



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:09 AM UTC

PDB ID : 1ARZ / pdb_00001arz
Title : ESCHERICHIA COLI DIHYDRODIPICOLINATE REDUCTASE IN COM-
PLEX WITH NADH AND 2,6 PYRIDINE DICARBOXYLATE
Authors : Scapin, G.; Reddy, S.G.; Zheng, R.; Blanchard, J.S.
Deposited on : 1997-08-08
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

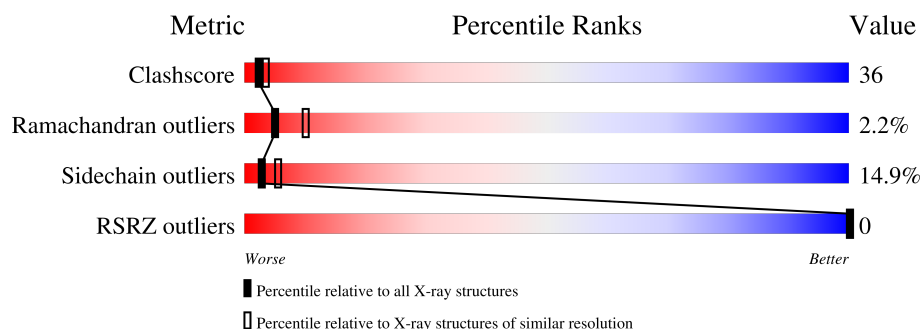
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	273	
1	B	273	
1	C	273	
1	D	273	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PDC	D	303	-	-	X	-

2 Entry composition [i](#)

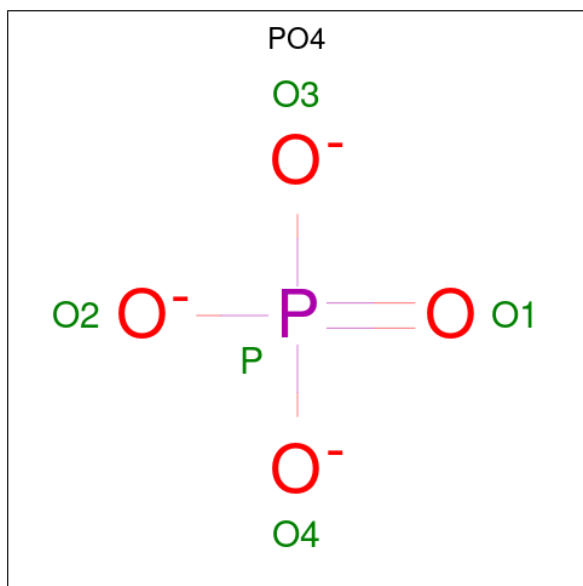
There are 6 unique types of molecules in this entry. The entry contains 8232 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DIHYDRODIPICOLINATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			1939	1207	344	378	10			
1	B	269	Total	C	N	O	S	0	0	0
			1975	1225	356	384	10			
1	C	271	Total	C	N	O	S	0	0	0
			1980	1229	357	384	10			
1	D	271	Total	C	N	O	S	0	0	0
			1984	1232	357	385	10			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

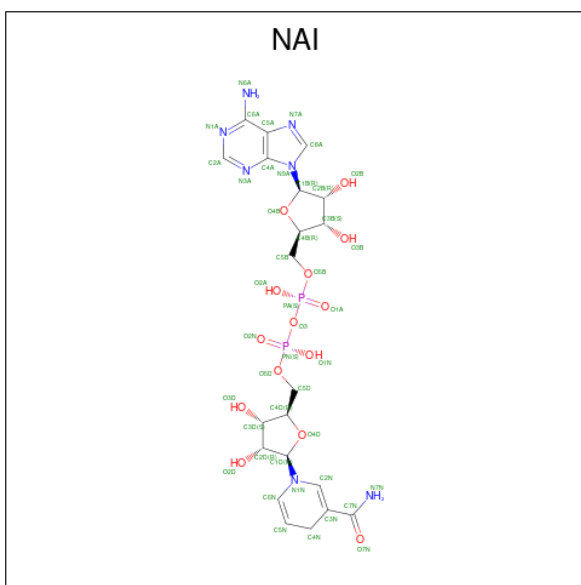


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O P	0	0
			5	4 1		

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

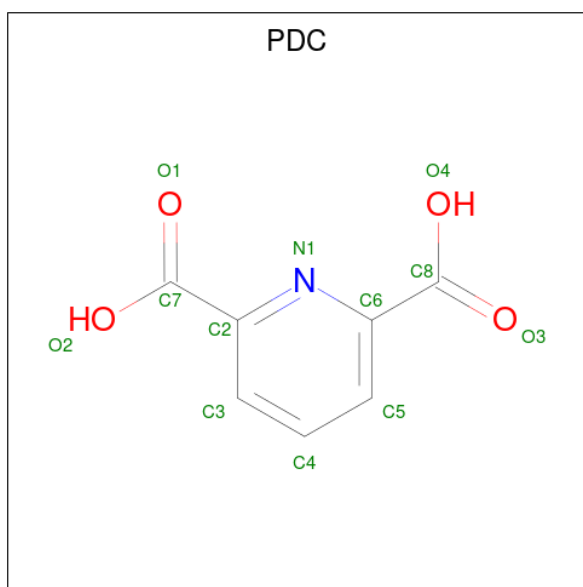
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total K 1 1	0	0
3	D	1	Total K 1 1	0	0

- Molecule 4 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $\text{C}_{21}\text{H}_{29}\text{N}_7\text{O}_{14}\text{P}_2$).



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

- Molecule 5 is PYRIDINE-2,6-DICARBOXYLIC ACID (CCD ID: PDC) (formula: $C_7H_5NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			12	7	1	4		
5	C	1	Total	C	N	O	0	0
			12	7	1	4		
5	D	1	Total	C	N	O	0	0
			12	7	1	4		

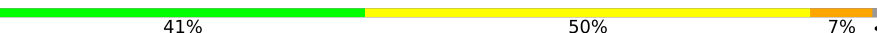
- Molecule 6 is water.

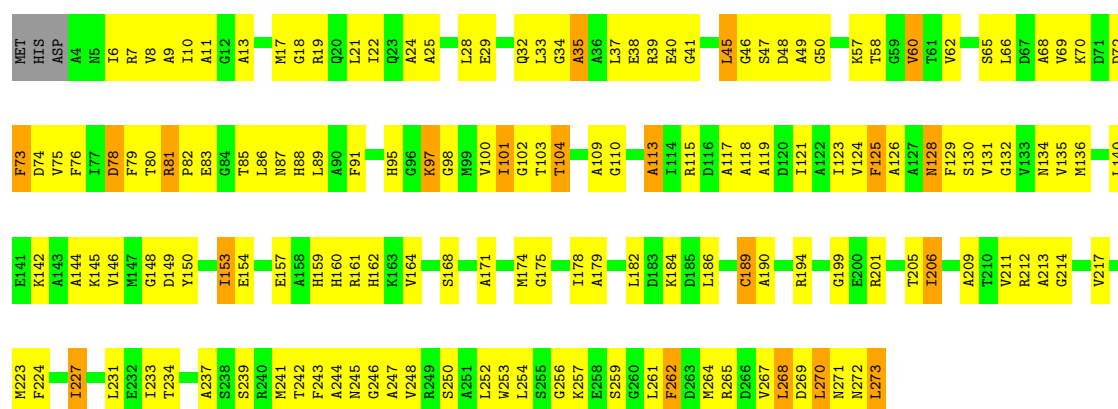
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	41	Total	O	0	0
			41	41		
6	B	47	Total	O	0	0
			47	47		
6	C	45	Total	O	0	0
			45	45		
6	D	46	Total	O	0	0
			46	46		

3 Residue-property plots

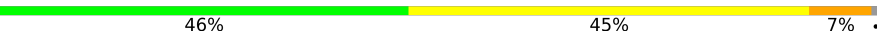
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

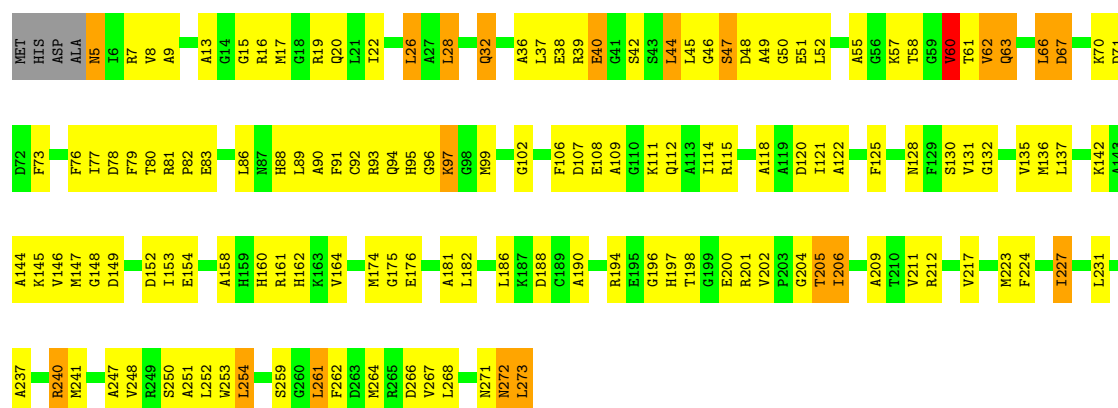
• Molecule 1: DIHYDRODIPICOLINATE REDUCTASE

Chain A: 

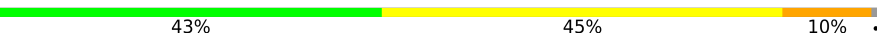


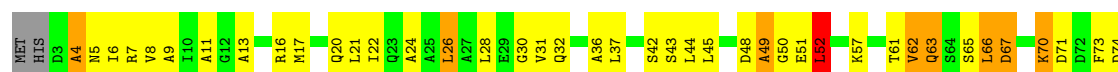
• Molecule 1: DIHYDRODIPICOLINATE REDUCTASE

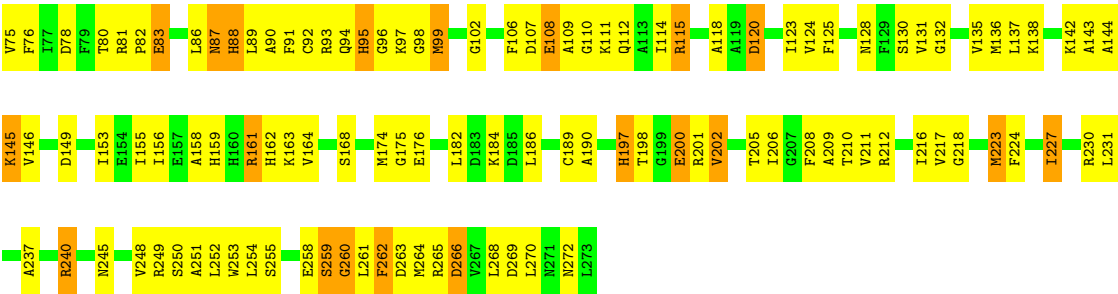
Chain B: 



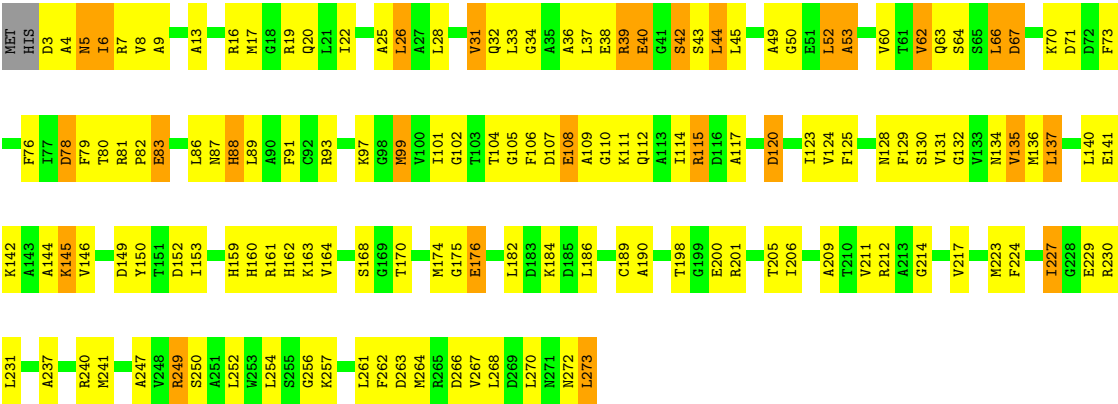
• Molecule 1: DIHYDRODIPICOLINATE REDUCTASE

