



#### • Molecule 1: D-LACTATE DEHYDROGENASE



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.35Å 60.70Å 130.39Å 90.00° 106.92° 90.00°	Depositor
Resolution (Å)	105.57 – 2.18 105.57 – 2.18	Depositor EDS
% Data completeness (in resolution range)	95.8 (105.57-2.18) 95.8 (105.57-2.18)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.01 (at 2.18Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.177 , 0.224 0.196 , 0.233	Depositor DCC
$R_{free}$ test set	4173 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtrriage
Anisotropy	0.041	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 39.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10931	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.25% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.90	75/2609 (2.9%)	1.26	22/3520 (0.6%)
1	B	1.98	76/2664 (2.9%)	1.21	12/3595 (0.3%)
1	C	2.02	93/2664 (3.5%)	1.22	17/3595 (0.5%)
1	D	2.04	107/2609 (4.1%)	1.24	17/3520 (0.5%)
All	All	1.99	351/10546 (3.3%)	1.23	68/14230 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	1
1	D	0	1
All	All	1	2

All (351) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	31	ASP	C-O	-8.74	1.13	1.24
1	C	161	ARG	C-O	-8.62	1.14	1.24
1	D	159	ALA	C-O	-8.06	1.14	1.24
1	B	58	ARG	C-O	-8.05	1.17	1.24
1	D	168	MET	C-O	-7.82	1.14	1.23
1	C	160	LEU	C-O	-7.78	1.15	1.24
1	A	115	THR	C-O	-7.77	1.15	1.24
1	D	69	VAL	C-O	-7.75	1.15	1.24
1	D	252	ILE	C-O	-7.68	1.16	1.24
1	D	181	ALA	C-O	-7.64	1.15	1.24
1	C	158	ALA	C-O	-7.62	1.15	1.24
1	D	301	ALA	C-O	-7.43	1.15	1.24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	198	SER	C-O	-7.41	1.15	1.24
1	B	164	LYS	C-O	-7.36	1.15	1.24
1	A	113	MET	C-O	-7.36	1.15	1.24
1	C	164	LYS	C-O	-7.30	1.15	1.24
1	D	194	LEU	C-O	-7.21	1.15	1.24
1	A	153	GLY	C-O	-7.17	1.16	1.23
1	D	196	ALA	C-O	-7.16	1.15	1.24
1	C	107	GLU	C-O	-7.16	1.15	1.24
1	B	302	GLU	C-O	-7.14	1.15	1.24
1	D	153	GLY	C-O	-7.08	1.16	1.23
1	B	51	PHE	C-O	-7.08	1.15	1.24
1	B	317	GLN	C-O	-7.06	1.15	1.24
1	D	302	GLU	C-O	-7.06	1.16	1.24
1	D	158	ALA	C-O	-7.06	1.15	1.24
1	A	196	ALA	C-O	-7.05	1.15	1.24
1	C	181	ALA	C-O	-7.05	1.15	1.24
1	A	143	HIS	C-O	-7.03	1.15	1.23
1	C	292	PHE	C-O	-7.02	1.15	1.24
1	A	182	LEU	C-O	-6.93	1.16	1.24
1	C	139	GLY	C-O	-6.89	1.17	1.24
1	A	104	ALA	C-O	-6.88	1.16	1.24
1	C	77	ALA	C-O	-6.86	1.16	1.24
1	D	205	CYS	C-O	-6.86	1.18	1.24
1	D	143	HIS	C-O	-6.82	1.15	1.23
1	D	14	LYS	C-O	-6.79	1.16	1.24
1	D	160	LEU	C-O	-6.79	1.16	1.24
1	B	205	CYS	C-O	-6.78	1.18	1.24
1	C	143	HIS	C-O	-6.77	1.15	1.23
1	D	124	TYR	C-O	-6.77	1.16	1.24
1	D	113	MET	C-O	-6.76	1.16	1.24
1	C	157	VAL	C-O	-6.74	1.16	1.24
1	A	107	GLU	C-O	-6.74	1.16	1.24
1	D	118	ARG	C-O	-6.73	1.15	1.24
1	D	107	GLU	C-O	-6.72	1.16	1.24
1	C	121	HIS	C-O	-6.72	1.16	1.24
1	A	111	GLY	C-O	-6.66	1.15	1.23
1	D	303	ALA	C-O	-6.63	1.16	1.24
1	D	126	ARG	C-O	-6.59	1.16	1.24
1	A	232	THR	C-O	-6.56	1.15	1.24
1	D	123	ALA	C-O	-6.54	1.16	1.24
1	D	19	VAL	C-O	-6.53	1.16	1.24
1	A	163	LEU	C-O	-6.53	1.16	1.24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159	ALA	C-O	-6.52	1.16	1.24
1	A	162	ILE	C-O	-6.49	1.16	1.24
1	C	120	ILE	C-O	-6.48	1.16	1.24
1	B	289	ASN	C-O	-6.47	1.16	1.23
1	D	110	ILE	C-O	-6.45	1.16	1.24
1	C	127	THR	C-O	-6.45	1.16	1.24
1	D	103	GLU	C-O	-6.44	1.16	1.24
1	D	112	MET	C-O	-6.44	1.16	1.24
1	B	304	LEU	C-O	-6.44	1.16	1.24
1	B	113	MET	C-O	-6.39	1.16	1.24
1	A	103	GLU	C-O	-6.39	1.16	1.24
1	D	52	VAL	C-O	-6.36	1.16	1.24
1	C	67	HIS	C-O	-6.36	1.15	1.24
1	D	175	PRO	C-O	-6.34	1.16	1.24
1	A	241	GLN	C-O	-6.32	1.16	1.24
1	B	161	ARG	C-O	-6.32	1.16	1.24
1	C	37	LYS	C-O	-6.30	1.16	1.24
1	C	180	ALA	C-O	-6.30	1.16	1.24
1	B	124	TYR	C-O	-6.29	1.16	1.24
1	C	138	THR	C-O	-6.28	1.16	1.23
1	A	161	ARG	C-O	-6.28	1.16	1.24
1	B	157	VAL	C-O	-6.23	1.16	1.24
1	D	120	ILE	C-O	-6.23	1.16	1.24
1	A	248	LYS	C-O	-6.22	1.16	1.24
1	C	194	LEU	C-O	-6.22	1.16	1.24
1	A	118	ARG	C-O	-6.21	1.15	1.24
1	A	158	ALA	C-O	-6.19	1.16	1.24
1	C	307	ILE	C-O	-6.17	1.17	1.24
1	A	114	MET	C-O	-6.17	1.16	1.24
1	D	16	LEU	C-O	-6.16	1.17	1.24
1	A	77	ALA	C-O	-6.16	1.16	1.24
1	C	10	GLN	C-O	-6.16	1.17	1.24
1	C	305	ILE	C-O	-6.15	1.17	1.24
1	C	115	THR	C-O	-6.13	1.17	1.24
1	C	243	ALA	C-O	-6.13	1.17	1.24
1	D	115	THR	C-O	-6.13	1.17	1.24
1	C	179	THR	C-O	-6.12	1.17	1.24
1	A	226	GLY	C-O	-6.11	1.16	1.24
1	B	290	VAL	C-O	-6.11	1.17	1.24
1	C	31	ASP	C-O	-6.11	1.16	1.24
1	C	296	GLN	C-O	-6.11	1.15	1.24
1	D	114	MET	C-O	-6.10	1.16	1.24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	38	THR	C-O	-6.10	1.15	1.23
1	C	5	VAL	C-O	-6.07	1.17	1.24
1	A	186	VAL	C-O	-6.07	1.17	1.24
1	A	142	MET	C-O	-6.05	1.17	1.24
1	B	182	LEU	C-O	-6.05	1.17	1.24
1	B	14	LYS	C-O	-6.02	1.17	1.24
1	B	307	ILE	C-O	-6.02	1.17	1.24
1	B	133	SER	C-O	-6.01	1.16	1.23
1	C	13	LYS	C-O	-6.01	1.17	1.24
1	C	36	GLU	C-O	-6.01	1.17	1.24
1	D	192	GLN	C-O	-6.01	1.17	1.24
1	C	163	LEU	C-O	-6.00	1.17	1.24
1	C	200	VAL	C-O	-5.99	1.17	1.24
1	B	252	ILE	C-O	-5.99	1.17	1.24
1	C	136	GLY	C-O	-5.98	1.16	1.24
1	D	127	THR	C-O	-5.98	1.16	1.24
1	C	302	GLU	C-O	-5.98	1.17	1.24
1	B	115	THR	C-O	-5.97	1.17	1.24
1	C	306	SER	C-O	-5.95	1.17	1.24
1	D	53	ASN	C-O	-5.94	1.16	1.24
1	D	195	PHE	C-O	-5.93	1.17	1.24
1	B	65	LYS	C-O	-5.92	1.17	1.24
1	D	34	LEU	C-O	-5.89	1.16	1.24
1	C	53	ASN	C-O	-5.89	1.16	1.24
1	B	62	GLU	C-O	-5.89	1.17	1.24
1	B	16	LEU	C-O	-5.89	1.17	1.24
1	A	179	THR	C-O	-5.87	1.17	1.24
1	C	116	LEU	C-O	-5.87	1.17	1.24
1	A	252	ILE	C-O	-5.86	1.18	1.24
1	D	311	THR	C-O	-5.86	1.17	1.24
1	D	319	GLU	C-O	-5.86	1.17	1.24
1	D	299	LEU	C-O	-5.86	1.17	1.23
1	D	86	ALA	C-O	-5.86	1.17	1.24
1	D	183	ASP	C-O	-5.84	1.16	1.24
1	D	152	THR	C-O	-5.84	1.15	1.23
1	A	198	SER	C-O	-5.83	1.16	1.24
1	D	156	GLY	C-O	-5.82	1.16	1.23
1	A	291	LEU	C-O	-5.82	1.17	1.24
1	B	127	THR	C-O	-5.81	1.16	1.24
1	D	15	TYR	C-O	-5.81	1.17	1.24
1	D	65	LYS	C-O	-5.81	1.17	1.24
1	D	162	ILE	C-O	-5.81	1.17	1.24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	164	LYS	C-O	-5.81	1.17	1.24
1	B	13	LYS	C-O	-5.81	1.17	1.24
1	B	306	SER	C-O	-5.81	1.17	1.24
1	C	294	GLY	C-O	-5.80	1.16	1.23
1	B	153	GLY	C-O	-5.80	1.18	1.23
1	C	303	ALA	C-O	-5.79	1.17	1.24
1	B	82	VAL	C-O	-5.78	1.17	1.24
1	D	242	ALA	C-O	-5.76	1.17	1.24
1	C	309	GLU	C-O	-5.76	1.17	1.24
1	C	16	LEU	C-O	-5.75	1.17	1.24
1	A	121	HIS	C-O	-5.74	1.17	1.24
1	B	146	THR	C-O	-5.72	1.17	1.24
1	D	67	HIS	C-O	-5.72	1.16	1.24
1	C	50	ILE	C-O	-5.71	1.17	1.23
1	C	40	LYS	C-O	-5.71	1.16	1.24
1	C	285	SER	C-O	-5.71	1.17	1.24
1	A	140	PHE	C-O	-5.70	1.17	1.23
1	B	205	CYS	CA-C	-5.70	1.47	1.52
1	C	103	GLU	C-O	-5.69	1.17	1.24
1	B	194	LEU	C-O	-5.68	1.17	1.24
