



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 10:44 AM BST

PDB ID : 2GRA  
Title : crystal structure of Human Pyrroline-5-carboxylate Reductase complexed with nadp  
Authors : Meng, Z.; Lou, Z.; Liu, Z.; Rao, Z.  
Deposited on : 2006-04-23  
Resolution : 3.10 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.4.dev1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

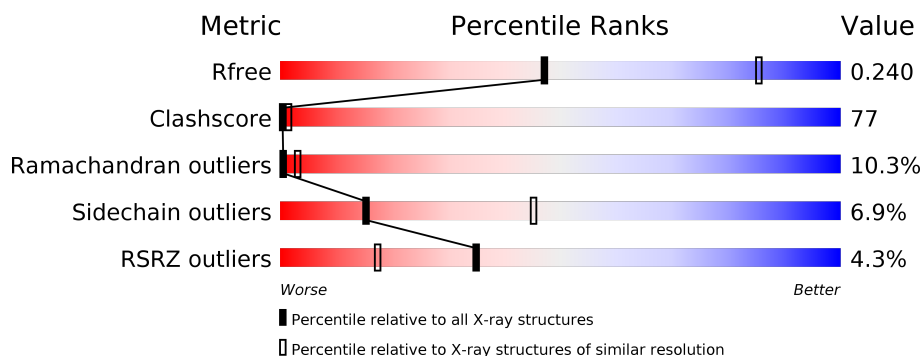
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	277	<div> <div></div> <div> <div>25%</div> <div>58%</div> <div>14%</div> <div>.</div> </div> </div>
1	B	277	<div> <div>11%</div> <div>21%</div> <div>64%</div> <div>15%</div> <div>.</div> </div>
1	C	277	<div> <div>10%</div> <div>27%</div> <div>64%</div> <div>9%</div> </div>
1	D	277	<div> <div>29%</div> <div>60%</div> <div>12%</div> </div>
1	E	277	<div> <div>25%</div> <div>64%</div> <div>11%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAP	A	1300	X	-	-	-
2	NAP	B	2300	-	-	-	X
2	NAP	C	3300	X	-	-	X
2	NAP	D	4300	-	-	-	X
2	NAP	E	5300	X	-	-	X
3	GLU	B	2301	-	-	-	X
3	GLU	C	3301	-	-	-	X
3	GLU	D	4301	-	-	-	X
3	GLU	E	5301	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11079 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 Pyrroline-5-carboxylate reductase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2038	1279	363	383	13			
1	B	276	Total	C	N	O	S	0	0	0
			2023	1270	358	382	13			
1	C	277	Total	C	N	O	S	0	0	0
			2032	1276	360	383	13			
1	D	277	Total	C	N	O	S	0	0	0
			2038	1279	363	383	13			
1	E	277	Total	C	N	O	S	0	0	0
			2038	1279	363	383	13			

There are 10 discrepancies between the modelled and reference sequences:

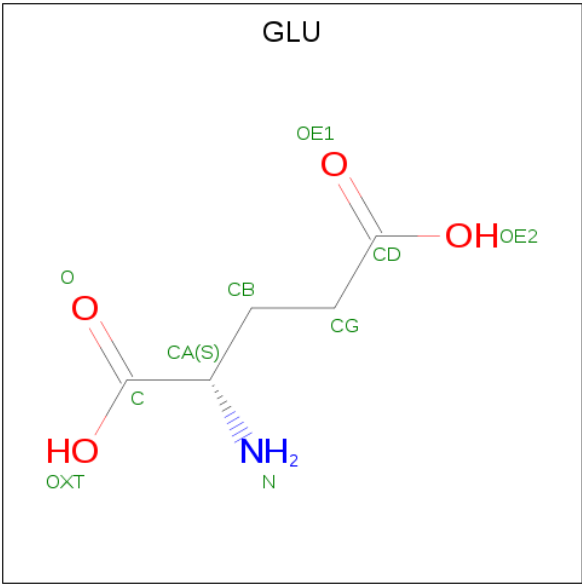
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ARG	-	CLONING ARTIFACT	UNP P32322
A	0	GLY	-	CLONING ARTIFACT	UNP P32322
B	-1	ARG	-	CLONING ARTIFACT	UNP P32322
B	0	GLY	-	CLONING ARTIFACT	UNP P32322
C	-1	ARG	-	CLONING ARTIFACT	UNP P32322
C	0	GLY	-	CLONING ARTIFACT	UNP P32322
D	-1	ARG	-	CLONING ARTIFACT	UNP P32322
D	0	GLY	-	CLONING ARTIFACT	UNP P32322
E	-1	ARG	-	CLONING ARTIFACT	UNP P32322
E	0	GLY	-	CLONING ARTIFACT	UNP P32322

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is GLUTAMIC ACID (three-letter code: GLU) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	5	1	4		
3	B	1	Total	C	N	O	0	0
			10	5	1	4		
3	C	1	Total	C	N	O	0	0
			10	5	1	4		
3	D	1	Total	C	N	O	0	0
			10	5	1	4		
3	E	1	Total	C	N	O	0	0
			10	5	1	4		

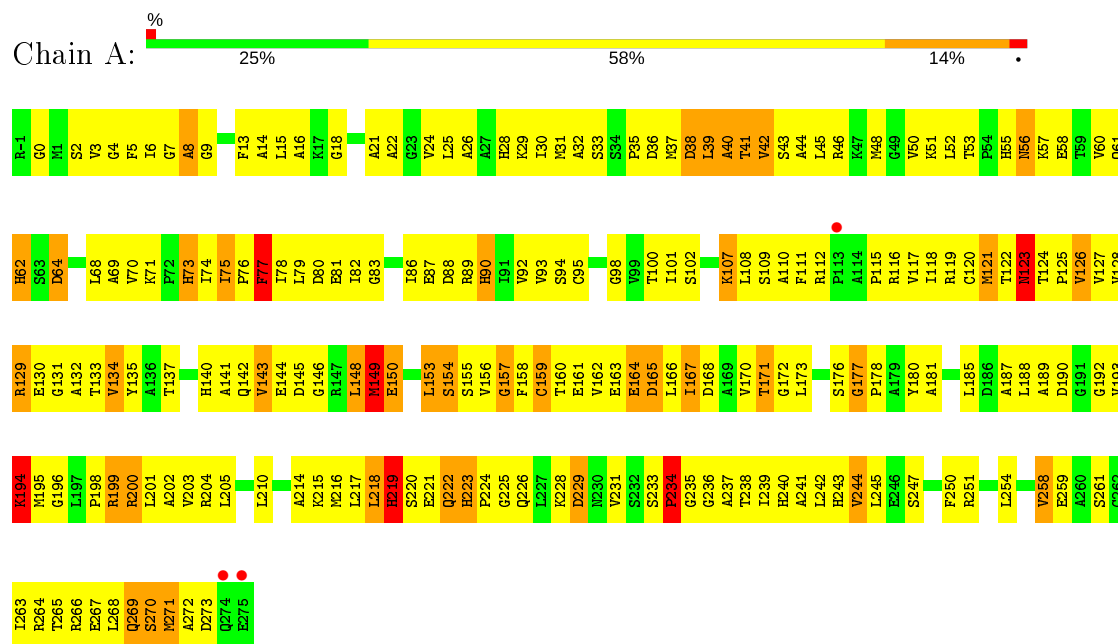
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	127	Total	O	0	0
			127	127		
4	B	100	Total	O	0	0
			100	100		
4	C	104	Total	O	0	0
			104	104		
4	D	125	Total	O	0	0
			125	125		
4	E	164	Total	O	0	0
			164	164		

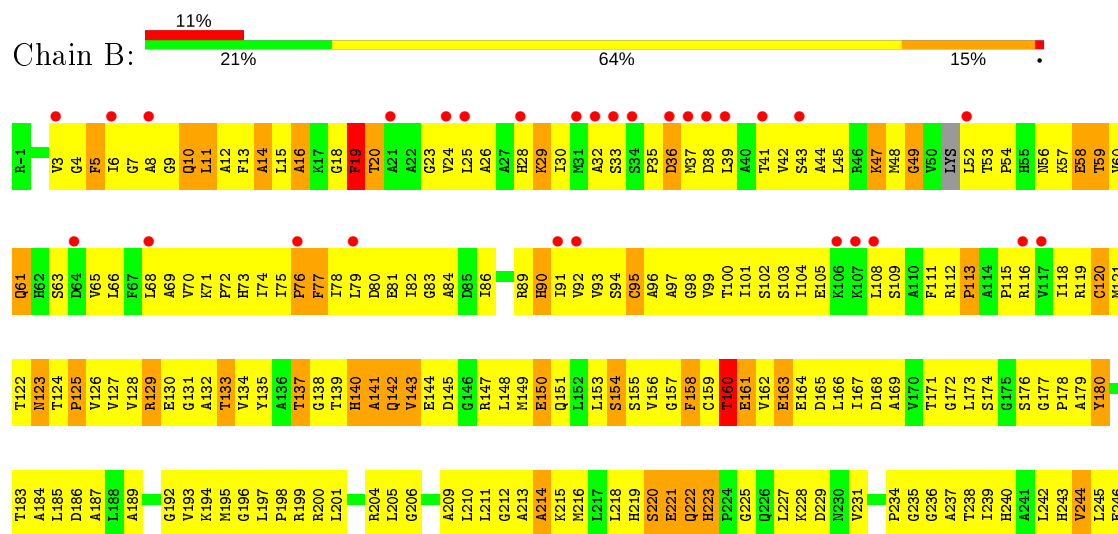
### 3 Residue-property plots

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: Pyrroline-5-carboxylate reductase 1

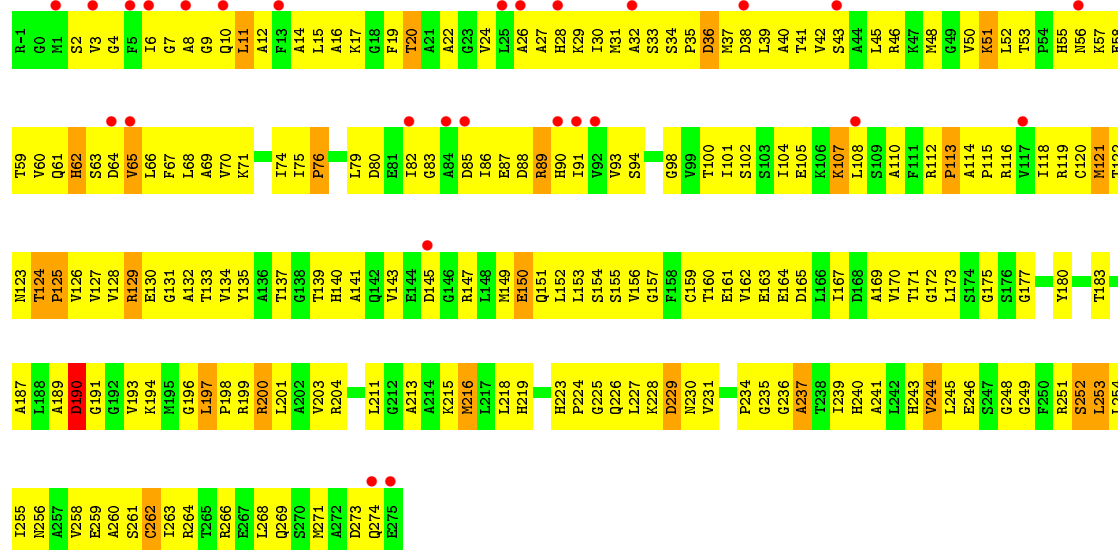


#### • Molecule 1: Pyrroline-5-carboxylate reductase 1

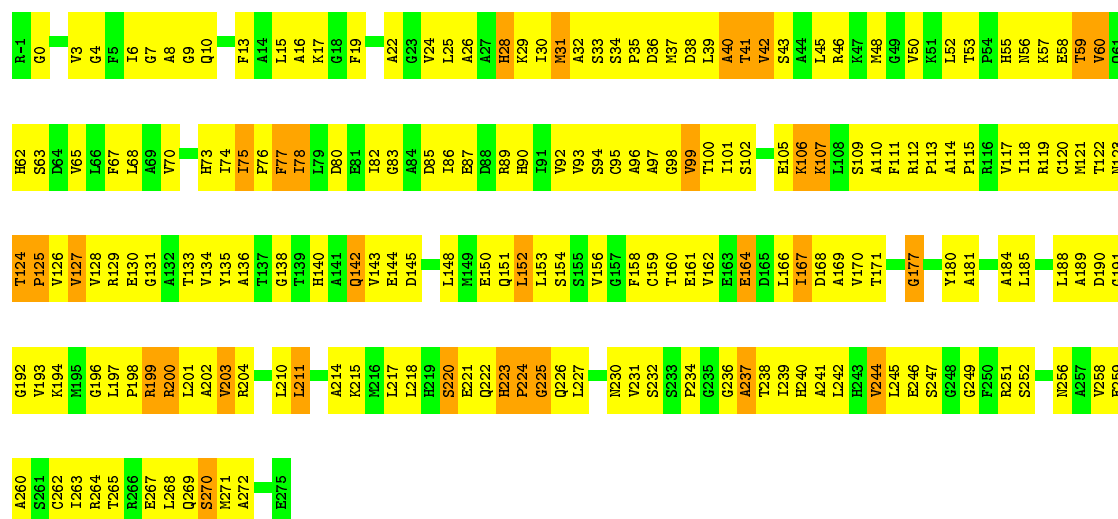




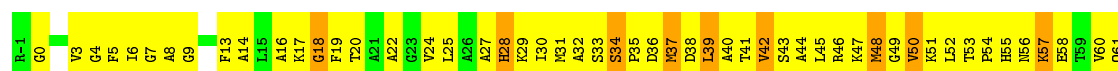
● Molecule 1: Pyrroline-5-carboxylate reductase 1



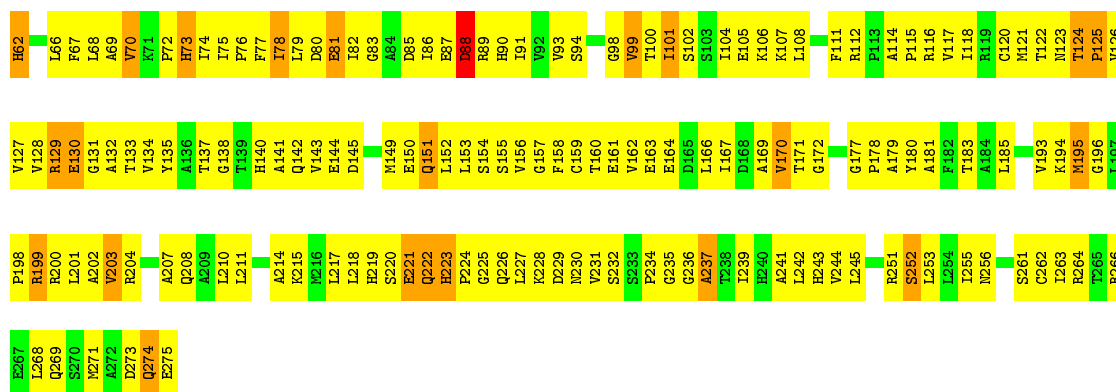
● Molecule 1: Pyrroline-5-carboxylate reductase 1



● Molecule 1: Pyrroline-5-carboxylate reductase 1







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	207.87Å 123.50Å 120.83Å 90.00° 121.97° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 48.42 – 3.01	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.10) 96.0 (48.42-3.01)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.228 , 0.249 0.223 , 0.240	Depositor DCC
$R_{free}$ test set	2528 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.0	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 126.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.017 for $-1/2^*h+1/2^*k+1, 1/2^*h-1/2^*k+1, 1/2^*h+1/2^*k$ 0.026 for $-1/2^*h-1/2^*k+1, -1/2^*h-1/2^*k-1, 1/2^*h-1/2^*k$	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11079	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAP

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	0.61	3/2069 (0.1%)	0.79	7/2800 (0.2%)
1	B	0.34	0/2053	0.65	1/2779 (0.0%)
1	C	0.35	0/2063	0.66	0/2793
1	D	0.36	0/2069	0.68	0/2800
1	E	0.39	0/2069	0.70	0/2800
All	All	0.42	3/10323 (0.0%)	0.70	8/13972 (0.1%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219	HIS	C-N	16.69	1.72	1.34
1	A	157	GLY	C-N	9.66	1.56	1.34
1	A	153	LEU	C-N	-9.30	1.12	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	HIS	O-C-N	-10.31	106.20	122.70
1	A	219	HIS	CA-C-N	7.21	133.06	117.20
1	A	157	GLY	O-C-N	7.14	134.12	122.70
1	A	219	HIS	C-N-CA	6.86	138.84	121.70
1	A	154	SER	O-C-N	6.26	132.72	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	157	GLY	CA-C-N	-5.41	105.30	117.20
1	A	154	SER	CA-C-N	-5.21	105.74	117.20
1	B	49	GLY	N-CA-C	-5.04	100.50	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	218	LEU	Mainchain

## 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	2038	0	2082	327	0
1	B	2023	0	2059	345	0
1	C	2032	0	2073	310	2
1	D	2038	0	2084	279	0
1	E	2038	0	2084	328	1
2	A	48	0	23	18	0
2	B	48	0	22	15	0
2	C	48	0	21	12	0
2	D	48	0	22	11	1
2	E	48	0	21	14	0
3	A	10	0	5	3	0
3	B	10	0	5	3	0
3	C	10	0	5	1	0
3	D	10	0	5	2	0
3	E	10	0	5	0	0
4	A	127	0	0	63	3
4	B	100	0	0	45	0
4	C	104	0	0	57	1
4	D	125	0	0	59	0
4	E	164	0	0	53	0
All	All	11079	0	10516	1619	4

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 77.