Chain C: 





● Molecule 1: DIHYDRODIPICOLINATE REDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	137.60Å 123.80Å 66.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	89.9 (20.00-2.60) 90.0 (20.00-2.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.53Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.214 , 0.297 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.437	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 77.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8232	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAI, PO4, PDC, K

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	0.99	1/1965 (0.1%)	1.37	25/2658 (0.9%)
1	B	0.93	1/2001 (0.0%)	1.33	21/2697 (0.8%)
1	C	0.94	0/2006	1.31	24/2705 (0.9%)
1	D	0.95	2/2010 (0.1%)	1.27	13/2710 (0.5%)
All	All	0.95	4/7982 (0.1%)	1.32	83/10770 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	ILE	CA-CB	-6.01	1.47	1.54
1	D	53	ALA	CA-CB	-5.84	1.44	1.53
1	D	267	VAL	CA-CB	-5.35	1.47	1.54
1	B	147	MET	CA-C	-5.07	1.45	1.52

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	ILE	N-CA-C	11.54	118.56	106.21
1	B	205	THR	N-CA-C	11.14	125.02	110.43
1	C	260	GLY	N-CA-C	10.31	121.74	111.95
1	B	60	VAL	N-CA-C	8.74	123.20	110.09
1	D	149	ASP	N-CA-C	8.49	121.29	111.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	ASP	N-CA-C	8.43	121.22	111.11
1	A	97	LYS	N-CA-C	8.37	123.61	113.23
1	D	6	ILE	N-CA-C	8.05	126.09	109.34
1	A	149	ASP	N-CA-C	7.84	120.52	111.11
1	C	149	ASP	N-CA-C	7.78	120.45	111.11
1	D	8	VAL	N-CA-C	7.64	118.80	108.11
1	C	8	VAL	N-CA-C	7.53	118.66	108.11
1	C	200	GLU	N-CA-C	-7.34	99.66	110.52
1	C	6	ILE	N-CA-C	7.18	121.12	109.78
1	B	202	VAL	CA-C-N	7.16	128.79	119.84
1	B	202	VAL	C-N-CA	7.16	128.79	119.84
1	C	31	VAL	N-CA-C	7.16	118.62	108.17
1	A	257	LYS	N-CA-C	7.14	120.78	109.50
1	B	161	ARG	N-CA-C	6.98	120.69	111.75
1	B	28	LEU	N-CA-C	6.87	120.44	109.24
1	A	72	ASP	N-CA-C	6.77	125.22	110.80
1	B	97	LYS	N-CA-C	6.67	120.10	109.24
1	B	8	VAL	N-CA-C	6.66	117.44	108.11
1	D	50	GLY	N-CA-C	6.55	121.67	114.40
1	A	60	VAL	N-CA-C	6.55	117.31	107.75
1	B	63	GLN	N-CA-C	6.53	118.13	108.60
1	C	250	SER	N-CA-C	-6.49	104.13	111.14
1	D	161	ARG	N-CA-C	6.44	119.11	111.71
1	C	161	ARG	N-CA-C	6.39	120.65	112.34
1	A	81	ARG	CA-C-N	6.34	127.76	119.84
1	A	81	ARG	C-N-CA	6.34	127.76	119.84
1	C	28	LEU	N-CA-C	6.29	119.15	108.90
1	A	272	ASN	N-CA-C	-6.28	105.56	112.72
1	B	272	ASN	N-CA-C	-6.19	99.15	109.24
1	D	28	LEU	N-CA-C	6.17	118.77	108.96
1	C	4	ALA	N-CA-C	6.09	123.78	110.80
1	B	206	ILE	CB-CA-C	-6.07	102.23	110.42
1	C	146	VAL	N-CA-C	6.00	116.06	110.42
1	A	78	ASP	N-CA-C	5.97	118.45	108.73
1	C	43	SER	N-CA-C	-5.95	106.37	113.21
1	C	259	SER	N-CA-C	5.82	117.62	108.96
1	C	50	GLY	N-CA-C	5.77	120.94	113.27
1	A	125	PHE	N-CA-C	5.75	117.75	107.80
1	B	146	VAL	N-CA-C	5.73	115.81	110.42
1	A	35	ALA	N-CA-C	5.69	116.91	108.60
1	A	270	LEU	N-CA-C	5.64	120.85	113.30
1	C	266	ASP	N-CA-C	-5.63	105.06	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	PHE	N-CA-C	5.62	117.78	109.69
1	A	146	VAL	N-CA-C	5.61	115.81	110.53
1	B	135	VAL	CB-CA-C	-5.58	104.74	111.88
1	A	161	ARG	N-CA-C	5.57	119.18	112.38
1	C	52	LEU	N-CA-C	-5.53	105.33	111.36
1	D	266	ASP	N-CA-C	-5.52	105.18	111.14
1	B	47	SER	N-CA-C	5.52	122.55	110.80
1	C	135	VAL	CB-CA-C	-5.50	104.84	111.88
1	C	78	ASP	N-CA-C	5.50	117.48	108.52
1	C	223	MET	N-CA-C	5.44	117.28	108.41
1	D	101	ILE	N-CA-C	5.41	116.10	108.36
1	D	146	VAL	N-CA-C	5.40	115.61	110.53
1	B	267	VAL	CB-CA-C	-5.25	104.97	111.70
1	D	135	VAL	CB-CA-C	-5.24	105.27	111.97
1	C	198	THR	N-CA-C	-5.22	102.29	110.17
1	C	202	VAL	CA-C-N	5.22	125.22	119.90
1	C	202	VAL	C-N-CA	5.22	125.22	119.90
1	C	65	SER	N-CA-C	5.20	117.89	108.69
1	A	128	ASN	N-CA-C	5.20	116.03	107.20
1	B	55	ALA	N-CA-C	5.19	117.88	110.24
1	D	78	ASP	N-CA-C	5.19	116.98	108.52
1	A	189	CYS	N-CA-C	5.19	119.18	111.87
1	B	57	LYS	N-CA-C	5.19	117.62	108.75
1	A	262	PHE	N-CA-C	5.18	115.13	108.34
1	D	40	GLU	N-CA-C	5.17	118.37	111.75
1	B	204	GLY	N-CA-C	5.15	120.39	114.16
1	A	206	ILE	CB-CA-C	-5.14	103.17	110.83
1	A	45	LEU	N-CA-C	-5.12	102.71	110.28
1	A	234	THR	N-CA-C	5.12	117.78	109.24
1	A	104	THR	N-CA-C	5.10	116.90	108.13
1	A	13	ALA	N-CA-C	5.08	121.63	110.80
1	B	164	VAL	N-CA-C	5.07	117.77	112.90
1	A	113	ALA	N-CA-C	-5.04	105.26	111.40
1	B	181	ALA	N-CA-C	-5.01	106.99	113.01
1	C	210	THR	N-CA-C	5.01	116.58	108.41
1	D	134	ASN	CB-CA-C	5.00	118.73	110.88

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	150	TYR	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1939	0	1871	162	0
1	B	1975	0	1943	141	0
1	C	1980	0	1941	147	0
1	D	1984	0	1953	135	0
2	A	5	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	B	44	0	27	6	0
4	C	44	0	27	3	0
4	D	44	0	27	5	0
5	B	12	0	4	0	0
5	C	12	0	3	2	0
5	D	12	0	3	4	0
6	A	41	0	0	1	0
6	B	47	0	0	5	0
6	C	45	0	0	5	0
6	D	46	0	0	7	0
All	All	8232	0	7799	565	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