1	D	10	GLN	C-O	-5.67	1.17	1.24
1	B	240	SER	C-O	-5.67	1.17	1.24
1	B	303	ALA	C-O	-5.67	1.17	1.24
1	B	43	ASN	C-O	-5.67	1.17	1.23
1	C	124	TYR	C-O	-5.67	1.17	1.24
1	B	52	VAL	C-O	-5.66	1.17	1.24
1	C	118	ARG	C-O	-5.64	1.16	1.24
1	A	238	ILE	C-O	-5.64	1.17	1.24
1	B	185	GLY	C-O	-5.64	1.16	1.24
1	C	301	ALA	C-O	-5.63	1.17	1.24
1	C	122	ARG	C-O	-5.63	1.17	1.24
1	B	285	SER	C-O	-5.62	1.17	1.24
1	A	289	ASN	C-O	-5.61	1.17	1.23
1	C	232	THR	C-O	-5.61	1.16	1.24
1	B	286	ALA	C-O	-5.60	1.17	1.24
1	A	296	GLN	C-O	-5.60	1.16	1.24
1	D	317	GLN	C-O	-5.59	1.17	1.24
1	A	154	LYS	C-O	-5.59	1.17	1.24
1	B	116	LEU	C-O	-5.59	1.17	1.24
1	C	123	ALA	C-O	-5.59	1.17	1.24
1	D	8	THR	C-O	-5.58	1.17	1.23
1	D	305	ILE	C-O	-5.58	1.17	1.24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	GLY	C-O	-5.57	1.19	1.24
1	A	170	LEU	C-O	-5.57	1.17	1.24
1	A	188	TYR	C-O	-5.57	1.17	1.23
1	D	141	THR	C-O	-5.57	1.17	1.24
1	A	174	ASP	C-O	-5.56	1.17	1.24
1	A	175	PRO	C-O	-5.55	1.16	1.24
1	C	241	GLN	C-O	-5.55	1.17	1.24
1	C	175	PRO	C-O	-5.55	1.17	1.24
1	B	309	GLU	C-O	-5.54	1.17	1.24
1	A	192	GLN	C-O	-5.54	1.17	1.24
1	C	182	LEU	C-O	-5.54	1.17	1.24
1	B	131	ASN	C-O	-5.53	1.17	1.24
1	A	164	LYS	C-O	-5.53	1.17	1.24
1	A	219	ALA	C-O	-5.53	1.17	1.24
1	A	16	LEU	C-O	-5.52	1.17	1.24
1	D	293	THR	C-O	-5.52	1.16	1.23
1	B	121	HIS	C-O	-5.51	1.17	1.24
1	D	165	GLY	C-O	-5.51	1.16	1.23
1	A	204	HIS	C-O	-5.50	1.17	1.23
1	D	228	MET	C-O	-5.50	1.17	1.24
1	C	125	GLN	C-O	-5.50	1.17	1.24
1	C	12	ASP	C-O	-5.49	1.17	1.24
1	D	94	VAL	C-O	-5.49	1.18	1.24
1	B	301	ALA	C-O	-5.49	1.17	1.24
1	A	123	ALA	C-O	-5.48	1.17	1.24
1	A	235	GLY	C-O	-5.47	1.17	1.23
1	D	221	ASP	C-O	-5.47	1.17	1.24
1	C	69	VAL	C-O	-5.46	1.17	1.24
1	C	168	MET	C-O	-5.46	1.17	1.23
1	A	286	ALA	C-O	-5.46	1.17	1.24
1	C	109	ALA	C-O	-5.46	1.17	1.24
1	C	128	ARG	C-O	-5.45	1.17	1.24
1	D	121	HIS	C-O	-5.44	1.17	1.24
1	B	53	ASN	C-O	-5.44	1.16	1.24
1	D	289	ASN	C-O	-5.44	1.17	1.23
1	B	10	GLN	C-O	-5.44	1.17	1.24
1	B	233	SER	C-O	-5.43	1.17	1.23
1	B	160	LEU	C-O	-5.43	1.17	1.24
1	D	39	ALA	C-O	-5.42	1.17	1.24
1	D	258	ASP	C-O	-5.42	1.17	1.24
1	A	193	THR	C-O	-5.42	1.17	1.24
1	A	225	ASN	C-O	-5.42	1.17	1.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	183	ASP	C-O	-5.41	1.17	1.24
1	D	155	ILE	C-O	-5.41	1.18	1.24
1	C	65	LYS	C-O	-5.40	1.17	1.24
1	B	179	THR	C-O	-5.39	1.17	1.24
1	D	77	ALA	C-O	-5.39	1.17	1.24
1	D	51	PHE	C-O	-5.38	1.16	1.23
1	B	173	PHE	C-O	-5.38	1.17	1.24
1	B	232	THR	C-O	-5.38	1.16	1.23
1	C	252	ILE	C-O	-5.38	1.17	1.23
1	B	107	GLU	C-O	-5.37	1.17	1.24
1	A	242	ALA	C-O	-5.37	1.17	1.24
1	C	315	LEU	C-O	-5.37	1.17	1.24
1	D	235	GLY	C-O	-5.37	1.17	1.23
1	D	163	LEU	C-O	-5.35	1.17	1.24
1	A	15	TYR	C-O	-5.35	1.17	1.24
1	D	111	GLY	C-O	-5.35	1.17	1.23
1	C	105	VAL	C-O	-5.34	1.18	1.24
1	B	40	LYS	C-O	-5.33	1.17	1.24
1	D	5	VAL	C-O	-5.33	1.18	1.24
1	C	113	MET	C-O	-5.33	1.18	1.24
1	C	130	ALA	C-O	-5.33	1.16	1.23
1	D	294	GLY	C-O	-5.33	1.16	1.23
1	C	286	ALA	C-O	-5.32	1.17	1.24
1	A	120	ILE	C-O	-5.32	1.18	1.24
1	B	85	ASP	C-O	-5.31	1.18	1.24
1	D	309	GLU	C-O	-5.31	1.18	1.24
1	B	97	VAL	N-CA	-5.30	1.42	1.46
1	B	162	ILE	C-O	-5.30	1.18	1.24
1	A	251	LYS	C-O	-5.30	1.18	1.24
1	A	167	GLY	C-O	-5.29	1.16	1.24
1	C	38	THR	C-O	-5.29	1.17	1.24
1	D	222	GLN	C-O	-5.29	1.17	1.24
1	D	104	ALA	C-O	-5.29	1.18	1.24
1	B	67	HIS	C-O	-5.28	1.17	1.24
1	B	142	MET	C-O	-5.28	1.18	1.24
1	D	281	PHE	C-O	-5.27	1.18	1.24
1	D	236	ALA	C-O	-5.27	1.17	1.24
1	C	63	GLU	C-O	-5.26	1.18	1.24
1	D	135	GLU	C-O	-5.26	1.17	1.23
1	D	167	GLY	C-O	-5.25	1.16	1.24
1	B	167	GLY	C-O	-5.25	1.16	1.24
1	C	196	ALA	C-O	-5.25	1.17	1.24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	97	VAL	N-CA	-5.25	1.42	1.46
1	D	68	GLY	C-O	-5.25	1.17	1.24
1	D	58	ARG	C-O	-5.25	1.19	1.24
1	C	155	ILE	C-O	-5.25	1.18	1.24
1	D	149	VAL	C-O	-5.24	1.18	1.24
1	D	188	TYR	C-O	-5.23	1.17	1.23
1	B	316	SER	C-O	-5.22	1.18	1.24
1	A	49	CYS	C-O	-5.22	1.18	1.24
1	D	248	LYS	C-O	-5.22	1.18	1.24
1	D	180	ALA	C-O	-5.22	1.18	1.24
1	C	192	GLN	C-O	-5.20	1.18	1.24
1	A	180	ALA	C-O	-5.20	1.18	1.24
1	C	19	VAL	C-O	-5.20	1.17	1.24
1	B	181	ALA	C-O	-5.19	1.18	1.24
1	A	212	TYR	C-O	-5.19	1.17	1.23
1	A	160	LEU	C-O	-5.19	1.18	1.24
1	A	290	VAL	C-O	-5.19	1.18	1.24
1	C	316	SER	C-O	-5.19	1.18	1.24
1	D	208	THR	C-O	-5.18	1.19	1.24
1	B	31	ASP	C-O	-5.18	1.17	1.24
1	B	99	ALA	C-O	-5.18	1.17	1.23
1	A	106	ALA	C-O	-5.17	1.18	1.24
1	D	88	LYS	C-O	-5.17	1.18	1.24
1	C	229	ILE	N-CA	-5.17	1.39	1.46
1	B	37	LYS	C-O	-5.17	1.17	1.24
1	B	205	CYS	N-CA	-5.17	1.41	1.45
1	C	17	GLN	C-O	-5.17	1.18	1.24
1	A	124	TYR	C-O	-5.16	1.18	1.24
1	B	103	GLU	C-O	-5.16	1.18	1.24
1	C	76	CYS	C-O	-5.16	1.17	1.23
1	C	81	ASN	C-O	-5.15	1.17	1.24
1	C	74	LEU	C-O	-5.15	1.17	1.24
1	D	140	PHE	C-O	-5.15	1.17	1.23
1	D	61	LEU	C-O	-5.14	1.18	1.24
1	A	5	VAL	C-O	-5.14	1.18	1.24
1	C	178	SER	C-O	-5.14	1.17	1.23
1	C	317	GLN	C-O	-5.14	1.18	1.24
1	C	11	TYR	C-O	-5.13	1.18	1.24
1	A	105	VAL	C-O	-5.13	1.18	1.24
1	B	21	GLU	C-O	-5.12	1.17	1.24
1	D	218	ALA	C-O	-5.12	1.18	1.24
1	A	197	GLU	C-O	-5.12	1.17	1.24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	PHE	C-O	-5.12	1.17	1.24
1	D	306	SER	C-O	-5.12	1.18	1.24
1	A	146	THR	C-O	-5.12	1.17	1.24
1	A	302	GLU	C-O	-5.12	1.18	1.24
1	D	174	ASP	C-O	-5.10	1.18	1.24
1	B	120	ILE	C-O	-5.10	1.18	1.24
1	A	214	LEU	C-O	-5.10	1.18	1.24
1	C	112	MET	C-O	-5.10	1.18	1.24
1	D	217	HIS	C-O	-5.09	1.18	1.24
1	B	319	GLU	C-O	-5.09	1.17	1.24
1	C	6	TYR	C-O	-5.09	1.17	1.23
1	C	324	CYS	C-O	-5.09	1.18	1.24
1	D	186	VAL	C-O	-5.09	1.18	1.24
1	D	288	HIS	C-O	-5.08	1.17	1.23
1	D	3	LEU	C-O	-5.08	1.18	1.24
1	D	62	GLU	C-O	-5.08	1.18	1.24
1	A	181	ALA	C-O	-5.08	1.18	1.24
1	C	106	ALA	C-O	-5.08	1.18	1.24
1	B	154	LYS	C-O	-5.07	1.18	1.24
1	C	159	ALA	C-O	-5.07	1.18	1.24
1	D	81	ASN	C-O	-5.07	1.17	1.24
1	D	136	GLY	C-O	-5.07	1.17	1.24
1	A	199	ASP	C-O	-5.07	1.18	1.24
1	D	125	GLN	C-O	-5.07	1.18	1.24
1	A	156	GLY	C-O	-5.07	1.17	1.23
1	C	144	GLY	C-O	-5.06	1.16	1.24
1	D	134	LEU	C-O	-5.06	1.17	1.24
1	D	307	ILE	C-O	-5.06	1.18	1.24
1	D	36	GLU	C-O	-5.05	1.18	1.24
1	B	166	PHE	C-O	-5.04	1.17	1.24
1	D	312	LEU	C-O	-5.04	1.18	1.24
1	B	86	ALA	C-O	-5.03	1.18	1.24
1	B	169	ARG	C-O	-5.03	1.18	1.23
1	D	232	THR	C-O	-5.03	1.17	1.24
1	C	233	SER	C-O	-5.03	1.18	1.23
1	B	87	ALA	C-O	-5.03	1.18	1.24
1	A	110	ILE	C-O	-5.03	1.18	1.24
1	A	297	ALA	C-O	-5.03	1.17	1.24
1	A	112	MET	C-O	-5.02	1.18	1.24
1	A	201	ILE	C-O	-5.01	1.18	1.24
1	C	33	LEU	C-O	-5.01	1.17	1.23
1	D	144	GLY	C-O	-5.01	1.17	1.24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	30	PHE	C-O	-5.00	1.18	1.24
1	C	319	GLU	C-O	-5.00	1.17	1.24
1	B	311	THR	C-O	-5.00	1.18	1.24