All (1619) 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)
2:E:5300:NAP:N7A	2:E:5300:NAP:C8A	1.72	1.51
2:A:1300:NAP:N7A	2:A:1300:NAP:C8A	1.72	1.49
2:C:3300:NAP:N7A	2:C:3300:NAP:C8A	1.72	1.45
2:D:4300:NAP:C8A	2:D:4300:NAP:N7A	1.71	1.40
2:B:2300:NAP:N7A	2:B:2300:NAP:C8A	1.72	1.40
1:A:219:HIS:C	1:A:220:SER:N	1.72	1.39
2:A:1300:NAP:C5D	2:A:1300:NAP:O5D	1.78	1.32
2:A:1300:NAP:C5D	2:A:1300:NAP:PN	2.22	1.27
1:A:215:LYS:NZ	4:A:1320:HOH:O	1.67	1.24
1:E:200:ARG:O	1:E:204:ARG:HG2	1.44	1.16
1:B:200:ARG:O	1:B:204:ARG:HG2	1.46	1.15
1:B:74:ILE:HD11	1:B:99:VAL:HG11	1.31	1.05
1:D:122:THR:HG22	1:D:133:THR:CB	1.86	1.05
1:A:129:ARG:HD2	4:A:1316:HOH:O	1.54	1.05
1:B:236:GLY:HA2	1:B:239:ILE:HG22	1.35	1.05
1:D:53:THR:HG22	1:D:55:HIS:H	1.16	1.04
1:D:87:GLU:H	1:D:90:HIS:HD2	1.04	1.02
1:D:122:THR:HG22	1:D:133:THR:HB	1.02	1.00
1:C:8:ALA:HB3	1:C:34:SER:HB2	1.41	0.98
1:D:122:THR:CG2	1:D:133:THR:HB	1.92	0.98
1:D:258:VAL:HA	4:D:4303:HOH:O	1.65	0.96
1:E:121:MET:HE2	1:E:122:THR:H	1.28	0.96
1:E:274:GLN:HG3	1:E:275:GLU:H	1.29	0.96
1:C:112:ARG:HH11	1:C:113:PRO:HD2	1.31	0.96
1:B:123:ASN:HB2	1:B:125:PRO:HD2	1.48	0.95
1:A:198:PRO:HG2	1:A:201:LEU:HB3	1.48	0.95
1:C:200:ARG:O	1:C:204:ARG:HG2	1.66	0.95
1:E:123:ASN:HD21	1:E:132:ALA:H	1.10	0.94
1:B:246:GLU:HB3	4:B:2331:HOH:O	1.66	0.94
1:B:79:LEU:HD11	1:B:104:ILE:HD12	1.48	0.94
4:B:2356:HOH:O	1:E:194:LYS:HD2	1.67	0.94
1:B:158:PHE:HB3	4:B:2359:HOH:O	1.65	0.93
1:B:74:ILE:HA	1:B:78:ILE:HG13	1.49	0.93
1:E:39:LEU:H	1:E:39:LEU:HD23	1.33	0.93
1:B:75:ILE:HB	1:B:76:PRO:HD3	1.49	0.93
1:D:37:MET:SD	1:D:42:VAL:HG11	2.07	0.93
1:D:121:MET:HG2	4:D:4405:HOH:O	1.69	0.92
1:D:30:ILE:HB	1:D:50:VAL:HG23	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:GLY:HA2	1:B:239:ILE:CG2	1.99	0.92
1:D:126:VAL:HG13	1:D:156:VAL:HG11	1.52	0.91
1:C:31:MET:HB3	1:C:59:THR:HG23	1.53	0.91
1:B:164:GLU:HG3	1:B:167:ILE:HD12	1.50	0.91
1:E:236:GLY:HA2	1:E:239:ILE:HG22	1.53	0.91
1:E:9:GLY:H	1:E:41:THR:HG21	1.31	0.91
2:A:1300:NAP:C4D	2:A:1300:NAP:O5D	2.18	0.90
1:B:122:THR:HG22	1:B:133:THR:HB	1.49	0.90
1:A:126:VAL:HG13	4:A:1401:HOH:O	1.72	0.90
1:D:200:ARG:O	1:D:204:ARG:HG3	1.73	0.89
1:A:37:MET:HA	1:A:42:VAL:HG21	1.53	0.89
1:B:125:PRO:HG2	1:B:131:GLY:HA2	1.55	0.88
1:E:57:LYS:HD3	1:E:57:LYS:H	1.39	0.88
1:B:83:GLY:HA2	1:B:86:ILE:HD12	1.54	0.88
1:A:204:ARG:HG2	4:A:1335:HOH:O	1.72	0.88
1:A:122:THR:HG22	1:A:123:ASN:H	1.38	0.87
1:A:118:ILE:HG22	1:A:137:THR:HA	1.57	0.87
1:D:180:TYR:HA	4:D:4333:HOH:O	1.74	0.87
1:E:14:ALA:HA	1:E:127:VAL:HG22	1.54	0.87
1:E:180:TYR:HA	4:E:5307:HOH:O	1.74	0.87
1:C:32:ALA:HB1	4:C:3383:HOH:O	1.75	0.86
1:B:45:LEU:HB2	1:B:52:LEU:HD21	1.56	0.86
1:D:162:VAL:HG13	1:D:166:LEU:HD12	1.58	0.86
1:D:17:LYS:HD2	1:D:127:VAL:HG12	1.57	0.86
1:A:128:VAL:O	1:A:129:ARG:HB2	1.72	0.86
1:C:86:ILE:HD11	1:C:108:LEU:HD22	1.56	0.85
1:B:79:LEU:HD13	1:B:104:ILE:HG23	1.58	0.85
1:D:124:THR:O	1:D:127:VAL:HG23	1.77	0.85
1:D:9:GLY:H	1:D:41:THR:HG21	1.41	0.85
1:B:147:ARG:HG3	1:B:151:GLN:HE21	1.42	0.84
1:E:245:LEU:HG	4:E:5420:HOH:O	1.77	0.84
1:C:112:ARG:HG3	1:C:113:PRO:HD2	1.57	0.84
1:B:143:VAL:HG12	1:B:144:GLU:H	1.42	0.83
2:A:1300:NAP:H52N	2:A:1300:NAP:PN	2.19	0.83
1:B:198:PRO:HG2	1:B:201:LEU:HB3	1.59	0.83
1:A:45:LEU:HB2	1:A:52:LEU:HD11	1.59	0.83
1:A:162:VAL:HG13	1:A:166:LEU:HD12	1.61	0.83
1:E:86:ILE:HG22	4:E:5449:HOH:O	1.79	0.83
1:A:126:VAL:HG22	1:A:156:VAL:HG12	1.60	0.83
1:C:26:ALA:HB3	1:C:29:LYS:HG2	1.59	0.83
1:A:234:PRO:HB3	1:C:196:GLY:O	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:LYS:HD3	1:C:71:LYS:H	1.42	0.83
1:C:234:PRO:HA	1:D:193:VAL:HG13	1.61	0.82
1:D:87:GLU:H	1:D:90:HIS:CD2	1.94	0.82
1:A:26:ALA:HB3	1:A:29:LYS:HB2	1.61	0.82
1:D:129:ARG:HA	1:D:156:VAL:HG13	1.62	0.82
1:C:252:SER:O	1:C:254:LEU:N	2.12	0.82
1:D:39:LEU:O	1:D:43:SER:HB3	1.81	0.81
1:E:9:GLY:N	1:E:41:THR:HG21	1.94	0.81
1:A:123:ASN:HD21	1:A:132:ALA:H	1.24	0.81
1:E:224:PRO:HA	4:E:5315:HOH:O	1.80	0.81
1:E:7:GLY:H	1:E:33:SER:HB2	1.46	0.81
1:A:269:GLN:HA	4:A:1386:HOH:O	1.81	0.81
1:E:53:THR:HG21	1:E:58:GLU:HB2	1.62	0.81
1:E:221:GLU:HA	2:E:5300:NAP:O2X	1.80	0.80
1:E:154:SER:O	2:E:5300:NAP:N7N	2.14	0.80
1:C:134:VAL:HB	4:C:3368:HOH:O	1.80	0.80
1:A:13:PHE:HA	1:A:45:LEU:HD21	1.61	0.80
1:E:217:LEU:HD21	1:E:224:PRO:HG3	1.63	0.80
1:B:138:GLY:HA3	4:B:2377:HOH:O	1.82	0.80
1:E:274:GLN:HG3	1:E:275:GLU:HG2	1.63	0.80
1:B:75:ILE:HD11	1:B:99:VAL:HG22	1.63	0.80
1:A:202:ALA:HB3	4:A:1313:HOH:O	1.82	0.79
1:E:37:MET:SD	1:E:42:VAL:HG11	2.23	0.79
1:A:89:ARG:HG3	1:A:90:HIS:H	1.47	0.79
1:C:53:THR:HG22	1:C:55:HIS:H	1.46	0.79
1:D:9:GLY:N	1:D:41:THR:HG21	1.96	0.79
1:A:121:MET:HB3	4:A:1352:HOH:O	1.82	0.79
1:B:124:THR:N	1:B:125:PRO:HD2	1.97	0.79
1:B:135:TYR:CE1	1:B:161:GLU:HB3	2.17	0.79
1:E:121:MET:HE2	1:E:122:THR:N	1.96	0.79
2:A:1300:NAP:C5N	3:A:1301:GLU:OXT	2.30	0.79
1:A:236:GLY:HA2	1:A:239:ILE:CG2	2.13	0.79
1:D:227:LEU:HB2	4:D:4321:HOH:O	1.81	0.79
1:B:200:ARG:HG2	1:B:204:ARG:HE	1.48	0.79
1:B:71:LYS:H	1:B:71:LYS:HD2	1.47	0.78
1:D:68:LEU:HD12	1:D:94:SER:HB2	1.64	0.78
1:B:123:ASN:HB3	4:B:2397:HOH:O	1.82	0.78
1:B:11:LEU:O	1:B:15:LEU:HD12	1.83	0.78
1:D:156:VAL:O	1:D:156:VAL:HG12	1.83	0.78
1:D:75:ILE:HB	1:D:76:PRO:HD3	1.66	0.78
1:C:29:LYS:HB3	4:C:3313:HOH:O	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:SER:HB3	1:C:62:HIS:O	1.84	0.78
1:E:55:HIS:HB3	1:E:57:LYS:HE2	1.63	0.78
1:B:79:LEU:CD1	1:B:104:ILE:HD12	2.13	0.77
1:C:155:SER:HA	2:C:3300:NAP:N7N	1.98	0.77
1:E:123:ASN:ND2	1:E:132:ALA:H	1.82	0.77
1:E:181:ALA:O	1:E:185:LEU:HD12	1.85	0.77
1:A:126:VAL:HG22	1:A:156:VAL:CG1	2.13	0.77
1:A:30:ILE:HB	1:A:50:VAL:HG13	1.66	0.77
1:B:93:VAL:HG12	1:B:95:CYS:SG	2.24	0.77
1:C:9:GLY:H	1:C:12:ALA:HB3	1.50	0.77
1:E:53:THR:HG22	1:E:55:HIS:H	1.49	0.77
1:B:71:LYS:HB3	1:B:72:PRO:HD2	1.64	0.77
1:C:198:PRO:HG2	1:C:201:LEU:HB3	1.66	0.77
1:A:128:VAL:HB	4:A:1338:HOH:O	1.84	0.76
1:A:68:LEU:HD12	1:A:94:SER:HB2	1.67	0.76
1:E:253:LEU:HD21	4:E:5458:HOH:O	1.83	0.76
1:E:274:GLN:HG3	1:E:275:GLU:N	2.00	0.76
1:B:70:VAL:HB	1:B:74:ILE:HG22	1.67	0.76
1:A:124:THR:O	1:A:127:VAL:HG23	1.86	0.75
1:A:270:SER:HA	1:A:273:ASP:OD2	1.85	0.75
1:E:236:GLY:HA2	1:E:239:ILE:CG2	2.15	0.75
1:E:172:GLY:HA2	1:E:261:SER:OG	1.85	0.75
1:E:203:VAL:HG12	1:E:204:ARG:HD3	1.68	0.75
1:B:126:VAL:HA	4:B:2313:HOH:O	1.85	0.75
1:A:218:LEU:HD13	2:A:1300:NAP:O1N	1.87	0.75
1:B:5:PHE:CE1	1:B:12:ALA:HA	2.21	0.75
1:A:199:ARG:HA	4:A:1313:HOH:O	1.85	0.75
1:B:222:GLN:O	1:B:223:HIS:HB2	1.86	0.75
1:C:118:ILE:HG22	1:C:137:THR:HA	1.67	0.75
1:D:153:LEU:HA	4:D:4410:HOH:O	1.85	0.75
1:D:198:PRO:HG2	1:D:201:LEU:HB3	1.69	0.75
1:C:63:SER:HB2	4:C:3321:HOH:O	1.87	0.74
1:A:60:VAL:HG21	1:A:82:ILE:HD12	1.70	0.74
2:A:1300:NAP:C5D	2:A:1300:NAP:O1N	2.35	0.74
1:B:71:LYS:O	1:B:74:ILE:HG23	1.86	0.74
1:C:51:LYS:H	1:C:51:LYS:HD3	1.52	0.74
1:D:133:THR:HG21	1:D:153:LEU:HB3	1.69	0.74
1:E:241:ALA:O	1:E:244:VAL:HG12	1.87	0.74
1:A:9:GLY:H	1:A:41:THR:HG21	1.52	0.74
1:A:135:TYR:HE2	1:A:150:GLU:HG2	1.52	0.74
1:C:8:ALA:HB1	4:C:3383:HOH:O	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:ILE:HG22	1:D:78:ILE:HG12	1.69	0.73
1:A:269:GLN:HG2	1:A:270:SER:N	2.02	0.73
1:B:134:VAL:HG13	1:B:160:THR:O	1.89	0.73
1:C:37:MET:HA	1:C:42:VAL:HG11	1.71	0.73
1:B:14:ALA:HA	1:B:127:VAL:HG22	1.70	0.73
1:E:215:LYS:HA	1:E:218:LEU:HD12	1.71	0.73
1:E:218:LEU:HD13	2:E:5300:NAP:O1N	1.89	0.73
1:A:198:PRO:HD2	1:A:201:LEU:HD23	1.68	0.73
1:A:198:PRO:HG2	1:A:201:LEU:CB	2.19	0.73
1:D:260:ALA:HA	4:D:4402:HOH:O	1.87	0.73
1:B:198:PRO:HD2	1:B:201:LEU:HD23	1.69	0.73
1:A:2:SER:H	1:A:64:ASP:HB2	1.53	0.73
1:B:58:GLU:O	1:B:61:GLN:HG3	1.88	0.73
1:D:267:GLU:HA	1:D:270:SER:HB2	1.69	0.73
1:A:193:VAL:HG13	1:E:234:PRO:HA	1.69	0.73
1:D:130:GLU:OE2	2:D:4300:NAP:H2D	1.88	0.73
1:A:135:TYR:CE2	1:A:150:GLU:HG2	2.24	0.73
1:A:89:ARG:HG3	1:A:90:HIS:N	2.02	0.73
1:A:123:ASN:HD21	1:A:132:ALA:N	1.87	0.72
1:D:224:PRO:HA	4:D:4321:HOH:O	1.89	0.72
1:E:198:PRO:HG2	1:E:201:LEU:HB3	1.69	0.72
1:A:167:ILE:HB	4:A:1369:HOH:O	1.88	0.72
1:E:231:VAL:HG12	4:E:5339:HOH:O	1.88	0.72
1:E:124:THR:O	1:E:127:VAL:HG23	1.90	0.72
1:E:183:THR:HB	4:E:5316:HOH:O	1.89	0.72
1:B:82:ILE:O	1:B:86:ILE:HG13	1.89	0.72
1:D:256:ASN:HA	4:D:4318:HOH:O	1.89	0.72
1:B:35:PRO:HG2	1:B:71:LYS:NZ	2.05	0.72
1:C:6:ILE:HG23	1:C:56:ASN:HB3	1.71	0.72
1:C:189:ALA:HA	4:C:3358:HOH:O	1.89	0.72
1:C:128:VAL:C	1:C:130:GLU:H	1.90	0.72
1:D:70:VAL:HG11	1:D:74:ILE:HG21	1.71	0.72
1:E:122:THR:HG22	1:E:133:THR:HG22	1.72	0.71
1:A:26:ALA:HB3	1:A:29:LYS:HE3	1.73	0.71
1:D:125:PRO:HB2	1:D:131:GLY:HA2	1.72	0.71
1:A:108:LEU:HA	4:A:1373:HOH:O	1.90	0.71
1:B:15:LEU:HB3	1:B:19:PHE:CZ	2.25	0.71
1:C:8:ALA:CB	1:C:34:SER:HB2	2.19	0.71
1:C:29:LYS:C	1:C:30:ILE:HD12	2.11	0.71
1:A:123:ASN:C	1:A:125:PRO:HD2	2.11	0.71
1:A:266:ARG:HG2	1:A:266:ARG:HH11	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ILE:HG22	1:B:86:ILE:HD11	1.72	0.71
1:B:239:ILE:HG21	4:E:5386:HOH:O	1.91	0.71
1:B:38:ASP:HB3	1:B:42:VAL:HG23	1.73	0.70
1:D:214:ALA:HA	4:D:4330:HOH:O	1.91	0.70
1:B:220:SER:O	1:B:221:GLU:HB3	1.90	0.70
1:D:203:VAL:O	1:D:204:ARG:HD3	1.91	0.70
1:B:100:THR:HB	1:B:103:SER:OG	1.92	0.70
1:C:28:HIS:HA	1:C:51:LYS:HE3	1.71	0.70
1:C:124:THR:N	1:C:125:PRO:HD2	2.07	0.70
1:C:45:LEU:O	1:C:48:MET:HB3	1.92	0.70
1:C:7:GLY:HA3	1:C:69:ALA:O	1.92	0.70
1:A:33:SER:HA	1:A:53:THR:O	1.92	0.70
1:E:30:ILE:HB	1:E:50:VAL:HG22	1.74	0.70
1:B:71:LYS:HB2	1:B:73:HIS:CE1	2.27	0.69
1:E:122:THR:HG22	1:E:133:THR:CG2	2.22	0.69
1:E:6:ILE:HD11	1:E:66:LEU:HD21	1.73	0.69
1:C:124:THR:O	1:C:127:VAL:HG23	1.92	0.69
1:D:239:ILE:HG22	4:D:4382:HOH:O	1.91	0.69
1:E:55:HIS:HB3	1:E:57:LYS:HG2	1.74	0.69
1:E:38:ASP:HB2	4:E:5379:HOH:O	1.93	0.69
1:C:52:LEU:HD23	1:C:52:LEU:O	1.92	0.69
1:D:200:ARG:O	1:D:204:ARG:CG	2.40	0.69
1:C:93:VAL:HG12	1:C:118:ILE:HD11	1.75	0.69
1:E:69:ALA:HB3	4:E:5454:HOH:O	1.91	0.69
1:A:236:GLY:HA2	1:A:239:ILE:HG22	1.75	0.69
1:B:215:LYS:HG3	4:B:2319:HOH:O	1.93	0.69
1:E:232:SER:HB3	4:E:5347:HOH:O	1.91	0.69
1:E:39:LEU:CD2	1:E:39:LEU:H	2.06	0.69
1:E:194:LYS:HB2	4:E:5398:HOH:O	1.92	0.69
1:B:153:LEU:C	1:B:155:SER:H	1.96	0.69
1:B:5:PHE:HZ	1:B:15:LEU:HB2	1.57	0.68
1:B:252:SER:HB3	4:B:2353:HOH:O	1.91	0.68
1:A:14:ALA:HA	1:A:127:VAL:HG22	1.76	0.68
1:A:6:ILE:HD12	1:A:56:ASN:HB2	1.76	0.68
1:B:33:SER:OG	1:B:56:ASN:HA	1.93	0.68
1:A:9:GLY:N	1:A:41:THR:HG21	2.08	0.68
1:A:122:THR:HG22	1:A:123:ASN:N	2.09	0.68
1:A:150:GLU:O	1:A:154:SER:HB2	1.93	0.68
1:E:73:HIS:O	1:E:74:ILE:HD13	1.94	0.68
2:B:2300:NAP:O1A	2:B:2300:NAP:H3B	1.93	0.68
1:C:48:MET:HG3	1:C:50:VAL:HG23	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:MET:HA	1:E:42:VAL:HG21	1.74	0.68
1:A:88:ASP:HB2	1:A:112:ARG:HH21	1.59	0.68
1:A:133:THR:HG21	1:A:153:LEU:HD13	1.76	0.68
2:C:3300:NAP:O1A	2:C:3300:NAP:H3B	1.94	0.68
1:D:240:HIS:HA	4:D:4382:HOH:O	1.94	0.68
1:C:3:VAL:HB	1:C:30:ILE:HG12	1.76	0.67
1:E:55:HIS:CB	1:E:57:LYS:HE2	2.23	0.67
1:E:123:ASN:HD21	1:E:132:ALA:N	1.89	0.67
1:E:0:GLY:HA3	4:E:5401:HOH:O	1.93	0.67
1:A:134:VAL:HG22	1:A:160:THR:HG23	1.76	0.67
1:B:74:ILE:O	1:B:79:LEU:HG	1.94	0.67
2:D:4300:NAP:H3B	2:D:4300:NAP:O1A	1.94	0.67
1:A:135:TYR:HA	4:A:1402:HOH:O	1.94	0.67
1:C:187:ALA:O	1:C:190:ASP:HB2	1.95	0.67
1:E:118:ILE:CD1	1:E:137:THR:HA	2.25	0.67
1:C:223:HIS:ND1	1:C:224:PRO:HD2	2.09	0.67
1:B:42:VAL:HG13	1:B:52:LEU:HG	1.75	0.67
1:A:25:LEU:HD11	1:A:29:LYS:HB3	1.75	0.67
1:C:46:ARG:HH22	1:C:52:LEU:HD22	1.60	0.67
1:C:11:LEU:O	1:C:15:LEU:HG	1.94	0.66
2:A:1300:NAP:H3B	2:A:1300:NAP:O1A	1.95	0.66
1:D:60:VAL:HG21	1:D:82:ILE:HG23	1.77	0.66
1:B:19:PHE:CD1	1:B:25:LEU:HD12	2.30	0.66
1:C:39:LEU:HA	1:C:43:SER:HB2	1.77	0.66
1:E:48:MET:O	1:E:48:MET:HG2	1.94	0.66
1:D:3:VAL:HG13	1:D:65:VAL:HG13	1.77	0.66
1:E:221:GLU:O	1:E:223:HIS:N	2.28	0.66
1:B:33:SER:HB2	1:B:59:THR:OG1	1.95	0.66
1:C:172:GLY:HA2	1:C:261:SER:OG	1.96	0.66
1:E:177:GLY:HA2	1:E:180:TYR:CD1	2.30	0.66
1:E:162:VAL:CG1	1:E:166:LEU:HD12	2.26	0.66
1:C:26:ALA:HB3	1:C:29:LYS:CG	2.26	0.66
1:C:8:ALA:HB3	1:C:34:SER:CB	2.21	0.66
1:B:53:THR:HG23	1:B:58:GLU:OE2	1.96	0.65
1:D:231:VAL:O	1:D:231:VAL:HG12	1.95	0.65
1:E:7:GLY:N	1:E:33:SER:HB2	2.11	0.65
2:E:5300:NAP:H3B	2:E:5300:NAP:O1A	1.96	0.65
1:D:202:ALA:C	1:D:204:ARG:H	2.00	0.65
1:C:118:ILE:HG13	1:C:118:ILE:O	1.95	0.65
1:E:122:THR:HG22	1:E:133:THR:CB	2.26	0.65
1:A:156:VAL:O	1:A:156:VAL:HG12	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:GLY:O	1:E:234:PRO:HB3	1.96	0.65
1:C:259:GLU:O	1:C:263:ILE:HG12	1.96	0.65
1:D:45:LEU:HB3	1:D:50:VAL:HG11	1.78	0.65
1:D:83:GLY:O	1:D:86:ILE:HG22	1.97	0.65
1:A:57:LYS:HG3	1:A:82:ILE:HD11	1.78	0.65
1:B:148:LEU:O	1:B:151:GLN:HB2	1.97	0.65
1:D:211:LEU:HB3	4:D:4325:HOH:O	1.97	0.65
1:A:217:LEU:HB3	4:A:1361:HOH:O	1.97	0.65
1:C:39:LEU:HA	1:C:43:SER:CB	2.27	0.65
1:B:101:ILE:HB	4:B:2377:HOH:O	1.96	0.65
1:D:211:LEU:HD12	1:D:211:LEU:O	1.97	0.64
1:E:193:VAL:HG12	4:E:5386:HOH:O	1.95	0.64
1:C:123:ASN:HB2	1:C:125:PRO:HD2	1.78	0.64
1:D:7:GLY:H	1:D:33:SER:HB2	1.62	0.64
1:E:177:GLY:O	1:E:180:TYR:HB2	1.97	0.64
1:A:199:ARG:HD3	4:A:1303:HOH:O	1.97	0.64
1:C:170:VAL:HG13	4:C:3324:HOH:O	1.97	0.64
1:D:264:ARG:HD3	4:D:4406:HOH:O	1.97	0.64
1:A:153:LEU:C	1:A:155:SER:H	1.99	0.64
1:A:39:LEU:O	1:A:43:SER:HB3	1.97	0.64
1:B:221:GLU:CG	1:B:222:GLN:N	2.60	0.64
1:A:9:GLY:CA	1:A:41:THR:HG21	2.27	0.64
1:C:46:ARG:NH2	1:C:52:LEU:HD22	2.12	0.64
1:E:42:VAL:HG12	1:E:46:ARG:NH1	2.12	0.64
1:A:134:VAL:HG22	1:A:160:THR:CG2	2.28	0.64
1:C:38:ASP:H	1:C:42:VAL:HB	1.63	0.64
1:D:53:THR:HG22	1:D:55:HIS:N	2.00	0.64
1:D:267:GLU:O	1:D:271:MET:HG2	1.97	0.63
1:C:135:TYR:HE2	1:C:150:GLU:HG3	1.63	0.63
1:A:39:LEU:HG	4:A:1416:HOH:O	1.97	0.63
1:E:33:SER:OG	1:E:56:ASN:HA	1.99	0.63
1:A:241:ALA:O	1:A:244:VAL:HG22	1.98	0.63
1:B:45:LEU:HA	1:B:48:MET:SD	2.39	0.63
1:B:66:LEU:HB2	1:B:92:VAL:HG22	1.81	0.63
1:C:46:ARG:NH1	1:C:52:LEU:HB3	2.14	0.63
1:B:5:PHE:CZ	1:B:15:LEU:HB2	2.33	0.63
1:C:196:GLY:O	1:C:197:LEU:O	2.17	0.63
1:C:82:ILE:O	1:C:86:ILE:HG13	1.98	0.63
1:A:101:ILE:HG13	1:A:164:GLU:OE1	1.98	0.63
1:B:128:VAL:HG12	1:B:129:ARG:N	2.13	0.63
1:C:249:GLY:O	1:C:253:LEU:HD13	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:VAL:HB	1:C:30:ILE:CG1	2.29	0.63
1:C:82:ILE:HA	1:C:85:ASP:HB2	1.81	0.63
1:E:122:THR:HG22	1:E:133:THR:HB	1.81	0.63
1:B:147:ARG:HG3	1:B:151:GLN:NE2	2.12	0.63
1:C:112:ARG:HH11	1:C:113:PRO:CD	2.09	0.63
1:B:15:LEU:HB3	1:B:19:PHE:HZ	1.64	0.63
1:A:95:CYS:HB2	4:A:1421:HOH:O	1.98	0.62
1:D:271:MET:HG3	4:D:4398:HOH:O	1.99	0.62
1:A:135:TYR:OH	1:A:150:GLU:HG3	1.99	0.62
1:C:239:ILE:HD13	4:D:4372:HOH:O	1.99	0.62
1:D:45:LEU:HB3	1:D:50:VAL:CG1	2.30	0.62
1:D:87:GLU:N	1:D:90:HIS:HD2	1.86	0.62
1:A:272:ALA:HB3	4:A:1386:HOH:O	1.98	0.62
1:C:161:GLU:HA	4:C:3374:HOH:O	1.99	0.62
1:D:124:THR:O	1:D:126:VAL:N	2.31	0.62
4:A:1388:HOH:O	1:E:228:LYS:HE3	1.99	0.62
1:C:231:VAL:O	1:C:231:VAL:HG12	1.99	0.62
1:C:53:THR:HG21	1:C:58:GLU:HB2	1.82	0.62
1:D:215:LYS:HE2	4:D:4331:HOH:O	1.99	0.62
1:E:169:ALA:C	1:E:171:THR:H	2.01	0.62
1:B:143:VAL:HG12	1:B:144:GLU:N	2.13	0.62
1:D:117:VAL:O	1:D:138:GLY:HA3	1.99	0.62
1:D:17:LYS:HD2	1:D:127:VAL:CG1	2.30	0.62
1:E:75:ILE:HG13	1:E:99:VAL:HG21	1.82	0.62
1:B:23:GLY:O	1:B:25:LEU:N	2.32	0.62
1:C:193:VAL:HG12	4:C:3322:HOH:O	1.99	0.62
1:C:57:LYS:O	1:C:60:VAL:N	2.32	0.62
1:D:211:LEU:HD12	1:D:211:LEU:C	2.19	0.62
1:A:93:VAL:HG22	1:A:118:ILE:HD11	1.82	0.62
1:B:15:LEU:HD23	1:B:19:PHE:CE2	2.34	0.62
1:B:269:GLN:HB3	4:B:2321:HOH:O	2.00	0.62
1:C:3:VAL:O	1:C:30:ILE:HG23	2.00	0.62
1:C:135:TYR:CZ	1:C:161:GLU:HB3	2.34	0.62
1:C:231:VAL:HB	4:C:3356:HOH:O	1.98	0.62
1:A:83:GLY:HA2	1:A:86:ILE:HG12	1.81	0.61
1:B:195:MET:HA	1:B:195:MET:HE2	1.82	0.61
1:D:60:VAL:HG21	1:D:82:ILE:CG2	2.29	0.61
1:A:217:LEU:HD12	4:A:1397:HOH:O	1.99	0.61
1:B:149:MET:C	1:B:151:GLN:H	2.03	0.61
1:B:19:PHE:CD2	1:B:156:VAL:HG21	2.36	0.61
1:C:266:ARG:HA	4:C:3335:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:VAL:HB	4:D:4410:HOH:O	1.99	0.61
1:E:75:ILE:HB	1:E:76:PRO:HD3	1.81	0.61
1:A:222:GLN:O	1:A:223:HIS:CB	2.48	0.61
1:C:177:GLY:HA2	1:C:180:TYR:CD1	2.36	0.61
1:A:146:GLY:O	1:A:150:GLU:HB2	2.01	0.61
1:E:79:LEU:HD12	1:E:107:LYS:HD2	1.82	0.61
2:A:1300:NAP:O4D	2:A:1300:NAP:O5D	2.19	0.61
1:D:92:VAL:HB	1:D:117:VAL:HG22	1.82	0.61
1:B:262:CYS:O	1:B:265:THR:HB	2.01	0.61
1:B:266:ARG:O	1:B:269:GLN:HG2	2.00	0.61
1:C:218:LEU:HB3	2:C:3300:NAP:O1N	2.01	0.61
1:A:163:GLU:O	1:A:165:ASP:N	2.34	0.61
1:B:42:VAL:HG11	4:B:2401:HOH:O	2.01	0.61
1:A:233:SER:O	1:A:235:GLY:N	2.34	0.61
1:B:221:GLU:HG3	1:B:222:GLN:N	2.16	0.61
1:B:47:LYS:HB3	1:B:47:LYS:NZ	2.16	0.61
1:B:220:SER:O	1:B:221:GLU:CB	2.49	0.61
1:A:150:GLU:O	1:A:154:SER:CB	2.49	0.61
1:B:122:THR:HG22	1:B:133:THR:CB	2.27	0.61
1:C:82:ILE:HG23	1:C:85:ASP:HB2	1.82	0.61
1:D:25:LEU:HD23	1:D:25:LEU:N	2.16	0.61
1:A:149:MET:CE	1:A:149:MET:HA	2.31	0.60
1:E:220:SER:O	1:E:221:GLU:HB2	2.02	0.60
1:A:74:ILE:HG22	1:A:78:ILE:HD11	1.82	0.60
1:B:4:GLY:HA3	1:B:66:LEU:HD23	1.83	0.60
1:B:162:VAL:HG12	1:B:163:GLU:OE2	2.01	0.60
1:D:220:SER:C	1:D:222:GLN:H	2.05	0.60
1:E:6:ILE:O	1:E:70:VAL:CG2	2.49	0.60
1:D:222:GLN:O	1:D:223:HIS:HB3	2.02	0.60
1:A:129:ARG:CD	4:A:1316:HOH:O	2.30	0.60
1:E:134:VAL:HG21	1:E:170:VAL:HG11	1.84	0.60
1:E:57:LYS:HD3	1:E:57:LYS:N	2.14	0.60
1:C:236:GLY:HA2	1:C:239:ILE:CG2	2.31	0.60