All (565) 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:C:89:LEU:HA	1:C:99:MET:HE1	1.18	1.11
1:C:264:MET:HE3	1:C:268:LEU:HD11	1.43	0.99
1:C:89:LEU:HA	1:C:99:MET:CE	1.93	0.99
1:C:45:LEU:HA	1:C:62:VAL:HG22	1.49	0.95
1:B:20:GLN:NE2	1:B:241:MET:HE2	1.87	0.90
1:C:245:ASN:O	1:C:249:ARG:HD2	1.71	0.89
1:C:102:GLY:O	4:C:301:NAI:H2N	1.72	0.88
1:C:86:LEU:O	1:C:89:LEU:HB3	1.74	0.88
1:C:108:GLU:HA	1:C:111:LYS:HD3	1.55	0.88
1:C:153:ILE:HG22	1:C:206:ILE:HG23	1.56	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:MET:HE3	1:B:174:MET:HE3	1.60	0.83
1:B:108:GLU:HA	1:B:111:LYS:HD3	1.60	0.83
1:D:108:GLU:HA	1:D:111:LYS:HD3	1.60	0.82
1:A:241:MET:HE3	1:A:245:ASN:HD21	1.45	0.82
1:A:101:ILE:N	1:A:101:ILE:HD12	1.95	0.81
1:C:218:GLY:HA3	6:C:412:HOH:O	1.77	0.81
1:D:102:GLY:O	4:D:302:NAI:H2N	1.82	0.79
1:C:48:ASP:HB3	1:C:51:GLU:HG2	1.62	0.79
1:C:89:LEU:CA	1:C:99:MET:HE1	2.07	0.79
1:C:138:LYS:HE2	1:C:272:ASN:HA	1.65	0.79
1:B:20:GLN:HE21	1:B:241:MET:HE2	1.47	0.78
1:B:86:LEU:O	1:B:89:LEU:HG	1.84	0.78
1:C:67:ASP:HA	1:C:70:LYS:HB3	1.65	0.78
1:D:39:ARG:HG2	1:D:39:ARG:HH11	1.49	0.77
1:D:186:LEU:HD23	1:D:190:ALA:HB2	1.65	0.77
1:B:67:ASP:HA	1:B:70:LYS:HB3	1.64	0.77
1:D:67:ASP:HA	1:D:70:LYS:HB3	1.65	0.77
1:A:201:ARG:HD3	1:C:212:ARG:O	1.83	0.77
1:A:73:PHE:CE1	1:A:97:LYS:HE3	2.19	0.77
1:C:73:PHE:O	1:C:97:LYS:HE2	1.85	0.77
1:C:136:MET:HE3	1:C:174:MET:HE3	1.67	0.77
1:A:186:LEU:HD23	1:A:190:ALA:HB2	1.67	0.77
1:B:186:LEU:HD23	1:B:190:ALA:HB2	1.66	0.76
1:B:38:GLU:HG3	1:B:42:SER:OG	1.84	0.76
1:A:45:LEU:HD12	1:A:62:VAL:O	1.85	0.76
1:B:13:ALA:O	1:B:52:LEU:HD11	1.86	0.76
1:B:88:HIS:O	1:B:92:CYS:HB2	1.85	0.76
1:D:7:ARG:HB2	1:D:73:PHE:HA	1.69	0.75
1:D:66:LEU:HB3	1:D:91:PHE:CE2	2.22	0.75
1:C:186:LEU:HD23	1:C:190:ALA:HB2	1.70	0.74
1:C:49:ALA:O	1:C:52:LEU:HB3	1.87	0.74
1:D:249:ARG:HG2	1:D:249:ARG:HH11	1.53	0.74
1:A:136:MET:HE3	1:A:174:MET:HE3	1.70	0.73
1:D:49:ALA:O	1:D:52:LEU:HG	1.88	0.72
1:A:241:MET:HE3	1:A:245:ASN:ND2	2.04	0.72
1:B:273:LEU:HA	6:B:438:HOH:O	1.89	0.72
1:A:129:PHE:O	1:A:246:GLY:HA3	1.90	0.72
1:C:216:ILE:HA	6:C:438:HOH:O	1.88	0.72
1:A:101:ILE:CD1	1:A:123:ILE:HG23	2.20	0.71
1:A:264:MET:HE3	1:A:268:LEU:HD22	1.71	0.71
1:B:76:PHE:HB2	1:B:92:CYS:SG	2.31	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:LYS:HE3	1:B:273:LEU:HG	1.71	0.70
1:A:80:THR:O	1:A:103:THR:HG23	1.92	0.69
1:C:48:ASP:OD2	1:C:57:LYS:HA	1.93	0.68
1:C:251:ALA:HA	1:C:254:LEU:HD12	1.74	0.68
1:A:73:PHE:HE1	1:A:97:LYS:HB3	1.58	0.68
1:B:93:ARG:HA	1:B:121:ILE:HG21	1.76	0.67
1:C:7:ARG:HB2	1:C:73:PHE:HA	1.76	0.67
1:A:11:ALA:HB2	1:A:76:PHE:CZ	2.29	0.67
1:B:114:ILE:HG22	1:B:261:LEU:HD11	1.76	0.67
1:B:273:LEU:HD12	1:C:142:LYS:HD2	1.76	0.67
1:A:89:LEU:HD23	1:A:89:LEU:O	1.95	0.67
1:B:7:ARG:HB2	1:B:73:PHE:HA	1.76	0.67
1:B:19:ARG:HD3	1:B:52:LEU:HD13	1.76	0.67
1:D:136:MET:HE3	1:D:174:MET:HE3	1.76	0.67
1:A:124:VAL:HG23	1:A:254:LEU:HD21	1.78	0.66
4:D:302:NAI:H4B	6:D:426:HOH:O	1.94	0.66
1:B:76:PHE:CB	1:B:92:CYS:SG	2.83	0.66
1:A:46:GLY:H	1:A:62:VAL:HG13	1.60	0.66
1:A:79:PHE:CE1	1:A:102:GLY:HA3	2.30	0.66
1:D:36:ALA:C	1:D:37:LEU:HD12	2.21	0.66
1:D:19:ARG:HB3	1:D:53:ALA:HB2	1.78	0.66
1:B:136:MET:CE	1:B:174:MET:HE3	2.26	0.66
1:C:17:MET:HB2	6:C:407:HOH:O	1.96	0.66
1:C:240:ARG:HD3	6:C:444:HOH:O	1.96	0.66
1:A:82:PRO:O	1:A:85:THR:N	2.29	0.66
1:B:89:LEU:HA	1:B:99:MET:HE1	1.79	0.65
1:C:262:PHE:HD1	1:C:262:PHE:N	1.94	0.65
1:C:264:MET:O	1:C:268:LEU:HD12	1.96	0.65
1:B:60:VAL:HG12	1:B:61:THR:H	1.60	0.65
1:D:89:LEU:HD12	1:D:99:MET:HE1	1.77	0.65
1:D:93:ARG:HD2	1:D:117:ALA:HA	1.79	0.65
1:C:227:ILE:HD13	1:C:227:ILE:H	1.62	0.65
1:C:80:THR:O	4:C:301:NAI:H4D	1.95	0.65
1:C:262:PHE:N	1:C:262:PHE:CD1	2.64	0.65
1:D:99:MET:O	1:D:254:LEU:HD11	1.96	0.65
1:B:247:ALA:O	1:B:250:SER:HB2	1.97	0.64
1:B:36:ALA:C	1:B:37:LEU:HD12	2.22	0.64
1:B:44:LEU:HD13	1:B:44:LEU:O	1.96	0.64
1:D:3:ASP:N	1:D:31:VAL:H	1.96	0.64
1:A:79:PHE:CZ	1:A:102:GLY:HA3	2.32	0.64
1:B:114:ILE:HG22	1:B:261:LEU:CD1	2.28	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:ASN:HD22	1:C:130:SER:H	1.45	0.64
1:A:47:SER:O	1:A:62:VAL:HG12	1.98	0.63
1:C:93:ARG:O	1:C:96:GLY:N	2.31	0.63
1:B:120:ASP:O	1:B:259:SER:HB3	1.98	0.63
1:A:89:LEU:HD21	1:A:117:ALA:CB	2.27	0.63
1:A:264:MET:O	1:A:268:LEU:HB2	1.99	0.62
1:A:91:PHE:HE1	1:A:95:HIS:CD2	2.17	0.62
1:C:138:LYS:HE2	1:C:272:ASN:H	1.64	0.62
1:C:265:ARG:HG2	1:C:270:LEU:HD12	1.81	0.62
1:D:128:ASN:HD22	1:D:130:SER:H	1.48	0.62
1:A:89:LEU:HD23	1:A:89:LEU:C	2.25	0.62
1:A:131:VAL:HG13	1:A:268:LEU:HD21	1.81	0.62
1:B:152:ASP:HA	6:B:443:HOH:O	1.99	0.62
1:B:120:ASP:C	1:B:259:SER:HB3	2.25	0.62
1:A:101:ILE:HD11	1:A:123:ILE:HG23	1.80	0.61
1:A:189:CYS:HB2	1:A:205:THR:HA	1.82	0.61
1:D:129:PHE:C	1:D:264:MET:HE2	2.25	0.61
1:A:126:ALA:HB3	1:A:129:PHE:CE1	2.36	0.61
1:B:153:ILE:CG2	1:B:206:ILE:HD13	2.30	0.61
1:A:46:GLY:N	1:A:62:VAL:HG13	2.15	0.61
1:B:227:ILE:HG12	1:B:227:ILE:O	1.99	0.61
1:B:112:GLN:HA	1:B:112:GLN:OE1	1.99	0.61
1:A:227:ILE:HD13	1:A:227:ILE:H	1.65	0.60
1:A:265:ARG:NH1	1:A:271:ASN:HD21	2.00	0.60
1:B:48:ASP:HA	1:B:60:VAL:O	2.01	0.60
1:B:227:ILE:HD13	1:B:227:ILE:H	1.67	0.60
1:B:194:ARG:HH22	1:B:201:ARG:NH1	2.00	0.60
1:D:79:PHE:CZ	1:D:102:GLY:HA3	2.37	0.60
1:C:89:LEU:HD22	1:C:99:MET:HE3	1.82	0.60
1:C:261:LEU:C	1:C:262:PHE:CD1	2.80	0.60
1:D:89:LEU:HD11	1:D:117:ALA:CB	2.31	0.60
1:D:227:ILE:HD13	1:D:227:ILE:H	1.66	0.60
1:B:112:GLN:O	1:B:115:ARG:HB3	2.02	0.60
1:B:28:LEU:HD12	1:B:248:VAL:HG11	1.84	0.59
1:C:261:LEU:C	1:C:262:PHE:HD1	2.09	0.59
1:C:227:ILE:O	1:C:227:ILE:HG12	2.02	0.59
1:B:118:ALA:HB1	1:B:261:LEU:N	2.17	0.59
1:B:36:ALA:C	1:B:62:VAL:HG13	2.28	0.59
1:B:60:VAL:HG12	1:B:61:THR:N	2.18	0.59
1:B:142:LYS:HE3	1:B:273:LEU:CG	2.32	0.59
1:B:223:MET:HE1	1:D:211:VAL:HG11	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ILE:N	1:A:201:ARG:HH21	2.01	0.58
1:A:273:LEU:HD22	1:D:142:LYS:HD2	1.86	0.58
1:C:138:LYS:HE2	1:C:272:ASN:CA	2.32	0.58
1:A:101:ILE:N	1:A:101:ILE:CD1	2.65	0.58
1:D:112:GLN:OE1	1:D:112:GLN:HA	2.02	0.58
1:A:91:PHE:CE1	1:A:95:HIS:CD2	2.91	0.58
1:A:78:ASP:OD2	1:A:85:THR:HG23	2.03	0.58
1:B:66:LEU:HB3	1:B:91:PHE:CZ	2.39	0.58
1:D:3:ASP:N	1:D:31:VAL:N	2.51	0.58
1:A:76:PHE:CZ	1:A:88:HIS:CD2	2.91	0.58
1:A:89:LEU:HD21	1:A:117:ALA:HB2	1.86	0.58
1:C:36:ALA:C	1:C:37:LEU:HD12	2.29	0.58
1:B:162:HIS:HA	1:D:200:GLU:OE1	2.04	0.58
1:D:227:ILE:HG12	1:D:227:ILE:O	2.04	0.58
1:C:112:GLN:HA	1:C:112:GLN:OE1	2.03	0.57
1:A:101:ILE:HD13	1:A:123:ILE:HG23	1.84	0.57
1:D:20:GLN:NE2	1:D:241:MET:HE2	2.20	0.57
1:C:66:LEU:HB3	1:C:91:PHE:CE1	2.40	0.57
1:C:74:ASP:O	1:C:97:LYS:HD3	2.04	0.57
1:C:251:ALA:CA	1:C:254:LEU:HD12	2.35	0.57
1:C:261:LEU:HD23	1:C:262:PHE:N	2.19	0.57
1:A:19:ARG:O	1:A:22:ILE:HB	2.05	0.57
1:A:153:ILE:H	1:A:201:ARG:NH2	2.03	0.57
1:B:76:PHE:HB3	1:B:99:MET:HG3	1.87	0.57
1:D:39:ARG:HH11	1:D:39:ARG:CG	2.16	0.57
1:A:125:PHE:CD1	1:A:125:PHE:C	2.80	0.56
1:C:66:LEU:HB3	1:C:91:PHE:CZ	2.40	0.56
1:A:8:VAL:HG22	1:A:33:LEU:HA	1.88	0.56
1:A:9:ALA:HB3	1:A:76:PHE:HA	1.87	0.56
1:D:26:LEU:CD1	1:D:33:LEU:HB2	2.35	0.56
1:A:22:ILE:O	1:A:25:ALA:HB3	2.05	0.56
1:B:142:LYS:O	1:B:145:LYS:HB3	2.05	0.56
1:C:88:HIS:O	1:C:92:CYS:SG	2.63	0.56
1:D:102:GLY:O	4:D:302:NAI:C2N	2.51	0.56
1:A:83:GLU:HA	1:A:86:LEU:HD23	1.86	0.56
1:B:106:PHE:CD2	1:B:125:PHE:HZ	2.24	0.56
1:B:128:ASN:HD22	1:B:130:SER:H	1.53	0.56
1:A:261:LEU:HD23	1:A:262:PHE:N	2.21	0.56
1:D:76:PHE:HB3	1:D:99:MET:HG3	1.88	0.55
1:A:78:ASP:CG	1:A:85:THR:HG23	2.31	0.55
1:D:5:ASN:N	1:D:5:ASN:HD22	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ASP:OD2	1:A:85:THR:HA	2.06	0.55
1:A:223:MET:HE1	1:C:211:VAL:HG11	1.87	0.55
1:D:160:HIS:CE1	6:D:413:HOH:O	2.60	0.55
1:A:136:MET:CE	1:A:174:MET:HE3	2.36	0.55
1:B:102:GLY:O	4:B:302:NAI:H2N	2.07	0.55
1:D:88:HIS:O	1:D:91:PHE:HB3	2.05	0.55
1:B:201:ARG:HG3	1:B:201:ARG:HH11	1.71	0.55
1:C:162:HIS:HE1	6:C:415:HOH:O	1.90	0.55
1:D:66:LEU:HB3	1:D:91:PHE:CZ	2.42	0.55
1:C:92:CYS:HB2	1:C:99:MET:HE2	1.90	0.54
1:C:112:GLN:O	1:C:115:ARG:HB3	2.06	0.54
1:B:153:ILE:HG21	1:B:206:ILE:HD13	1.89	0.54
1:D:136:MET:CE	1:D:174:MET:HE3	2.38	0.54
1:A:65:SER:HB3	1:A:68:ALA:HB2	1.90	0.54
1:A:79:PHE:CD1	1:A:102:GLY:HA3	2.43	0.54
1:D:249:ARG:HG2	1:D:249:ARG:NH1	2.19	0.54
1:A:73:PHE:CE1	1:A:97:LYS:HB3	2.42	0.54
1:A:268:LEU:HB3	1:A:270:LEU:HG	1.88	0.54
1:D:186:LEU:CD2	1:D:190:ALA:HB2	2.38	0.54
1:B:252:LEU:C	1:B:252:LEU:HD23	2.32	0.54
1:C:136:MET:CE	1:C:174:MET:HE3	2.37	0.54
1:A:131:VAL:O	1:A:132:GLY:C	2.51	0.53
1:B:175:GLY:C	1:B:186:LEU:HD12	2.33	0.53
1:C:142:LYS:O	1:C:145:LYS:HB3	2.07	0.53
1:C:265:ARG:NH1	1:C:265:ARG:HB2	2.22	0.53
1:D:13:ALA:HB1	1:D:22:ILE:HD11	1.91	0.53
1:A:175:GLY:HA3	1:A:186:LEU:HD11	1.90	0.53
1:B:211:VAL:HG11	1:D:223:MET:HE1	1.90	0.53
1:C:128:ASN:ND2	1:C:130:SER:H	2.06	0.53
1:C:13:ALA:HB1	1:C:22:ILE:HD11	1.91	0.53
1:D:104:THR:HG21	5:D:303:PDC:C7	2.39	0.53
1:B:252:LEU:HD23	1:B:253:TRP:N	2.23	0.53
1:C:45:LEU:HA	1:C:62:VAL:CG2	2.32	0.53
1:D:81:ARG:HB3	1:D:82:PRO:HD2	1.90	0.53
1:B:88:HIS:N	1:B:88:HIS:CD2	2.73	0.53
1:B:194:ARG:NH2	1:B:201:ARG:NH1	2.55	0.53
1:A:245:ASN:N	1:A:245:ASN:HD22	2.06	0.53
1:B:186:LEU:CD2	1:B:190:ALA:HB2	2.38	0.53
1:A:75:VAL:HG23	1:A:98:GLY:O	2.08	0.53
1:A:242:THR:HG23	1:D:229:GLU:CD	2.34	0.53
1:C:251:ALA:HA	1:C:254:LEU:CD1	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:TRP:HZ3	1:C:262:PHE:CD2	2.27	0.53
1:D:142:LYS:O	1:D:145:LYS:HB3	2.09	0.53
1:D:272:ASN:HB2	6:D:423:HOH:O	2.09	0.53
1:C:253:TRP:CZ3	1:C:262:PHE:CD2	2.97	0.52
1:C:87:ASN:O	1:C:88:HIS:C	2.52	0.52
1:D:19:ARG:CB	1:D:53:ALA:HB2	2.39	0.52
1:D:170:THR:N	5:D:303:PDC:O1	2.42	0.52
1:A:175:GLY:C	1:A:186:LEU:HD12	2.34	0.52
1:A:227:ILE:HG12	1:A:227:ILE:O	2.09	0.52
1:B:81:ARG:HB3	1:B:82:PRO:HD2	1.91	0.52
1:C:189:CYS:HB2	1:C:205:THR:HA	1.91	0.52
1:C:201:ARG:HG2	1:C:201:ARG:HH11	1.73	0.52
1:A:65:SER:HB3	1:A:68:ALA:CB	2.39	0.52
1:A:100:VAL:HG12	1:A:100:VAL:O	2.08	0.52
1:A:243:PHE:CD1	1:A:243:PHE:N	2.78	0.52
1:B:115:ARG:HA	1:B:261:LEU:HD12	1.92	0.52
1:C:175:GLY:C	1:C:186:LEU:HD12	2.35	0.52
1:D:152:ASP:CG	1:D:201:ARG:HE	2.17	0.52
1:A:209:ALA:HB1	1:C:209:ALA:HB1	1.92	0.52
1:A:273:LEU:HD22	1:D:142:LYS:CD	2.39	0.52
1:C:106:PHE:CD2	1:C:125:PHE:HZ	2.28	0.52
1:C:138:LYS:HE2	1:C:272:ASN:N	2.24	0.52
1:C:186:LEU:CD2	1:C:190:ALA:HB2	2.38	0.52
1:B:26:LEU:HD21	1:B:58:THR:HG21	1.91	0.52
1:B:38:GLU:OE1	4:B:302:NAI:H1B	2.10	0.52
1:B:194:ARG:NH2	1:B:201:ARG:HH11	2.08	0.52
1:A:142:LYS:O	1:A:145:LYS:HB3	2.10	0.52
1:A:79:PHE:CE2	1:A:102:GLY:HA3	2.45	0.52
1:A:186:LEU:CD2	1:A:190:ALA:HB2	2.38	0.52
1:D:112:GLN:O	1:D:115:ARG:HB3	2.10	0.52
1:B:264:MET:HE3	1:B:268:LEU:HD11	1.93	0.51
1:C:95:HIS:N	1:C:95:HIS:ND1	2.56	0.51
1:B:67:ASP:O	1:B:70:LYS:HG2	2.11	0.51
1:D:19:ARG:HB3	1:D:53:ALA:CB	2.41	0.51
1:A:118:ALA:O	1:A:121:ILE:O	2.28	0.51
1:B:212:ARG:O	1:D:201:ARG:HD2	2.11	0.51
1:B:50:GLY:HA3	1:B:58:THR:HG23	1.93	0.51
1:A:128:ASN:O	1:A:134:ASN:ND2	2.44	0.51
1:B:39:ARG:O	1:B:40:GLU:C	2.54	0.51
1:B:88:HIS:CD2	1:B:88:HIS:H	2.27	0.51
1:D:175:GLY:C	1:D:186:LEU:HD12	2.36	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:ARG:O	1:C:269:ASP:N	2.43	0.51
1:D:106:PHE:CD2	1:D:125:PHE:HZ	2.28	0.51
1:A:119:ALA:O	1:A:259:SER:HB2	2.10	0.51
1:B:209:ALA:HB1	1:D:209:ALA:HB1	1.93	0.50
1:A:124:VAL:HG22	1:A:262:PHE:HB2	1.93	0.50
1:C:21:LEU:O	1:C:24:ALA:HB3	2.12	0.50
1:C:131:VAL:O	1:C:132:GLY:C	2.54	0.50
1:C:153:ILE:O	1:C:206:ILE:HA	2.11	0.50
1:D:7:ARG:CB	1:D:73:PHE:HA	2.40	0.50
1:C:89:LEU:HD22	1:C:99:MET:CE	2.42	0.50
1:A:144:ALA:O	1:A:182:LEU:HD21	2.12	0.50
1:C:42:SER:C	1:C:44:LEU:H	2.18	0.50
1:C:163:LYS:NZ	5:C:302:PDC:N1	2.56	0.50
1:A:160:HIS:HB2	1:A:214:GLY:O	2.11	0.50
1:C:73:PHE:CE1	1:C:97:LYS:HD2	2.47	0.50
1:B:46:GLY:O	1:B:61:THR:HB	2.11	0.50
1:B:106:PHE:HD2	1:B:125:PHE:HZ	1.58	0.50
1:C:5:ASN:HB2	1:C:30:GLY:O	2.12	0.50
1:D:152:ASP:HA	1:D:201:ARG:HH21	1.76	0.50
1:A:265:ARG:HH11	1:A:271:ASN:HD21	1.60	0.49
1:A:109:ALA:O	1:A:113:ALA:HB2	2.12	0.49
1:A:153:ILE:HG12	1:A:224:PHE:CD1	2.48	0.49
1:B:106:PHE:CD2	1:B:125:PHE:CZ	3.01	0.49
1:B:125:PHE:CB	1:B:261:LEU:HD21	2.41	0.49
1:D:9:ALA:HB2	1:D:73:PHE:CD2	2.47	0.49
1:D:17:MET:HE2	1:D:79:PHE:CE2	2.47	0.49