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	LEU	N-CA-C	9.38	121.27	111.14
1	A	27	LEU	CA-C-N	8.92	137.75	121.70
1	A	27	LEU	C-N-CA	8.92	137.75	121.70
1	C	269	GLU	N-CA-C	8.35	120.30	111.03
1	A	286	ALA	N-CA-C	8.32	120.13	111.14
1	B	274	ASP	N-CA-C	8.04	122.67	113.02
1	B	286	ALA	N-CA-C	7.62	119.37	111.14
1	C	37	LYS	N-CA-C	7.54	120.56	111.82
1	A	28	GLU	N-CA-C	7.38	131.68	111.00
1	A	314	ASN	N-CA-C	-7.28	103.35	111.28
1	A	52	VAL	N-CA-C	7.20	120.09	111.09
1	B	77	ALA	N-CA-C	7.17	118.88	111.14
1	A	37	LYS	N-CA-C	7.12	120.08	111.82
1	D	170	LEU	N-CA-C	6.97	119.89	108.52
1	C	286	ALA	N-CA-C	6.88	118.86	111.36
1	A	317	GLN	N-CA-C	-6.74	103.94	111.28
1	A	32	PHE	N-CA-C	6.71	119.18	110.53
1	B	330	LYS	N-CA-C	6.52	119.39	111.82
1	D	286	ALA	N-CA-C	6.49	118.15	111.14
1	D	266	LEU	N-CA-C	-6.47	99.70	108.24
1	A	170	LEU	N-CA-C	6.36	118.78	108.41
1	D	31	ASP	N-CA-C	6.34	118.27	111.36
1	C	126	ARG	N-CA-C	6.31	117.95	111.14
1	D	77	ALA	N-CA-C	6.29	118.22	111.36
1	B	268	PHE	N-CA-C	6.22	119.48	110.28
1	C	52	VAL	N-CA-C	6.19	118.78	111.05
1	C	22	ALA	N-CA-C	6.16	118.96	111.82
1	B	334	HIS	N-CA-C	6.14	120.08	111.30
1	C	46	GLU	N-CA-C	6.10	118.89	111.82
1	B	37	LYS	N-CA-C	6.09	118.89	111.82
1	A	269	GLU	N-CA-C	-6.09	104.56	111.07
1	D	68	GLY	N-CA-C	6.07	123.73	115.30
1	D	15	TYR	N-CA-C	6.04	117.94	111.36
1	B	52	VAL	N-CA-C	6.04	118.59	111.05
1	B	105	VAL	N-CA-C	6.03	116.20	110.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	203	LEU	N-CA-C	5.94	118.40	108.96
1	D	37	LYS	N-CA-C	5.90	117.79	111.36
1	D	24	GLY	N-CA-C	5.75	124.11	113.76
1	D	287	CYS	N-CA-C	5.75	118.49	111.82
1	B	191	LEU	N-CA-C	5.73	117.53	111.28
1	C	15	TYR	N-CA-C	5.72	117.59	111.36
1	B	197	GLU	N-CA-C	5.68	120.22	113.28
1	A	2	LYS	N-CA-C	-5.55	100.14	109.07
1	B	15	TYR	N-CA-C	5.52	117.38	111.36
1	D	276	ILE	N-CA-C	-5.52	100.38	108.11
1	C	196	ALA	N-CA-C	5.49	117.34	111.36
1	A	257	MET	N-CA-C	5.44	117.26	108.34
1	D	126	ARG	N-CA-C	5.43	117.06	111.03
1	C	97	VAL	CA-C-O	5.39	122.33	119.15
1	A	94	VAL	N-CA-C	5.38	115.73	107.77
1	A	77	ALA	N-CA-C	5.36	117.20	111.36
1	D	197	GLU	N-CA-C	5.33	119.94	113.38
1	A	72	ILE	N-CA-C	5.30	115.21	107.37
1	D	277	GLN	N-CA-C	5.27	117.32	108.73
1	C	105	VAL	N-CA-C	5.20	115.41	110.42
1	C	164	LYS	CA-C-N	5.19	126.62	120.14
1	C	164	LYS	C-N-CA	5.19	126.62	120.14
1	C	94	VAL	N-CA-C	5.12	115.28	108.11
1	A	122	ARG	N-CA-C	5.12	116.94	111.36
1	C	255	LEU	N-CA-C	5.07	116.65	108.34
1	C	77	ALA	N-CA-C	5.06	116.88	111.36
1	C	197	GLU	N-CA-C	5.06	119.61	113.38
1	A	279	ASP	N-CA-C	-5.05	105.90	111.71
1	A	71	TYR	N-CA-C	5.03	117.10	108.90
1	A	299	LEU	N-CA-C	5.03	117.26	108.52
1	D	114	MET	N-CA-C	5.02	116.83	111.36
1	D	127	THR	N-CA-C	5.02	117.64	111.82
1	A	27	LEU	O-C-N	-5.01	117.45	123.31

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	28	GLU	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	27	LEU	Peptide
1	D	275	VAL	Peptide

## 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	2565	0	2553	110	0
1	B	2615	0	2592	67	0
1	C	2615	0	2591	63	0
1	D	2565	0	2557	72	3
2	A	44	0	27	3	0
2	D	44	0	27	6	0
3	A	104	0	0	2	0
3	B	125	0	0	1	0
3	C	148	0	0	3	0
3	D	106	0	0	1	0
All	All	10931	0	10347	305	3

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 15.