1:D:193:VAL:HA	1:D:197:LEU:O	2.01	0.60
1:D:56:ASN:O	1:D:60:VAL:HG23	2.01	0.60
1:C:163:GLU:HB2	1:C:165:ASP:OD2	2.01	0.60
1:C:2:SER:HA	4:C:3313:HOH:O	2.01	0.60
1:E:170:VAL:HG12	1:E:170:VAL:O	2.00	0.60
1:B:73:HIS:C	1:B:75:ILE:H	2.05	0.60
1:D:218:LEU:HD13	2:D:4300:NAP:O1N	2.01	0.60
1:E:88:ASP:N	4:E:5449:HOH:O	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:THR:O	1:B:127:VAL:HG23	2.02	0.59
1:B:221:GLU:O	1:B:223:HIS:N	2.35	0.59
1:C:128:VAL:C	1:C:130:GLU:N	2.56	0.59
1:A:124:THR:N	1:A:125:PRO:HD2	2.17	0.59
1:B:112:ARG:HG3	1:B:113:PRO:HD2	1.84	0.59
1:C:14:ALA:CB	1:C:127:VAL:HG22	2.33	0.59
1:D:46:ARG:HG2	1:D:52:LEU:HD12	1.84	0.59
1:A:76:PRO:C	1:A:78:ILE:H	2.04	0.59
1:C:100:THR:HG22	1:C:101:ILE:N	2.18	0.59
1:C:156:VAL:HG12	1:C:156:VAL:O	2.02	0.59
1:D:73:HIS:O	1:D:76:PRO:HD2	2.02	0.59
1:E:19:PHE:O	1:E:24:VAL:HG23	2.02	0.59
1:A:269:GLN:C	1:A:271:MET:H	2.04	0.59
1:A:31:MET:HA	1:A:51:LYS:O	2.02	0.59
1:A:87:GLU:H	1:A:90:HIS:CE1	2.20	0.59
1:B:222:GLN:HG2	4:B:2369:HOH:O	2.02	0.59
1:B:39:LEU:HD12	1:B:43:SER:HB2	1.84	0.59
1:C:236:GLY:HA2	1:C:239:ILE:HG22	1.83	0.59
1:B:150:GLU:O	1:B:154:SER:HB3	2.03	0.59
1:C:266:ARG:HD2	4:C:3345:HOH:O	2.02	0.59
1:E:17:LYS:O	1:E:18:GLY:C	2.41	0.59
1:A:188:LEU:HA	4:A:1315:HOH:O	2.01	0.59
1:A:55:HIS:C	1:A:57:LYS:H	2.06	0.59
1:D:185:LEU:HD21	1:D:210:LEU:HD12	1.84	0.59
2:A:1300:NAP:H5N	3:A:1301:GLU:OXT	2.02	0.59
1:E:31:MET:HG2	1:E:51:LYS:HB2	1.83	0.59
1:A:112:ARG:HG3	4:A:1404:HOH:O	2.01	0.59
2:A:1300:NAP:H8A	2:A:1300:NAP:O3X	2.03	0.59
1:C:133:THR:O	1:C:159:CYS:HA	2.03	0.59
1:C:42:VAL:HA	4:C:3344:HOH:O	2.03	0.59
1:E:169:ALA:O	1:E:171:THR:N	2.36	0.59
1:E:43:SER:O	1:E:46:ARG:HB2	2.02	0.59
1:E:7:GLY:HA3	1:E:70:VAL:HG22	1.84	0.59
1:B:93:VAL:HA	1:B:118:ILE:O	2.03	0.58
1:E:121:MET:CE	1:E:122:THR:H	2.07	0.58
1:A:13:PHE:CA	1:A:45:LEU:HD21	2.30	0.58
1:C:269:GLN:C	1:C:271:MET:H	2.05	0.58
1:E:222:GLN:O	1:E:223:HIS:HB2	2.03	0.58
1:A:4:GLY:HA2	1:A:31:MET:O	2.04	0.58
1:B:172:GLY:HA2	1:B:261:SER:OG	2.02	0.58
1:C:152:LEU:HG	1:C:153:LEU:HG	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:GLY:O	1:C:237:ALA:HB3	2.03	0.58
1:C:46:ARG:CZ	1:C:52:LEU:HD13	2.34	0.58
1:D:244:VAL:HA	4:D:4352:HOH:O	2.02	0.58
1:E:101:ILE:HG22	1:E:102:SER:N	2.17	0.58
1:E:101:ILE:HG23	1:E:105:GLU:HG3	1.84	0.58
1:E:227:LEU:O	1:E:231:VAL:HG23	2.03	0.58
1:B:95:CYS:HA	1:B:120:CYS:O	2.04	0.58
1:C:33:SER:HA	1:C:53:THR:O	2.04	0.58
1:A:80:ASP:OD2	1:A:107:LYS:NZ	2.36	0.58
1:A:123:ASN:ND2	1:A:132:ALA:H	1.98	0.58
1:A:134:VAL:HB	4:A:1352:HOH:O	2.04	0.58
1:C:200:ARG:C	1:C:204:ARG:HG2	2.24	0.58
1:C:87:GLU:H	1:C:90:HIS:CE1	2.21	0.58
1:D:102:SER:OG	1:D:106:LYS:HE3	2.02	0.58
1:B:74:ILE:HA	1:B:78:ILE:CG1	2.28	0.58
1:D:191:GLY:HA2	4:D:4346:HOH:O	2.03	0.58
1:A:121:MET:HE2	4:A:1384:HOH:O	2.03	0.58
1:A:133:THR:HG22	1:A:134:VAL:N	2.19	0.58
1:D:199:ARG:O	1:D:203:VAL:HG12	2.04	0.58
1:D:22:ALA:HA	1:D:129:ARG:NH1	2.18	0.58
1:E:132:ALA:HB1	4:E:5429:HOH:O	2.03	0.58
1:A:57:LYS:HE3	1:A:81:GLU:OE1	2.04	0.58
1:B:16:ALA:O	1:B:20:THR:HG23	2.03	0.58
1:B:19:PHE:O	1:B:25:LEU:HB2	2.03	0.58
1:E:38:ASP:H	1:E:42:VAL:CG2	2.16	0.58
1:A:79:LEU:HB2	4:A:1413:HOH:O	2.04	0.58
1:B:38:ASP:O	1:B:42:VAL:HB	2.03	0.58
1:D:238:THR:HA	4:D:4342:HOH:O	2.04	0.58
1:E:227:LEU:HD12	4:E:5315:HOH:O	2.04	0.58
1:E:172:GLY:HA2	1:E:261:SER:CB	2.33	0.58
1:A:214:ALA:HA	4:A:1361:HOH:O	2.04	0.58
1:A:222:GLN:HB2	4:A:1397:HOH:O	2.02	0.58
1:A:239:ILE:HD11	1:C:190:ASP:O	2.04	0.58
1:D:263:ILE:HD13	4:D:4419:HOH:O	2.03	0.58
1:E:154:SER:HB3	4:E:5448:HOH:O	2.03	0.58
1:E:5:PHE:O	1:E:32:ALA:HA	2.04	0.58
1:C:108:LEU:HB3	4:C:3398:HOH:O	2.04	0.57
1:C:33:SER:HB2	1:C:59:THR:OG1	2.03	0.57
1:E:121:MET:HA	1:E:121:MET:HE3	1.85	0.57
1:A:26:ALA:CB	1:A:29:LYS:HE3	2.34	0.57
1:B:84:ALA:HB3	4:B:2393:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:ARG:NE	1:C:90:HIS:HD2	2.02	0.57
1:D:30:ILE:HB	1:D:50:VAL:CG2	2.27	0.57
1:A:38:ASP:O	1:A:39:LEU:C	2.42	0.57
1:A:77:PHE:H	1:A:77:PHE:HD1	1.50	0.57
1:C:30:ILE:HA	1:C:62:HIS:NE2	2.19	0.57
1:D:97:ALA:HB1	1:D:265:THR:HG23	1.86	0.57
1:E:114:ALA:HB1	1:E:140:HIS:ND1	2.19	0.57
1:A:200:ARG:O	1:A:204:ARG:HG2	2.04	0.57
1:A:41:THR:O	1:A:44:ALA:HB3	2.04	0.57
1:A:243:HIS:HD2	1:C:194:LYS:NZ	2.02	0.57
1:C:66:LEU:HD23	1:C:67:PHE:N	2.17	0.57
1:E:87:GLU:O	1:E:89:ARG:N	2.36	0.57
1:B:255:ILE:O	1:B:258:VAL:HG12	2.04	0.57
1:C:105:GLU:HA	4:C:3329:HOH:O	2.05	0.57
1:D:135:TYR:HE2	1:D:150:GLU:HG2	1.69	0.57
1:B:101:ILE:HG22	1:B:119:ARG:HB2	1.86	0.57
1:B:122:THR:CG2	1:B:133:THR:HB	2.28	0.57
1:C:160:THR:CG2	1:C:161:GLU:N	2.66	0.57
1:D:247:SER:HB2	4:D:4352:HOH:O	2.05	0.57
1:A:193:VAL:C	1:A:195:MET:H	2.08	0.57
1:D:232:SER:HB3	1:D:239:ILE:HD11	1.87	0.57
1:A:202:ALA:HB1	4:A:1415:HOH:O	2.04	0.57
1:D:203:VAL:HG22	1:D:203:VAL:O	2.05	0.57
1:E:28:HIS:C	1:E:28:HIS:CD2	2.78	0.57
3:B:2301:GLU:HG2	3:B:2301:GLU:OXT	2.05	0.57
1:B:78:ILE:O	1:B:82:ILE:HG13	2.05	0.57
1:C:189:ALA:HB3	4:C:3359:HOH:O	2.04	0.57
1:C:31:MET:HG2	1:C:53:THR:OG1	2.05	0.57
1:A:200:ARG:O	1:A:204:ARG:CG	2.53	0.56
1:A:231:VAL:HB	4:A:1359:HOH:O	2.05	0.56
1:B:198:PRO:CG	1:B:201:LEU:HB3	2.33	0.56
1:B:162:VAL:HB	1:B:166:LEU:HD12	1.87	0.56
1:B:3:VAL:O	1:B:30:ILE:HG23	2.06	0.56
1:C:100:THR:HG22	1:C:101:ILE:H	1.70	0.56
1:C:82:ILE:HB	4:C:3338:HOH:O	2.05	0.56
1:B:198:PRO:CD	1:B:201:LEU:HD23	2.35	0.56
1:C:172:GLY:HA2	1:C:261:SER:CB	2.35	0.56
1:D:38:ASP:OD2	1:D:40:ALA:HB3	2.05	0.56
1:E:118:ILE:HD12	1:E:137:THR:HA	1.87	0.56
1:B:251:ARG:O	1:B:254:LEU:N	2.38	0.56
1:B:38:ASP:HB3	1:B:42:VAL:CG2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3:VAL:O	1:E:30:ILE:HA	2.06	0.56
1:A:203:VAL:HG12	1:A:204:ARG:HD3	1.88	0.56
1:A:135:TYR:CD1	1:A:135:TYR:C	2.78	0.56
1:A:9:GLY:O	1:A:41:THR:HG23	2.06	0.56
1:B:130:GLU:OE2	2:B:2300:NAP:H2D	2.06	0.56
1:B:220:SER:HB3	4:B:2369:HOH:O	2.04	0.56
1:C:53:THR:HG23	1:C:58:GLU:OE2	2.06	0.56
1:C:71:LYS:CD	1:C:71:LYS:H	2.18	0.56
1:D:236:GLY:CA	1:D:240:HIS:HD2	2.18	0.56
4:B:2306:HOH:O	1:E:203:VAL:HG21	2.04	0.56
1:E:239:ILE:HD13	4:E:5424:HOH:O	2.04	0.56
1:C:240:HIS:HB3	4:C:3363:HOH:O	2.05	0.56
1:C:29:LYS:HG3	4:C:3390:HOH:O	2.05	0.56
1:C:35:PRO:O	1:C:36:ASP:HB2	2.05	0.56
1:D:63:SER:O	1:D:90:HIS:CE1	2.59	0.56
1:A:130:GLU:HG2	4:A:1374:HOH:O	2.05	0.56
1:B:141:ALA:O	1:B:145:ASP:HB3	2.06	0.56
1:B:154:SER:O	2:B:2300:NAP:N7N	2.39	0.56
1:B:200:ARG:C	1:B:204:ARG:HG2	2.24	0.56
1:B:258:VAL:HG13	1:B:259:GLU:N	2.20	0.56
1:C:153:LEU:C	1:C:155:SER:H	2.08	0.56
1:B:201:LEU:O	1:B:204:ARG:HB2	2.05	0.56
1:B:84:ALA:N	1:B:111:PHE:HD2	2.04	0.56
1:C:61:GLN:C	1:C:63:SER:H	2.10	0.56
1:D:133:THR:O	1:D:159:CYS:HA	2.05	0.56
1:D:236:GLY:HA3	1:D:240:HIS:HD2	1.71	0.56
1:D:109:SER:C	1:D:111:PHE:H	2.10	0.56
1:D:15:LEU:HB3	1:D:19:PHE:CE1	2.41	0.56
1:B:153:LEU:C	1:B:155:SER:N	2.59	0.55
1:B:57:LYS:HG3	1:B:58:GLU:N	2.21	0.55
1:A:193:VAL:HG23	4:A:1313:HOH:O	2.05	0.55
1:B:204:ARG:N	1:B:204:ARG:HD3	2.19	0.55
1:B:7:GLY:HA3	1:B:69:ALA:C	2.26	0.55
1:D:105:GLU:O	1:D:107:LYS:N	2.34	0.55
1:D:133:THR:N	4:D:4418:HOH:O	2.39	0.55
1:D:236:GLY:HA3	1:D:240:HIS:CD2	2.42	0.55
1:E:100:THR:HG22	1:E:101:ILE:N	2.20	0.55
1:E:124:THR:N	1:E:125:PRO:HD2	2.21	0.55
1:E:144:GLU:OE1	1:E:144:GLU:HA	2.07	0.55
1:E:18:GLY:O	1:E:22:ALA:N	2.38	0.55
1:A:149:MET:HE3	1:A:149:MET:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:THR:HG21	1:B:58:GLU:HB2	1.89	0.55
1:B:264:ARG:O	1:B:268:LEU:HG	2.06	0.55
1:D:251:ARG:HH11	1:D:251:ARG:HG2	1.71	0.55
1:E:126:VAL:HG22	1:E:131:GLY:HA3	1.88	0.55
1:E:46:ARG:O	1:E:49:GLY:N	2.40	0.55
1:C:154:SER:O	2:C:3300:NAP:N7N	2.39	0.55
1:E:153:LEU:HD12	1:E:153:LEU:N	2.21	0.55
1:E:82:ILE:HA	1:E:85:ASP:OD2	2.06	0.55
1:B:121:MET:HE3	1:B:171:THR:HG23	1.88	0.55
1:B:18:GLY:O	1:B:20:THR:N	2.38	0.55
1:C:126:VAL:C	1:C:128:VAL:H	2.09	0.55
1:E:42:VAL:HG12	1:E:46:ARG:HH12	1.72	0.55
1:E:53:THR:HG21	1:E:58:GLU:CB	2.35	0.55
1:B:218:LEU:HB3	2:B:2300:NAP:O1N	2.05	0.55
1:C:101:ILE:HB	1:C:164:GLU:OE1	2.07	0.55
1:D:269:GLN:O	1:D:271:MET:N	2.39	0.55
1:A:107:LYS:HB3	4:A:1308:HOH:O	2.07	0.55
1:A:129:ARG:CG	4:A:1316:HOH:O	2.52	0.55
1:A:244:VAL:CG2	1:A:245:LEU:N	2.69	0.55
1:B:274:GLN:HG2	1:B:275:GLU:HG3	1.87	0.55
1:C:124:THR:O	1:C:126:VAL:N	2.40	0.55
1:C:180:TYR:O	1:C:183:THR:HB	2.07	0.55
1:C:51:LYS:NZ	1:C:51:LYS:HB2	2.21	0.55
1:E:181:ALA:C	1:E:185:LEU:HD12	2.27	0.55
2:E:5300:NAP:H4N	4:E:5448:HOH:O	2.07	0.55
1:B:204:ARG:NH2	4:B:2339:HOH:O	2.34	0.55
1:B:43:SER:HB3	4:B:2352:HOH:O	2.05	0.55
1:C:259:GLU:HG2	1:C:259:GLU:O	2.05	0.55
1:C:33:SER:OG	1:C:56:ASN:HA	2.06	0.55
1:C:86:ILE:HD13	4:C:3398:HOH:O	2.05	0.55
1:E:243:HIS:HB3	4:E:5324:HOH:O	2.07	0.55
2:E:5300:NAP:H8A	2:E:5300:NAP:O3X	2.07	0.55
1:B:201:LEU:HD11	1:B:205:LEU:HD11	1.89	0.55
1:B:254:LEU:HB2	4:B:2357:HOH:O	2.07	0.55
1:D:32:ALA:HB3	1:D:52:LEU:CD2	2.37	0.55
1:E:118:ILE:HD13	1:E:138:GLY:H	1.71	0.55
1:B:251:ARG:O	1:B:252:SER:C	2.45	0.54
1:D:231:VAL:HA	4:D:4425:HOH:O	2.07	0.54
1:B:195:MET:HA	1:B:195:MET:CE	2.36	0.54
1:E:45:LEU:HA	1:E:48:MET:HE3	1.88	0.54
1:B:174:SER:O	4:B:2397:HOH:O	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:GLY:CA	1:B:239:ILE:HG22	2.25	0.54
1:D:128:VAL:HG13	1:D:130:GLU:HB2	1.90	0.54
1:D:203:VAL:HG13	1:D:204:ARG:NE	2.22	0.54
1:D:31:MET:HG2	1:D:59:THR:HA	1.88	0.54
1:D:77:PHE:N	1:D:77:PHE:CD1	2.74	0.54
1:E:124:THR:O	1:E:126:VAL:N	2.40	0.54
1:A:16:ALA:C	1:A:48:MET:HE1	2.28	0.54
1:B:140:HIS:CE1	1:B:142:GLN:HB2	2.43	0.54
1:B:157:GLY:O	1:B:158:PHE:HB2	2.07	0.54
1:C:41:THR:O	1:C:45:LEU:HB2	2.08	0.54
1:D:153:LEU:HB2	1:D:159:CYS:SG	2.47	0.54
1:D:193:VAL:O	1:D:196:GLY:N	2.41	0.54
1:D:217:LEU:HB3	4:D:4330:HOH:O	2.08	0.54
1:E:162:VAL:HG13	1:E:166:LEU:HD12	1.90	0.54
1:C:101:ILE:HG23	1:C:102:SER:N	2.21	0.54
2:D:4300:NAP:O3X	2:D:4300:NAP:H8A	2.07	0.54
1:E:44:ALA:O	1:E:48:MET:HE3	2.07	0.54
1:A:236:GLY:C	1:A:238:THR:H	2.11	0.54
1:D:154:SER:OG	1:D:159:CYS:HB3	2.07	0.54
1:D:60:VAL:O	1:D:90:HIS:HE1	1.89	0.54
1:E:129:ARG:HA	1:E:156:VAL:HG13	1.90	0.54
1:A:125:PRO:HG2	1:A:131:GLY:HA2	1.89	0.54
1:A:33:SER:O	1:A:35:PRO:HD3	2.08	0.54
1:C:14:ALA:HB1	1:C:127:VAL:HG22	1.89	0.54
1:C:189:ALA:CB	1:C:203:VAL:HA	2.37	0.54
1:C:243:HIS:HB2	4:C:3389:HOH:O	2.07	0.54
1:C:258:VAL:CG1	1:C:258:VAL:O	2.56	0.54
1:E:134:VAL:HG12	4:E:5329:HOH:O	2.07	0.54
1:E:153:LEU:HB2	4:E:5465:HOH:O	2.08	0.54
1:E:34:SER:HB3	1:E:54:PRO:HA	1.89	0.54
1:A:129:ARG:HB2	4:A:1316:HOH:O	2.08	0.54
1:B:167:ILE:HD13	4:B:2354:HOH:O	2.07	0.54
1:B:3:VAL:HG13	1:B:65:VAL:O	2.07	0.54
1:C:228:LYS:HD3	4:C:3392:HOH:O	2.08	0.54
1:E:53:THR:C	1:E:55:HIS:H	2.09	0.54
1:A:122:THR:HG23	1:A:133:THR:OG1	2.08	0.54
1:A:171:THR:C	1:A:173:LEU:H	2.12	0.54
1:A:55:HIS:HB3	1:A:57:LYS:HD3	1.90	0.54
2:B:2300:NAP:O2D	3:B:2301:GLU:CD	2.46	0.54
1:C:128:VAL:O	1:C:130:GLU:N	2.40	0.54
1:C:51:LYS:N	1:C:51:LYS:HD3	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:ILE:O	1:C:82:ILE:HG22	2.08	0.54
1:D:77:PHE:HD1	1:D:77:PHE:N	2.05	0.54
1:A:215:LYS:O	1:A:216:MET:C	2.46	0.54
1:A:76:PRO:O	1:A:78:ILE:N	2.41	0.54
1:A:95:CYS:HB3	4:A:1384:HOH:O	2.07	0.54
1:D:121:MET:CE	1:D:171:THR:HG23	2.37	0.54
1:D:232:SER:HB3	1:D:239:ILE:CD1	2.38	0.54
1:A:259:GLU:HG2	1:A:263:ILE:CD1	2.38	0.53
1:A:77:PHE:CD1	1:A:77:PHE:N	2.75	0.53
1:B:71:LYS:H	1:B:71:LYS:CD	2.19	0.53
1:B:83:GLY:CA	1:B:108:LEU:HD22	2.38	0.53
1:C:204:ARG:HD3	1:C:204:ARG:N	2.23	0.53
1:D:125:PRO:O	1:D:128:VAL:HG12	2.08	0.53
1:D:199:ARG:O	1:D:201:LEU:N	2.41	0.53
1:E:17:LYS:HB2	4:E:5389:HOH:O	2.08	0.53
1:E:22:ALA:HB3	1:E:24:VAL:HG23	1.91	0.53
1:A:194:LYS:CG	1:E:239:ILE:HG13	2.38	0.53
1:A:172:GLY:HA2	1:A:261:SER:OG	2.08	0.53
1:A:194:LYS:HG2	1:E:239:ILE:HG13	1.89	0.53
1:A:7:GLY:O	1:A:8:ALA:HB2	2.07	0.53
1:A:87:GLU:N	1:A:90:HIS:CE1	2.76	0.53
1:B:83:GLY:HA3	1:B:111:PHE:CB	2.38	0.53
1:C:147:ARG:HA	4:C:3380:HOH:O	2.08	0.53
1:C:241:ALA:O	1:C:244:VAL:HG12	2.08	0.53
1:C:253:LEU:HD12	1:C:253:LEU:H	1.73	0.53
1:D:177:GLY:HA2	1:D:180:TYR:CD1	2.44	0.53
1:E:131:GLY:O	1:E:158:PHE:N	2.42	0.53
1:E:7:GLY:HA3	1:E:70:VAL:CG2	2.38	0.53
1:E:70:VAL:HG12	1:E:70:VAL:O	2.07	0.53
1:B:221:GLU:CG	1:B:222:GLN:H	2.21	0.53
1:C:261:SER:N	4:C:3302:HOH:O	2.41	0.53
1:C:262:CYS:N	4:C:3302:HOH:O	2.25	0.53
1:C:27:ALA:HB1	1:C:50:VAL:HG22	1.90	0.53
1:C:53:THR:CG2	1:C:58:GLU:HB2	2.38	0.53
1:E:77:PHE:HD1	1:E:77:PHE:H	1.55	0.53
1:A:271:MET:CE	1:A:272:ALA:HB2	2.38	0.53
1:C:31:MET:HB2	1:C:62:HIS:CE1	2.43	0.53
2:E:5300:NAP:O3X	2:E:5300:NAP:C8A	2.56	0.53
1:A:92:VAL:O	1:A:117:VAL:HG23	2.08	0.53
1:C:189:ALA:HB2	1:C:203:VAL:HA	1.91	0.53
1:D:129:ARG:HB3	4:D:4315:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:ARG:HB3	1:D:136:ALA:HB3	1.91	0.53
1:D:77:PHE:HD1	1:D:77:PHE:H	1.56	0.53
1:A:149:MET:HE2	1:A:153:LEU:HG	1.91	0.53
1:A:259:GLU:HG2	1:A:263:ILE:HD11	1.91	0.53
1:A:33:SER:OG	1:A:56:ASN:HB3	2.09	0.53
1:B:139:THR:HG22	1:B:139:THR:O	2.07	0.53
1:B:180:TYR:CD2	1:B:180:TYR:N	2.71	0.53
1:B:28:HIS:HD2	1:B:49:GLY:O	1.90	0.53
2:E:5300:NAP:H6N	2:E:5300:NAP:PN	2.49	0.53
1:E:72:PRO:C	1:E:74:ILE:H	2.11	0.53
1:A:271:MET:HE2	1:A:272:ALA:HB2	1.91	0.53
1:B:132:ALA:HA	4:B:2359:HOH:O	2.08	0.53
1:B:239:ILE:HG23	1:B:240:HIS:HD2	1.72	0.53
1:D:124:THR:C	1:D:126:VAL:H	2.09	0.53
1:D:272:ALA:HA	4:D:4335:HOH:O	2.08	0.53
1:E:128:VAL:O	1:E:128:VAL:HG12	2.09	0.53
1:E:8:ALA:HB1	1:E:41:THR:HG21	1.91	0.53
1:E:6:ILE:O	1:E:70:VAL:HG23	2.08	0.53
1:A:231:VAL:O	1:A:231:VAL:HG12	2.08	0.53
1:B:72:PRO:HA	4:B:2322:HOH:O	2.08	0.53
1:D:237:ALA:H	1:D:240:HIS:HD2	1.55	0.53
1:E:149:MET:O	1:E:152:LEU:HB3	2.07	0.53
1:A:201:LEU:O	1:A:205:LEU:HG	2.08	0.53
1:C:271:MET:HA	1:C:274:GLN:HB3	1.89	0.53
1:D:25:LEU:H	1:D:25:LEU:HD23	1.74	0.53
1:D:70:VAL:HG11	1:D:74:ILE:CG2	2.39	0.53
1:E:114:ALA:HB1	1:E:140:HIS:CG	2.43	0.53
1:E:129:ARG:NE	2:E:5300:NAP:O7N	2.42	0.53
1:A:128:VAL:HG12	4:A:1374:HOH:O	2.08	0.53
1:A:25:LEU:CD1	1:A:29:LYS:HB3	2.39	0.53
1:B:100:THR:HG22	1:B:102:SER:H	1.74	0.53
1:B:35:PRO:HG2	1:B:71:LYS:HZ2	1.72	0.53
1:B:73:HIS:C	1:B:75:ILE:N	2.62	0.53
1:C:143:VAL:HG12	1:C:143:VAL:O	2.09	0.53
4:A:1321:HOH:O	1:C:194:LYS:HA	2.08	0.53
1:C:191:GLY:O	1:C:194:LYS:N	2.42	0.53
1:C:6:ILE:HG12	1:C:66:LEU:HD11	1.91	0.53
1:E:13:PHE:O	1:E:16:ALA:HB3	2.08	0.53
1:A:166:LEU:O	1:A:170:VAL:HG23	2.09	0.52
1:B:119:ARG:CD	1:B:164:GLU:OE2	2.57	0.52
1:B:13:PHE:O	1:B:16:ALA:HB3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ALA:HB3	1:B:29:LYS:HB2	1.91	0.52
1:D:236:GLY:CA	1:D:240:HIS:CD2	2.92	0.52
1:B:194:LYS:HE3	1:D:240:HIS:ND1	2.23	0.52
1:E:45:LEU:O	1:E:49:GLY:O	2.27	0.52
1:E:5:PHE:HB3	4:E:5454:HOH:O	2.09	0.52
1:D:269:GLN:C	1:D:271:MET:H	2.13	0.52
1:D:59:THR:O	1:D:62:HIS:N	2.43	0.52
1:E:214:ALA:O	1:E:218:LEU:HG	2.09	0.52
2:A:1300:NAP:O3X	2:A:1300:NAP:C8A	2.57	0.52
1:A:266:ARG:HG2	1:A:266:ARG:NH1	2.24	0.52
1:A:45:LEU:O	1:A:48:MET:HB3	2.09	0.52
1:C:213:ALA:O	1:C:216:MET:HB2	2.09	0.52
1:C:61:GLN:O	1:C:89:ARG:NH2	2.43	0.52
1:D:121:MET:HE1	1:D:171:THR:HG23	1.90	0.52
1:E:83:GLY:HA3	1:E:111:PHE:CD1	2.44	0.52
1:B:155:SER:HA	2:B:2300:NAP:N7N	2.25	0.52
1:D:26:ALA:HB3	1:D:28:HIS:CD2	2.45	0.52
1:A:240:HIS:CD2	1:C:194:LYS:HE2	2.44	0.52
1:C:126:VAL:CG1	4:C:3387:HOH:O	2.57	0.52
1:C:75:ILE:N	1:C:76:PRO:CD	2.72	0.52
1:D:164:GLU:HA	1:D:167:ILE:HG12	1.91	0.52
1:A:121:MET:SD	1:A:171:THR:HG22	2.50	0.52
1:A:70:VAL:HG21	1:A:78:ILE:HD12	1.92	0.52
1:B:3:VAL:HG22	1:B:65:VAL:HB	1.92	0.52
1:C:130:GLU:HA	1:C:130:GLU:OE2	2.10	0.52
1:D:191:GLY:O	1:D:192:GLY:C	2.48	0.52
1:E:67:PHE:HA	1:E:93:VAL:O	2.10	0.52
1:B:100:THR:HG22	1:B:101:ILE:N	2.25	0.52
1:B:12:ALA:HB3	4:B:2360:HOH:O	2.10	0.52
1:D:35:PRO:HG3	4:D:4394:HOH:O	2.09	0.52
1:E:169:ALA:C	1:E:171:THR:N	2.63	0.52
1:A:15:LEU:O	1:A:16:ALA:C	2.48	0.52
1:B:142:GLN:HG2	1:B:143:VAL:H	1.75	0.52
1:B:168:ASP:HB2	4:B:2365:HOH:O	2.09	0.52
1:D:134:VAL:HG11	1:D:170:VAL:HG11	1.91	0.52
1:D:74:ILE:O	1:D:75:ILE:C	2.49	0.52
1:E:118:ILE:HD13	1:E:137:THR:HA	1.92	0.52
1:A:18:GLY:HA3	4:A:1401:HOH:O	2.08	0.52
1:A:226:GLN:HA	1:A:226:GLN:OE1	2.08	0.52
1:B:103:SER:C	1:B:104:ILE:HD13	2.29	0.52
1:B:135:TYR:OH	1:B:150:GLU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:GLU:HB2	1:C:90:HIS:NE2	2.24	0.52
1:E:185:LEU:CD2	1:E:207:ALA:HA	2.40	0.52
1:E:33:SER:HB3	1:E:56:ASN:OD1	2.09	0.52
1:A:153:LEU:O	1:A:155:SER:N	2.43	0.52
1:E:13:PHE:O	1:E:16:ALA:N	2.43	0.52
1:A:268:LEU:HB2	4:A:1412:HOH:O	2.10	0.51
1:B:109:SER:HA	1:B:115:PRO:CD	2.40	0.51
1:B:25:LEU:HD22	1:B:30:ILE:HD11	1.92	0.51
1:C:193:VAL:HG23	4:C:3358:HOH:O	2.11	0.51
1:C:68:LEU:HB3	1:C:94:SER:HB2	1.91	0.51
1:D:156:VAL:HG23	4:D:4347:HOH:O	2.10	0.51
1:B:142:GLN:HG2	1:B:143:VAL:N	2.26	0.51
1:C:160:THR:HG22	1:C:161:GLU:N	2.24	0.51
1:D:134:VAL:HG21	1:D:162:VAL:CG2	2.41	0.51
1:D:13:PHE:HA	1:D:45:LEU:HD21	1.93	0.51
1:E:117:VAL:O	1:E:138:GLY:HA3	2.10	0.51
1:B:124:THR:N	1:B:125:PRO:CD	2.70	0.51
1:B:186:ASP:HB3	4:B:2304:HOH:O	2.11	0.51
1:B:243:HIS:O	1:B:247:SER:HB2	2.09	0.51
1:E:79:LEU:HD13	1:E:107:LYS:HB2	1.93	0.51
1:B:105:GLU:HA	1:B:105:GLU:OE1	2.10	0.51
1:B:158:PHE:CE2	2:B:2300:NAP:H51A	2.44	0.51
1:D:268:LEU:HD11	4:D:4358:HOH:O	2.10	0.51
1:A:233:SER:C	1:A:235:GLY:H	2.12	0.51
1:A:38:ASP:H	1:A:42:VAL:HG23	1.76	0.51
1:A:87:GLU:N	1:A:90:HIS:HE1	2.09	0.51
1:B:105:GLU:CG	1:B:139:THR:OG1	2.59	0.51
1:D:98:GLY:HA3	1:D:269:GLN:HB2	1.93	0.51
1:E:68:LEU:HA	4:E:5377:HOH:O	2.11	0.51