1:A:86:LEU:O	1:A:89:LEU:HB3	2.13	0.49
1:C:75:VAL:HG13	1:C:98:GLY:O	2.11	0.49
1:C:87:ASN:C	1:C:89:LEU:N	2.68	0.49
1:C:120:ASP:C	1:C:259:SER:HB2	2.37	0.49
1:B:95:HIS:ND1	1:B:95:HIS:N	2.60	0.49
1:B:153:ILE:HG12	1:B:224:PHE:CD1	2.48	0.49
1:C:73:PHE:CD1	1:C:97:LYS:HD2	2.47	0.49
1:B:217:VAL:HB	1:B:237:ALA:O	2.12	0.49
1:D:86:LEU:O	1:D:89:LEU:HB3	2.13	0.49
1:D:263:ASP:HB2	6:D:416:HOH:O	2.12	0.49
1:A:18:GLY:O	1:A:19:ARG:C	2.56	0.48
1:A:102:GLY:O	1:A:104:THR:HG22	2.13	0.48
1:A:199:GLY:C	1:C:164:VAL:HG12	2.38	0.48
1:B:153:ILE:H	1:B:201:ARG:HH21	1.61	0.48
1:D:40:GLU:N	1:D:40:GLU:CD	2.70	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ARG:O	1:B:20:GLN:HG2	2.12	0.48
1:B:47:SER:O	1:B:61:THR:HA	2.13	0.48
1:B:83:GLU:O	1:B:86:LEU:HB2	2.13	0.48
6:B:409:HOH:O	1:C:230:ARG:HG2	2.13	0.48
1:D:39:ARG:O	1:D:42:SER:OG	2.32	0.48
1:D:150:TYR:HE2	6:D:432:HOH:O	1.96	0.48
1:A:162:HIS:HD2	1:C:200:GLU:OE1	1.97	0.48
1:D:36:ALA:CB	1:D:62:VAL:HG23	2.44	0.48
1:D:163:LYS:NZ	5:D:303:PDC:O2	2.47	0.48
1:D:249:ARG:HH11	1:D:249:ARG:CG	2.25	0.48
1:B:154:GLU:HB2	1:B:223:MET:HE2	1.95	0.48
1:B:201:ARG:HD2	1:D:212:ARG:O	2.13	0.48
1:C:82:PRO:HA	1:C:106:PHE:CE1	2.49	0.48
1:A:101:ILE:HD12	1:A:101:ILE:H	1.74	0.48
1:B:188:ASP:HA	6:B:428:HOH:O	2.13	0.48
1:D:129:PHE:CA	1:D:264:MET:HE2	2.44	0.48
1:B:201:ARG:NH2	1:B:205:THR:O	2.46	0.48
1:D:42:SER:C	1:D:44:LEU:H	2.22	0.48
1:A:48:ASP:OD1	1:A:58:THR:HB	2.14	0.48
1:A:153:ILE:H	1:A:201:ARG:HH21	1.58	0.48
1:A:241:MET:CE	1:A:245:ASN:HD21	2.21	0.48
1:A:48:ASP:O	1:A:50:GLY:N	2.46	0.47
1:B:125:PHE:N	1:B:262:PHE:O	2.47	0.47
1:A:10:ILE:HD13	1:A:22:ILE:HA	1.96	0.47
1:C:163:LYS:NZ	5:C:302:PDC:O2	2.47	0.47
1:D:20:GLN:HE21	1:D:241:MET:HE2	1.79	0.47
1:D:129:PHE:O	1:D:264:MET:HE2	2.15	0.47
1:A:123:ILE:HG22	1:A:124:VAL:N	2.27	0.47
1:B:7:ARG:CB	1:B:73:PHE:HA	2.42	0.47
1:D:128:ASN:ND2	1:D:130:SER:H	2.10	0.47
1:C:76:PHE:CZ	1:C:88:HIS:CD2	3.02	0.47
1:B:107:ASP:OD1	1:B:109:ALA:HB3	2.14	0.47
1:B:120:ASP:C	1:B:259:SER:CB	2.87	0.47
1:C:44:LEU:H	1:C:44:LEU:HD23	1.79	0.47
1:A:123:ILE:CG2	1:A:124:VAL:N	2.77	0.47
1:A:140:LEU:HD12	1:A:233:ILE:HD12	1.97	0.47
1:A:243:PHE:HD1	1:A:243:PHE:H	1.61	0.47
1:B:131:VAL:O	1:B:132:GLY:C	2.57	0.47
1:B:266:ASP:HA	1:B:271:ASN:ND2	2.30	0.47
1:B:273:LEU:HD22	6:B:438:HOH:O	2.14	0.47
1:C:90:ALA:O	1:C:93:ARG:HG3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:ILE:HG12	1:C:224:PHE:CD1	2.49	0.47
1:C:270:LEU:O	1:C:272:ASN:N	2.47	0.47
1:A:38:GLU:HG3	1:A:39:ARG:N	2.30	0.47
1:A:82:PRO:O	1:A:83:GLU:C	2.57	0.47
1:B:125:PHE:HB3	1:B:261:LEU:HD21	1.96	0.47
1:B:144:ALA:O	1:B:182:LEU:HD21	2.14	0.47
1:A:65:SER:O	1:A:69:VAL:HG22	2.15	0.47
1:A:100:VAL:HG11	1:A:247:ALA:HB1	1.97	0.47
1:B:15:GLY:HA2	4:B:302:NAI:O1A	2.15	0.47
1:D:105:GLY:HA3	6:D:441:HOH:O	2.15	0.47
1:A:154:GLU:HB2	1:A:223:MET:HE2	1.97	0.46
1:C:83:GLU:O	1:C:86:LEU:HB2	2.16	0.46
1:C:107:ASP:OD1	1:C:109:ALA:HB3	2.14	0.46
1:C:118:ALA:O	1:C:260:GLY:N	2.48	0.46
1:A:6:ILE:O	1:A:32:GLN:N	2.47	0.46
1:A:18:GLY:O	1:A:22:ILE:HD12	2.14	0.46
1:B:89:LEU:O	1:B:92:CYS:N	2.48	0.46
1:D:7:ARG:HG3	1:D:7:ARG:HH11	1.80	0.46
1:D:175:GLY:HA3	1:D:186:LEU:HD11	1.96	0.46
1:A:9:ALA:HB2	1:A:73:PHE:CD2	2.50	0.46
1:C:90:ALA:O	1:C:93:ARG:HB2	2.15	0.46
1:A:7:ARG:HB3	1:A:34:GLY:HA3	1.98	0.46
1:A:160:HIS:HA	1:A:213:ALA:O	2.15	0.46
1:B:91:PHE:C	1:B:93:ARG:H	2.23	0.46
1:C:16:ARG:O	1:C:20:GLN:HG2	2.13	0.46
1:D:107:ASP:OD1	1:D:109:ALA:HB3	2.16	0.46
1:A:115:ARG:O	1:A:118:ALA:HB3	2.16	0.46
1:A:250:SER:O	1:A:253:TRP:HB3	2.16	0.46
1:C:144:ALA:O	1:C:182:LEU:HD21	2.16	0.46
1:C:175:GLY:HA3	1:C:186:LEU:HD11	1.98	0.46
1:A:89:LEU:C	1:A:89:LEU:CD2	2.89	0.46
1:C:44:LEU:HD23	1:C:44:LEU:N	2.31	0.46
1:D:93:ARG:HG3	1:D:120:ASP:OD1	2.16	0.46
1:A:7:ARG:HB2	1:A:73:PHE:HA	1.97	0.46
1:B:196:GLY:O	1:B:198:THR:HG23	2.16	0.46
1:B:200:GLU:CD	1:D:162:HIS:HD2	2.24	0.46
1:C:9:ALA:HB2	1:C:73:PHE:CG	2.51	0.46
1:A:33:LEU:O	1:A:60:VAL:HG21	2.16	0.45
1:B:118:ALA:CB	1:B:261:LEU:HB2	2.46	0.45
1:B:45:LEU:HD11	1:B:63:GLN:C	2.41	0.45
1:C:45:LEU:HD12	1:C:63:GLN:HA	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:ALA:O	1:D:37:LEU:HD12	2.16	0.45
1:A:85:THR:OG1	1:A:103:THR:HG21	2.17	0.45
1:A:153:ILE:HA	1:A:223:MET:O	2.16	0.45
1:A:217:VAL:HB	1:A:237:ALA:O	2.17	0.45
1:B:20:GLN:HG3	1:B:240:ARG:HB3	1.98	0.45
1:B:80:THR:O	4:B:302:NAI:H4D	2.17	0.45
1:B:9:ALA:HB3	1:B:76:PHE:HA	1.97	0.45
1:A:73:PHE:CD1	1:A:73:PHE:C	2.94	0.45
1:B:17:MET:HE2	1:B:79:PHE:CE2	2.51	0.45
1:A:18:GLY:O	1:A:21:LEU:HB2	2.16	0.45
1:B:48:ASP:C	1:B:50:GLY:N	2.72	0.45
1:B:89:LEU:HB2	1:B:90:ALA:H	1.65	0.45
1:C:61:THR:O	1:C:63:GLN:HG2	2.17	0.45
1:C:89:LEU:O	1:C:93:ARG:HG3	2.17	0.45
1:D:144:ALA:O	1:D:182:LEU:HD21	2.17	0.45
1:A:28:LEU:HG	1:A:248:VAL:HG12	1.99	0.45
1:B:13:ALA:HB1	1:B:22:ILE:HD11	1.98	0.45
1:B:251:ALA:O	1:B:252:LEU:C	2.60	0.45
1:C:48:ASP:HB3	1:C:51:GLU:CG	2.42	0.45
1:C:143:ALA:O	1:C:144:ALA:C	2.59	0.45
1:C:201:ARG:NH1	1:C:205:THR:OG1	2.49	0.45
1:D:176:GLU:N	1:D:186:LEU:HD12	2.32	0.45
1:D:206:ILE:HD12	1:D:206:ILE:N	2.31	0.45
1:D:25:ALA:O	1:D:31:VAL:HG12	2.17	0.45
1:D:106:PHE:HD2	1:D:125:PHE:HZ	1.64	0.45
1:D:256:GLY:O	1:D:257:LYS:C	2.60	0.45
1:A:37:LEU:HD21	1:A:66:LEU:HD13	1.99	0.45
1:B:76:PHE:HB3	1:B:92:CYS:SG	2.57	0.45
1:B:197:HIS:HA	1:D:164:VAL:O	2.17	0.45
1:B:261:LEU:O	1:B:262:PHE:CD1	2.70	0.45
1:C:201:ARG:HG2	1:C:201:ARG:NH1	2.31	0.45
1:A:48:ASP:O	1:A:49:ALA:C	2.60	0.45
1:B:118:ALA:HB2	1:B:261:LEU:HB2	1.99	0.45
1:D:153:ILE:HG12	1:D:224:PHE:CD1	2.51	0.45
1:A:33:LEU:HD21	1:A:35:ALA:O	2.16	0.44
1:B:175:GLY:HA3	1:B:186:LEU:HD11	1.98	0.44
1:D:106:PHE:CD2	1:D:125:PHE:CZ	3.05	0.44
1:A:97:LYS:HD2	1:A:97:LYS:HA	1.76	0.44
1:C:81:ARG:HB3	1:C:82:PRO:HD2	1.98	0.44
1:D:247:ALA:O	1:D:250:SER:HB2	2.17	0.44
4:D:302:NAI:H2D	4:D:302:NAI:H6N	1.64	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ALA:O	1:A:174:MET:HB2	2.17	0.44
1:C:248:VAL:O	1:C:251:ALA:HB3	2.16	0.44
1:D:45:LEU:HD12	1:D:63:GLN:HA	2.00	0.44
1:D:97:LYS:HA	6:D:428:HOH:O	2.16	0.44
1:A:17:MET:HE3	1:A:17:MET:HA	1.99	0.44
1:A:110:GLY:O	1:A:113:ALA:HB3	2.18	0.44
4:B:302:NAI:H2B	4:B:302:NAI:H8A	1.64	0.44
1:D:135:VAL:O	1:D:136:MET:C	2.60	0.44
1:A:40:GLU:HG3	1:A:41:GLY:N	2.32	0.44
1:A:118:ALA:HA	1:A:123:ILE:HD12	2.00	0.44
1:D:82:PRO:HA	1:D:106:PHE:CE1	2.53	0.44
1:A:58:THR:C	1:A:60:VAL:H	2.26	0.44
1:A:201:ARG:HB3	1:C:161:ARG:HB2	1.99	0.44
1:C:158:ALA:HA	1:C:211:VAL:O	2.18	0.44
1:D:129:PHE:HA	1:D:264:MET:HE2	1.99	0.44
1:B:44:LEU:HD11	1:B:47:SER:HB2	2.00	0.44
1:C:106:PHE:CD2	1:C:125:PHE:CZ	3.06	0.44
1:C:17:MET:HB2	4:C:301:NAI:O2N	2.17	0.43
1:D:31:VAL:HG23	1:D:252:LEU:HD11	1.99	0.43
1:D:38:GLU:HG3	1:D:42:SER:OG	2.17	0.43
1:C:67:ASP:O	1:C:70:LYS:HG2	2.17	0.43
1:D:159:HIS:CE1	1:D:168:SER:HB3	2.53	0.43
1:B:38:GLU:HG3	1:B:42:SER:CB	2.48	0.43
1:C:202:VAL:O	1:C:205:THR:HG23	2.18	0.43
1:D:4:ALA:HB1	1:D:5:ASN:HD22	1.83	0.43
1:A:144:ALA:O	1:A:148:GLY:HA3	2.18	0.43
1:B:94:GLN:C	1:B:96:GLY:H	2.26	0.43
1:B:137:LEU:HD12	1:B:137:LEU:HA	1.67	0.43
1:A:69:VAL:O	1:A:70:LYS:C	2.62	0.43
1:A:87:ASN:O	1:A:88:HIS:C	2.59	0.43
1:A:24:ALA:HB1	1:A:248:VAL:HG21	2.01	0.43
1:A:135:VAL:O	1:A:136:MET:C	2.61	0.43
1:A:211:VAL:HG11	1:C:223:MET:HE1	2.00	0.43
1:A:252:LEU:O	1:A:252:LEU:HD12	2.18	0.43
1:B:60:VAL:CG1	1:B:61:THR:H	2.30	0.43
1:C:159:HIS:CE1	1:C:168:SER:HB3	2.53	0.43
1:A:10:ILE:HD11	1:A:25:ALA:HB2	2.00	0.43
1:B:48:ASP:O	1:B:49:ALA:C	2.62	0.43
1:B:48:ASP:O	1:B:50:GLY:N	2.52	0.43
1:C:7:ARG:CB	1:C:73:PHE:HA	2.47	0.43
1:C:86:LEU:O	1:C:89:LEU:CB	2.55	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:ALA:HB2	1:D:73:PHE:CG	2.53	0.43
1:D:52:LEU:HD23	1:D:52:LEU:H	1.83	0.43
1:B:7:ARG:HG3	1:B:7:ARG:HH11	1.83	0.43
1:B:122:ALA:O	1:B:254:LEU:HD11	2.18	0.43
1:D:153:ILE:H	1:D:201:ARG:NH2	2.16	0.43
1:D:264:MET:O	1:D:268:LEU:HD23	2.18	0.43
1:B:273:LEU:CD1	1:C:142:LYS:HD2	2.47	0.43
1:C:11:ALA:HB2	1:C:76:PHE:CZ	2.54	0.43
1:C:93:ARG:O	1:C:94:GLN:C	2.62	0.43
1:C:138:LYS:CE	1:C:272:ASN:H	2.32	0.43
1:D:80:THR:O	4:D:302:NAI:H4D	2.19	0.43
1:A:89:LEU:HD21	1:A:117:ALA:HB1	2.01	0.42
1:C:7:ARG:HA	1:C:32:GLN:O	2.19	0.42
1:C:89:LEU:CD2	1:C:99:MET:HE3	2.49	0.42
1:D:42:SER:C	1:D:44:LEU:N	2.77	0.42
1:D:78:ASP:C	1:D:79:PHE:HD1	2.26	0.42
1:D:87:ASN:O	1:D:88:HIS:C	2.62	0.42
1:D:16:ARG:H	1:D:16:ARG:HG2	1.61	0.42
1:D:270:LEU:O	1:D:272:ASN:N	2.52	0.42
1:B:42:SER:C	1:B:44:LEU:N	2.76	0.42
1:C:42:SER:C	1:C:44:LEU:N	2.78	0.42
1:D:42:SER:O	1:D:45:LEU:HD23	2.20	0.42
1:A:83:GLU:CA	1:A:86:LEU:HD23	2.48	0.42
1:C:16:ARG:H	1:C:16:ARG:HG2	1.67	0.42
1:C:155:ILE:O	1:C:208:PHE:HA	2.19	0.42
1:D:163:LYS:NZ	5:D:303:PDC:N1	2.65	0.42
1:B:77:ILE:O	1:B:77:ILE:HG22	2.17	0.42
1:C:114:ILE:H	1:C:114:ILE:HD12	1.85	0.42
1:D:42:SER:O	1:D:45:LEU:CD2	2.67	0.42
1:A:57:LYS:O	1:A:58:THR:C	2.62	0.42
1:A:241:MET:O	1:A:244:ALA:N	2.53	0.42
1:A:160:HIS:CB	1:A:214:GLY:O	2.67	0.42
1:B:92:CYS:O	1:B:97:LYS:O	2.37	0.42
1:D:131:VAL:O	1:D:132:GLY:C	2.62	0.42
1:A:65:SER:CB	1:A:68:ALA:HB2	2.50	0.42
1:D:123:ILE:HG22	1:D:124:VAL:N	2.34	0.42
1:B:158:ALA:HA	1:B:211:VAL:O	2.20	0.42
1:D:160:HIS:HB2	1:D:214:GLY:O	2.20	0.42
1:D:33:LEU:O	1:D:60:VAL:HG21	2.20	0.41
1:C:83:GLU:CD	1:C:83:GLU:H	2.26	0.41
1:C:261:LEU:C	1:C:261:LEU:HD23	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:LEU:HD11	1:D:64:SER:HB3	2.02	0.41
1:D:110:GLY:O	1:D:114:ILE:HD12	2.21	0.41
1:A:28:LEU:HD13	1:A:29:GLU:O	2.21	0.41
1:A:75:VAL:HG23	1:A:98:GLY:C	2.44	0.41
1:A:254:LEU:O	1:A:256:GLY:N	2.53	0.41
1:C:93:ARG:C	1:C:96:GLY:H	2.27	0.41
1:D:5:ASN:N	1:D:5:ASN:ND2	2.67	0.41
1:D:19:ARG:HA	1:D:53:ALA:CB	2.50	0.41
1:A:57:LYS:O	1:A:58:THR:O	2.38	0.41
1:A:124:VAL:CG2	1:A:254:LEU:HD21	2.47	0.41
1:A:201:ARG:NH2	1:A:205:THR:O	2.52	0.41
1:D:67:ASP:O	1:D:70:LYS:HG2	2.20	0.41
1:D:189:CYS:HB2	1:D:205:THR:HA	2.03	0.41
1:A:130:SER:OG	1:D:229:GLU:OE1	2.37	0.41
1:A:212:ARG:HD3	1:A:212:ARG:HA	1.87	0.41
1:B:78:ASP:C	1:B:79:PHE:HD1	2.28	0.41
1:C:87:ASN:O	1:C:90:ALA:N	2.53	0.41
1:C:110:GLY:O	1:C:114:ILE:HD12	2.21	0.41
1:A:154:GLU:OE1	1:A:194:ARG:NH1	2.44	0.41
1:A:265:ARG:O	1:A:269:ASP:N	2.54	0.41
1:A:267:VAL:HG12	6:A:430:HOH:O	2.21	0.41
1:B:67:ASP:HB3	1:B:70:LYS:HD3	2.02	0.41
1:B:82:PRO:HA	1:B:106:PHE:CE1	2.56	0.41
1:C:67:ASP:HB3	1:C:70:LYS:HD3	2.03	0.41
1:D:83:GLU:CD	1:D:83:GLU:H	2.29	0.41
1:C:26:LEU:HD12	1:C:26:LEU:HA	1.85	0.41
1:C:217:VAL:HB	1:C:237:ALA:O	2.20	0.41
1:D:140:LEU:O	1:D:141:GLU:C	2.64	0.41
1:A:81:ARG:O	1:A:85:THR:OG1	2.39	0.41
1:A:159:HIS:CE1	1:A:168:SER:HB3	2.56	0.41
1:B:5:ASN:HA	1:B:32:GLN:OE1	2.20	0.41
1:B:79:PHE:CZ	1:B:102:GLY:HA3	2.56	0.41
1:B:114:ILE:CG2	1:B:261:LEU:HD11	2.47	0.41
1:B:197:HIS:ND1	1:B:197:HIS:C	2.78	0.41
1:C:263:ASP:N	1:C:266:ASP:OD1	2.54	0.41
1:D:32:GLN:O	1:D:34:GLY:N	2.54	0.41
1:D:76:PHE:HB3	1:D:99:MET:CG	2.50	0.41
1:D:137:LEU:HD12	1:D:137:LEU:HA	1.72	0.41
1:D:217:VAL:HB	1:D:237:ALA:O	2.21	0.41
1:C:82:PRO:O	1:C:86:LEU:HG	2.21	0.41
1:D:16:ARG:O	1:D:20:GLN:HG2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:ILE:HD12	1:D:114:ILE:H	1.85	0.41
1:B:26:LEU:HA	1:B:26:LEU:HD12	1.80	0.40
1:D:88:HIS:N	1:D:88:HIS:ND1	2.60	0.40
1:D:273:LEU:HD22	1:D:273:LEU:OXT	2.21	0.40
1:A:273:LEU:HA	1:A:273:LEU:HD23	1.37	0.40
1:B:60:VAL:CG1	1:B:61:THR:N	2.84	0.40
1:B:154:GLU:OE2	1:B:201:ARG:NH1	2.55	0.40
1:A:164:VAL:O	1:C:197:HIS:HA	2.21	0.40
1:B:266:ASP:HA	1:B:271:ASN:HD21	1.86	0.40
1:C:123:ILE:HG22	1:C:124:VAL:N	2.36	0.40
1:A:21:LEU:HD23	1:A:21:LEU:HA	1.84	0.40
1:A:157:GLU:CD	1:A:212:ARG:HH12	2.29	0.40
1:A:178:ILE:O	1:A:179:ALA:C	2.63	0.40
1:A:199:GLY:O	1:C:164:VAL:HA	2.21	0.40
1:B:15:GLY:HA3	4:B:302:NAI:H4B	2.02	0.40
1:C:91:PHE:CZ	1:C:95:HIS:CD2	3.10	0.40
1:C:156:ILE:HG23	1:C:209:ALA:HB3	2.02	0.40
1:D:25:ALA:HA	1:D:31:VAL:CG1	2.52	0.40
1:A:74:ASP:O	1:A:97:LYS:O	2.39	0.40
1:A:79:PHE:CD2	1:A:102:GLY:HA3	2.56	0.40
1:B:144:ALA:O	1:B:148:GLY:HA3	2.22	0.40
1:C:265:ARG:O	1:C:269:ASP:CA	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	117/273 (43%)	102 (87%)	14 (12%)	1 (1%)	14	30
1	C	69/273 (25%)	57 (83%)	9 (13%)	3 (4%)	2	2
All	All	186/546 (34%)	159 (86%)	23 (12%)	4 (2%)	5	10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	4	ALA
1	C	70	LYS
1	C	49	ALA
1	B	160	HIS