All (305) 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:A:317:GLN:NE2	1:A:324:CYS:CA	1.68	1.29
1:D:265:ASP:O	1:D:266:LEU:HD12	1.29	1.25
1:D:269:GLU:OE1	1:D:283:ARG:NH2	1.78	1.15
1:B:274:ASP:N	1:B:275:VAL:HA	1.55	1.12
1:A:269:GLU:HG2	1:A:280:VAL:HG21	1.35	1.08
1:A:257:MET:HE1	1:A:267:PHE:HE1	1.14	1.08
1:A:275:VAL:O	1:A:277:GLN:OE1	1.71	1.08
1:A:268:PHE:HB3	1:A:270:ASP:HB3	1.11	1.06
1:A:268:PHE:CB	1:A:270:ASP:HB3	1.84	1.05
1:C:275:VAL:C	1:C:276:ILE:HD12	1.82	1.05
1:C:241:GLN:HG2	1:C:269:GLU:O	1.55	1.04
1:D:270:ASP:OD1	1:D:271:LYS:HD3	1.57	1.03

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:GLN:HB2	1:C:280:VAL:HB	1.36	1.02
1:D:260:TYR:HB2	1:D:263:GLU:HG3	1.38	1.02
1:B:273:VAL:C	1:B:275:VAL:HA	1.85	1.01
1:A:268:PHE:HB3	1:A:270:ASP:CB	1.91	1.00
1:A:324:CYS:HB3	1:A:327:ALA:HB2	1.42	0.99
1:A:269:GLU:OE1	1:A:271:LYS:N	1.96	0.99
1:D:265:ASP:O	1:D:266:LEU:CD1	2.12	0.98
1:A:269:GLU:HG2	1:A:280:VAL:CG2	1.93	0.98
1:C:277:GLN:HG3	1:C:278:ASP:C	1.90	0.97
1:B:273:VAL:HB	1:B:274:ASP:OD1	1.64	0.96
1:B:241:GLN:NE2	1:B:268:PHE:O	1.98	0.96
1:D:53:ASN:HD21	1:D:261:GLU:HB3	1.29	0.95
1:A:257:MET:HE1	1:A:267:PHE:CE1	2.01	0.94
1:C:276:ILE:HG22	1:C:277:GLN:H	1.32	0.92
1:D:277:GLN:HG3	1:D:279:ASP:H	1.30	0.92
1:D:277:GLN:CG	1:D:279:ASP:HB2	1.99	0.92
1:A:2:LYS:HG2	1:A:45:CYS:SG	2.10	0.91
1:A:269:GLU:CG	1:A:280:VAL:HG21	2.00	0.90
1:D:260:TYR:CB	1:D:263:GLU:HG3	2.00	0.90
1:D:53:ASN:HD21	1:D:261:GLU:CB	1.85	0.90
1:B:192:GLN:OE1	1:B:222:GLN:NE2	2.05	0.89
1:A:266:LEU:HD12	1:A:268:PHE:CZ	2.07	0.88
1:C:275:VAL:C	1:C:276:ILE:CD1	2.47	0.87
1:B:269:GLU:HB2	1:B:270:ASP:HA	1.56	0.87
1:C:277:GLN:CB	1:C:280:VAL:HB	2.00	0.86
1:A:85:ASP:O	1:A:88:LYS:HG3	1.74	0.86
1:D:245:GLU:OE2	1:D:248:LYS:NZ	2.09	0.85
1:C:234:ARG:HH12	1:C:262:ASN:HD21	1.23	0.85
1:C:267:PHE:C	1:C:268:PHE:HD1	1.85	0.85
1:D:260:TYR:HB2	1:D:263:GLU:CG	2.06	0.84
1:A:245:GLU:HG2	3:A:2094:HOH:O	1.78	0.84
1:D:272:SER:O	1:D:273:VAL:HB	1.78	0.82
1:A:88:LYS:HE3	1:A:89:GLU:HG2	1.61	0.82
1:C:264:ARG:O	1:C:266:LEU:O	1.97	0.81
1:C:277:GLN:HA	1:C:279:ASP:N	1.96	0.79
1:A:320:LYS:NZ	1:A:320:LYS:HB3	1.96	0.79
1:A:85:ASP:O	1:A:88:LYS:CG	2.30	0.79
1:B:271:LYS:O	1:B:273:VAL:N	2.15	0.79
1:A:85:ASP:O	1:A:89:GLU:HG3	1.84	0.78
1:A:257:MET:HE3	3:A:2091:HOH:O	1.85	0.77
1:A:1:MET:HE2	1:A:71:TYR:CE2	2.21	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:ILE:HG22	1:C:277:GLN:N	1.98	0.75
1:C:113:MET:HG3	1:C:230:ILE:HG13	1.68	0.75
1:D:277:GLN:HG3	1:D:279:ASP:N	2.01	0.75
1:D:277:GLN:HG3	1:D:279:ASP:HB2	1.69	0.75
1:C:277:GLN:HA	1:C:280:VAL:H	1.52	0.74
1:A:268:PHE:CA	1:A:270:ASP:HB3	2.16	0.74
1:A:65:LYS:O	1:A:65:LYS:HD3	1.88	0.74
1:A:58:ARG:O	1:A:62:GLU:HG2	1.88	0.74
1:C:276:ILE:HD12	1:C:276:ILE:N	2.03	0.73
1:A:88:LYS:HE3	1:A:89:GLU:CG	2.18	0.73
1:A:257:MET:CE	1:A:267:PHE:HE1	1.99	0.72
1:A:266:LEU:N	1:A:266:LEU:HD22	2.03	0.72
1:B:274:ASP:N	1:B:275:VAL:CA	2.44	0.72
1:D:275:VAL:HG12	1:D:276:ILE:H	1.54	0.72
1:D:245:GLU:OE2	1:D:248:LYS:CE	2.37	0.72
1:B:190:ASP:OD1	1:B:193:THR:OG1	2.07	0.71
1:C:271:LYS:HG3	3:C:2126:HOH:O	1.89	0.71
1:A:209:PRO:HB2	1:A:210:GLU:OE2	1.90	0.70
1:A:273:VAL:O	1:A:274:ASP:HB2	1.91	0.70
1:D:53:ASN:ND2	1:D:261:GLU:HB3	2.06	0.70
1:A:88:LYS:HG3	1:A:89:GLU:N	2.04	0.70
1:B:271:LYS:HB2	1:B:273:VAL:HG13	1.73	0.69
1:C:276:ILE:CG2	1:C:277:GLN:H	2.06	0.69
1:A:317:GLN:NE2	1:A:324:CYS:HA	1.04	0.69
1:A:88:LYS:CE	1:A:89:GLU:HG2	2.22	0.68
1:D:245:GLU:OE2	1:D:248:LYS:HE2	1.95	0.67
1:D:100:TYR:CD2	2:D:1331:NAI:H42N	2.30	0.67
1:C:276:ILE:O	1:C:279:ASP:HB2	1.95	0.66
1:D:275:VAL:HG12	1:D:276:ILE:N	2.09	0.66
1:D:275:VAL:HG12	1:D:276:ILE:O	1.96	0.66
1:D:100:TYR:HD2	2:D:1331:NAI:H42N	1.61	0.66
1:B:241:GLN:HE21	1:B:268:PHE:C	2.02	0.66
1:A:59:PRO:HA	1:A:62:GLU:HG3	1.78	0.65
1:C:269:GLU:N	1:C:270:ASP:HB3	2.10	0.65
1:B:19:VAL:HG12	1:B:312:LEU:HD12	1.79	0.65
1:C:269:GLU:CB	1:C:270:ASP:HA	2.27	0.64
1:A:320:LYS:NZ	1:A:322:GLU:HB2	2.11	0.64
1:C:241:GLN:CG	1:C:269:GLU:O	2.40	0.64
1:D:277:GLN:CD	1:D:279:ASP:HB2	2.23	0.64
1:A:269:GLU:OE1	1:A:270:ASP:HA	1.98	0.64
1:D:265:ASP:C	1:D:266:LEU:HD12	2.20	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LYS:CE	1:B:330:LYS:HE3	2.28	0.63
1:B:272:SER:O	1:B:276:ILE:HG12	1.99	0.63
1:A:320:LYS:HZ1	1:A:322:GLU:HB2	1.63	0.62
1:B:208:THR:HB	1:B:209:PRO:HD2	1.82	0.62
1:A:88:LYS:HG3	1:A:89:GLU:HG3	1.80	0.62
1:B:241:GLN:HE22	1:B:269:GLU:C	2.07	0.62
1:B:268:PHE:HB3	1:B:270:ASP:OD1	2.00	0.62
1:C:277:GLN:HG3	1:C:278:ASP:O	1.98	0.62
1:D:260:TYR:HB2	1:D:263:GLU:OE2	1.99	0.62
1:A:324:CYS:HB3	1:A:327:ALA:CB	2.25	0.62
1:A:88:LYS:HG3	1:A:89:GLU:H	1.65	0.61
1:B:269:GLU:OE2	1:B:276:ILE:HG23	2.00	0.61
1:D:260:TYR:OH	2:D:1331:NAI:H2N	2.01	0.61
1:D:208:THR:HB	1:D:209:PRO:CD	2.31	0.61
1:B:275:VAL:C	1:B:276:ILE:CG1	2.72	0.61
1:B:164:LYS:HD2	1:B:184:LEU:HD22	1.81	0.61
1:D:260:TYR:CG	1:D:263:GLU:OE2	2.54	0.61
1:B:274:ASP:N	1:B:274:ASP:OD1	2.34	0.60
1:C:267:PHE:C	1:C:268:PHE:CD1	2.75	0.60
1:A:320:LYS:NZ	1:A:322:GLU:CB	2.64	0.60
1:B:88:LYS:HE3	1:B:330:LYS:HE3	1.83	0.60
1:D:266:LEU:O	1:D:267:PHE:HB2	2.01	0.60
1:A:1:MET:HE2	1:A:71:TYR:HE2	1.64	0.60
1:C:277:GLN:HB2	1:C:280:VAL:CB	2.23	0.59
1:D:58:ARG:N	1:D:59:PRO:HD2	2.17	0.59
1:A:266:LEU:HD12	1:A:268:PHE:HZ	1.67	0.59
1:A:269:GLU:CB	1:A:270:ASP:HA	2.32	0.59
1:B:270:ASP:O	1:B:271:LYS:HG3	2.03	0.59
1:C:277:GLN:HG3	1:C:278:ASP:CA	2.32	0.59
1:D:245:GLU:CD	1:D:248:LYS:HE2	2.27	0.59
1:B:270:ASP:O	1:B:271:LYS:CG	2.50	0.59
1:A:208:THR:HB	1:A:209:PRO:CD	2.32	0.59
1:B:192:GLN:OE1	1:B:222:GLN:CD	2.46	0.58
1:D:260:TYR:HB2	1:D:263:GLU:CD	2.29	0.58
1:C:273:VAL:HG12	1:C:274:ASP:N	2.17	0.58
1:A:23:PHE:HZ	1:A:313:GLN:HG2	1.69	0.57
1:A:57:SER:O	1:A:61:LEU:HG	2.03	0.57
1:A:98:PRO:HG2	1:A:99:ALA:H	1.70	0.57
1:D:268:PHE:CE1	1:D:277:GLN:O	2.57	0.57
1:D:205:CYS:C	2:D:1331:NAI:H4D	2.29	0.57
1:B:28:GLU:OE2	1:C:37:LYS:NZ	2.36	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:ARG:O	1:C:268:PHE:CE1	2.58	0.56
1:C:267:PHE:O	1:C:268:PHE:HD1	1.86	0.56
1:D:208:THR:HB	1:D:209:PRO:HD2	1.88	0.56
1:D:277:GLN:OE1	1:D:277:GLN:HA	2.06	0.56
1:A:268:PHE:HB3	1:A:270:ASP:CG	2.31	0.56
1:B:273:VAL:HG23	1:B:276:ILE:H	1.69	0.56
1:A:72:ILE:HB	1:A:94:VAL:HG22	1.88	0.56
1:A:265:ASP:C	1:A:266:LEU:HD22	2.31	0.55
1:A:65:LYS:HD3	1:A:65:LYS:C	2.30	0.55
1:A:322:GLU:CG	1:A:323:ALA:N	2.70	0.55
1:A:58:ARG:N	1:A:59:PRO:CD	2.70	0.55
1:A:232:THR:O	2:A:1331:NAI:H2N	2.06	0.54
1:B:272:SER:C	1:B:273:VAL:HG22	2.32	0.54
1:C:268:PHE:HB3	1:C:270:ASP:HB3	1.89	0.54
1:A:93:GLN:NE2	1:A:318:LEU:HD22	2.22	0.54
1:A:320:LYS:HB3	1:A:320:LYS:HZ2	1.70	0.54
1:D:330:LYS:HE2	1:D:330:LYS:O	2.07	0.54
1:C:268:PHE:HD2	1:C:276:ILE:HG21	1.71	0.54
1:A:85:ASP:HA	1:A:88:LYS:HG2	1.90	0.54