1:A:57:LYS:N	1:A:57:LYS:HD2	2.25	0.51
1:C:28:HIS:CA	1:C:51:LYS:HE3	2.40	0.51
1:D:200:ARG:NH1	1:D:204:ARG:NH2	2.59	0.51
1:E:123:ASN:OD1	1:E:125:PRO:HG2	2.10	0.51
1:E:130:GLU:OE2	2:E:5300:NAP:H2D	2.09	0.51
1:E:43:SER:HB3	4:E:5423:HOH:O	2.10	0.51
1:E:44:ALA:C	1:E:48:MET:HE3	2.31	0.51
1:A:221:GLU:O	1:A:223:HIS:N	2.44	0.51
1:A:83:GLY:HA2	1:A:86:ILE:CG1	2.40	0.51
1:C:225:GLY:HA2	4:C:3367:HOH:O	2.10	0.51
1:C:155:SER:CA	2:C:3300:NAP:N7N	2.72	0.51
1:C:218:LEU:HD13	2:C:3300:NAP:O1N	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ALA:HB1	1:A:28:HIS:CE1	2.46	0.51
1:B:15:LEU:O	1:B:19:PHE:CE1	2.63	0.51
1:C:251:ARG:O	1:C:252:SER:O	2.28	0.51
1:D:115:PRO:HD2	4:D:4370:HOH:O	2.10	0.51
1:A:233:SER:C	1:A:235:GLY:N	2.64	0.51
1:C:203:VAL:HG22	4:C:3359:HOH:O	2.10	0.51
1:D:202:ALA:O	1:D:204:ARG:N	2.43	0.51
1:A:135:TYR:CE1	1:A:161:GLU:HG2	2.46	0.51
1:A:162:VAL:CG1	1:A:166:LEU:HB2	2.41	0.51
1:D:101:ILE:HG12	1:D:164:GLU:OE1	2.11	0.51
1:D:246:GLU:HG3	4:D:4337:HOH:O	2.11	0.51
1:E:123:ASN:O	1:E:126:VAL:HG23	2.11	0.51
1:E:118:ILE:HD11	1:E:141:ALA:HB1	1.92	0.51
1:A:225:GLY:O	1:A:228:LYS:HB3	2.10	0.50
1:A:228:LYS:HE2	1:A:229:ASP:OD1	2.10	0.50
1:B:102:SER:HA	1:B:105:GLU:HB2	1.92	0.50
1:B:6:ILE:HA	1:B:33:SER:HB3	1.92	0.50
1:B:68:LEU:HD13	1:B:74:ILE:HB	1.92	0.50
1:B:70:VAL:HG12	1:B:71:LYS:N	2.27	0.50
1:B:76:PRO:HB2	1:B:77:PHE:CD1	2.46	0.50
1:D:124:THR:C	1:D:126:VAL:N	2.64	0.50
1:D:134:VAL:HG23	1:D:160:THR:O	2.11	0.50
1:E:122:THR:CG2	1:E:133:THR:HG22	2.40	0.50
1:A:149:MET:CE	1:A:153:LEU:HG	2.41	0.50
1:B:258:VAL:CG1	1:B:259:GLU:N	2.75	0.50
1:B:83:GLY:N	1:B:108:LEU:HD22	2.27	0.50
1:D:134:VAL:HG21	1:D:162:VAL:HG21	1.93	0.50
1:E:200:ARG:C	1:E:204:ARG:HG2	2.25	0.50
1:E:33:SER:O	1:E:35:PRO:CD	2.59	0.50
1:A:101:ILE:HG12	1:A:119:ARG:HB2	1.93	0.50
1:A:121:MET:O	1:A:133:THR:HG23	2.12	0.50
1:A:153:LEU:C	1:A:155:SER:N	2.64	0.50
1:A:199:ARG:NH1	4:A:1343:HOH:O	2.44	0.50
1:B:45:LEU:O	1:B:48:MET:HB2	2.11	0.50
1:B:74:ILE:O	1:B:78:ILE:HB	2.11	0.50
1:C:19:PHE:O	1:C:22:ALA:HB3	2.11	0.50
1:D:127:VAL:HG12	4:D:4415:HOH:O	2.11	0.50
2:A:1300:NAP:H52N	2:A:1300:NAP:O2N	2.12	0.50
1:A:64:ASP:O	1:A:90:HIS:HB3	2.11	0.50
2:B:2300:NAP:O3X	2:B:2300:NAP:H8A	2.12	0.50
1:B:29:LYS:O	1:B:30:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:THR:HG23	4:C:3317:HOH:O	2.10	0.50
1:C:135:TYR:CE1	1:C:161:GLU:HB3	2.47	0.50
1:D:22:ALA:HA	1:D:129:ARG:CZ	2.41	0.50
1:D:38:ASP:OD1	1:D:42:VAL:HG23	2.12	0.50
1:E:34:SER:HB3	1:E:54:PRO:CA	2.41	0.50
1:A:236:GLY:O	1:A:237:ALA:HB3	2.12	0.50
1:B:124:THR:H	1:B:125:PRO:HD2	1.74	0.50
1:B:7:GLY:HA3	1:B:69:ALA:HB3	1.93	0.50
1:A:223:HIS:ND1	1:A:224:PRO:HD2	2.25	0.50
1:B:123:ASN:ND2	1:B:132:ALA:H	2.10	0.50
1:C:126:VAL:C	1:C:128:VAL:N	2.65	0.50
1:C:114:ALA:HB1	1:C:140:HIS:ND1	2.27	0.50
1:C:255:ILE:O	1:C:256:ASN:C	2.50	0.50
1:D:223:HIS:ND1	1:D:224:PRO:HD2	2.27	0.50
1:D:218:LEU:HB3	2:D:4300:NAP:O1N	2.11	0.50
1:E:211:LEU:C	1:E:211:LEU:HD13	2.32	0.50
1:E:46:ARG:O	1:E:47:LYS:C	2.50	0.50
1:A:189:ALA:CB	1:A:203:VAL:HG22	2.42	0.50
1:B:14:ALA:CA	1:B:127:VAL:HG22	2.41	0.50
1:B:177:GLY:HA2	1:B:180:TYR:CD1	2.47	0.50
1:C:79:LEU:HD22	1:C:108:LEU:HD11	1.93	0.50
1:A:33:SER:HB3	1:A:56:ASN:HA	1.94	0.50
1:C:87:GLU:N	1:C:90:HIS:CE1	2.78	0.50
1:E:53:THR:C	1:E:55:HIS:N	2.64	0.50
1:A:122:THR:CG2	1:A:123:ASN:H	2.07	0.50
1:C:108:LEU:HD21	4:C:3338:HOH:O	2.12	0.50
1:C:11:LEU:HD12	1:C:14:ALA:HB3	1.94	0.50
1:C:22:ALA:O	1:C:24:VAL:HG23	2.12	0.50
1:C:172:GLY:HA2	1:C:261:SER:HB3	1.94	0.50
1:C:45:LEU:O	1:C:45:LEU:HD23	2.12	0.50
1:D:264:ARG:CD	4:D:4406:HOH:O	2.56	0.50
1:D:33:SER:HA	1:D:53:THR:O	2.12	0.50
1:A:193:VAL:HG11	4:E:5424:HOH:O	2.11	0.49
1:B:121:MET:O	1:B:133:THR:HB	2.12	0.49
1:C:259:GLU:C	4:C:3302:HOH:O	2.49	0.49
1:E:67:PHE:O	1:E:68:LEU:HD23	2.12	0.49
1:E:70:VAL:HB	4:E:5428:HOH:O	2.12	0.49
1:B:8:ALA:HA	1:B:12:ALA:CB	2.42	0.49
1:C:122:THR:CG2	1:C:133:THR:HG22	2.42	0.49
2:C:3300:NAP:C8A	2:C:3300:NAP:O3X	2.61	0.49
1:E:123:ASN:OD1	1:E:131:GLY:HA2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:THR:HG22	1:E:55:HIS:N	2.24	0.49
1:A:123:ASN:HD22	1:A:123:ASN:N	2.09	0.49
1:A:251:ARG:HG3	4:A:1403:HOH:O	2.11	0.49
1:B:123:ASN:HD21	1:B:132:ALA:H	1.61	0.49
1:C:91:ILE:HD11	1:C:116:ARG:CZ	2.42	0.49
1:C:98:GLY:O	1:C:269:GLN:HA	2.11	0.49
1:D:156:VAL:CG1	1:D:156:VAL:O	2.56	0.49
1:D:220:SER:O	1:D:222:GLN:N	2.39	0.49
1:D:262:CYS:HA	4:D:4354:HOH:O	2.12	0.49
1:D:98:GLY:O	1:D:99:VAL:C	2.51	0.49
1:E:91:ILE:HD11	1:E:116:ARG:CZ	2.42	0.49
1:A:122:THR:CG2	1:A:123:ASN:N	2.74	0.49
1:A:219:HIS:O	1:A:220:SER:N	2.38	0.49
1:A:264:ARG:CZ	1:A:268:LEU:HD21	2.43	0.49
1:B:258:VAL:HA	4:B:2347:HOH:O	2.11	0.49
1:C:134:VAL:CG1	4:C:3374:HOH:O	2.60	0.49
1:D:222:GLN:O	1:D:223:HIS:CB	2.59	0.49
1:E:125:PRO:HB2	1:E:130:GLU:O	2.13	0.49
1:E:262:CYS:HA	4:E:5320:HOH:O	2.12	0.49
1:E:36:ASP:OD1	1:E:37:MET:N	2.45	0.49
1:A:71:LYS:HB2	1:A:74:ILE:HG12	1.94	0.49
1:C:112:ARG:HG3	1:C:113:PRO:CD	2.36	0.49
1:C:236:GLY:HA2	1:C:240:HIS:HD2	1.78	0.49
1:D:162:VAL:HG11	1:D:166:LEU:HB2	1.93	0.49
1:D:201:LEU:O	1:D:204:ARG:HB2	2.12	0.49
1:D:80:ASP:HB2	4:D:4386:HOH:O	2.11	0.49
1:E:215:LYS:O	1:E:219:HIS:CD2	2.65	0.49
1:A:148:LEU:HD23	4:A:1423:HOH:O	2.13	0.49
1:B:221:GLU:HA	2:B:2300:NAP:O2X	2.12	0.49
1:B:221:GLU:O	1:B:222:GLN:C	2.50	0.49
2:D:4300:NAP:C8A	2:D:4300:NAP:O3X	2.60	0.49
1:D:60:VAL:O	1:D:90:HIS:CE1	2.66	0.49
1:E:124:THR:C	1:E:126:VAL:H	2.14	0.49
1:E:43:SER:HA	1:E:46:ARG:HH11	1.77	0.49
1:A:242:LEU:O	1:A:243:HIS:C	2.50	0.49
1:B:45:LEU:HD11	4:B:2360:HOH:O	2.12	0.49
1:B:76:PRO:C	1:B:78:ILE:H	2.15	0.49
1:B:66:LEU:HD12	1:B:92:VAL:HG22	1.95	0.49
1:C:127:VAL:O	1:C:127:VAL:HG12	2.13	0.49
1:C:256:ASN:HB3	4:C:3312:HOH:O	2.12	0.49
1:D:258:VAL:HG12	1:D:259:GLU:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:HIS:ND1	1:D:62:HIS:O	2.45	0.49
1:E:25:LEU:N	1:E:25:LEU:HD23	2.27	0.49
1:A:112:ARG:HG2	4:A:1424:HOH:O	2.13	0.49
1:A:71:LYS:HB2	1:A:73:HIS:CD2	2.48	0.49
1:B:156:VAL:HG22	4:B:2358:HOH:O	2.12	0.49
1:D:16:ALA:HB3	4:D:4329:HOH:O	2.13	0.49
1:D:82:ILE:HA	1:D:85:ASP:OD2	2.13	0.49
1:E:195:MET:SD	1:E:195:MET:N	2.85	0.49
1:A:143:VAL:O	1:A:143:VAL:HG12	2.12	0.49
1:A:83:GLY:O	1:A:86:ILE:HG12	2.12	0.49
1:B:105:GLU:CD	1:B:139:THR:OG1	2.51	0.49
1:B:73:HIS:O	1:B:76:PRO:HD2	2.13	0.49
1:B:9:GLY:O	1:B:13:PHE:HB2	2.13	0.49
1:C:215:LYS:HG3	1:C:219:HIS:CE1	2.47	0.49
1:A:164:GLU:C	1:A:166:LEU:H	2.16	0.49
1:A:203:VAL:HG11	4:A:1398:HOH:O	2.13	0.49
1:B:222:GLN:HB2	4:B:2303:HOH:O	2.13	0.49
1:B:225:GLY:O	1:B:228:LYS:HB3	2.13	0.49
1:C:107:LYS:O	1:C:110:ALA:HB3	2.12	0.49
1:D:19:PHE:HD2	4:D:4347:HOH:O	1.96	0.49
1:D:34:SER:C	1:D:36:ASP:H	2.15	0.49
2:D:4300:NAP:PN	2:D:4300:NAP:H6N	2.53	0.49
1:E:121:MET:CE	1:E:121:MET:HA	2.43	0.49
1:E:152:LEU:O	1:E:155:SER:HB2	2.13	0.49
1:E:55:HIS:HB3	1:E:57:LYS:CG	2.42	0.49
1:A:25:LEU:HD12	1:A:26:ALA:H	1.78	0.48
1:A:75:ILE:HG22	1:A:76:PRO:N	2.27	0.48
1:A:77:PHE:HD1	1:A:77:PHE:N	2.08	0.48
1:B:253:LEU:HB2	4:B:2342:HOH:O	2.13	0.48
1:C:56:ASN:O	1:C:82:ILE:HD11	2.13	0.48
1:C:7:GLY:HA2	1:C:70:VAL:HG22	1.95	0.48
1:D:67:PHE:HA	1:D:93:VAL:O	2.12	0.48
1:E:101:ILE:CG2	1:E:102:SER:N	2.75	0.48
1:C:122:THR:HB	4:C:3387:HOH:O	2.13	0.48
1:C:29:LYS:HG2	4:C:3346:HOH:O	2.12	0.48
2:C:3300:NAP:C3N	3:C:3301:GLU:N	2.76	0.48
1:C:6:ILE:HD11	1:C:60:VAL:HG22	1.94	0.48
1:C:83:GLY:O	1:C:86:ILE:HD12	2.12	0.48
1:D:189:ALA:HA	4:D:4326:HOH:O	2.12	0.48
1:D:202:ALA:C	1:D:204:ARG:N	2.66	0.48
1:E:3:VAL:HG12	1:E:4:GLY:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:GLY:HA2	1:C:108:LEU:CD2	2.43	0.48
1:C:122:THR:HB	1:C:133:THR:HG22	1.96	0.48
1:D:162:VAL:CG1	1:D:166:LEU:HB2	2.43	0.48
1:E:100:THR:HG22	1:E:101:ILE:H	1.78	0.48
1:E:83:GLY:HA2	1:E:86:ILE:CG1	2.43	0.48
1:B:147:ARG:O	1:B:151:GLN:HG3	2.14	0.48
1:B:221:GLU:HG2	1:B:222:GLN:H	1.79	0.48
1:B:239:ILE:HG23	1:B:240:HIS:N	2.28	0.48
1:D:119:ARG:HG2	4:D:4421:HOH:O	2.11	0.48
1:D:3:VAL:HG22	1:D:65:VAL:CG1	2.43	0.48
1:E:222:GLN:HG3	1:E:227:LEU:HD21	1.94	0.48
1:E:266:ARG:HD2	4:E:5337:HOH:O	2.14	0.48
1:A:178:PRO:O	1:A:181:ALA:HB3	2.13	0.48
1:A:29:LYS:HG2	4:A:1305:HOH:O	2.12	0.48
1:B:44:ALA:O	1:B:48:MET:HG3	2.13	0.48
1:C:30:ILE:N	1:C:30:ILE:HD12	2.27	0.48
1:D:148:LEU:O	1:D:148:LEU:HD12	2.14	0.48
1:D:45:LEU:O	1:D:50:VAL:HG12	2.14	0.48
2:C:3300:NAP:H8A	2:C:3300:NAP:O3X	2.14	0.48
1:E:162:VAL:HG12	1:E:163:GLU:N	2.28	0.48
1:B:119:ARG:HD2	1:B:164:GLU:OE2	2.13	0.48
1:B:42:VAL:C	1:B:44:ALA:H	2.15	0.48
1:C:171:THR:O	1:C:175:GLY:HA3	2.14	0.48
1:C:70:VAL:HG12	1:C:74:ILE:HB	1.96	0.48
1:A:187:ALA:O	1:A:190:ASP:HB2	2.14	0.48
1:A:38:ASP:H	1:A:42:VAL:CG2	2.27	0.48
1:A:71:LYS:HB2	1:A:73:HIS:HD2	1.78	0.48
1:B:104:ILE:HD13	1:B:104:ILE:N	2.29	0.48
1:B:13:PHE:HB2	1:B:41:THR:HG21	1.96	0.48
1:D:100:THR:HG22	1:D:101:ILE:N	2.28	0.48
1:D:244:VAL:HG12	1:D:245:LEU:N	2.28	0.48
1:D:39:LEU:HA	1:D:43:SER:HB2	1.95	0.48
1:E:150:GLU:O	1:E:152:LEU:N	2.46	0.48
1:E:31:MET:HG3	1:E:62:HIS:CE1	2.49	0.48
1:E:56:ASN:O	1:E:60:VAL:HG23	2.14	0.48
1:A:251:ARG:O	1:A:254:LEU:N	2.44	0.48
1:C:121:MET:HB2	4:C:3368:HOH:O	2.14	0.48
1:C:125:PRO:C	1:C:127:VAL:N	2.67	0.48
1:C:134:VAL:HG12	4:C:3374:HOH:O	2.14	0.48
1:C:153:LEU:C	1:C:155:SER:N	2.68	0.48
1:C:172:GLY:O	1:C:258:VAL:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:ARG:NH2	1:C:52:LEU:HD13	2.28	0.48
1:D:57:LYS:HE2	1:D:85:ASP:OD2	2.13	0.48
1:A:135:TYR:OH	1:A:150:GLU:CG	2.61	0.48
1:A:203:VAL:HB	4:A:1335:HOH:O	2.14	0.48
1:A:18:GLY:HA2	1:A:21:ALA:HB3	1.95	0.48
1:B:194:LYS:HG2	1:B:195:MET:CE	2.44	0.48
1:B:231:VAL:HG12	1:B:231:VAL:O	2.14	0.48
1:C:162:VAL:HG22	4:C:3374:HOH:O	2.14	0.48
1:D:251:ARG:NH1	1:D:251:ARG:HG2	2.29	0.48
1:A:134:VAL:HG13	1:A:162:VAL:HB	1.95	0.47
1:B:79:LEU:CD1	1:B:104:ILE:HG23	2.35	0.47
1:B:125:PRO:CG	1:B:131:GLY:HA2	2.37	0.47
1:B:84:ALA:H	1:B:111:PHE:HD2	1.62	0.47
1:C:6:ILE:HD12	1:C:56:ASN:HB3	1.95	0.47
4:B:2309:HOH:O	1:D:239:ILE:HD12	2.14	0.47
1:D:45:LEU:O	1:D:48:MET:HB3	2.14	0.47
1:E:83:GLY:HA2	1:E:86:ILE:HG12	1.94	0.47
1:B:194:LYS:HG2	1:B:195:MET:HE3	1.96	0.47
1:B:229:ASP:HA	4:E:5317:HOH:O	2.14	0.47
1:D:93:VAL:HG12	1:D:118:ILE:HB	1.95	0.47
1:D:22:ALA:HB3	1:D:24:VAL:HG23	1.96	0.47
1:A:137:THR:HB	1:A:141:ALA:CB	2.44	0.47
1:B:184:ALA:O	1:B:187:ALA:HB3	2.14	0.47
1:B:15:LEU:HD23	1:B:19:PHE:HE2	1.76	0.47
1:B:58:GLU:O	1:B:60:VAL:N	2.47	0.47
1:B:84:ALA:N	4:B:2393:HOH:O	2.46	0.47
1:C:141:ALA:HA	1:C:145:ASP:OD1	2.13	0.47
1:C:227:LEU:O	1:C:231:VAL:HG23	2.14	0.47
1:D:96:ALA:N	4:D:4413:HOH:O	2.46	0.47
1:E:107:LYS:O	1:E:111:PHE:HE1	1.97	0.47
1:E:217:LEU:HD13	1:E:227:LEU:HD12	1.95	0.47
1:E:226:GLN:HG2	4:E:5392:HOH:O	2.14	0.47
1:E:236:GLY:O	1:E:237:ALA:HB3	2.15	0.47
1:E:274:GLN:CG	1:E:275:GLU:HG2	2.40	0.47
1:B:141:ALA:O	1:B:142:GLN:O	2.32	0.47
1:B:150:GLU:O	1:B:150:GLU:HG2	2.15	0.47
1:B:83:GLY:HA3	1:B:111:PHE:HB2	1.96	0.47
1:C:51:LYS:CD	1:C:51:LYS:H	2.24	0.47
1:C:3:VAL:HA	1:C:65:VAL:O	2.14	0.47
1:D:203:VAL:O	1:D:204:ARG:CD	2.62	0.47
1:D:263:ILE:O	1:D:267:GLU:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:GLU:O	1:E:151:GLN:C	2.51	0.47
1:B:142:GLN:O	1:B:145:ASP:HB3	2.14	0.47
1:E:131:GLY:H	1:E:157:GLY:HA3	1.77	0.47
1:E:131:GLY:H	1:E:157:GLY:CA	2.28	0.47
1:E:222:GLN:O	1:E:223:HIS:CB	2.62	0.47
1:A:158:PHE:CE1	2:A:1300:NAP:H51A	2.49	0.47
1:B:153:LEU:O	1:B:155:SER:N	2.47	0.47
1:C:11:LEU:HD13	1:C:124:THR:HA	1.97	0.47
1:B:239:ILE:HG12	4:E:5386:HOH:O	2.15	0.47
1:B:196:GLY:O	1:D:234:PRO:HB3	2.15	0.47
1:E:123:ASN:HB2	1:E:125:PRO:HD2	1.96	0.47
1:E:57:LYS:H	1:E:57:LYS:CD	2.07	0.47
1:E:70:VAL:HG12	4:E:5441:HOH:O	2.14	0.47
1:A:115:PRO:O	1:A:140:HIS:HB2	2.15	0.47
1:C:71:LYS:N	1:C:71:LYS:HD3	2.19	0.47
1:A:39:LEU:O	1:A:43:SER:CB	2.63	0.47
1:A:7:GLY:HA3	1:A:69:ALA:HB3	1.95	0.47
1:A:73:HIS:O	1:A:76:PRO:HD2	2.15	0.47
1:B:122:THR:OG1	1:B:123:ASN:N	2.47	0.47
1:B:200:ARG:CG	1:B:204:ARG:HE	2.24	0.47
1:B:29:LYS:C	1:B:30:ILE:HG13	2.34	0.47
1:B:71:LYS:HB2	1:B:73:HIS:ND1	2.29	0.47
1:D:166:LEU:O	1:D:168:ASP:N	2.48	0.47
1:A:109:SER:C	1:A:111:PHE:H	2.18	0.47
1:A:133:THR:HG21	1:A:153:LEU:CD1	2.43	0.47
1:A:238:THR:C	1:A:240:HIS:N	2.63	0.47
1:C:79:LEU:HA	4:C:3338:HOH:O	2.14	0.47
1:C:83:GLY:HA2	1:C:108:LEU:HD22	1.96	0.47
1:D:33:SER:HB3	1:D:56:ASN:OD1	2.14	0.47
1:E:102:SER:C	1:E:104:ILE:N	2.68	0.47
1:E:77:PHE:N	1:E:77:PHE:HD1	2.12	0.47
1:A:144:GLU:CD	1:A:144:GLU:H	2.18	0.47
1:B:157:GLY:O	1:B:158:PHE:CB	2.63	0.47
1:C:223:HIS:ND1	1:C:224:PRO:CD	2.77	0.47
1:D:124:THR:N	1:D:125:PRO:CD	2.77	0.47
1:D:115:PRO:O	1:D:140:HIS:HB2	2.15	0.47
1:D:188:LEU:O	1:D:191:GLY:N	2.48	0.47
1:D:258:VAL:O	1:D:259:GLU:C	2.53	0.47
1:A:221:GLU:HG3	1:A:222:GLN:N	2.30	0.46
1:A:222:GLN:O	1:A:223:HIS:HB3	2.14	0.46
1:A:264:ARG:NH2	1:A:268:LEU:HD21	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:GLY:HA2	1:B:119:ARG:NH2	2.30	0.46
1:B:137:THR:HG22	1:B:138:GLY:N	2.30	0.46
1:B:74:ILE:C	1:B:74:ILE:HD12	2.35	0.46
1:C:149:MET:C	1:C:151:GLN:H	2.19	0.46
1:C:245:LEU:O	1:C:248:GLY:N	2.35	0.46
1:D:237:ALA:O	1:D:240:HIS:N	2.48	0.46
1:E:121:MET:SD	1:E:171:THR:HG23	2.55	0.46
1:A:22:ALA:CB	1:A:24:VAL:HG23	2.45	0.46
1:B:43:SER:O	1:B:47:LYS:HE2	2.14	0.46
1:B:52:LEU:O	1:B:54:PRO:HD3	2.15	0.46
1:B:74:ILE:C	1:B:78:ILE:HB	2.35	0.46
1:B:63:SER:O	1:B:89:ARG:NH1	2.49	0.46
1:C:79:LEU:HD11	1:C:104:ILE:HG12	1.97	0.46
1:C:57:LYS:O	1:C:61:GLN:OE1	2.32	0.46
1:C:86:ILE:HG22	1:C:87:GLU:N	2.30	0.46
1:E:185:LEU:HG	1:E:210:LEU:CD1	2.45	0.46
1:E:98:GLY:HA2	4:E:5346:HOH:O	2.14	0.46
1:A:74:ILE:HG22	1:A:78:ILE:CD1	2.46	0.46
1:B:101:ILE:HG13	1:B:102:SER:H	1.80	0.46
1:B:140:HIS:O	1:B:141:ALA:HB2	2.15	0.46
1:B:180:TYR:O	1:B:183:THR:HB	2.15	0.46
1:B:28:HIS:C	1:B:30:ILE:H	2.19	0.46
1:C:123:ASN:O	1:C:126:VAL:HG13	2.16	0.46
1:C:17:LYS:O	1:C:20:THR:HB	2.15	0.46
1:C:31:MET:N	1:C:62:HIS:NE2	2.63	0.46
1:E:220:SER:O	1:E:221:GLU:CB	2.64	0.46
1:E:39:LEU:N	1:E:39:LEU:HD23	2.15	0.46
1:E:77:PHE:N	1:E:77:PHE:CD1	2.82	0.46
1:E:82:ILE:O	1:E:86:ILE:HG12	2.16	0.46
1:A:76:PRO:C	1:A:78:ILE:N	2.68	0.46
1:B:70:VAL:HG11	1:B:78:ILE:HD11	1.96	0.46
1:D:22:ALA:HB2	1:D:129:ARG:HD3	1.97	0.46
1:D:34:SER:C	1:D:36:ASP:N	2.68	0.46
1:D:73:HIS:C	1:D:76:PRO:HD2	2.35	0.46
1:E:55:HIS:HB3	1:E:57:LYS:CE	2.40	0.46
1:E:8:ALA:HB1	1:E:41:THR:CG2	2.45	0.46
1:A:117:VAL:HG22	1:A:118:ILE:N	2.30	0.46
1:A:70:VAL:HG21	1:A:78:ILE:CD1	2.45	0.46
1:C:2:SER:O	1:C:65:VAL:HG12	2.14	0.46
1:D:114:ALA:HB1	1:D:140:HIS:CG	2.51	0.46
1:E:128:VAL:O	1:E:129:ARG:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLY:O	1:A:178:PRO:C	2.54	0.46
2:B:2300:NAP:O2D	3:B:2301:GLU:OE1	2.33	0.46
1:B:71:LYS:HD2	1:B:71:LYS:N	2.24	0.46
1:D:203:VAL:HG13	1:D:204:ARG:HG2	1.97	0.46
1:E:74:ILE:HG13	4:E:5441:HOH:O	2.16	0.46
1:A:194:LYS:O	1:A:195:MET:SD	2.74	0.46
1:A:217:LEU:CD1	4:A:1397:HOH:O	2.60	0.46
1:B:242:LEU:O	1:B:245:LEU:N	2.49	0.46
1:C:89:ARG:HE	1:C:90:HIS:HD2	1.64	0.46
1:D:112:ARG:HB3	4:D:4351:HOH:O	2.16	0.46
1:D:87:GLU:HG3	1:D:89:ARG:HH12	1.80	0.46
1:A:13:PHE:HB2	1:A:45:LEU:HD21	1.97	0.46
1:A:164:GLU:O	1:A:166:LEU:N	2.49	0.46
1:A:199:ARG:O	1:A:201:LEU:N	2.48	0.46
1:B:91:ILE:HG12	1:B:116:ARG:HD2	1.96	0.46
2:B:2300:NAP:H6N	2:B:2300:NAP:PN	2.55	0.46
1:E:115:PRO:O	1:E:140:HIS:HD2	1.99	0.46
1:B:149:MET:C	1:B:151:GLN:N	2.68	0.46
1:C:200:ARG:NH2	4:C:3379:HOH:O	2.49	0.46
1:D:190:ASP:C	4:D:4346:HOH:O	2.55	0.46
1:D:237:ALA:H	1:D:240:HIS:CD2	2.34	0.46
1:D:33:SER:CB	1:D:56:ASN:OD1	2.64	0.46
1:E:82:ILE:O	1:E:85:ASP:N	2.44	0.46
1:A:25:LEU:CD1	1:A:29:LYS:HD2	2.46	0.46
1:A:62:HIS:C	1:A:62:HIS:ND1	2.69	0.46
1:A:135:TYR:HE1	1:A:161:GLU:HG2	1.78	0.45
1:A:204:ARG:NH2	4:A:1341:HOH:O	2.48	0.45
1:B:193:VAL:HB	4:B:2309:HOH:O	2.15	0.45
1:B:200:ARG:O	1:B:201:LEU:C	2.54	0.45
1:B:206:GLY:O	1:B:209:ALA:HB3	2.16	0.45
1:C:252:SER:HB3	4:C:3361:HOH:O	2.16	0.45
1:D:220:SER:C	1:D:222:GLN:N	2.69	0.45
1:E:200:ARG:O	1:E:201:LEU:C	2.55	0.45
1:A:60:VAL:HG11	1:A:82:ILE:HG23	1.98	0.45
1:A:61:GLN:O	1:A:89:ARG:NH2	2.49	0.45
1:B:179:ALA:HB2	4:B:2371:HOH:O	2.16	0.45
1:B:189:ALA:HB1	1:B:199:ARG:NH1	2.32	0.45
1:C:162:VAL:HG21	4:C:3351:HOH:O	2.15	0.45
1:D:249:GLY:O	1:D:252:SER:HB3	2.16	0.45
1:E:142:GLN:HB2	1:E:145:ASP:OD2	2.15	0.45
1:E:16:ALA:O	1:E:20:THR:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:ASP:HB3	1:E:40:ALA:H	1.81	0.45
1:E:48:MET:CG	1:E:48:MET:O	2.62	0.45
1:E:33:SER:HA	1:E:53:THR:O	2.16	0.45
1:B:26:ALA:HB3	1:B:29:LYS:CG	2.47	0.45
1:B:83:GLY:C	1:B:111:PHE:HB3	2.36	0.45
1:C:125:PRO:HB2	1:C:130:GLU:O	2.17	0.45
1:C:122:THR:HG22	1:C:133:THR:HG22	1.97	0.45
1:C:52:LEU:HD12	4:C:3343:HOH:O	2.16	0.45
1:E:126:VAL:HG13	1:E:156:VAL:HG12	1.99	0.45
1:E:162:VAL:HG11	1:E:166:LEU:HD12	1.97	0.45
1:E:185:LEU:HG	1:E:210:LEU:HD11	1.99	0.45
1:E:230:ASN:N	1:E:230:ASN:OD1	2.50	0.45
1:A:192:GLY:HA3	4:A:1415:HOH:O	2.17	0.45
1:A:203:VAL:N	4:A:1335:HOH:O	2.49	0.45
1:A:36:ASP:C	1:A:37:MET:HG3	2.37	0.45
1:B:109:SER:OG	1:B:115:PRO:HD2	2.17	0.45
1:B:242:LEU:O	1:B:243:HIS:C	2.53	0.45
1:C:60:VAL:HG12	1:C:60:VAL:O	2.16	0.45
1:D:19:PHE:CE2	1:D:152:LEU:HD13	2.51	0.45
1:D:236:GLY:O	1:D:237:ALA:HB3	2.16	0.45
1:E:48:MET:HE3	1:E:48:MET:HB3	1.83	0.45
1:A:13:PHE:CB	1:A:45:LEU:HD21	2.45	0.45
1:A:258:VAL:HG12	1:A:259:GLU:N	2.32	0.45
1:B:189:ALA:O	1:B:193:VAL:HG23	2.15	0.45
1:D:111:PHE:O	1:D:112:ARG:C	2.55	0.45