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	69/201 (34%)	62 (90%)	7 (10%)	7	15
1	B	112/201 (56%)	93 (83%)	19 (17%)	2	4
1	C	193/201 (96%)	166 (86%)	27 (14%)	3	6
1	D	195/201 (97%)	163 (84%)	32 (16%)	2	4
All	All	569/804 (71%)	484 (85%)	85 (15%)	3	5

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	LYS
1	A	206	ILE
1	A	227	ILE
1	A	231	LEU
1	A	239	SER
1	A	268	LEU
1	A	273	LEU
1	B	5	ASN
1	B	26	LEU
1	B	32	GLN
1	B	40	GLU
1	B	44	LEU
1	B	51	GLU
1	B	60	VAL
1	B	62	VAL
1	B	66	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	67	ASP
1	B	71	ASP
1	B	176	GLU
1	B	227	ILE
1	B	231	LEU
1	B	240	ARG
1	B	254	LEU
1	B	261	LEU
1	B	272	ASN
1	B	273	LEU
1	C	26	LEU
1	C	52	LEU
1	C	62	VAL
1	C	63	GLN
1	C	66	LEU
1	C	67	ASP
1	C	71	ASP
1	C	83	GLU
1	C	87	ASN
1	C	88	HIS
1	C	95	HIS
1	C	99	MET
1	C	108	GLU
1	C	115	ARG
1	C	120	ASP
1	C	137	LEU
1	C	145	LYS
1	C	176	GLU
1	C	184	LYS
1	C	197	HIS
1	C	227	ILE
1	C	231	LEU
1	C	240	ARG
1	C	252	LEU
1	C	255	SER
1	C	258	GLU
1	C	262	PHE
1	D	5	ASN
1	D	6	ILE
1	D	26	LEU
1	D	31	VAL
1	D	39	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	42	SER
1	D	43	SER
1	D	44	LEU
1	D	52	LEU
1	D	62	VAL
1	D	66	LEU
1	D	67	ASP
1	D	71	ASP
1	D	83	GLU
1	D	88	HIS
1	D	99	MET
1	D	108	GLU
1	D	115	ARG
1	D	120	ASP
1	D	137	LEU
1	D	145	LYS
1	D	176	GLU
1	D	184	LYS
1	D	198	THR
1	D	227	ILE
1	D	230	ARG
1	D	231	LEU
1	D	240	ARG
1	D	249	ARG
1	D	261	LEU
1	D	262	PHE
1	D	273	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	ASN
1	A	271	ASN
1	A	272	ASN
1	B	20	GLN
1	B	159	HIS
1	B	271	ASN
1	C	20	GLN
1	C	32	GLN
1	C	88	HIS
1	C	128	ASN
1	C	162	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	197	HIS
1	C	272	ASN
1	D	5	ASN
1	D	20	GLN
1	D	32	GLN
1	D	128	ASN
1	D	162	HIS
1	D	197	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	NAI	D	302	-	47,48,48	1.56	9 (19%)	64,73,73	1.92	10 (15%)
5	PDC	B	303	-	12,12,12	4.74	7 (58%)	16,16,16	1.07	0
5	PDC	C	302	-	12,12,12	4.45	7 (58%)	16,16,16	1.49	3 (18%)
5	PDC	D	303	-	12,12,12	3.66	6 (50%)	16,16,16	1.80	6 (37%)
4	NAI	B	302	-	47,48,48	1.57	11 (23%)	64,73,73	1.91	11 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAI	C	301	-	47,48,48	1.88	12 (25%)	64,73,73	1.82	13 (20%)
2	PO4	A	301	-	4,4,4	1.06	1 (25%)	6,6,6	0.45	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	NAI	D	302	-	-	17/29/72/72	0/5/5/5
5	PDC	B	303	-	-	0/8/8/8	0/1/1/1
5	PDC	C	302	-	-	0/8/8/8	0/1/1/1
5	PDC	D	303	-	-	0/8/8/8	0/1/1/1
4	NAI	B	302	-	-	18/29/72/72	0/5/5/5
4	NAI	C	301	-	-	16/29/72/72	0/5/5/5