1:D:268:PHE:HB3	1:D:270:ASP:HB2	1.90	0.54
1:B:271:LYS:C	1:B:273:VAL:N	2.65	0.53
1:A:96:ARG:O	1:A:314:ASN:ND2	2.41	0.53
1:C:1:MET:CE	1:C:319:GLU:HB3	2.38	0.53
1:C:268:PHE:CD2	1:C:276:ILE:CG2	2.92	0.53
1:D:260:TYR:OH	2:D:1331:NAI:C2N	2.57	0.53
1:D:270:ASP:OD1	1:D:271:LYS:CD	2.46	0.52
1:A:12:ASP:O	1:A:16:LEU:HB2	2.09	0.52
1:A:85:ASP:O	1:A:88:LYS:HG2	2.09	0.52
1:A:10:GLN:HE22	1:B:136:GLY:H	1.58	0.52
1:B:192:GLN:OE1	1:B:222:GLN:OE1	2.27	0.52
1:C:277:GLN:CA	1:C:280:VAL:H	2.22	0.52
1:B:269:GLU:CB	1:B:270:ASP:HA	2.25	0.51
1:B:272:SER:C	1:B:273:VAL:CG2	2.84	0.51
1:D:53:ASN:HD21	1:D:261:GLU:HB2	1.71	0.51
1:A:161:ARG:HG2	1:A:184:LEU:HD11	1.92	0.51
1:B:275:VAL:C	1:B:276:ILE:HG12	2.35	0.51
1:D:241:GLN:HB3	3:D:2098:HOH:O	2.11	0.51
1:C:277:GLN:HA	1:C:278:ASP:C	2.36	0.51
1:D:268:PHE:CZ	1:D:277:GLN:O	2.64	0.51
1:A:320:LYS:HZ2	1:A:322:GLU:HB3	1.76	0.50
1:A:320:LYS:HB3	1:A:320:LYS:HZ3	1.73	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ILE:HG12	1:B:162:ILE:HG21	1.94	0.50
1:B:208:THR:HB	1:B:209:PRO:CD	2.40	0.50
1:A:58:ARG:NH2	1:A:89:GLU:OE1	2.44	0.50
1:B:267:PHE:HD1	1:B:267:PHE:O	1.95	0.50
1:C:266:LEU:O	1:C:268:PHE:CD1	2.65	0.50
1:B:278:ASP:CA	1:B:278:ASP:CG	2.85	0.49
1:A:269:GLU:HB2	1:A:270:ASP:HA	1.94	0.49
1:A:322:GLU:HG2	1:A:323:ALA:N	2.27	0.49
1:A:266:LEU:N	1:A:266:LEU:CD2	2.73	0.49
1:A:268:PHE:HB3	1:A:270:ASP:OD2	2.12	0.49
1:D:278:ASP:CA	1:D:278:ASP:CG	2.85	0.49
1:A:160:LEU:HD13	1:A:186:VAL:HG21	1.93	0.49
1:B:266:LEU:O	1:B:267:PHE:HB3	2.13	0.48
1:A:314:ASN:O	1:A:317:GLN:HG2	2.13	0.48
1:B:2:LYS:HG3	1:B:26:GLU:HB3	1.95	0.48
1:C:113:MET:SD	1:C:200:VAL:HG11	2.53	0.48
1:B:28:GLU:OE2	1:C:37:LYS:CE	2.61	0.48
1:D:260:TYR:CB	1:D:263:GLU:OE2	2.61	0.48
1:A:328:LEU:HD12	1:A:328:LEU:N	2.28	0.48
1:B:287:CYS:SG	1:D:283:ARG:HB2	2.53	0.48
1:D:265:ASP:C	1:D:266:LEU:CD1	2.85	0.48
1:A:62:GLU:HG2	1:A:62:GLU:H	1.53	0.48
1:B:58:ARG:NH2	1:B:89:GLU:OE1	2.47	0.48
1:C:132:PHE:CE2	1:D:264:ARG:HD2	2.48	0.47
1:C:267:PHE:O	1:C:267:PHE:HD1	1.97	0.47
1:A:234:ARG:HH12	1:A:262:ASN:HD21	1.62	0.47
1:C:192:GLN:HG3	1:C:222:GLN:HE22	1.80	0.47
1:B:1:MET:CE	1:B:319:GLU:HB3	2.45	0.47
1:B:113:MET:SD	1:B:200:VAL:HG11	2.55	0.47
1:A:94:VAL:O	1:A:328:LEU:HD13	2.13	0.47
1:A:268:PHE:C	1:A:270:ASP:HB3	2.39	0.47
1:A:269:GLU:HG3	1:A:280:VAL:HG21	1.91	0.47
1:A:320:LYS:NZ	1:A:320:LYS:CB	2.73	0.46
1:C:288:HIS:HB2	1:C:290:VAL:HG23	1.96	0.46
1:A:268:PHE:CB	1:A:270:ASP:CB	2.69	0.46
1:C:268:PHE:HD2	1:C:276:ILE:CG2	2.28	0.46
1:D:277:GLN:HG3	1:D:279:ASP:CB	2.43	0.46
1:C:160:LEU:HD13	1:C:186:VAL:HG21	1.97	0.46
1:D:174:ASP:OD2	2:D:1331:NAI:H1B	2.16	0.46
1:A:3:LEU:HD12	1:A:47:ALA:C	2.41	0.46
1:A:276:ILE:HG12	1:A:277:GLN:N	2.31	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:TYR:HD1	1:A:307:ILE:HD11	1.81	0.45
1:B:270:ASP:HB3	1:B:271:LYS:H	1.58	0.45
1:C:266:LEU:O	1:C:267:PHE:CB	2.62	0.45
1:D:275:VAL:CG1	1:D:276:ILE:O	2.64	0.45
1:A:320:LYS:NZ	1:A:322:GLU:HB3	2.31	0.45
1:A:114:MET:SD	1:A:142:MET:HE2	2.57	0.45
1:C:276:ILE:CG2	1:C:277:GLN:N	2.68	0.45
1:A:269:GLU:CD	1:A:270:ASP:HA	2.42	0.45
1:B:275:VAL:O	1:B:276:ILE:CB	2.64	0.45
1:C:264:ARG:O	1:C:268:PHE:HE1	1.99	0.45
1:B:267:PHE:O	1:B:267:PHE:CD1	2.70	0.45
1:D:36:GLU:OE2	1:D:37:LYS:HD2	2.17	0.45
1:D:269:GLU:HB3	1:D:270:ASP:HA	1.99	0.45
1:A:271:LYS:HD2	1:A:272:SER:C	2.42	0.45
1:B:241:GLN:NE2	1:B:268:PHE:C	2.68	0.45
1:B:266:LEU:O	1:B:267:PHE:CB	2.64	0.45
1:A:267:PHE:O	1:A:267:PHE:CD2	2.71	0.45
1:B:246:ALA:HB1	1:B:251:LYS:HB3	1.99	0.45
1:B:271:LYS:CB	1:B:273:VAL:HG13	2.45	0.45
1:C:136:GLY:H	1:D:10:GLN:HE22	1.65	0.45
1:D:1:MET:CE	1:D:319:GLU:HB2	2.47	0.44
1:A:174:ASP:OD2	2:A:1331:NAI:H1B	2.18	0.44
1:B:331:HIS:H	1:B:331:HIS:CD2	2.33	0.44
1:C:268:PHE:CD2	1:C:276:ILE:HG22	2.53	0.44
1:D:58:ARG:N	1:D:59:PRO:CD	2.81	0.44
1:A:268:PHE:CD1	1:A:270:ASP:CG	2.96	0.44
1:B:113:MET:HG3	1:B:230:ILE:HG13	1.98	0.44
1:C:267:PHE:O	1:C:267:PHE:CD1	2.70	0.44
1:A:269:GLU:HG2	1:A:280:VAL:HG22	1.93	0.44
1:B:58:ARG:N	1:B:59:PRO:CD	2.81	0.44
1:D:80:ASN:H	1:D:80:ASN:ND2	2.16	0.44
1:A:271:LYS:HZ3	1:A:274:ASP:N	2.16	0.44
1:C:46:GLU:HG3	3:C:2002:HOH:O	2.17	0.44
1:C:276:ILE:CD1	1:C:276:ILE:N	2.73	0.44
1:C:266:LEU:O	1:C:268:PHE:CE1	2.71	0.43
1:D:269:GLU:N	1:D:270:ASP:HB2	2.33	0.43
1:A:208:THR:HB	1:A:209:PRO:HD2	1.99	0.43
1:A:298:PHE:CD1	1:A:298:PHE:C	2.95	0.43
1:C:234:ARG:HH12	1:C:262:ASN:ND2	2.03	0.43
1:A:1:MET:HE2	1:A:71:TYR:CD2	2.52	0.43
1:A:260:TYR:HB2	1:A:263:GLU:HB2	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:LYS:HB2	1:C:170:LEU:HD11	2.00	0.43
1:D:266:LEU:C	1:D:268:PHE:N	2.76	0.43
1:C:266:LEU:O	1:C:267:PHE:HB3	2.19	0.43
1:A:2:LYS:HA	1:A:26:GLU:O	2.18	0.43
1:D:279:ASP:OD1	1:D:282:ARG:NH1	2.51	0.43
1:C:114:MET:SD	1:C:142:MET:HE2	2.59	0.43
1:A:113:MET:HG3	1:A:230:ILE:HG13	2.01	0.43
1:B:329:PHE:CD1	1:B:329:PHE:N	2.87	0.43
1:A:2:LYS:HD2	1:A:26:GLU:CD	2.44	0.42
1:A:51:PHE:CE1	1:A:76:CYS:HB3	2.55	0.42
1:A:93:GLN:NE2	1:A:318:LEU:CD2	2.81	0.42
1:A:100:TYR:CD2	2:A:1331:NAI:H42N	2.54	0.42
1:B:160:LEU:HD13	1:B:186:VAL:HG21	2.00	0.42
1:B:275:VAL:O	1:B:276:ILE:HB	2.19	0.42
1:C:126:ARG:HB3	1:C:131:ASN:O	2.19	0.42
1:D:134:LEU:HA	1:D:137:LEU:HD12	2.01	0.42
1:D:260:TYR:HB3	1:D:263:GLU:HG3	1.90	0.42
1:B:58:ARG:NH1	1:B:62:GLU:OE2	2.52	0.42
1:D:244:ILE:HG12	1:D:284:LEU:HD11	2.02	0.42
1:B:334:HIS:N	1:B:335:HIS:HA	2.35	0.42
1:A:272:SER:HA	1:A:273:VAL:HB	2.03	0.41
1:C:277:GLN:HA	1:C:279:ASP:H	1.79	0.41
1:C:313:GLN:HB2	3:C:2135:HOH:O	2.20	0.41
1:B:257:MET:HE3	3:B:2099:HOH:O	2.20	0.41
1:D:113:MET:HE2	1:D:200:VAL:CG1	2.50	0.41
1:A:23:PHE:CZ	1:A:313:GLN:HG2	2.54	0.41
1:A:103:GLU:O	1:A:107:GLU:HG3	2.20	0.41
1:D:160:LEU:HD13	1:D:186:VAL:HG21	2.02	0.41
1:D:277:GLN:HG2	1:D:279:ASP:HB2	1.97	0.41
1:A:171:LEU:HD23	1:A:187:GLU:HG2	2.03	0.41
1:A:277:GLN:HG3	1:A:279:ASP:HB2	2.03	0.41
1:B:269:GLU:OE2	1:B:276:ILE:CG2	2.68	0.41
1:D:266:LEU:O	1:D:267:PHE:CB	2.65	0.41
1:B:1:MET:HE2	1:B:319:GLU:HB3	2.02	0.41
1:A:318:LEU:HD23	1:A:318:LEU:HA	1.88	0.40
1:B:267:PHE:CD1	1:B:267:PHE:C	2.98	0.40
1:D:270:ASP:CG	1:D:271:LYS:H	2.29	0.40
1:B:241:GLN:NE2	1:B:269:GLU:C	2.76	0.40
1:A:138:THR:HA	1:B:299:LEU:HD23	2.04	0.40
1:B:234:ARG:HH12	1:B:262:ASN:HD21	1.70	0.40
1:C:49:CYS:HA	1:C:73:ALA:O	2.22	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:ILE:HG12	1:D:162:ILE:HG21	2.04	0.40
1:D:263:GLU:O	1:D:266:LEU:HB2	2.20	0.40
1:A:280:VAL:O	1:A:284:LEU:HG	2.21	0.40
1:C:150:ILE:HB	1:C:203:LEU:HD23	2.03	0.40
1:C:275:VAL:CA	1:C:276:ILE:HD12	2.51	0.40
1:D:53:ASN:ND2	1:D:261:GLU:CB	2.67	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MET:N	1:D:58:ARG:NH1[2_858]	0.74	1.46
1:D:1:MET:N	1:D:58:ARG:CZ[2_858]	2.07	0.13
1:D:1:MET:CA	1:D:58:ARG:NH1[2_858]	2.11	0.09