1:D:143:VAL:C	1:D:145:ASP:N	2.68	0.45
1:D:98:GLY:CA	1:D:269:GLN:HB2	2.47	0.45
1:D:3:VAL:HG12	1:D:4:GLY:N	2.32	0.45
1:E:153:LEU:H	1:E:153:LEU:HD12	1.80	0.45
1:E:241:ALA:O	1:E:242:LEU:C	2.55	0.45
1:E:268:LEU:HD12	4:E:5360:HOH:O	2.15	0.45
1:E:43:SER:HB2	4:E:5335:HOH:O	2.15	0.45
1:A:22:ALA:HB1	1:A:24:VAL:HG23	1.98	0.45
1:B:244:VAL:HA	4:B:2394:HOH:O	2.15	0.45
1:B:41:THR:O	1:B:45:LEU:HG	2.16	0.45
1:C:125:PRO:C	1:C:127:VAL:H	2.20	0.45
1:E:104:ILE:HG21	1:E:117:VAL:HG11	1.98	0.45
1:E:125:PRO:C	1:E:127:VAL:N	2.70	0.45
1:E:179:ALA:HB1	4:E:5310:HOH:O	2.15	0.45
1:E:224:PRO:HD2	4:E:5453:HOH:O	2.16	0.45
1:A:129:ARG:O	1:A:157:GLY:HA2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:PRO:HG2	4:B:2397:HOH:O	2.16	0.45
1:C:124:THR:C	1:C:126:VAL:H	2.20	0.45
1:D:87:GLU:HB2	1:D:90:HIS:CD2	2.52	0.45
1:E:202:ALA:C	1:E:204:ARG:N	2.69	0.45
1:E:55:HIS:CG	1:E:57:LYS:HE2	2.52	0.45
1:A:40:ALA:HB1	4:A:1422:HOH:O	2.17	0.45
1:B:162:VAL:O	1:B:163:GLU:C	2.56	0.45
1:B:72:PRO:O	1:B:75:ILE:HD12	2.17	0.45
1:B:94:SER:O	1:B:96:ALA:N	2.50	0.45
1:C:123:ASN:O	1:C:126:VAL:HG22	2.16	0.45
1:C:167:ILE:N	4:C:3351:HOH:O	2.50	0.45
1:C:253:LEU:HD12	1:C:253:LEU:N	2.32	0.45
1:D:199:ARG:NH1	4:D:4372:HOH:O	2.49	0.45
1:A:71:LYS:HD2	1:A:73:HIS:NE2	2.32	0.45
1:A:83:GLY:CA	1:A:86:ILE:HG12	2.45	0.45
1:B:123:ASN:CG	1:B:132:ALA:H	2.19	0.45
2:A:1300:NAP:C6N	3:A:1301:GLU:OXT	2.65	0.45
1:A:130:GLU:HB2	4:A:1338:HOH:O	2.16	0.45
1:A:133:THR:CG2	1:A:134:VAL:N	2.80	0.45
1:A:177:GLY:HA2	1:A:180:TYR:CD1	2.52	0.45
1:B:79:LEU:O	1:B:108:LEU:HD21	2.16	0.45
2:B:2300:NAP:O3X	2:B:2300:NAP:C8A	2.64	0.45
1:C:128:VAL:HG12	1:C:129:ARG:N	2.32	0.45
1:D:19:PHE:HA	4:D:4347:HOH:O	2.16	0.45
1:B:41:THR:O	1:B:44:ALA:HB3	2.17	0.44
1:D:75:ILE:HB	1:D:76:PRO:CD	2.42	0.44
1:E:263:ILE:O	1:E:266:ARG:N	2.48	0.44
1:E:13:PHE:HD1	1:E:48:MET:HE1	1.83	0.44
1:A:265:THR:N	4:A:1405:HOH:O	2.50	0.44
1:B:219:HIS:O	1:B:220:SER:O	2.36	0.44
1:C:116:ARG:HA	1:C:140:HIS:O	2.18	0.44
2:C:3300:NAP:H6N	2:C:3300:NAP:PN	2.57	0.44
1:D:15:LEU:O	1:D:16:ALA:C	2.55	0.44
1:E:102:SER:C	1:E:104:ILE:H	2.20	0.44
1:A:238:THR:O	1:A:241:ALA:N	2.50	0.44
1:A:46:ARG:HG3	1:A:52:LEU:HD12	1.99	0.44
1:A:74:ILE:CG2	1:A:78:ILE:HD11	2.48	0.44
1:B:101:ILE:HG13	1:B:102:SER:N	2.31	0.44
1:B:105:GLU:CD	1:B:139:THR:HG1	2.20	0.44
1:B:218:LEU:HD13	2:B:2300:NAP:O1N	2.16	0.44
1:B:227:LEU:HD21	4:B:2303:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:ALA:HB1	1:D:203:VAL:HB	1.99	0.44
1:E:252:SER:O	1:E:255:ILE:HB	2.17	0.44
1:E:19:PHE:HB3	1:E:25:LEU:HD21	1.98	0.44
1:D:111:PHE:HB2	4:D:4387:HOH:O	2.17	0.44
1:E:124:THR:C	1:E:126:VAL:N	2.71	0.44
1:A:36:ASP:O	1:A:37:MET:CB	2.65	0.44
1:B:151:GLN:HA	4:B:2323:HOH:O	2.16	0.44
1:C:198:PRO:HD2	1:C:201:LEU:HD23	1.99	0.44
1:C:43:SER:O	1:C:46:ARG:HB2	2.18	0.44
1:D:15:LEU:HD12	1:D:126:VAL:HG11	1.99	0.44
1:D:77:PHE:O	1:D:78:ILE:C	2.55	0.44
1:E:4:GLY:HA2	1:E:31:MET:O	2.16	0.44
1:E:42:VAL:HG13	1:E:52:LEU:HD13	1.99	0.44
1:A:55:HIS:HB2	1:A:58:GLU:HG3	1.99	0.44
1:A:7:GLY:HA3	1:A:69:ALA:C	2.37	0.44
1:B:253:LEU:HD23	1:B:253:LEU:N	2.32	0.44
1:D:115:PRO:HG3	4:D:4403:HOH:O	2.18	0.44
1:D:161:GLU:O	1:D:162:VAL:HG23	2.18	0.44
1:D:264:ARG:CZ	4:D:4391:HOH:O	2.66	0.44
1:E:162:VAL:CG1	1:E:163:GLU:N	2.81	0.44
1:A:116:ARG:NH2	1:A:145:ASP:OD1	2.49	0.44
1:A:193:VAL:C	1:A:195:MET:N	2.70	0.44
1:A:25:LEU:HD23	1:A:30:ILE:HG12	1.99	0.44
1:B:35:PRO:HG2	1:B:71:LYS:HZ3	1.82	0.44
1:B:57:LYS:O	1:B:58:GLU:C	2.55	0.44
1:B:75:ILE:HB	1:B:76:PRO:CD	2.35	0.44
1:C:75:ILE:HB	1:C:76:PRO:HD3	2.00	0.44
1:A:243:HIS:HD2	1:C:194:LYS:HZ2	1.64	0.44
1:A:244:VAL:HG23	1:A:245:LEU:N	2.33	0.44
1:B:244:VAL:HG12	1:B:245:LEU:N	2.33	0.44
1:C:53:THR:HG22	1:C:55:HIS:N	2.25	0.44
1:D:0:GLY:HA2	4:D:4350:HOH:O	2.17	0.44
1:E:172:GLY:HA2	1:E:261:SER:HB3	2.00	0.44
1:E:6:ILE:HA	1:E:33:SER:OG	2.17	0.44
1:E:78:ILE:HG13	4:E:5428:HOH:O	2.17	0.44
1:A:73:HIS:CD2	1:A:74:ILE:HG12	2.53	0.44
1:B:149:MET:CE	1:B:149:MET:HA	2.48	0.44
1:B:155:SER:CA	2:B:2300:NAP:N7N	2.81	0.44
1:B:166:LEU:O	1:B:169:ALA:N	2.51	0.44
1:B:86:ILE:CD1	1:B:108:LEU:HD13	2.48	0.44
1:C:88:ASP:OD2	1:C:112:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:HIS:ND1	1:D:224:PRO:N	2.65	0.44
1:D:9:GLY:CA	1:D:41:THR:HG21	2.48	0.44
1:A:142:GLN:HB3	1:A:144:GLU:OE1	2.18	0.43
1:A:134:VAL:CG2	1:A:160:THR:CG2	2.96	0.43
1:B:236:GLY:O	1:B:238:THR:N	2.39	0.43
1:B:238:THR:C	1:B:240:HIS:N	2.70	0.43
1:B:86:ILE:HA	1:B:90:HIS:NE2	2.32	0.43
1:B:93:VAL:CG1	1:B:95:CYS:SG	3.03	0.43
1:C:134:VAL:CG1	1:C:162:VAL:HG22	2.48	0.43
1:A:229:ASP:HB3	1:C:199:ARG:HG2	2.00	0.43
1:C:39:LEU:HA	1:C:43:SER:HB3	2.00	0.43
1:D:63:SER:HB3	4:D:4390:HOH:O	2.18	0.43
1:E:135:TYR:CE1	1:E:161:GLU:HB3	2.53	0.43
1:E:33:SER:O	1:E:35:PRO:HD3	2.18	0.43
1:E:6:ILE:HD12	1:E:68:LEU:CD2	2.48	0.43
1:A:33:SER:CB	1:A:56:ASN:HB3	2.48	0.43
1:B:109:SER:HA	1:B:115:PRO:HD2	2.00	0.43
1:B:150:GLU:HG3	1:B:159:CYS:HB2	2.00	0.43
1:B:160:THR:CG2	1:B:161:GLU:N	2.80	0.43
1:C:249:GLY:O	1:C:252:SER:HB2	2.18	0.43
2:A:1300:NAP:H6N	2:A:1300:NAP:PN	2.58	0.43
1:A:142:GLN:O	1:A:144:GLU:N	2.51	0.43
1:A:185:LEU:HA	1:A:188:LEU:HD12	2.00	0.43
1:B:4:GLY:HA2	1:B:59:THR:HG22	2.00	0.43
1:C:268:LEU:O	1:C:271:MET:HB3	2.17	0.43
1:E:121:MET:O	1:E:133:THR:HA	2.18	0.43
1:E:269:GLN:C	1:E:271:MET:H	2.22	0.43
1:A:164:GLU:HA	1:A:167:ILE:HG12	2.00	0.43
1:B:123:ASN:OD1	1:B:132:ALA:N	2.49	0.43
1:B:139:THR:HG22	4:B:2382:HOH:O	2.17	0.43
1:C:124:THR:N	1:C:125:PRO:CD	2.80	0.43
1:C:82:ILE:CG2	1:C:85:ASP:HB2	2.47	0.43
1:D:171:THR:N	4:D:4405:HOH:O	2.51	0.43
1:D:224:PRO:O	1:D:225:GLY:C	2.55	0.43
1:D:238:THR:HG22	4:D:4313:HOH:O	2.18	0.43
1:A:238:THR:O	1:A:240:HIS:N	2.52	0.43
1:B:14:ALA:O	1:B:18:GLY:N	2.46	0.43
1:C:199:ARG:HD2	1:C:199:ARG:HA	1.89	0.43
1:D:242:LEU:HA	1:D:242:LEU:HD23	1.82	0.43
1:E:134:VAL:HA	1:E:160:THR:O	2.18	0.43
1:E:271:MET:C	1:E:273:ASP:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:VAL:O	1:E:61:GLN:C	2.57	0.43
1:A:123:ASN:N	1:A:123:ASN:ND2	2.66	0.43
1:B:105:GLU:HG2	4:B:2368:HOH:O	2.18	0.43
1:B:148:LEU:HA	1:B:151:GLN:NE2	2.33	0.43
1:B:212:GLY:O	1:B:213:ALA:C	2.57	0.43
1:B:268:LEU:HD12	4:B:2366:HOH:O	2.18	0.43
1:C:17:LYS:HD2	1:C:127:VAL:HG13	2.01	0.43
1:D:74:ILE:O	1:D:77:PHE:N	2.52	0.43
1:E:135:TYR:CZ	1:E:161:GLU:HB3	2.54	0.43
1:E:211:LEU:HD13	1:E:211:LEU:O	2.19	0.43
1:D:36:ASP:OD1	1:D:37:MET:N	2.51	0.43
1:E:178:PRO:O	1:E:179:ALA:C	2.57	0.43
1:E:53:THR:HG22	1:E:55:HIS:HB2	2.00	0.43
1:B:119:ARG:HD3	1:B:164:GLU:OE2	2.17	0.43
1:B:176:SER:HB2	1:B:180:TYR:OH	2.19	0.43
1:B:35:PRO:O	1:B:36:ASP:HB2	2.19	0.43
1:C:251:ARG:HB2	4:C:3304:HOH:O	2.18	0.43
1:E:125:PRO:C	1:E:127:VAL:H	2.22	0.43
1:A:250:PHE:HB3	4:A:1403:HOH:O	2.18	0.43
1:B:124:THR:O	1:B:126:VAL:N	2.52	0.43
1:B:16:ALA:O	1:B:20:THR:CG2	2.67	0.43
1:C:123:ASN:HD21	1:C:132:ALA:HB3	1.84	0.43
1:C:15:LEU:O	1:C:19:PHE:CD1	2.72	0.43
1:C:260:ALA:N	4:C:3302:HOH:O	2.52	0.43
1:C:30:ILE:O	1:C:51:LYS:NZ	2.52	0.43
1:C:89:ARG:HE	1:C:90:HIS:CD2	2.37	0.43
1:D:135:TYR:CE2	1:D:150:GLU:HG2	2.52	0.43
1:E:199:ARG:O	1:E:200:ARG:C	2.57	0.43
1:E:220:SER:HB2	1:E:222:GLN:HG2	2.01	0.43
1:E:34:SER:O	1:E:54:PRO:HA	2.19	0.43
1:E:41:THR:HG22	1:E:45:LEU:HD11	2.00	0.43
1:B:130:GLU:HA	1:B:130:GLU:OE2	2.18	0.43
1:B:101:ILE:HG23	1:B:164:GLU:CD	2.40	0.43
1:C:80:ASP:OD2	1:C:107:LYS:HE3	2.18	0.43
1:C:150:GLU:C	1:C:154:SER:HB2	2.40	0.43
1:C:266:ARG:NE	4:C:3306:HOH:O	2.52	0.43
1:A:267:GLU:O	1:A:271:MET:HB3	2.19	0.42
1:A:37:MET:CA	1:A:42:VAL:HG21	2.37	0.42
1:C:115:PRO:HB3	4:C:3398:HOH:O	2.19	0.42
1:C:124:THR:C	1:C:126:VAL:N	2.72	0.42
1:C:199:ARG:NH2	4:C:3359:HOH:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:VAL:HG12	4:C:3369:HOH:O	2.19	0.42
1:E:79:LEU:HD21	1:E:104:ILE:HG12	2.00	0.42
1:E:223:HIS:ND1	1:E:225:GLY:N	2.65	0.42
1:E:227:LEU:O	1:E:229:ASP:N	2.52	0.42
1:E:89:ARG:HG3	1:E:90:HIS:N	2.34	0.42
1:A:100:THR:HG22	1:A:101:ILE:N	2.32	0.42
1:B:101:ILE:O	1:B:105:GLU:HB2	2.19	0.42
1:B:215:LYS:HE3	4:B:2319:HOH:O	2.19	0.42
1:C:269:GLN:C	1:C:271:MET:N	2.71	0.42
1:D:15:LEU:HD23	1:D:19:PHE:CZ	2.54	0.42
1:D:190:ASP:OD1	1:D:199:ARG:NH2	2.50	0.42
1:D:52:LEU:HB3	4:D:4362:HOH:O	2.19	0.42
1:E:227:LEU:C	1:E:229:ASP:N	2.71	0.42
1:E:44:ALA:C	1:E:46:ARG:N	2.72	0.42
1:E:79:LEU:HD22	1:E:108:LEU:HD21	2.01	0.42
1:A:129:ARG:HG3	1:A:156:VAL:HA	2.00	0.42
1:A:172:GLY:O	1:A:258:VAL:HA	2.19	0.42
1:A:189:ALA:HB1	1:A:199:ARG:NH1	2.34	0.42
1:A:200:ARG:O	1:A:204:ARG:HG3	2.19	0.42
1:A:269:GLN:C	1:A:271:MET:N	2.71	0.42
1:B:234:PRO:HB3	1:E:196:GLY:C	2.40	0.42
1:C:149:MET:SD	1:C:152:LEU:HD23	2.58	0.42
1:C:55:HIS:C	1:C:57:LYS:H	2.20	0.42
3:D:4301:GLU:O	3:D:4301:GLU:CG	2.66	0.42
1:E:219:HIS:HB3	4:E:5459:HOH:O	2.18	0.42
1:A:55:HIS:C	1:A:57:LYS:N	2.72	0.42
1:A:6:ILE:HA	1:A:6:ILE:HD13	1.85	0.42
1:B:18:GLY:O	1:B:20:THR:HG23	2.19	0.42
1:D:223:HIS:N	4:D:4336:HOH:O	2.48	0.42
1:D:6:ILE:HD12	1:D:56:ASN:HB3	2.01	0.42
1:E:44:ALA:C	1:E:46:ARG:H	2.22	0.42
1:E:60:VAL:HG21	1:E:82:ILE:HG23	2.01	0.42
1:B:76:PRO:HB2	1:B:77:PHE:H	1.62	0.42
1:C:112:ARG:HG3	1:C:112:ARG:HH11	1.84	0.42
1:D:119:ARG:HD2	1:D:164:GLU:OE1	2.20	0.42
1:D:269:GLN:C	1:D:271:MET:N	2.73	0.42
1:E:45:LEU:O	1:E:50:VAL:HB	2.19	0.42
1:E:75:ILE:O	1:E:79:LEU:HG	2.19	0.42
1:A:121:MET:HG3	1:A:171:THR:HG23	2.01	0.42
1:A:7:GLY:O	1:A:8:ALA:CB	2.67	0.42
1:B:100:THR:O	1:B:103:SER:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:ARG:HA	1:C:140:HIS:HB2	2.00	0.42
1:C:3:VAL:HB	1:C:30:ILE:HG13	2.02	0.42
1:C:91:ILE:HD11	1:C:116:ARG:NH2	2.35	0.42
1:E:200:ARG:HD3	4:E:5318:HOH:O	2.19	0.42
1:E:242:LEU:O	1:E:243:HIS:C	2.56	0.42
1:E:256:ASN:N	1:E:256:ASN:OD1	2.48	0.42
1:A:89:ARG:O	1:A:116:ARG:NH1	2.52	0.42
1:A:3:VAL:HG12	1:A:4:GLY:N	2.35	0.42
1:B:268:LEU:HD11	4:B:2317:HOH:O	2.19	0.42
1:C:264:ARG:O	1:C:268:LEU:HG	2.19	0.42
1:E:81:GLU:C	1:E:82:ILE:HG13	2.40	0.42
1:B:149:MET:O	1:B:151:GLN:N	2.53	0.42
1:B:201:LEU:O	1:B:205:LEU:HD12	2.20	0.42
1:B:228:LYS:HE2	1:B:229:ASP:OD1	2.19	0.42
1:B:236:GLY:O	1:B:237:ALA:HB3	2.18	0.42
1:B:274:GLN:C	1:B:275:GLU:HG3	2.40	0.42
1:B:80:ASP:HB2	1:B:81:GLU:OE2	2.19	0.42
1:C:162:VAL:CG2	4:C:3351:HOH:O	2.68	0.42
1:D:150:GLU:O	1:D:151:GLN:C	2.57	0.42
1:D:152:LEU:HD22	1:D:152:LEU:HA	1.80	0.42
1:D:177:GLY:O	1:D:180:TYR:N	2.53	0.42
1:D:237:ALA:N	1:D:240:HIS:HD2	2.18	0.42
1:E:36:ASP:O	1:E:37:MET:HE2	2.19	0.42
1:E:3:VAL:CG1	1:E:4:GLY:N	2.83	0.42
1:E:5:PHE:CD2	1:E:67:PHE:HB2	2.55	0.42
1:B:153:LEU:HB2	1:B:159:CYS:SG	2.59	0.42
1:C:31:MET:HB3	1:C:59:THR:CG2	2.37	0.42
1:C:53:THR:HG22	1:C:55:HIS:O	2.20	0.42
1:D:15:LEU:HD23	1:D:19:PHE:CE1	2.55	0.42
1:D:169:ALA:HA	1:D:262:CYS:SG	2.59	0.42
1:D:25:LEU:CD2	1:D:25:LEU:N	2.83	0.42
1:D:31:MET:HE2	1:D:62:HIS:HB3	2.02	0.42
1:E:177:GLY:O	1:E:180:TYR:N	2.53	0.42
1:E:264:ARG:O	1:E:268:LEU:HG	2.19	0.42
1:E:80:ASP:O	1:E:81:GLU:HG3	2.20	0.42
1:A:43:SER:O	1:A:46:ARG:HB2	2.20	0.42
1:C:228:LYS:HA	4:C:3356:HOH:O	2.19	0.42
1:C:53:THR:HG23	1:C:58:GLU:CD	2.40	0.42
1:D:123:ASN:HB2	1:D:125:PRO:HD2	2.02	0.42
1:D:199:ARG:O	1:D:200:ARG:C	2.58	0.42
1:A:137:THR:HB	1:A:141:ALA:HB1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:THR:O	1:A:239:ILE:C	2.58	0.41
1:B:185:LEU:HD21	1:B:210:LEU:HD12	2.01	0.41
1:B:32:ALA:O	1:B:53:THR:HB	2.20	0.41
1:C:114:ALA:HB1	1:C:140:HIS:CE1	2.55	0.41
1:C:9:GLY:H	1:C:12:ALA:CB	2.26	0.41
1:D:135:TYR:CD1	1:D:135:TYR:C	2.93	0.41
1:E:89:ARG:CZ	1:E:90:HIS:CE1	3.03	0.41
1:A:60:VAL:HG21	1:A:82:ILE:CG2	2.50	0.41
1:B:192:GLY:O	1:B:195:MET:N	2.53	0.41
1:C:27:ALA:HB1	1:C:50:VAL:CG2	2.49	0.41
1:C:35:PRO:O	1:C:36:ASP:CB	2.67	0.41
1:D:24:VAL:HB	1:D:25:LEU:HD23	2.02	0.41
1:D:268:LEU:HD12	1:D:268:LEU:HA	1.89	0.41
1:A:15:LEU:HD23	1:A:126:VAL:HG11	2.02	0.41
1:A:153:LEU:HB2	1:A:159:CYS:SG	2.60	0.41
1:A:229:ASP:N	1:A:229:ASP:OD1	2.53	0.41
1:B:118:ILE:HD13	1:B:137:THR:O	2.19	0.41
1:D:112:ARG:HB2	4:D:4403:HOH:O	2.20	0.41
1:D:129:ARG:HD2	4:D:4315:HOH:O	2.19	0.41
1:D:199:ARG:C	1:D:201:LEU:N	2.73	0.41
1:D:267:GLU:CA	1:D:270:SER:HB2	2.44	0.41
1:E:200:ARG:HG3	4:E:5336:HOH:O	2.20	0.41
2:E:5300:NAP:H6N	2:E:5300:NAP:O5D	2.19	0.41
1:E:68:LEU:HD12	1:E:94:SER:HB2	2.01	0.41
1:A:180:TYR:N	1:A:180:TYR:CD2	2.88	0.41
1:A:250:PHE:N	4:A:1403:HOH:O	2.54	0.41
1:B:171:THR:O	1:B:172:GLY:C	2.58	0.41
1:C:6:ILE:HD11	1:C:60:VAL:CG2	2.50	0.41
1:B:197:LEU:O	1:D:234:PRO:HB3	2.20	0.41
1:D:26:ALA:O	1:D:29:LYS:HB2	2.19	0.41
1:D:130:GLU:CD	2:D:4300:NAP:H2D	2.41	0.41
1:E:167:ILE:N	4:E:5388:HOH:O	2.52	0.41
1:E:219:HIS:NE2	2:E:5300:NAP:H51N	2.35	0.41
1:E:35:PRO:HB3	4:E:5462:HOH:O	2.19	0.41
1:A:101:ILE:O	1:A:102:SER:C	2.58	0.41
1:A:193:VAL:O	1:A:195:MET:N	2.53	0.41
1:B:214:ALA:O	1:B:215:LYS:C	2.58	0.41
1:B:38:ASP:OD2	1:B:39:LEU:N	2.54	0.41
1:C:131:GLY:O	1:C:157:GLY:HA3	2.20	0.41
1:D:181:ALA:O	1:D:184:ALA:N	2.54	0.41
2:D:4300:NAP:N1N	3:D:4301:GLU:HG2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:LYS:N	1:E:57:LYS:CD	2.79	0.41
1:A:190:ASP:HA	4:A:1343:HOH:O	2.20	0.41
1:A:201:LEU:C	4:A:1335:HOH:O	2.58	0.41
1:A:244:VAL:O	1:A:247:SER:HB2	2.20	0.41
1:A:55:HIS:O	1:A:57:LYS:N	2.52	0.41
1:B:123:ASN:HD21	1:B:132:ALA:HB3	1.85	0.41
1:B:143:VAL:CG1	1:B:144:GLU:H	2.15	0.41
1:B:195:MET:CE	1:B:195:MET:CA	2.98	0.41
1:B:41:THR:HG22	1:B:45:LEU:HD21	2.03	0.41
1:B:6:ILE:O	1:B:6:ILE:HG22	2.19	0.41
1:C:86:ILE:HG22	1:C:112:ARG:HG2	2.02	0.41
1:D:202:ALA:HB1	4:D:4326:HOH:O	2.20	0.41
1:E:106:LYS:HB3	4:E:5419:HOH:O	2.21	0.41
1:E:143:VAL:HG12	1:E:143:VAL:O	2.21	0.41
1:A:129:ARG:CB	4:A:1316:HOH:O	2.68	0.41
1:A:9:GLY:HA2	1:A:41:THR:HG21	2.03	0.41
1:C:119:ARG:HH11	1:C:164:GLU:CG	2.34	0.41
1:D:239:ILE:O	1:D:242:LEU:HB2	2.20	0.41
1:D:86:ILE:HG21	4:D:4387:HOH:O	2.21	0.41
1:E:150:GLU:HA	4:E:5465:HOH:O	2.21	0.41
1:E:27:ALA:C	1:E:29:LYS:H	2.23	0.41
1:E:41:THR:HG22	1:E:45:LEU:CD1	2.51	0.41
1:E:31:MET:HA	1:E:51:LYS:O	2.21	0.41
1:A:168:ASP:HB2	4:A:1385:HOH:O	2.21	0.41
1:A:200:ARG:C	4:A:1335:HOH:O	2.59	0.41
1:A:226:GLN:C	1:A:228:LYS:N	2.73	0.41
1:C:243:HIS:CG	4:C:3389:HOH:O	2.74	0.41
1:E:121:MET:HE2	1:E:122:THR:O	2.21	0.41
1:E:14:ALA:CA	1:E:127:VAL:HG22	2.40	0.41
1:E:133:THR:O	1:E:159:CYS:HA	2.20	0.41
1:E:17:LYS:HE3	1:E:17:LYS:HB2	1.80	0.41
1:E:185:LEU:HD21	1:E:210:LEU:HD12	2.03	0.41
1:E:221:GLU:HG2	2:E:5300:NAP:O1X	2.20	0.41
1:A:13:PHE:HA	1:A:45:LEU:CD2	2.43	0.41
1:B:79:LEU:HA	1:B:82:ILE:HD12	2.01	0.41
1:C:226:GLN:O	1:C:230:ASN:OD1	2.38	0.41
1:C:67:PHE:HZ	1:C:152:LEU:HD21	1.85	0.41
1:E:177:GLY:O	1:E:180:TYR:CB	2.67	0.41
1:E:237:ALA:HB3	4:E:5430:HOH:O	2.19	0.41
1:E:74:ILE:O	1:E:75:ILE:C	2.60	0.41
1:B:150:GLU:O	1:B:154:SER:CB	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ALA:O	1:B:216:MET:HB3	2.21	0.41
1:B:239:ILE:CG2	1:B:240:HIS:N	2.84	0.41
1:C:24:VAL:HG12	1:C:24:VAL:O	2.21	0.41
2:C:3300:NAP:H6N	2:C:3300:NAP:O5D	2.20	0.41
1:C:3:VAL:HG22	1:C:65:VAL:CG1	2.51	0.41
1:D:128:VAL:HG22	1:D:128:VAL:O	2.20	0.41
1:D:133:THR:HG22	1:D:158:PHE:O	2.21	0.41
1:D:19:PHE:HB3	1:D:25:LEU:HD21	2.03	0.41
1:A:176:SER:O	1:A:177:GLY:C	2.59	0.41
1:C:10:GLN:C	1:C:12:ALA:H	2.22	0.41
1:D:68:LEU:CD1	1:D:94:SER:HB2	2.42	0.41
1:E:127:VAL:HG12	1:E:127:VAL:O	2.19	0.41
1:A:0:GLY:HA2	4:A:1358:HOH:O	2.20	0.40
1:B:101:ILE:CG1	1:B:102:SER:N	2.85	0.40
1:C:123:ASN:HD21	1:C:132:ALA:H	1.68	0.40
1:C:165:ASP:OD2	1:C:165:ASP:N	2.53	0.40
1:C:171:THR:O	1:C:175:GLY:CA	2.69	0.40
1:C:169:ALA:O	1:C:172:GLY:N	2.55	0.40
1:C:57:LYS:O	1:C:60:VAL:HG23	2.21	0.40
1:D:142:GLN:N	1:D:145:ASP:OD2	2.53	0.40
1:D:241:ALA:O	1:D:244:VAL:HB	2.22	0.40
1:D:158:PHE:CZ	2:D:4300:NAP:H51A	2.56	0.40
1:E:102:SER:HA	1:E:105:GLU:HB2	2.03	0.40
1:E:44:ALA:O	1:E:48:MET:HB3	2.21	0.40
2:A:1300:NAP:H3B	2:A:1300:NAP:PA	2.61	0.40
1:A:171:THR:HA	4:A:1355:HOH:O	2.20	0.40
1:A:189:ALA:CB	1:A:199:ARG:NH1	2.84	0.40
1:A:7:GLY:HA2	1:A:70:VAL:HG12	2.03	0.40
1:A:60:VAL:HG21	1:A:82:ILE:HG23	2.04	0.40
1:B:161:GLU:O	1:B:162:VAL:HG22	2.20	0.40
1:B:19:PHE:N	4:B:2373:HOH:O	2.54	0.40
1:C:101:ILE:HG21	4:C:3328:HOH:O	2.22	0.40
1:C:193:VAL:N	4:C:3358:HOH:O	2.49	0.40
1:C:61:GLN:C	1:C:63:SER:N	2.73	0.40
1:D:105:GLU:HB3	4:D:4370:HOH:O	2.20	0.40
1:E:225:GLY:CA	4:E:5416:HOH:O	2.69	0.40
1:A:41:THR:HG22	1:A:42:VAL:N	2.37	0.40
1:A:88:ASP:HA	4:A:1424:HOH:O	2.20	0.40
1:B:75:ILE:CB	1:B:76:PRO:HD3	2.32	0.40
1:C:149:MET:HA	1:C:152:LEU:HB3	2.03	0.40
1:C:3:VAL:HG12	1:C:4:GLY:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101:ILE:HB	1:E:164:GLU:OE2	2.21	0.40
1:E:202:ALA:O	1:E:204:ARG:N	2.54	0.40
1:E:271:MET:C	1:E:273:ASP:N	2.75	0.40
1:E:40:ALA:HB3	4:E:5379:HOH:O	2.20	0.40
1:E:45:LEU:HA	1:E:48:MET:CE	2.52	0.40
1:E:76:PRO:O	1:E:77:PHE:C	2.60	0.40
1:A:25:LEU:CD2	1:A:30:ILE:HG12	2.51	0.40
1:A:5:PHE:O	1:A:32:ALA:HA	2.21	0.40
1:A:46:ARG:CG	1:A:52:LEU:HD12	2.51	0.40
1:B:247:SER:HB3	4:B:2394:HOH:O	2.22	0.40
1:B:274:GLN:HE21	1:B:275:GLU:CD	2.25	0.40
1:B:45:LEU:HD12	1:B:52:LEU:HD11	2.03	0.40
1:C:115:PRO:O	1:C:140:HIS:CD2	2.74	0.40
1:C:211:LEU:C	1:C:211:LEU:HD13	2.40	0.40
1:C:228:LYS:NZ	1:C:229:ASP:OD1	2.54	0.40
1:C:246:GLU:HA	1:C:246:GLU:OE2	2.21	0.40
1:C:262:CYS:O	1:C:263:ILE:C	2.59	0.40
1:C:2:SER:HB2	1:C:64:ASP:HB2	2.04	0.40
1:E:167:ILE:HG12	4:E:5388:HOH:O	2.21	0.40
1:A:187:ALA:O	1:A:188:LEU:C	2.60	0.40
1:A:98:GLY:O	1:A:269:GLN:HB2	2.22	0.40
1:D:193:VAL:O	1:D:194:LYS:C	2.59	0.40
1:D:53:THR:HG21	1:D:58:GLU:OE1	2.21	0.40