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	303	PDC	C2-C7	-9.19	1.34	1.50
5	B	303	PDC	C6-C8	-8.45	1.35	1.50
5	C	302	PDC	C2-C7	-7.52	1.37	1.50
5	D	303	PDC	C2-C7	-7.41	1.37	1.50
5	C	302	PDC	C6-C8	-7.05	1.38	1.50
4	C	301	NAI	C4N-C3N	-5.70	1.39	1.50
5	D	303	PDC	C6-C8	-5.68	1.40	1.50
5	C	302	PDC	C6-N1	5.68	1.42	1.34
5	C	302	PDC	O1-C7	5.37	1.38	1.22
5	C	302	PDC	O3-C8	5.27	1.37	1.22
5	C	302	PDC	C2-N1	5.27	1.42	1.34
5	B	303	PDC	C6-N1	5.19	1.42	1.34
5	B	303	PDC	C2-N1	5.09	1.42	1.34
5	B	303	PDC	O3-C8	5.09	1.37	1.22
5	D	303	PDC	O3-C8	4.73	1.36	1.22
5	B	303	PDC	O1-C7	4.65	1.36	1.22
4	D	302	NAI	C4N-C3N	-4.43	1.41	1.50
5	D	303	PDC	C6-N1	4.09	1.40	1.34
4	C	301	NAI	C4A-N9A	-3.99	1.29	1.37
4	C	301	NAI	C7N-C3N	-3.98	1.40	1.48
4	C	301	NAI	C4N-C5N	-3.89	1.38	1.49
5	D	303	PDC	O1-C7	3.68	1.33	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	303	PDC	C2-N1	3.57	1.39	1.34
4	B	302	NAI	C6N-C5N	3.50	1.43	1.33
4	C	301	NAI	C5A-C4A	-3.48	1.32	1.39
4	D	302	NAI	C5A-C4A	-3.39	1.33	1.39
4	D	302	NAI	C7N-C3N	-3.34	1.41	1.48
4	D	302	NAI	C4N-C5N	-3.23	1.40	1.49
4	B	302	NAI	C5A-N7A	-3.06	1.33	1.39
4	C	301	NAI	O5B-C5B	2.89	1.55	1.44
4	B	302	NAI	C2N-C3N	2.83	1.43	1.35
4	B	302	NAI	C8A-N7A	2.82	1.37	1.31
4	D	302	NAI	C4A-N9A	-2.79	1.31	1.37
4	B	302	NAI	C1D-N1N	2.78	1.54	1.46
4	B	302	NAI	C1B-N9A	2.49	1.53	1.46
4	B	302	NAI	C4N-C3N	-2.47	1.45	1.50
4	B	302	NAI	O5B-C5B	2.46	1.53	1.44
4	C	301	NAI	C6N-C5N	2.45	1.40	1.33
4	C	301	NAI	C2B-C1B	-2.45	1.45	1.53
4	B	302	NAI	C2A-N1A	2.45	1.38	1.33
4	B	302	NAI	C5A-C4A	-2.41	1.34	1.39
4	C	301	NAI	C8A-N7A	2.35	1.36	1.31
5	B	303	PDC	O4-C8	2.34	1.37	1.30
4	D	302	NAI	O5B-C5B	2.32	1.53	1.44
4	C	301	NAI	PN-O3	-2.30	1.57	1.59
4	B	302	NAI	C6N-N1N	2.25	1.42	1.37
5	C	302	PDC	C4-C5	2.22	1.42	1.38
4	D	302	NAI	C6N-C5N	2.20	1.39	1.33
4	C	301	NAI	C5B-C4B	2.19	1.58	1.51
4	C	301	NAI	C2N-C3N	2.16	1.41	1.35
4	D	302	NAI	C5A-N7A	-2.07	1.35	1.39
2	A	301	PO4	P-O1	2.06	1.55	1.50
4	D	302	NAI	O5D-C5D	2.06	1.52	1.44