## 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	328/338 (97%)	321 (98%)	6 (2%)	1 (0%)	36	39
1	B	333/338 (98%)	324 (97%)	6 (2%)	3 (1%)	14	12
1	C	333/338 (98%)	328 (98%)	3 (1%)	2 (1%)	21	20
1	D	328/338 (97%)	322 (98%)	4 (1%)	2 (1%)	21	20
All	All	1322/1352 (98%)	1295 (98%)	19 (1%)	8 (1%)	21	20

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	ASP
1	C	276	ILE

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	275	VAL
1	B	267	PHE
1	B	276	ILE
1	D	273	VAL
1	B	273	VAL
1	C	273	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/281 (96%)	251 (93%)	20 (7%)	13	13
1	B	276/281 (98%)	265 (96%)	11 (4%)	28	35
1	C	276/281 (98%)	268 (97%)	8 (3%)	37	47
1	D	271/281 (96%)	261 (96%)	10 (4%)	30	38
All	All	1094/1124 (97%)	1045 (96%)	49 (4%)	24	30

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

Mol	Chain	Res	Type
1	A	1	MET
1	A	21	GLU
1	A	27	LEU
1	A	28	GLU
1	A	46	GLU
1	A	62	GLU
1	A	65	LYS
1	A	88	LYS
1	A	110	ILE
1	A	178	SER
1	A	210	GLU
1	A	265	ASP
1	A	269	GLU
1	A	270	ASP
1	A	271	LYS

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	273	VAL
1	A	275	VAL
1	A	276	ILE
1	A	316	SER
1	A	320	LYS
1	B	37	LYS
1	B	84	LEU
1	B	170	LEU
1	B	171	LEU
1	B	248	LYS
1	B	270	ASP
1	B	272	SER
1	B	274	ASP
1	B	276	ILE
1	B	277	GLN
1	B	330	LYS
1	C	28	GLU
1	C	110	ILE
1	C	179	THR
1	C	248	LYS
1	C	269	GLU
1	C	271	LYS
1	C	276	ILE
1	C	277	GLN
1	D	28	GLU
1	D	36	GLU
1	D	84	LEU
1	D	128	ARG
1	D	264	ARG
1	D	271	LYS
1	D	272	SER
1	D	274	ASP
1	D	276	ILE
1	D	330	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	93	GLN
1	A	277	GLN
1	A	296	GLN
1	B	43	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	67	HIS
1	B	217	HIS
1	B	241	GLN
1	B	249	ASN
1	B	277	GLN
1	B	296	GLN
1	B	331	HIS
1	B	334	HIS
1	C	143	HIS
1	C	213	HIS
1	C	262	ASN
1	C	296	GLN
1	D	18	GLN
1	D	53	ASN
1	D	108	HIS
1	D	296	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAI	A	1331	-	47,48,48	1.63	8 (17%)	64,73,73	2.16	24 (37%)
2	NAI	D	1331	-	47,48,48	1.86	8 (17%)	64,73,73	2.16	19 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAI	A	1331	-	-	7/29/72/72	0/5/5/5
2	NAI	D	1331	-	-	5/29/72/72	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1331	NAI	C5A-C4A	6.56	1.50	1.39
2	A	1331	NAI	C5A-C4A	5.53	1.48	1.39
2	D	1331	NAI	PN-O3	4.67	1.64	1.59
2	A	1331	NAI	PN-O3	4.54	1.64	1.59
2	D	1331	NAI	PA-O3	4.54	1.64	1.59
2	D	1331	NAI	C5A-C6A	3.64	1.51	1.41
2	A	1331	NAI	PA-O3	3.39	1.63	1.59
2	A	1331	NAI	C8A-N7A	3.23	1.37	1.31
2	A	1331	NAI	C5A-C6A	3.04	1.49	1.41
2	D	1331	NAI	C8A-N7A	2.89	1.37	1.31
2	A	1331	NAI	C2N-C3N	2.48	1.42	1.35
2	D	1331	NAI	C2N-C3N	2.39	1.41	1.35
2	D	1331	NAI	C7N-C3N	2.33	1.53	1.48
2	A	1331	NAI	C4A-N9A	-2.29	1.32	1.37
2	A	1331	NAI	C7N-C3N	2.24	1.53	1.48
2	D	1331	NAI	C4A-N9A	-2.02	1.33	1.37

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1331	NAI	O7N-C7N-C3N	-6.92	107.87	120.90
2	D	1331	NAI	C3N-C7N-N7N	6.03	128.38	117.67
2	A	1331	NAI	C3N-C7N-N7N	5.45	127.35	117.67
2	A	1331	NAI	O7N-C7N-C3N	-5.09	111.31	120.90
2	D	1331	NAI	C5A-C4A-N3A	-4.46	120.58	126.72
2	A	1331	NAI	C5A-C4A-N3A	-4.17	120.97	126.72