All (4) 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)
4:A:1340:HOH:O	4:C:3362:HOH:O[2_555]	1.63	0.57
1:C:129:ARG:CG	4:A:1320:HOH:O[2_555]	2.05	0.15
1:E:208:GLN:OE1	2:D:4300:NAP:O2N[2_555]	2.16	0.04
1:C:129:ARG:CD	4:A:1320:HOH:O[2_555]	2.19	0.01

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	275/277 (99%)	188 (68%)	62 (22%)	25 (9%)	1	4
1	B	272/277 (98%)	167 (61%)	67 (25%)	38 (14%)	0	1
1	C	275/277 (99%)	193 (70%)	59 (22%)	23 (8%)	1	5
1	D	275/277 (99%)	193 (70%)	51 (18%)	31 (11%)	0	2
1	E	275/277 (99%)	185 (67%)	66 (24%)	24 (9%)	1	4
All	All	1372/1385 (99%)	926 (68%)	305 (22%)	141 (10%)	0	3

All (141) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ALA
1	A	39	LEU
1	A	107	LYS
1	A	129	ARG
1	A	143	VAL
1	A	164	GLU
1	A	222	GLN
1	A	223	HIS
1	B	10	GLN
1	B	19	PHE
1	B	24	VAL
1	B	36	ASP
1	B	37	MET
1	B	61	GLN
1	B	113	PRO
1	B	137	THR
1	B	141	ALA
1	B	142	GLN
1	B	220	SER
1	B	221	GLU
1	B	222	GLN
1	B	223	HIS
1	C	197	LEU
1	C	252	SER
1	C	253	LEU
1	D	40	ALA
1	D	142	GLN
1	D	203	VAL