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	302	NAI	C4A-N9A-C1B	7.51	144.19	126.63
4	D	302	NAI	C4A-N9A-C1B	7.42	143.99	126.63
4	D	302	NAI	C1B-N9A-C8A	-6.97	111.62	127.09
4	B	302	NAI	C1B-N9A-C8A	-6.27	113.18	127.09
4	C	301	NAI	C1B-N9A-C8A	-5.88	114.05	127.09
4	C	301	NAI	C4A-N9A-C1B	5.76	140.11	126.63
4	D	302	NAI	O5B-C5B-C4B	4.44	124.12	108.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	301	NAI	O5B-C5B-C4B	4.38	123.91	108.99
4	C	301	NAI	O5D-C5D-C4D	4.25	123.47	108.99
4	B	302	NAI	O5D-C5D-C4D	3.75	121.75	108.99
4	B	302	NAI	C5A-C4A-N3A	-3.60	121.76	126.72
4	B	302	NAI	O5B-C5B-C4B	3.57	121.15	108.99
4	D	302	NAI	C6N-N1N-C2N	3.54	123.11	119.32
4	B	302	NAI	C6A-C5A-C4A	3.35	121.75	117.18
5	D	303	PDC	C5-C6-N1	-3.31	119.06	122.92
4	D	302	NAI	C6A-C5A-C4A	3.19	121.54	117.18
4	B	302	NAI	C5A-C4A-N9A	3.10	109.19	105.81
4	D	302	NAI	C5A-C4A-N3A	-2.99	122.59	126.72
4	B	302	NAI	C6A-C5A-N7A	-2.99	126.33	132.09
4	C	301	NAI	O4B-C1B-N9A	2.98	113.82	108.09
4	B	302	NAI	C4A-N9A-C8A	-2.98	102.61	105.74
4	C	301	NAI	O3B-C3B-C4B	-2.85	102.89	111.08
5	D	303	PDC	O2-C7-C2	2.85	121.48	114.71
5	C	302	PDC	C5-C6-N1	-2.81	119.64	122.92
4	D	302	NAI	O5D-C5D-C4D	2.80	118.54	108.99
4	D	302	NAI	C5A-C4A-N9A	2.77	108.83	105.81
4	D	302	NAI	C6A-C5A-N7A	-2.74	126.81	132.09
4	C	301	NAI	C5A-C4A-N9A	2.71	108.77	105.81
4	C	301	NAI	C6A-C5A-N7A	-2.59	127.09	132.09
4	C	301	NAI	O4D-C1D-N1N	-2.59	103.15	108.08
5	D	303	PDC	C6-N1-C2	2.41	120.52	117.54
5	C	302	PDC	C3-C2-N1	-2.40	120.12	122.92
4	C	301	NAI	O4B-C4B-C5B	2.36	116.89	109.33
4	B	302	NAI	O4B-C1B-N9A	2.32	112.54	108.09
5	D	303	PDC	O4-C8-C6	2.25	120.05	114.71
4	C	301	NAI	C5A-N7A-C8A	-2.22	99.96	103.45
5	D	303	PDC	O4-C8-O3	-2.20	118.63	123.35
4	C	301	NAI	C6A-C5A-C4A	2.17	120.14	117.18
5	C	302	PDC	C6-N1-C2	2.14	120.18	117.54
5	D	303	PDC	C3-C2-N1	-2.12	120.45	122.92
4	D	302	NAI	O3B-C3B-C4B	-2.10	105.06	111.08
4	C	301	NAI	N3A-C2A-N1A	-2.09	125.41	128.58
4	B	302	NAI	C2D-C3D-C4D	-2.02	98.71	102.61

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	302	NAI	C5B-O5B-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	302	NAI	C5B-O5B-PA-O3
4	B	302	NAI	O4B-C4B-C5B-O5B
4	B	302	NAI	C5D-O5D-PN-O3
4	B	302	NAI	C5D-O5D-PN-O2N
4	C	301	NAI	C5B-O5B-PA-O1A
4	C	301	NAI	C5B-O5B-PA-O2A
4	C	301	NAI	C5B-O5B-PA-O3
4	C	301	NAI	O4B-C4B-C5B-O5B
4	C	301	NAI	C5D-O5D-PN-O2N
4	D	302	NAI	C5D-O5D-PN-O3
4	D	302	NAI	C5D-O5D-PN-O2N
4	D	302	NAI	O4D-C4D-C5D-O5D
4	C	301	NAI	O4D-C4D-C5D-O5D
4	D	302	NAI	O4B-C4B-C5B-O5B
4	B	302	NAI	C3B-C4B-C5B-O5B
4	C	301	NAI	C3B-C4B-C5B-O5B
4	C	301	NAI	C3D-C4D-C5D-O5D
4	D	302	NAI	C3B-C4B-C5B-O5B
4	D	302	NAI	C3D-C4D-C5D-O5D
4	D	302	NAI	C2D-C1D-N1N-C2N
4	C	301	NAI	C2D-C1D-N1N-C2N
4	D	302	NAI	C2D-C1D-N1N-C6N
4	B	302	NAI	O4D-C4D-C5D-O5D
4	C	301	NAI	C2D-C1D-N1N-C6N
4	D	302	NAI	C4B-C5B-O5B-PA
4	B	302	NAI	C2B-C1B-N9A-C8A
4	D	302	NAI	C2B-C1B-N9A-C8A
4	B	302	NAI	PA-O3-PN-O2N
4	D	302	NAI	PN-O3-PA-O1A
4	B	302	NAI	C5D-O5D-PN-O1N
4	C	301	NAI	C5D-O5D-PN-O3
4	C	301	NAI	C5D-O5D-PN-O1N
4	D	302	NAI	C5D-O5D-PN-O1N
4	C	301	NAI	O4D-C1D-N1N-C2N
4	D	302	NAI	O4D-C1D-N1N-C2N
4	D	302	NAI	O4D-C1D-N1N-C6N
4	B	302	NAI	PA-O3-PN-O1N
4	B	302	NAI	O4D-C1D-N1N-C2N
4	B	302	NAI	C2D-C1D-N1N-C2N
4	B	302	NAI	C3D-C4D-C5D-O5D
4	B	302	NAI	C2N-C3N-C7N-N7N
4	C	301	NAI	O4D-C1D-N1N-C6N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	301	NAI	C2N-C3N-C7N-N7N
4	D	302	NAI	C2N-C3N-C7N-N7N
4	B	302	NAI	O4B-C1B-N9A-C8A
4	B	302	NAI	C2B-C1B-N9A-C4A
4	D	302	NAI	O4B-C1B-N9A-C8A
4	B	302	NAI	C4B-C5B-O5B-PA
4	C	301	NAI	PN-O3-PA-O2A
4	D	302	NAI	PN-O3-PA-O2A

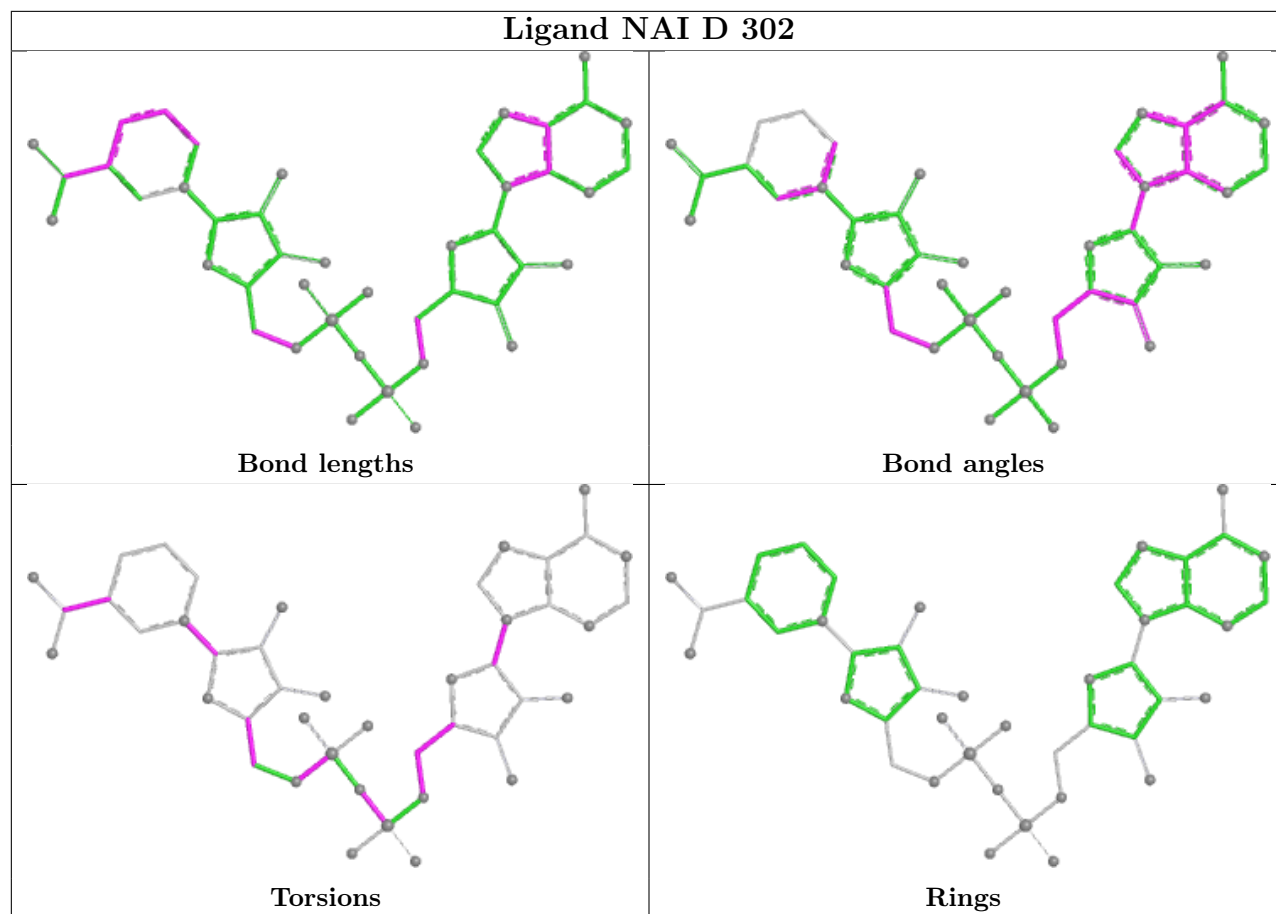
There are no ring outliers.