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1331	NAI	O4D-C1D-N1N	4.09	115.88	108.08
2	A	1331	NAI	N3A-C2A-N1A	-3.88	122.72	128.58
2	A	1331	NAI	O4B-C1B-N9A	3.79	115.37	108.09
2	D	1331	NAI	N3A-C2A-N1A	-3.74	122.91	128.58
2	D	1331	NAI	O4B-C1B-N9A	3.59	114.98	108.09
2	D	1331	NAI	C2A-N3A-C4A	3.58	120.57	111.83
2	A	1331	NAI	C2A-N3A-C4A	3.54	120.47	111.83
2	A	1331	NAI	C6A-C5A-N7A	3.52	138.88	132.09
2	A	1331	NAI	C4A-N9A-C1B	-3.52	118.40	126.63
2	D	1331	NAI	C4A-C5A-N7A	-3.50	106.58	110.58
2	A	1331	NAI	C4A-C5A-N7A	-3.49	106.59	110.58
2	D	1331	NAI	C2A-N1A-C6A	3.43	124.36	118.73
2	A	1331	NAI	O2A-PA-O1A	3.39	128.21	112.44
2	D	1331	NAI	O2A-PA-O1A	3.35	128.04	112.44
2	D	1331	NAI	N3A-C4A-N9A	3.33	132.82	127.17
2	D	1331	NAI	O4B-C4B-C3B	3.27	111.64	105.15
2	A	1331	NAI	O4B-C4B-C3B	3.11	111.32	105.15
2	D	1331	NAI	C6A-C5A-N7A	3.04	137.94	132.09
2	A	1331	NAI	N3A-C4A-N9A	2.96	132.21	127.17
2	A	1331	NAI	C2D-C1D-N1N	-2.91	106.16	113.31
2	A	1331	NAI	C4A-N9A-C8A	2.86	108.74	105.74
2	A	1331	NAI	C2A-N1A-C6A	2.77	123.28	118.73
2	A	1331	NAI	O5B-PA-O1A	-2.66	98.41	108.94
2	D	1331	NAI	O1N-PN-O2N	2.65	124.76	112.44
2	D	1331	NAI	C4A-N9A-C1B	-2.57	120.62	126.63
2	A	1331	NAI	C1B-N9A-C8A	2.53	132.70	127.09
2	A	1331	NAI	C5A-N7A-C8A	2.52	107.41	103.45
2	A	1331	NAI	N9A-C8A-N7A	-2.48	110.42	113.94
2	D	1331	NAI	C5B-C4B-C3B	-2.36	106.70	115.21
2	D	1331	NAI	C2D-C1D-N1N	-2.33	107.57	113.31
2	D	1331	NAI	C5A-N7A-C8A	2.28	107.04	103.45
2	A	1331	NAI	C5B-C4B-C3B	-2.25	107.11	115.21
2	D	1331	NAI	C4A-N9A-C8A	2.09	107.93	105.74
2	A	1331	NAI	C4B-O4B-C1B	-2.07	104.89	109.47
2	D	1331	NAI	O5B-C5B-C4B	-2.05	102.00	108.99
2	A	1331	NAI	O1N-PN-O2N	2.05	121.99	112.44
2	A	1331	NAI	C6A-C5A-C4A	-2.00	114.45	117.18

There are no chirality outliers.

All (12) torsion outliers are listed below:

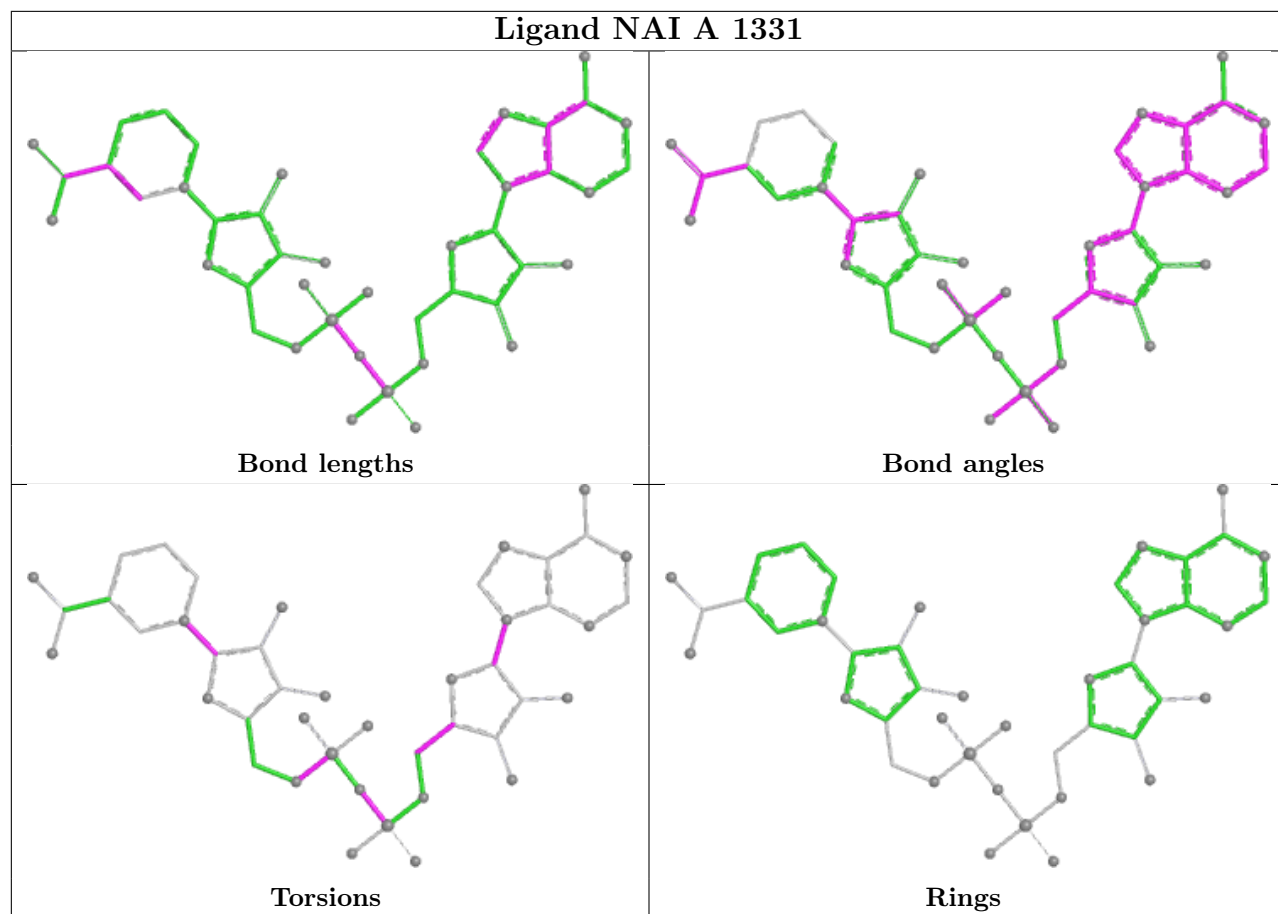
Mol	Chain	Res	Type	Atoms
2	D	1331	NAI	C2N-C3N-C7N-N7N
2	A	1331	NAI	O4B-C4B-C5B-O5B
2	D	1331	NAI	O4D-C4D-C5D-O5D
2	D	1331	NAI	O4D-C1D-N1N-C2N
2	A	1331	NAI	C5D-O5D-PN-O2N
2	A	1331	NAI	O4D-C1D-N1N-C2N
2	A	1331	NAI	C2B-C1B-N9A-C8A
2	A	1331	NAI	O4B-C1B-N9A-C8A
2	D	1331	NAI	O4B-C1B-N9A-C8A
2	D	1331	NAI	C2B-C1B-N9A-C8A
2	A	1331	NAI	C3B-C4B-C5B-O5B
2	A	1331	NAI	PN-O3-PA-O2A

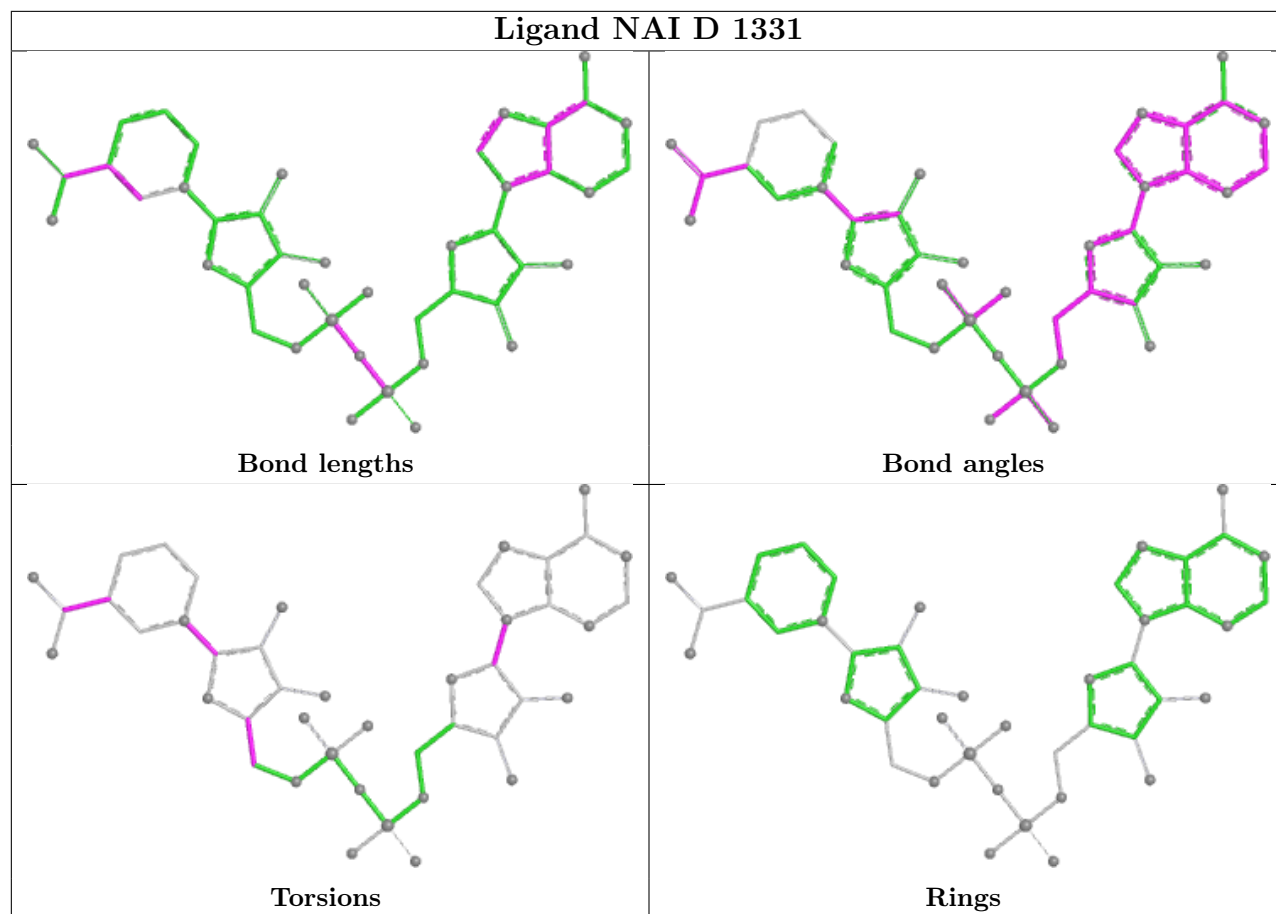
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1331	NAI	3	0
2	D	1331	NAI	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	330/338 (97%)	0.78	46 (13%) <b>6</b> <b>5</b>	14, 29, 75, 137	1 (0%)
1	B	335/338 (99%)	0.31	17 (5%) <b>33</b> <b>33</b>	13, 24, 56, 142	1 (0%)
1	C	335/338 (99%)	0.19	19 (5%) <b>29</b> <b>28</b>	9, 21, 50, 151	1 (0%)
1	D	330/338 (97%)	0.22	20 (6%) <b>27</b> <b>26</b>	11, 21, 54, 134	1 (0%)
All	All	1330/1352 (98%)	0.38	102 (7%) <b>19</b> <b>18</b>	9, 23, 65, 151	4 (0%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	276	ILE	10.2
1	A	276	ILE	9.6
1	C	275	VAL	8.3
1	A	268	PHE	8.3
1	B	276	ILE	8.3
1	B	268	PHE	8.1
1	B	275	VAL	8.0
1	B	273	VAL	7.8
1	A	273	VAL	7.8
1	A	275	VAL	7.8
1	D	275	VAL	7.6
1	B	267	PHE	7.5
1	C	267	PHE	7.3
1	C	273	VAL	7.3
1	A	267	PHE	7.0
1	D	273	VAL	6.8
1	C	276	ILE	6.6
1	D	267	PHE	6.4
1	B	274	ASP	6.4
1	C	269	GLU	6.4
1	B	266	LEU	6.2