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Mol	Chain	Res	Type
1	E	223	HIS
1	A	40	ALA
1	A	41	THR
1	A	77	PHE
1	A	165	ASP
1	A	219	HIS
1	B	16	ALA
1	B	59	THR
1	B	76	PRO
1	B	77	PHE
1	B	97	ALA
1	B	129	ARG
1	B	158	PHE
1	B	173	LEU
1	C	20	THR
1	C	36	ASP
1	C	40	ALA
1	C	139	THR
1	C	150	GLU
1	C	235	GLY
1	D	8	ALA
1	D	10	GLN
1	D	42	VAL
1	D	99	VAL
1	D	164	GLU
1	D	167	ILE
1	D	177	GLY
1	D	200	ARG
1	D	270	SER
1	E	42	VAL
1	E	50	VAL
1	E	88	ASP
1	E	99	VAL
1	E	130	GLU
1	E	170	VAL
1	E	222	GLN
1	E	274	GLN
1	A	177	GLY
1	A	200	ARG
1	B	29	LYS
1	B	140	HIS
1	B	143	VAL

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Mol	Chain	Res	Type
1	B	150	GLU
1	B	160	THR
1	C	11	LEU
1	C	113	PRO
1	C	129	ARG
1	C	173	LEU
1	C	190	ASP
1	C	200	ARG
1	C	237	ALA
1	D	107	LYS
1	D	125	PRO
1	D	199	ARG
1	D	221	GLU
1	E	73	HIS
1	E	78	ILE
1	A	149	MET
1	A	194	LYS
1	A	199	ARG
1	A	234	PRO
1	A	270	SER
1	B	11	LEU
1	B	14	ALA
1	B	214	ALA
1	B	252	SER
1	C	107	LYS
1	C	125	PRO
1	C	229	ASP
1	D	41	THR
1	D	106	LYS
1	D	110	ALA
1	D	223	HIS
1	D	224	PRO
1	D	226	GLN
1	D	230	ASN
1	D	237	ALA
1	E	34	SER
1	E	37	MET
1	E	125	PRO
1	E	129	ARG
1	E	151	GLN
1	E	221	GLU
1	E	235	GLY

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Mol	Chain	Res	Type
1	A	110	ALA
1	B	20	THR
1	B	58	GLU
1	B	154	SER
1	B	165	ASP
1	C	16	ALA
1	C	62	HIS
1	D	59	THR
1	D	113	PRO
1	D	220	SER
1	E	81	GLU
1	E	199	ARG
1	E	237	ALA
1	A	56	ASN
1	A	123	ASN
1	B	95	CYS
1	B	235	GLY
1	A	42	VAL
1	B	125	PRO
1	C	76	PRO
1	D	60	VAL
1	E	203	VAL
1	A	167	ILE
1	C	65	VAL
1	D	78	ILE
1	D	225	GLY
1	E	70	VAL
1	E	18	GLY
1	D	75	ILE

### 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	215/215 (100%)	190 (88%)	25 (12%)	5	22
1	B	213/215 (99%)	198 (93%)	15 (7%)	15	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	214/215 (100%)	204 (95%)	10 (5%)	26	59
1	D	215/215 (100%)	204 (95%)	11 (5%)	24	56
1	E	215/215 (100%)	202 (94%)	13 (6%)	19	49
All	All	1072/1075 (100%)	998 (93%)	74 (7%)	15	45

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
1	A	62	HIS
1	A	64	ASP
1	A	73	HIS
1	A	75	ILE
1	A	77	PHE
1	A	90	HIS
1	A	120	CYS
1	A	121	MET
1	A	123	ASN
1	A	126	VAL
1	A	134	VAL
1	A	148	LEU
1	A	149	MET
1	A	150	GLU
1	A	159	CYS
1	A	171	THR
1	A	194	LYS
1	A	210	LEU
1	A	229	ASP
1	A	234	PRO
1	A	244	VAL
1	A	258	VAL
1	A	269	GLN
1	A	271	MET
1	B	5	PHE
1	B	10	GLN
1	B	19	PHE
1	B	47	LYS
1	B	90	HIS
1	B	120	CYS
1	B	123	ASN
1	B	133	THR

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Mol	Chain	Res	Type
1	B	160	THR
1	B	161	GLU
1	B	163	GLU
1	B	180	TYR
1	B	211	LEU
1	B	244	VAL
1	B	273	ASP
1	C	51	LYS
1	C	89	ARG
1	C	120	CYS
1	C	121	MET
1	C	124	THR
1	C	190	ASP
1	C	216	MET
1	C	244	VAL
1	C	262	CYS
1	C	273	ASP
1	D	28	HIS
1	D	31	MET
1	D	77	PHE
1	D	95	CYS
1	D	120	CYS
1	D	124	THR
1	D	127	VAL
1	D	144	GLU
1	D	152	LEU
1	D	211	LEU
1	D	244	VAL
1	E	28	HIS
1	E	39	LEU
1	E	48	MET
1	E	57	LYS
1	E	62	HIS
1	E	88	ASP
1	E	101	ILE
1	E	112	ARG
1	E	120	CYS
1	E	124	THR
1	E	195	MET
1	E	251	ARG
1	E	252	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	HIS
1	A	123	ASN
1	A	140	HIS
1	A	208	GLN
1	A	240	HIS
1	A	243	HIS
1	A	269	GLN
1	B	28	HIS
1	B	55	HIS
1	B	151	GLN
1	B	240	HIS
1	B	243	HIS
1	B	274	GLN
1	C	90	HIS
1	C	240	HIS
1	C	274	GLN
1	D	28	HIS
1	D	55	HIS
1	D	90	HIS
1	D	140	HIS
1	D	142	GLN
1	D	240	HIS
1	E	28	HIS
1	E	140	HIS
1	E	219	HIS
1	E	226	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

10 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
3	GLU	C	3301	-	2,9,9	0.47	0	2,11,11	0.35	0
3	GLU	B	2301	-	2,9,9	0.24	0	2,11,11	0.81	0
2	NAP	D	4300	1	45,52,52	4.79	24 (53%)	56,80,80	3.15	23 (41%)
2	NAP	E	5300	-	45,52,52	4.75	23 (51%)	56,80,80	3.29	22 (39%)
3	GLU	A	1301	-	2,9,9	0.22	0	2,11,11	0.39	0
3	GLU	D	4301	-	2,9,9	0.26	0	2,11,11	0.63	0
2	NAP	B	2300	-	45,52,52	4.95	25 (55%)	56,80,80	3.16	23 (41%)
2	NAP	A	1300	-	45,52,52	5.33	25 (55%)	56,80,80	4.16	31 (55%)
3	GLU	E	5301	-	2,9,9	0.24	0	2,11,11	0.34	0
2	NAP	C	3300	-	45,52,52	4.88	24 (53%)	56,80,80	3.64	22 (39%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLU	C	3301	-	-	0/3/9/9	-
3	GLU	B	2301	-	-	2/3/9/9	-
2	NAP	D	4300	1	-	6/31/67/67	0/5/5/5
2	NAP	E	5300	-	1/1/12/12	6/31/67/67	0/5/5/5
3	GLU	A	1301	-	-	1/3/9/9	-
3	GLU	D	4301	-	-	2/3/9/9	-
2	NAP	B	2300	-	-	6/31/67/67	0/5/5/5
2	NAP	A	1300	-	1/1/12/12	5/31/67/67	0/5/5/5
3	GLU	E	5301	-	-	0/3/9/9	-
2	NAP	C	3300	-	1/1/12/12	6/31/67/67	0/5/5/5

All (121) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2300	NAP	C8A-N7A	21.40	1.72	1.34
2	E	5300	NAP	C8A-N7A	21.32	1.72	1.34
2	A	1300	NAP	C8A-N7A	21.10	1.72	1.34
2	C	3300	NAP	C8A-N7A	20.98	1.72	1.34
2	D	4300	NAP	C8A-N7A	20.86	1.71	1.34
2	A	1300	NAP	O7N-C7N	10.78	1.44	1.24
2	C	3300	NAP	C2N-N1N	9.71	1.46	1.35
2	D	4300	NAP	C2N-N1N	9.70	1.46	1.35
2	E	5300	NAP	C2N-N1N	9.70	1.46	1.35
2	B	2300	NAP	C2N-N1N	9.69	1.46	1.35
2	A	1300	NAP	C3N-C7N	-9.48	1.36	1.50
2	A	1300	NAP	O5D-C5D	8.64	1.78	1.44
2	A	1300	NAP	C2D-C1D	-7.90	1.41	1.53
2	B	2300	NAP	P2B-O2B	7.63	1.73	1.59
2	D	4300	NAP	O7N-C7N	7.42	1.38	1.24
2	B	2300	NAP	O7N-C7N	7.40	1.38	1.24
2	C	3300	NAP	O7N-C7N	7.40	1.38	1.24
2	E	5300	NAP	O7N-C7N	7.39	1.38	1.24
2	A	1300	NAP	P2B-O1X	7.21	1.73	1.50
2	A	1300	NAP	C6N-N1N	7.19	1.53	1.35
2	D	4300	NAP	P2B-O2B	7.16	1.72	1.59
2	E	5300	NAP	C4N-C3N	7.07	1.51	1.39
2	C	3300	NAP	C4N-C3N	7.06	1.51	1.39
2	B	2300	NAP	C4N-C3N	7.05	1.51	1.39
2	D	4300	NAP	C4N-C3N	6.99	1.51	1.39
2	C	3300	NAP	C5D-C4D	-6.80	1.30	1.51
2	C	3300	NAP	O4D-C1D	6.62	1.50	1.41
2	C	3300	NAP	P2B-O2B	6.39	1.71	1.59
2	A	1300	NAP	PN-O1N	6.34	1.73	1.50
2	B	2300	NAP	O4D-C4D	-6.24	1.31	1.45
2	E	5300	NAP	P2B-O2B	6.23	1.71	1.59
2	D	4300	NAP	PN-O1N	6.11	1.72	1.50
2	E	5300	NAP	PN-O1N	6.05	1.72	1.50
2	E	5300	NAP	C5D-C4D	-6.00	1.32	1.51
2	A	1300	NAP	P2B-O2B	-5.97	1.48	1.59
2	B	2300	NAP	PN-O1N	5.97	1.72	1.50
2	A	1300	NAP	C3D-C4D	-5.90	1.37	1.53
2	C	3300	NAP	PN-O1N	5.82	1.71	1.50
2	B	2300	NAP	C5N-C4N	5.71	1.50	1.38
2	D	4300	NAP	C5N-C4N	5.69	1.50	1.38
2	C	3300	NAP	C5N-C4N	5.68	1.50	1.38
2	E	5300	NAP	C5N-C4N	5.65	1.50	1.38
2	D	4300	NAP	O4D-C4D	-5.64	1.32	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1300	NAP	P2B-O2X	5.55	1.76	1.54
2	B	2300	NAP	O4D-C1D	-5.53	1.33	1.41
2	A	1300	NAP	C5N-C4N	5.30	1.50	1.38
2	C	3300	NAP	P2B-O2X	5.06	1.74	1.54
2	A	1300	NAP	C5D-C4D	-5.05	1.35	1.51
2	D	4300	NAP	P2B-O2X	4.98	1.74	1.54
2	B	2300	NAP	C4A-N3A	4.95	1.42	1.35
2	B	2300	NAP	P2B-O2X	4.93	1.73	1.54
2	A	1300	NAP	P2B-O3X	4.87	1.73	1.54
2	D	4300	NAP	C4A-N3A	4.83	1.42	1.35
2	C	3300	NAP	C7N-N7N	-4.80	1.23	1.33
2	B	2300	NAP	C7N-N7N	-4.78	1.23	1.33
2	D	4300	NAP	C7N-N7N	-4.78	1.23	1.33
2	E	5300	NAP	C7N-N7N	-4.77	1.23	1.33
2	E	5300	NAP	P2B-O1X	4.72	1.65	1.50
2	B	2300	NAP	P2B-O1X	4.72	1.65	1.50
2	B	2300	NAP	C2A-N3A	4.68	1.39	1.32
2	C	3300	NAP	C4A-N3A	4.68	1.42	1.35
2	E	5300	NAP	P2B-O2X	4.65	1.72	1.54
2	B	2300	NAP	C6N-N1N	4.61	1.46	1.35
2	C	3300	NAP	P2B-O1X	4.60	1.65	1.50
2	E	5300	NAP	C6N-N1N	4.58	1.46	1.35
2	D	4300	NAP	C6N-N1N	4.58	1.46	1.35
2	C	3300	NAP	C6N-N1N	4.56	1.46	1.35
2	D	4300	NAP	P2B-O1X	4.48	1.65	1.50
2	C	3300	NAP	C2A-N3A	4.45	1.39	1.32
2	E	5300	NAP	PA-O2A	4.33	1.75	1.55
2	B	2300	NAP	PA-O2A	4.31	1.75	1.55
2	D	4300	NAP	PA-O2A	4.27	1.75	1.55
2	E	5300	NAP	C4A-N3A	4.27	1.41	1.35
2	D	4300	NAP	O4D-C1D	-4.24	1.35	1.41
2	C	3300	NAP	PA-O2A	4.20	1.75	1.55
2	A	1300	NAP	C4A-N3A	4.19	1.41	1.35
2	C	3300	NAP	O5B-C5B	-4.16	1.28	1.44
2	D	4300	NAP	C2A-N3A	4.14	1.38	1.32
2	A	1300	NAP	PA-O2A	4.12	1.74	1.55
2	B	2300	NAP	PA-O1A	4.03	1.65	1.50
2	C	3300	NAP	PA-O1A	3.93	1.64	1.50
2	E	5300	NAP	C2A-N3A	3.91	1.38	1.32
2	A	1300	NAP	PA-O1A	3.91	1.64	1.50
2	D	4300	NAP	PA-O1A	3.86	1.64	1.50
2	A	1300	NAP	C2A-N3A	3.84	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	5300	NAP	PA-O1A	3.78	1.64	1.50
2	A	1300	NAP	O4D-C1D	3.58	1.46	1.41
2	A	1300	NAP	O3D-C3D	3.49	1.51	1.43
2	A	1300	NAP	C6A-N6A	3.45	1.46	1.34
2	A	1300	NAP	O4D-C4D	-3.43	1.37	1.45
2	E	5300	NAP	C6A-N6A	3.41	1.46	1.34
2	D	4300	NAP	C6A-N6A	3.41	1.46	1.34
2	A	1300	NAP	O2D-C2D	3.24	1.50	1.43
2	B	2300	NAP	C6A-N6A	3.24	1.45	1.34
2	C	3300	NAP	C6A-N6A	3.22	1.45	1.34
2	A	1300	NAP	C2N-N1N	3.00	1.38	1.35
2	B	2300	NAP	C5D-C4D	-2.96	1.42	1.51
2	B	2300	NAP	C2D-C1D	2.85	1.58	1.53
2	E	5300	NAP	C3D-C4D	-2.65	1.46	1.53
2	D	4300	NAP	C5D-C4D	-2.63	1.43	1.51
2	B	2300	NAP	O5B-C5B	2.32	1.53	1.44
2	B	2300	NAP	C5A-N7A	2.28	1.48	1.39
2	C	3300	NAP	C2N-C3N	2.24	1.42	1.39
2	D	4300	NAP	C2N-C3N	2.23	1.42	1.39
2	B	2300	NAP	C2N-C3N	2.22	1.42	1.39
2	E	5300	NAP	C2N-C3N	2.21	1.42	1.39
2	C	3300	NAP	C2D-C1D	-2.17	1.50	1.53
2	D	4300	NAP	O4B-C4B	-2.17	1.40	1.45
2	E	5300	NAP	O4D-C1D	2.13	1.44	1.41
2	E	5300	NAP	C5A-N7A	2.12	1.47	1.39
2	B	2300	NAP	C6N-C5N	-2.10	1.34	1.38
2	E	5300	NAP	C6N-C5N	-2.08	1.34	1.38
2	C	3300	NAP	C6N-C5N	-2.08	1.34	1.38
2	E	5300	NAP	PA-O5B	2.08	1.67	1.59
2	D	4300	NAP	C3D-C4D	-2.07	1.47	1.53
2	A	1300	NAP	C5A-N7A	2.06	1.47	1.39
2	D	4300	NAP	C5A-N7A	2.06	1.47	1.39
2	C	3300	NAP	C5A-N7A	2.05	1.47	1.39
2	D	4300	NAP	C6N-C5N	-2.05	1.34	1.38
2	B	2300	NAP	O2D-C2D	-2.02	1.38	1.43
2	C	3300	NAP	O4D-C4D	-2.02	1.40	1.45

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3300	NAP	O5B-C5B-C4B	12.75	152.88	108.99
2	C	3300	NAP	C2N-N1N-C1D	-12.18	92.01	119.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1300	NAP	O7N-C7N-N7N	-11.61	106.09	122.58
2	E	5300	NAP	C2N-N1N-C1D	-11.05	94.53	119.14
2	A	1300	NAP	O5B-C5B-C4B	10.13	143.86	108.99
2	D	4300	NAP	C2N-N1N-C1D	-9.27	98.48	119.14
2	B	2300	NAP	C2N-N1N-C1D	-8.95	99.21	119.14
2	A	1300	NAP	C2N-N1N-C1D	-8.94	99.23	119.14
2	A	1300	NAP	C3N-C7N-N7N	8.48	127.93	117.75
2	C	3300	NAP	O4D-C1D-C2D	-8.34	94.74	106.93
2	E	5300	NAP	O5B-C5B-C4B	8.27	137.44	108.99
2	A	1300	NAP	C3B-C2B-C1B	-7.98	87.89	102.89
2	D	4300	NAP	C3B-C2B-C1B	-7.98	87.89	102.89
2	B	2300	NAP	C3B-C2B-C1B	-7.87	88.09	102.89
2	A	1300	NAP	C2N-C3N-C4N	7.86	127.17	118.26
2	C	3300	NAP	C3B-C2B-C1B	-7.35	89.06	102.89
2	E	5300	NAP	O4D-C1D-C2D	-7.33	96.21	106.93
2	E	5300	NAP	C3B-C2B-C1B	-7.20	89.36	102.89
2	B	2300	NAP	PN-O3-PA	-7.10	108.46	132.83
2	C	3300	NAP	PN-O3-PA	-6.87	109.25	132.83
2	A	1300	NAP	PN-O5D-C5D	-6.76	82.03	121.68
2	D	4300	NAP	PN-O3-PA	-6.72	109.78	132.83
2	E	5300	NAP	PN-O3-PA	-6.56	110.33	132.83
2	D	4300	NAP	O5B-C5B-C4B	6.47	131.25	108.99
2	A	1300	NAP	PN-O3-PA	-6.46	110.66	132.83
2	B	2300	NAP	O5B-C5B-C4B	6.40	131.01	108.99
2	A	1300	NAP	O5D-C5D-C4D	-6.37	87.06	108.99
2	B	2300	NAP	O4D-C1D-C2D	-6.31	97.71	106.93
2	D	4300	NAP	O4D-C1D-C2D	-6.01	98.15	106.93
2	B	2300	NAP	O7N-C7N-C3N	-5.91	112.56	119.63
2	C	3300	NAP	O7N-C7N-C3N	-5.91	112.56	119.63
2	D	4300	NAP	O7N-C7N-C3N	-5.89	112.59	119.63
2	E	5300	NAP	O7N-C7N-C3N	-5.88	112.59	119.63
2	E	5300	NAP	C5D-C4D-C3D	5.79	136.87	115.18
2	B	2300	NAP	O4B-C4B-C5B	5.70	128.14	109.37
2	A	1300	NAP	O4D-C4D-C5D	-5.60	90.96	109.37
2	B	2300	NAP	C2B-C3B-C4B	5.23	113.35	101.99
2	C	3300	NAP	C2B-C3B-C4B	5.22	113.33	101.99
2	A	1300	NAP	O7N-C7N-C3N	5.21	125.87	119.63
2	A	1300	NAP	C2B-C3B-C4B	5.16	113.20	101.99
2	E	5300	NAP	C2B-C3B-C4B	5.12	113.11	101.99
2	D	4300	NAP	C2B-C3B-C4B	5.09	113.04	101.99
2	D	4300	NAP	O4B-C4B-C5B	5.06	126.03	109.37
2	D	4300	NAP	C2D-C3D-C4D	-4.90	93.13	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1300	NAP	O3D-C3D-C4D	-4.86	97.01	111.05
2	A	1300	NAP	O3X-P2B-O1X	-4.81	91.84	110.68
2	B	2300	NAP	C3N-C7N-N7N	4.61	123.28	117.75
2	D	4300	NAP	C3N-C7N-N7N	4.60	123.28	117.75
2	A	1300	NAP	C5N-C6N-N1N	-4.59	113.82	120.40
2	C	3300	NAP	C3N-C7N-N7N	4.59	123.26	117.75
2	E	5300	NAP	C3N-C7N-N7N	4.59	123.26	117.75
2	A	1300	NAP	C5N-C4N-C3N	-4.53	114.98	120.34
2	C	3300	NAP	O4B-C4B-C3B	-4.50	96.20	105.11
2	C	3300	NAP	C5D-C4D-C3D	4.45	131.88	115.18
2	B	2300	NAP	O4B-C4B-C3B	-4.19	96.82	105.11
2	D	4300	NAP	O5D-C5D-C4D	-4.14	94.76	108.99
2	B	2300	NAP	O5D-C5D-C4D	-4.09	94.92	108.99
2	D	4300	NAP	O4B-C4B-C3B	-4.05	97.11	105.11
2	B	2300	NAP	C2D-C3D-C4D	-4.01	94.86	102.64
2	C	3300	NAP	O3X-P2B-O2X	3.95	122.73	107.64
2	C	3300	NAP	O5D-C5D-C4D	-3.94	95.43	108.99
2	A	1300	NAP	C5B-C4B-C3B	-3.91	100.51	115.18
2	E	5300	NAP	O4B-C4B-C3B	-3.89	97.42	105.11
2	A	1300	NAP	O4B-C4B-C3B	-3.85	97.49	105.11
2	B	2300	NAP	O3X-P2B-O2X	3.80	122.17	107.64
2	D	4300	NAP	O3X-P2B-O2X	3.77	122.03	107.64
2	E	5300	NAP	O3X-P2B-O2X	3.76	122.02	107.64
2	E	5300	NAP	O4B-C4B-C5B	3.67	121.43	109.37
2	D	4300	NAP	C5B-C4B-C3B	-3.60	101.69	115.18
2	B	2300	NAP	C5B-C4B-C3B	-3.59	101.72	115.18
2	A	1300	NAP	O3D-C3D-C2D	3.45	122.97	111.82
2	E	5300	NAP	C5B-C4B-C3B	-3.31	102.80	115.18
2	C	3300	NAP	O4D-C4D-C3D	-3.23	98.73	105.11
2	C	3300	NAP	C5A-C6A-N6A	-3.17	115.53	120.35
2	A	1300	NAP	O2D-C2D-C3D	-2.98	102.17	111.82
2	E	5300	NAP	C1B-N9A-C4A	-2.96	121.43	126.64
2	B	2300	NAP	O2B-C2B-C1B	2.91	120.58	110.10
2	D	4300	NAP	C5A-C6A-N6A	-2.86	116.00	120.35
2	E	5300	NAP	O2B-C2B-C1B	2.86	120.40	110.10
2	B	2300	NAP	C3D-C2D-C1D	-2.85	96.68	100.98
2	D	4300	NAP	O2B-C2B-C1B	2.85	120.37	110.10
2	C	3300	NAP	O2B-C2B-C1B	2.85	120.37	110.10
2	A	1300	NAP	O4B-C4B-C5B	2.84	118.72	109.37
2	B	2300	NAP	C5A-C6A-N6A	-2.81	116.08	120.35
2	A	1300	NAP	O2B-C2B-C1B	2.80	120.18	110.10
2	A	1300	NAP	C3N-C2N-N1N	-2.77	117.72	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5300	NAP	C5A-C6A-N6A	-2.71	116.24	120.35
2	C	3300	NAP	O4B-C1B-C2B	-2.71	101.89	106.59
2	A	1300	NAP	C6N-C5N-C4N	2.70	123.36	119.44
2	C	3300	NAP	C5B-C4B-C3B	-2.68	105.15	115.18
2	B	2300	NAP	O3X-P2B-O1X	-2.65	100.29	110.68
2	E	5300	NAP	O5D-C5D-C4D	-2.65	99.86	108.99
2	D	4300	NAP	O3X-P2B-O1X	-2.65	100.31	110.68
2	A	1300	NAP	C5A-C6A-N6A	-2.62	116.37	120.35
2	A	1300	NAP	PA-O5B-C5B	-2.62	106.31	121.68
2	A	1300	NAP	C1B-N9A-C4A	-2.55	122.16	126.64
2	C	3300	NAP	O3X-P2B-O1X	-2.54	100.73	110.68
2	E	5300	NAP	O3X-P2B-O1X	-2.54	100.76	110.68
2	A	1300	NAP	O2X-P2B-O2B	2.50	117.19	105.99
2	D	4300	NAP	C5D-C4D-C3D	2.50	124.53	115.18
2	D	4300	NAP	C1B-N9A-C4A	-2.46	122.32	126.64
2	D	4300	NAP	C3D-C2D-C1D	-2.41	97.34	100.98
2	B	2300	NAP	PA-O5B-C5B	-2.37	107.80	121.68
2	E	5300	NAP	O4D-C4D-C3D	-2.36	100.45	105.11
2	D	4300	NAP	PA-O5B-C5B	-2.28	108.32	121.68
2	A	1300	NAP	O4D-C1D-C2D	-2.28	103.60	106.93
2	C	3300	NAP	N6A-C6A-N1A	2.27	123.28	118.57
2	B	2300	NAP	C1B-N9A-C4A	-2.24	122.70	126.64
2	C	3300	NAP	C1B-N9A-C4A	-2.24	122.71	126.64
2	D	4300	NAP	N6A-C6A-N1A	2.23	123.21	118.57
2	E	5300	NAP	N6A-C6A-N1A	2.20	123.14	118.57
2	C	3300	NAP	C6N-N1N-C2N	2.19	123.97	121.97
2	B	2300	NAP	C6N-N1N-C2N	2.16	123.94	121.97
2	C	3300	NAP	C2D-C3D-C4D	-2.16	98.45	102.64
2	B	2300	NAP	O4B-C1B-C2B	-2.15	102.85	106.59
2	A	1300	NAP	N6A-C6A-N1A	2.15	123.03	118.57
2	E	5300	NAP	C6N-N1N-C2N	2.14	123.93	121.97
2	E	5300	NAP	O4B-C1B-C2B	-2.12	102.90	106.59
2	D	4300	NAP	C6N-N1N-C2N	2.12	123.90	121.97
2	B	2300	NAP	C5D-C4D-C3D	2.09	123.01	115.18
2	A	1300	NAP	C4N-C3N-C7N	-2.01	115.67	121.04

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	5300	NAP	C1D
2	A	1300	NAP	C1D
2	C	3300	NAP	C1D

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2301	GLU	N-CA-CB-CG
3	B	2301	GLU	C-CA-CB-CG
2	D	4300	NAP	C5B-O5B-PA-O1A
2	D	4300	NAP	C2D-C1D-N1N-C2N
2	D	4300	NAP	C2D-C1D-N1N-C6N
2	E	5300	NAP	C2D-C1D-N1N-C2N
2	E	5300	NAP	C2D-C1D-N1N-C6N
3	A	1301	GLU	C-CA-CB-CG
2	B	2300	NAP	C2D-C1D-N1N-C2N
2	B	2300	NAP	C2D-C1D-N1N-C6N
2	A	1300	NAP	C2D-C1D-N1N-C2N
2	A	1300	NAP	C2D-C1D-N1N-C6N
2	C	3300	NAP	C4B-C5B-O5B-PA
2	C	3300	NAP	C2D-C1D-N1N-C2N
2	C	3300	NAP	C2D-C1D-N1N-C6N
2	C	3300	NAP	O4B-C4B-C5B-O5B
2	C	3300	NAP	C3B-C4B-C5B-O5B
3	D	4301	GLU	CA-CB-CG-CD
2	B	2300	NAP	O4B-C4B-C5B-O5B
2	D	4300	NAP	C4B-C5B-O5B-PA
2	B	2300	NAP	C4B-C5B-O5B-PA
2	A	1300	NAP	C4B-C5B-O5B-PA
2	E	5300	NAP	C4B-C5B-O5B-PA
2	E	5300	NAP	C5D-O5D-PN-O2N
3	D	4301	GLU	C-CA-CB-CG
2	D	4300	NAP	O4B-C4B-C5B-O5B
2	D	4300	NAP	C3B-C2B-O2B-P2B
2	E	5300	NAP	C3B-C2B-O2B-P2B
2	B	2300	NAP	C3B-C2B-O2B-P2B
2	C	3300	NAP	C3B-C2B-O2B-P2B
2	A	1300	NAP	C3B-C2B-O2B-P2B
2	E	5300	NAP	C5B-O5B-PA-O1A
2	B	2300	NAP	C5B-O5B-PA-O1A
2	A	1300	NAP	C5B-O5B-PA-O1A

There are no ring outliers.