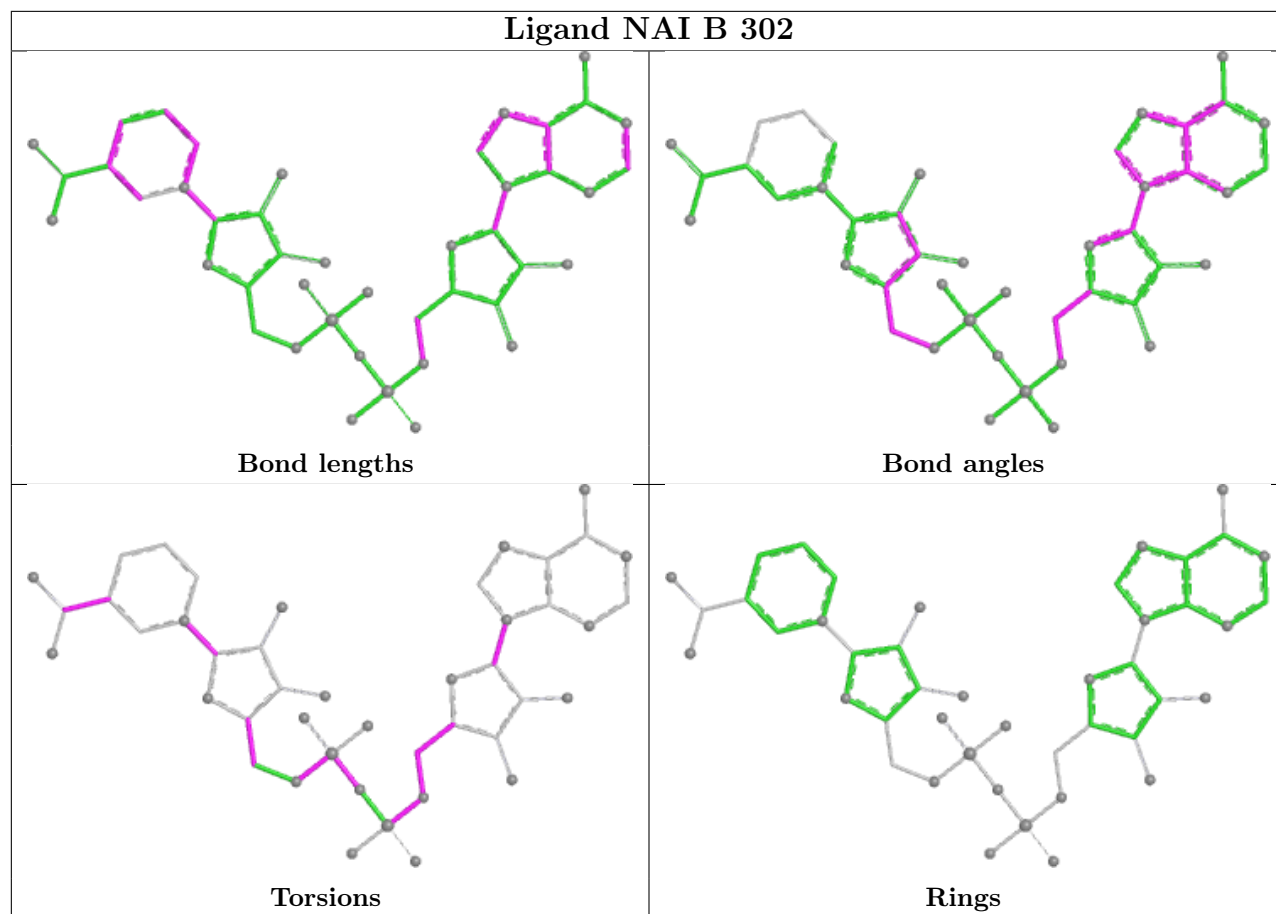
5 monomers are involved in 20 short contacts:

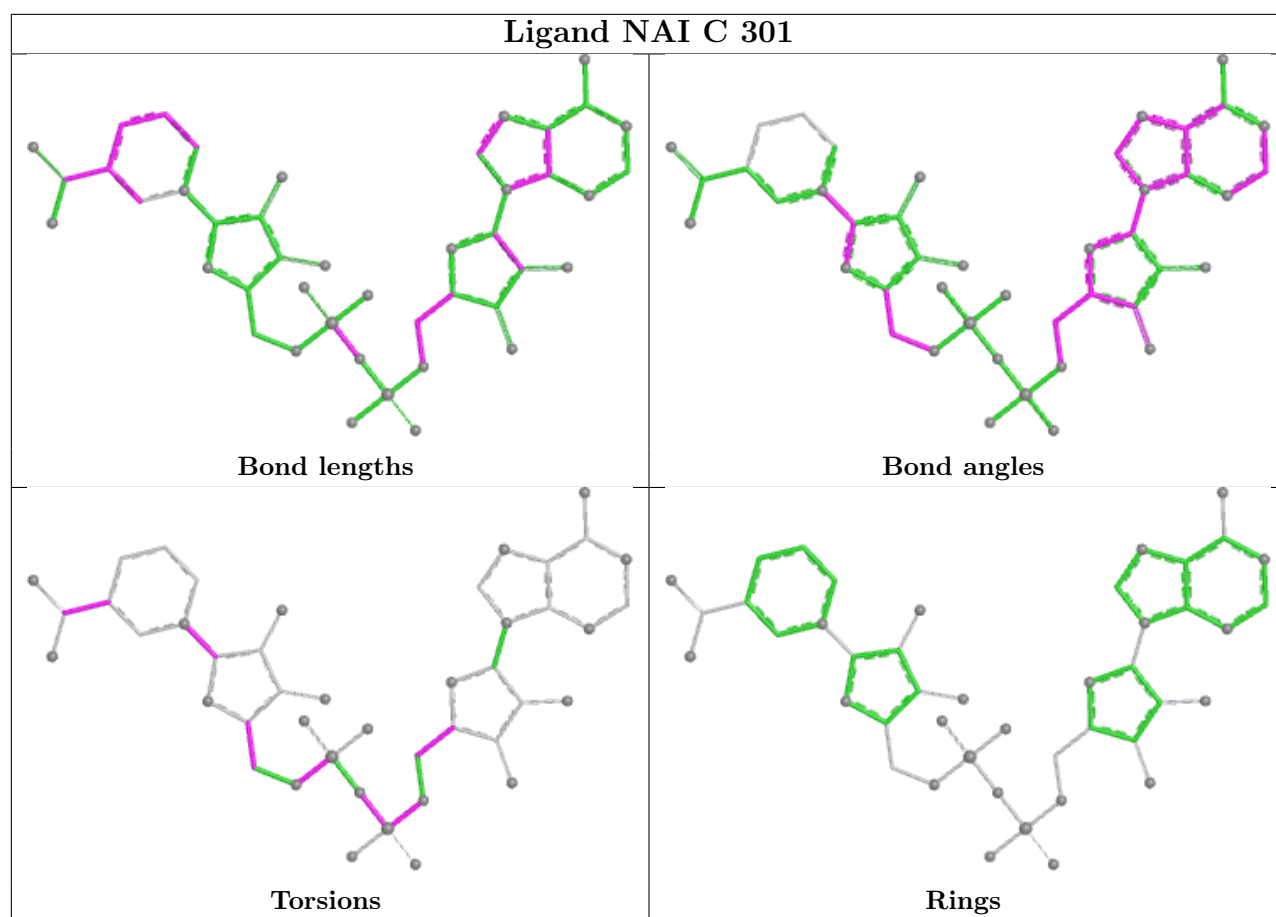
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	302	NAI	5	0
5	C	302	PDC	2	0
5	D	303	PDC	4	0
4	B	302	NAI	6	0
4	C	301	NAI	3	0

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.

Ligand NAI D 302







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	270/273 (98%)	-0.47	0 100 100	5, 30, 64, 87	0
1	B	269/273 (98%)	-0.25	0 100 100	8, 31, 64, 77	0
1	C	271/273 (99%)	-0.34	0 100 100	8, 28, 62, 91	0
1	D	271/273 (99%)	-0.36	0 100 100	9, 29, 62, 77	0
All	All	1081/1092 (98%)	-0.36	0 100 100	5, 30, 63, 91	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PO4	A	301	5/5	0.86	0.13	37,41,50,56	0
4	NAI	B	302	44/44	0.92	0.08	4,32,49,51	0
4	NAI	D	302	44/44	0.94	0.08	2,25,51,52	0
5	PDC	D	303	12/12	0.94	0.10	2,17,22,29	0

Continued on next page...

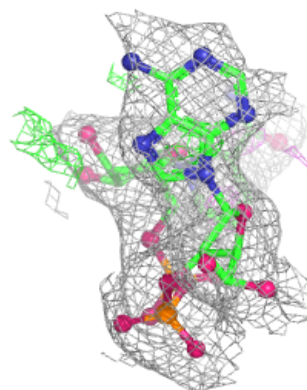
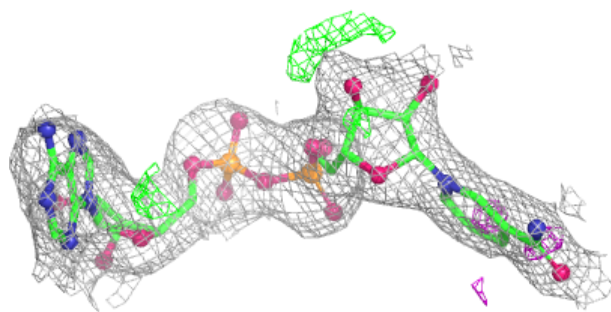
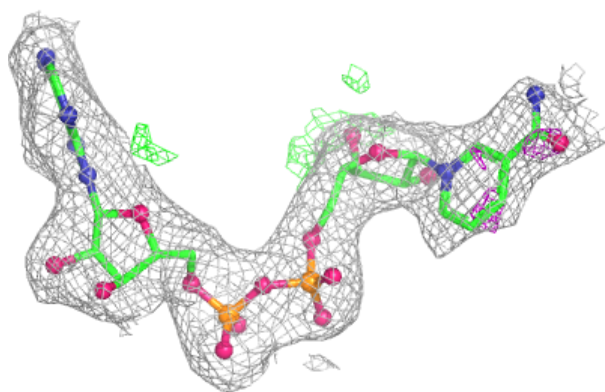
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PDC	C	302	12/12	0.95	0.09	2,11,15,15	0
4	NAI	C	301	44/44	0.96	0.06	7,15,32,35	0
3	K	D	301	1/1	0.96	0.11	24,24,24,24	0
5	PDC	B	303	12/12	0.97	0.08	2,4,12,14	0
3	K	B	301	1/1	0.99	0.04	29,29,29,29	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.

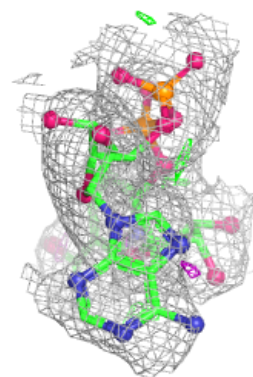
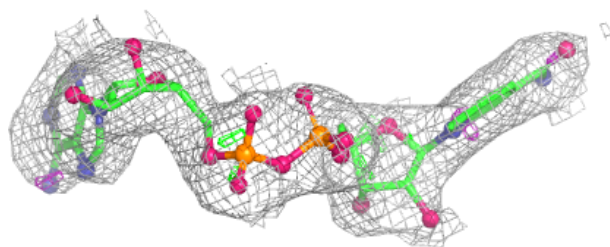
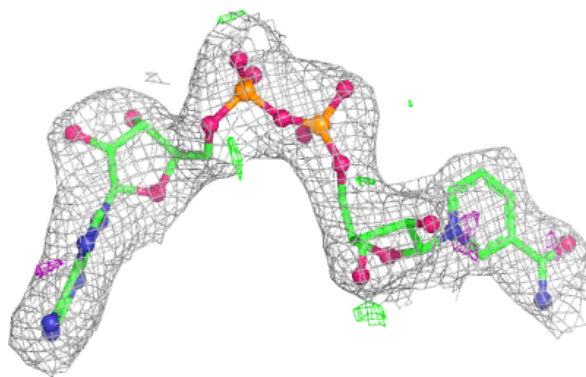
Electron density around NAI B 302:

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

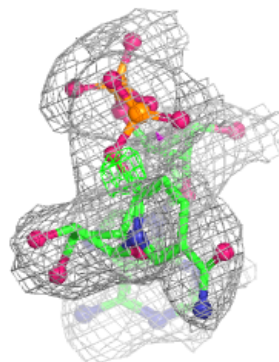
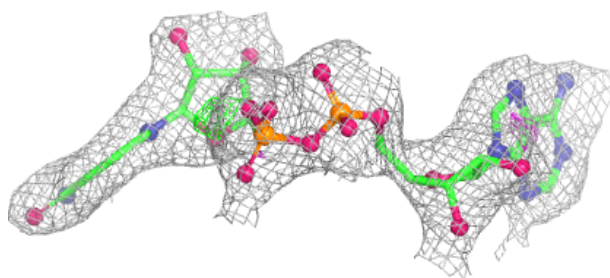
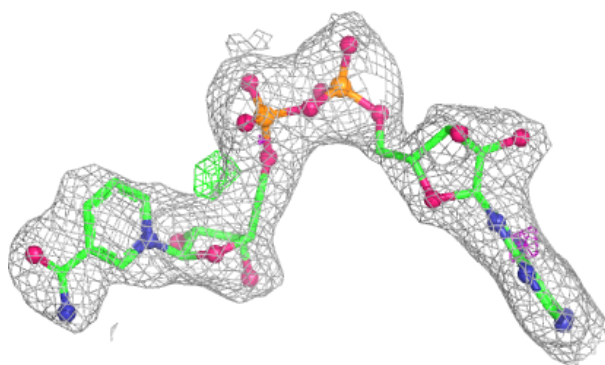


Electron density around NAI D 302:

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

**Electron density around NAI C 301:**

$2mF_o-DF_c$ (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.