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	266	LEU	6.2
1	D	268	PHE	6.2
1	B	271	LYS	5.9
1	C	274	ASP	5.4
1	A	266	LEU	5.4
1	C	268	PHE	5.4
1	A	329	PHE	5.0
1	B	272	SER	4.8
1	C	272	SER	4.8
1	B	270	ASP	4.7
1	B	269	GLU	4.7
1	A	269	GLU	4.7
1	D	272	SER	4.5
1	A	265	ASP	4.4
1	C	270	ASP	4.4
1	A	330	LYS	4.4
1	D	271	LYS	4.3
1	D	265	ASP	4.3
1	B	335	HIS	4.3
1	D	266	LEU	4.3
1	A	271	LYS	4.2
1	C	271	LYS	4.1
1	D	277	GLN	3.9
1	D	269	GLU	3.9
1	A	270	ASP	3.9
1	A	277	GLN	3.8
1	A	320	LYS	3.8
1	A	272	SER	3.6
1	A	78	GLY	3.5
1	A	274	ASP	3.5
1	B	277	GLN	3.4
1	A	318	LEU	3.4
1	A	97	VAL	3.4
1	C	277	GLN	3.3
1	D	270	ASP	3.2
1	A	77	ALA	3.1
1	A	84	LEU	3.1
1	A	317	GLN	3.1
1	A	264	ARG	3.1
1	A	323	ALA	3.1
1	D	330	LYS	3.1
1	A	82	VAL	3.0

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	334	HIS	3.0
1	C	262	ASN	2.9
1	D	274	ASP	2.8
1	A	79	PHE	2.8
1	C	334	HIS	2.8
1	D	58	ARG	2.8
1	C	280	VAL	2.8
1	A	324	CYS	2.8
1	C	335	HIS	2.8
1	A	328	LEU	2.8
1	D	249	ASN	2.7
1	A	315	LEU	2.7
1	A	98	PRO	2.7
1	A	87	ALA	2.6
1	B	265	ASP	2.6
1	A	27	LEU	2.6
1	B	262	ASN	2.5
1	A	69	VAL	2.5
1	C	209	PRO	2.5
1	D	261	GLU	2.5
1	B	280	VAL	2.5
1	A	24	GLY	2.5
1	C	264	ARG	2.4
1	A	94	VAL	2.4
1	A	80	ASN	2.4
1	A	326	ASN	2.4
1	C	278	ASP	2.4
1	A	316	SER	2.4
1	D	279	ASP	2.3
1	D	264	ARG	2.3
1	A	71	TYR	2.3
1	A	92	LEU	2.3
1	A	278	ASP	2.2
1	A	22	ALA	2.2
1	A	95	VAL	2.1
1	D	10	GLN	2.1
1	A	65	LYS	2.1
1	A	81	ASN	2.1
1	A	99	ALA	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

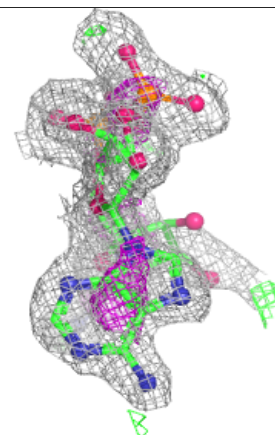
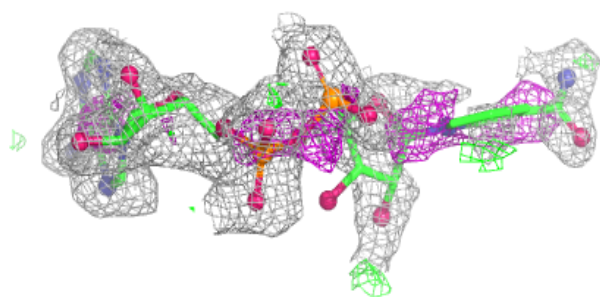
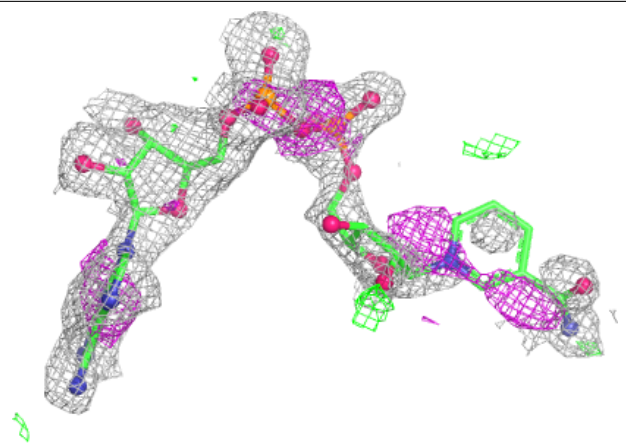
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

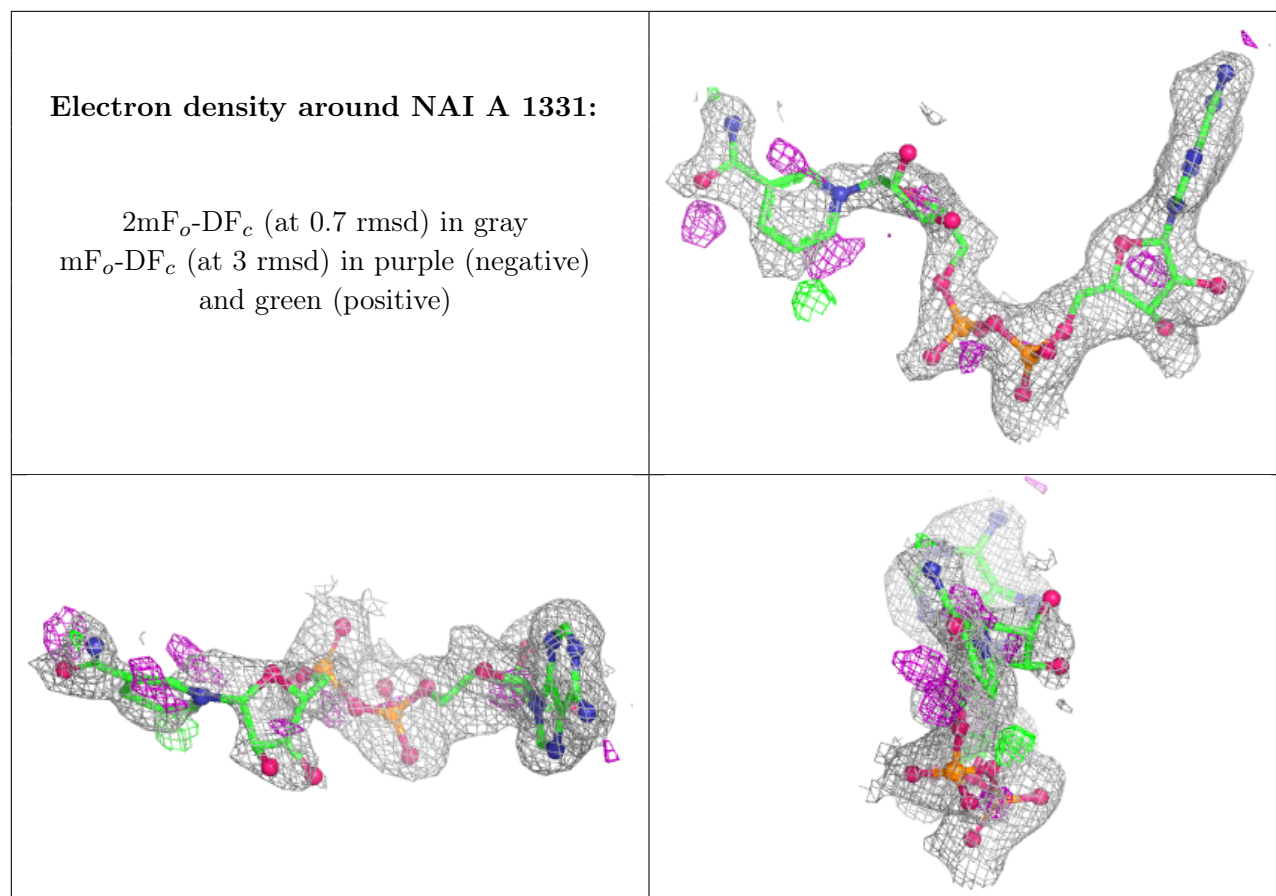
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAI	D	1331	44/44	0.81	0.19	34,49,85,89	0
2	NAI	A	1331	44/44	0.87	0.14	30,40,63,64	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around NAI D 1331:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.