9 monomers are involved in 73 short contacts:

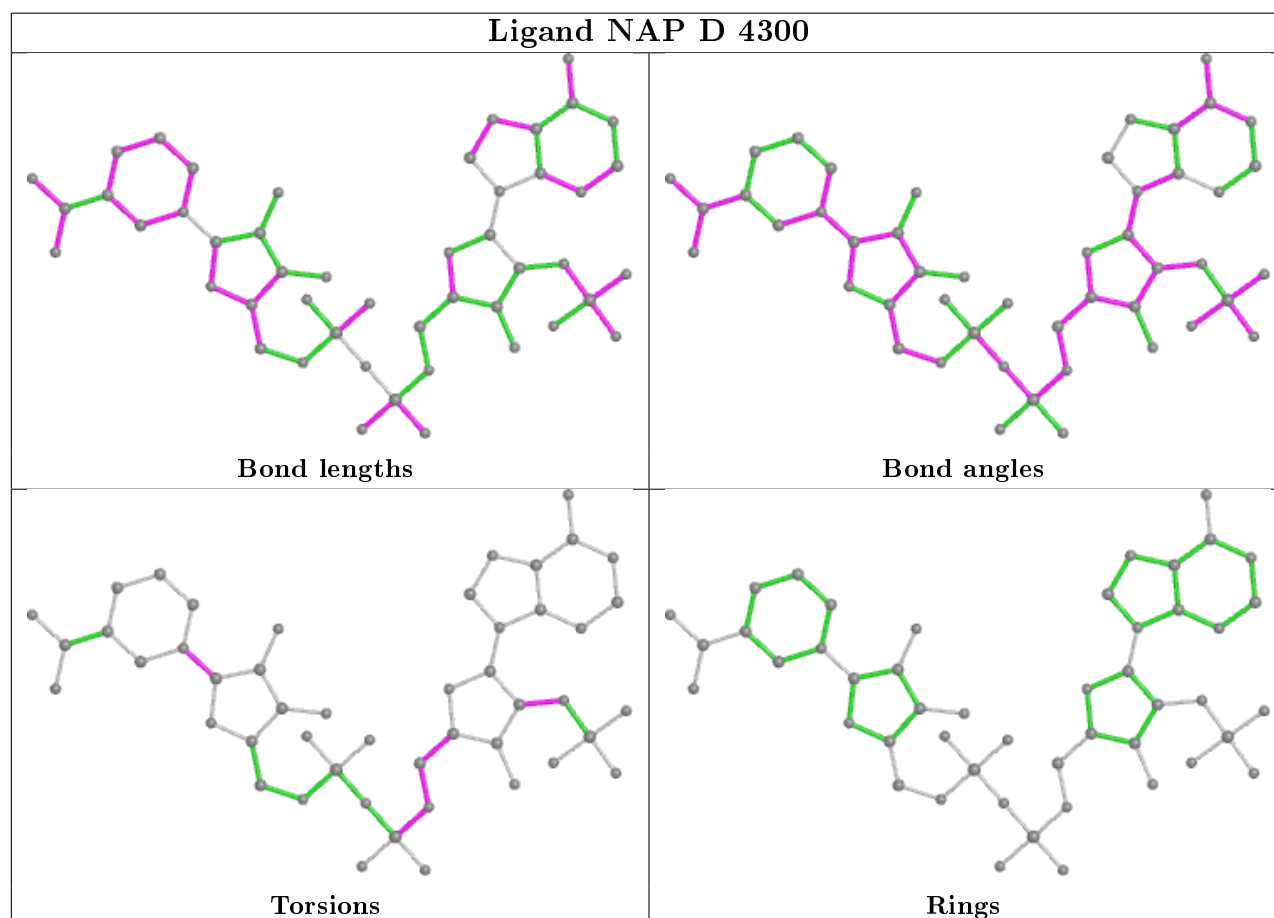
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3301	GLU	1	0
3	B	2301	GLU	3	0

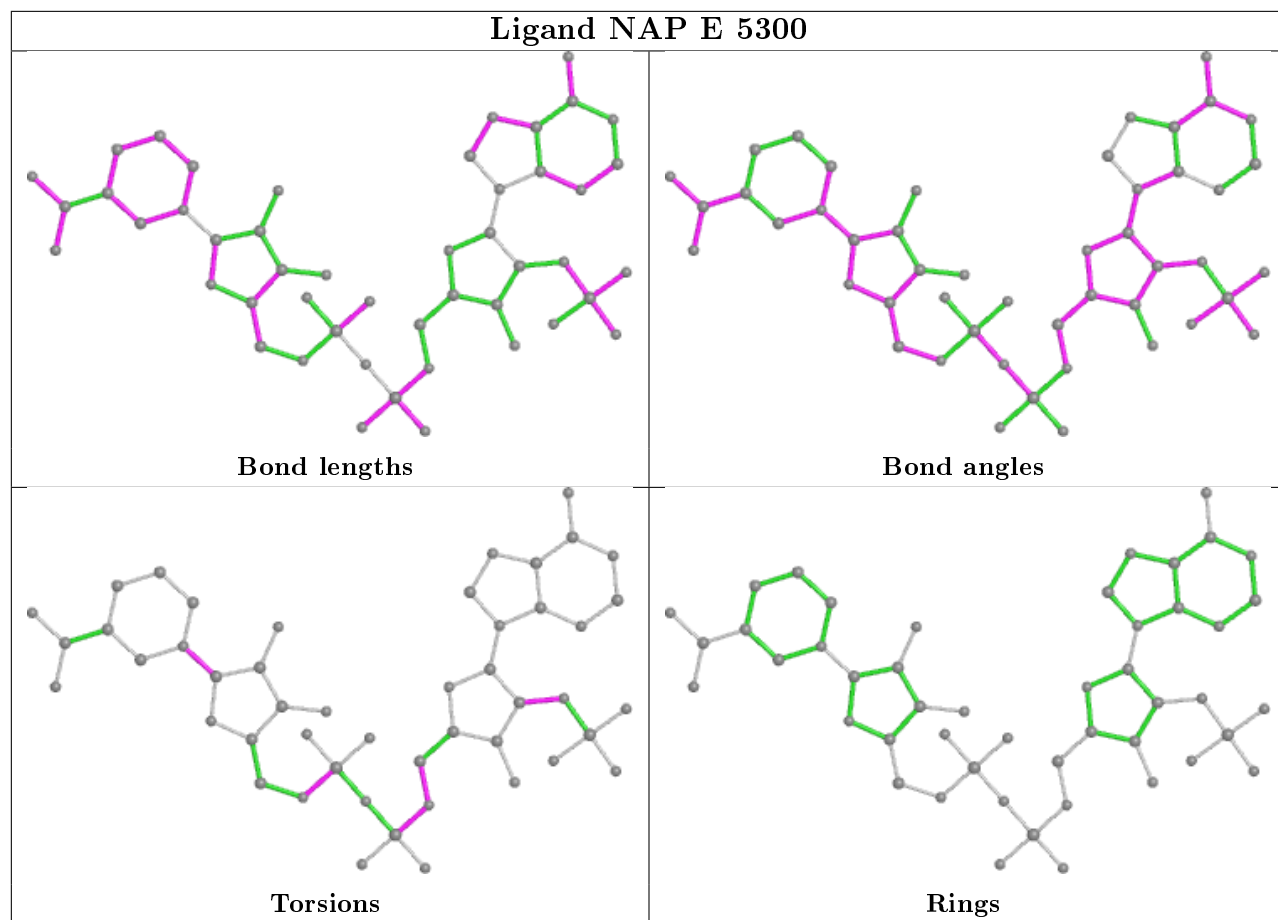
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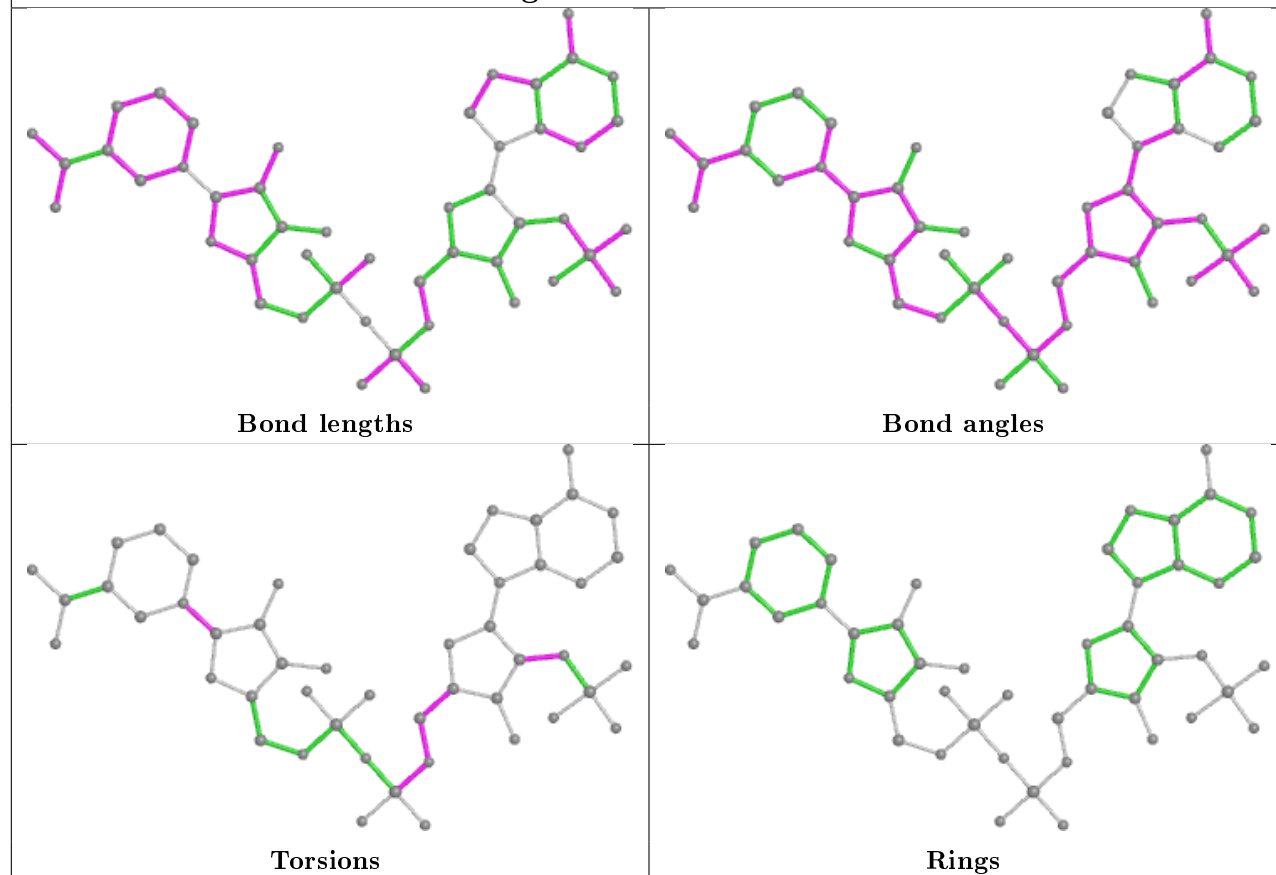
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	4300	NAP	11	1
2	E	5300	NAP	14	0
3	A	1301	GLU	3	0
3	D	4301	GLU	2	0
2	B	2300	NAP	15	0
2	A	1300	NAP	18	0
2	C	3300	NAP	12	0

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.

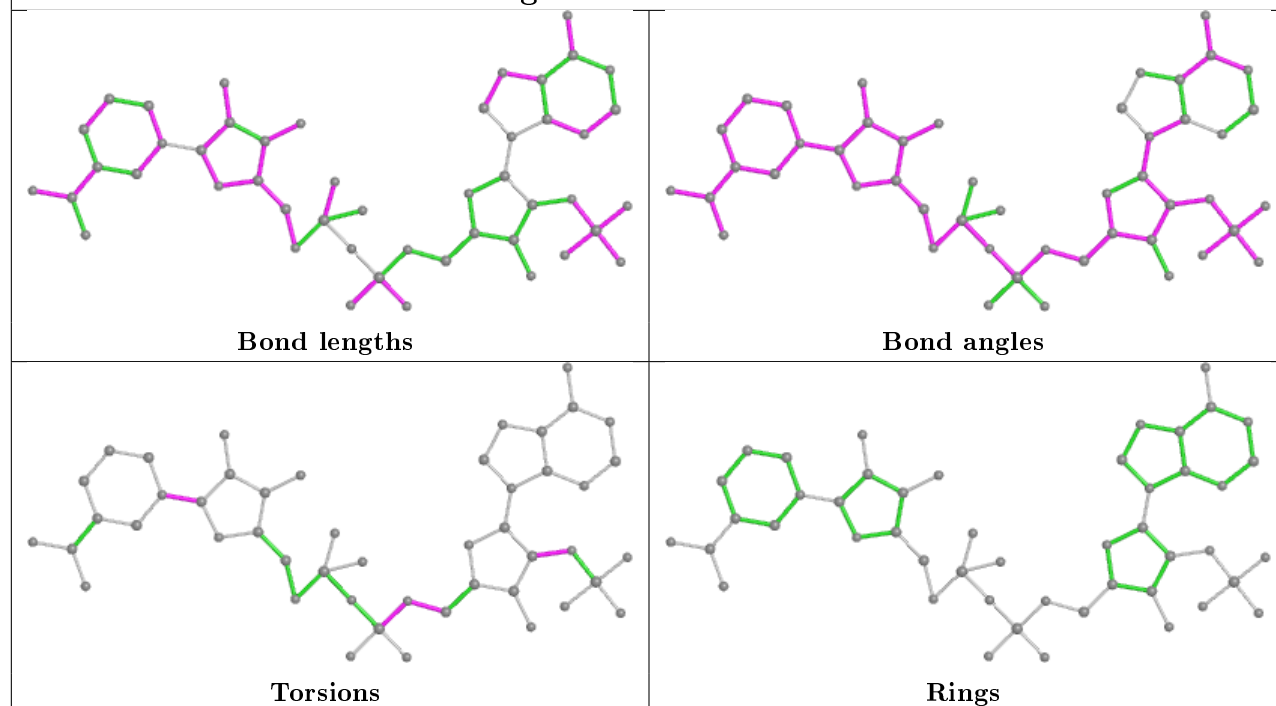


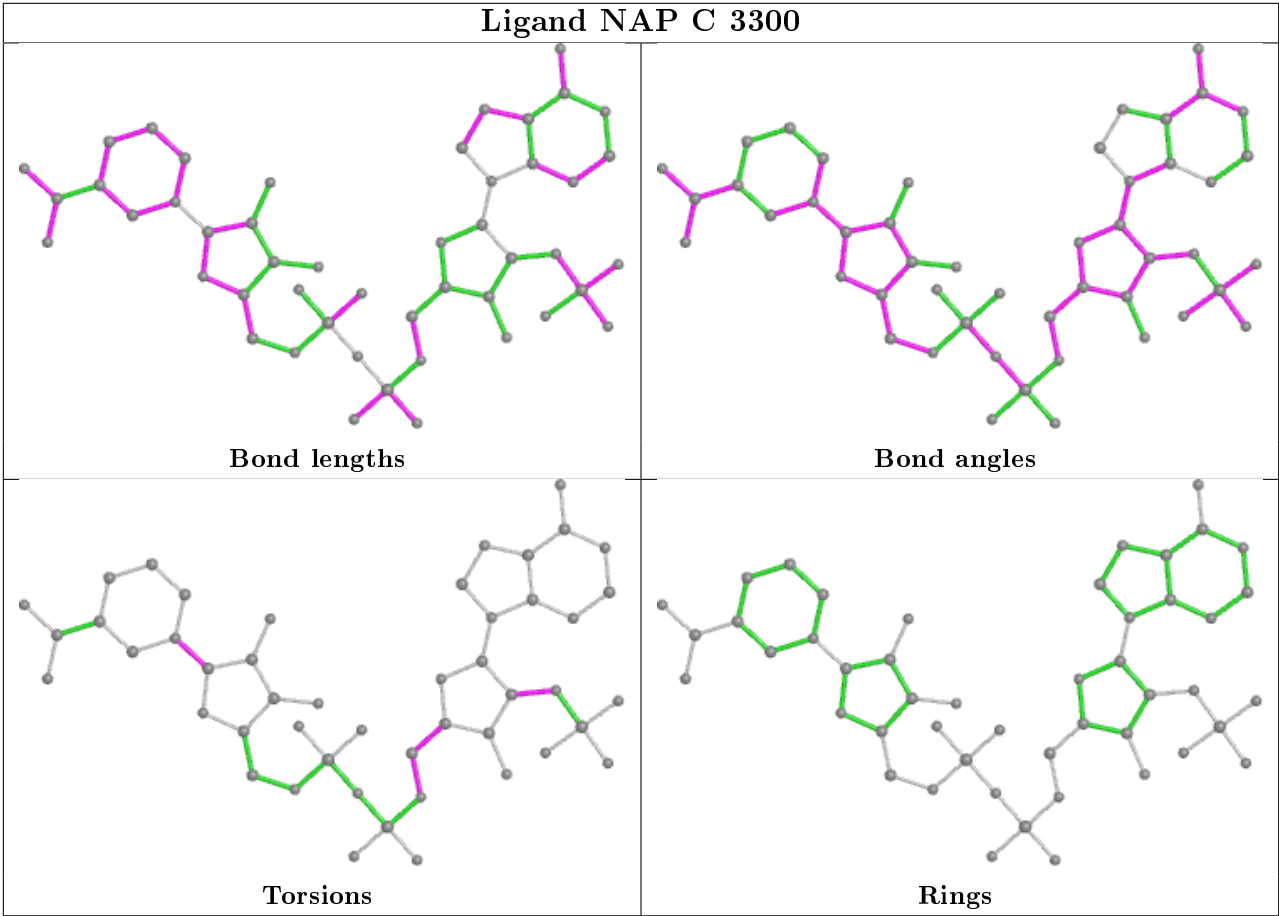


## Ligand NAP B 2300



## Ligand NAP A 1300





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	219:HIS	C	220:SER	N	1.72
1	A	153:LEU	C	154:SER	N	1.12

## 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	277/277 (100%)	-0.47	3 (1%) 80 64	20, 68, 115, 173	0
1	B	276/277 (99%)	0.28	30 (10%) 5 2	19, 115, 183, 200	0
1	C	277/277 (100%)	0.24	27 (9%) 7 2	16, 112, 178, 200	0
1	D	277/277 (100%)	-0.56	0 100 100	15, 62, 113, 178	0
1	E	277/277 (100%)	-0.53	0 100 100	14, 67, 124, 175	0
All	All	1384/1385 (99%)	-0.21	60 (4%) 35 17	14, 73, 170, 200	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	91	ILE	4.5
1	B	38	ASP	4.4
1	B	52	LEU	4.2
1	C	25	LEU	4.1
1	C	91	ILE	3.9
1	C	32	ALA	3.8
1	B	32	ALA	3.7
1	B	36	ASP	3.6
1	B	116	ARG	3.6
1	C	6	ILE	3.5
1	B	33	SER	3.0
1	C	90	HIS	2.9
1	B	108	LEU	2.9
1	C	38	ASP	2.9
1	C	145	ASP	2.8
1	C	28	HIS	2.8
1	C	92	VAL	2.8
1	C	1	MET	2.5
1	B	31	MET	2.5
1	C	13	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	21	ALA	2.5
1	C	82	ILE	2.5
1	B	107	LYS	2.5
1	B	8	ALA	2.5
1	C	64	ASP	2.4
1	C	84	ALA	2.4
1	B	37	MET	2.4
1	B	34	SER	2.4
1	B	25	LEU	2.4
1	C	117	VAL	2.4
1	B	39	LEU	2.4
1	B	41	THR	2.3
1	A	113	PRO	2.3
1	C	8	ALA	2.3
1	A	275	GLU	2.3
1	B	79	LEU	2.3
1	B	92	VAL	2.3
1	B	106	LYS	2.3
1	C	85	ASP	2.2
1	B	117	VAL	2.2
1	A	274	GLN	2.2
1	B	28	HIS	2.2
1	B	68	LEU	2.2
1	C	274	GLN	2.2
1	C	5	PHE	2.2
1	C	26	ALA	2.2
1	B	6	ILE	2.2
1	C	65	VAL	2.2
1	B	76	PRO	2.2
1	B	275	GLU	2.2
1	B	24	VAL	2.2
1	C	3	VAL	2.2
1	C	108	LEU	2.1
1	B	3	VAL	2.1
1	C	275	GLU	2.1
1	C	56	ASN	2.1
1	B	43	SER	2.1
1	C	43	SER	2.1
1	B	64	ASP	2.1
1	C	10	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

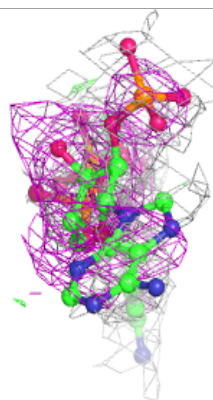
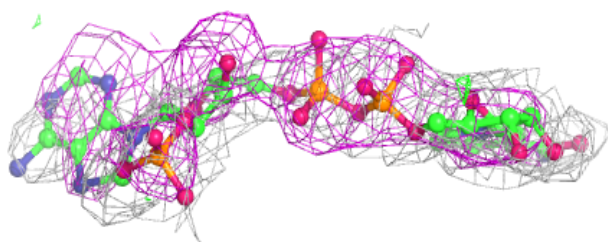
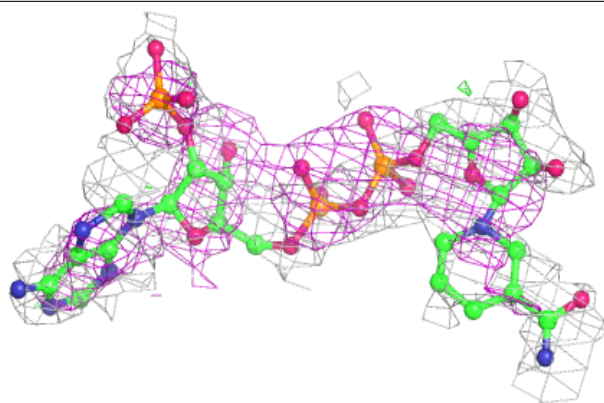
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	GLU	B	2301	10/10	0.36	0.52	132,200,200,200	0
3	GLU	E	5301	10/10	0.42	0.59	157,188,190,191	0
3	GLU	C	3301	10/10	0.45	0.67	144,195,198,199	0
3	GLU	D	4301	10/10	0.55	0.51	142,156,157,158	0
3	GLU	A	1301	10/10	0.64	0.34	120,122,125,126	0
2	NAP	C	3300	48/48	0.68	0.49	79,94,101,106	0
2	NAP	D	4300	48/48	0.73	0.50	63,90,97,99	0
2	NAP	E	5300	48/48	0.74	0.50	71,90,95,99	0
2	NAP	B	2300	48/48	0.76	0.44	61,86,91,94	0
2	NAP	A	1300	48/48	0.80	0.40	55,76,86,88	0

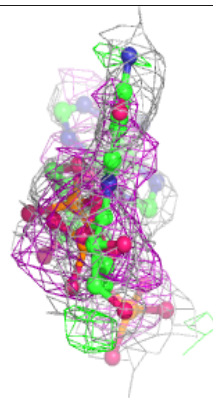
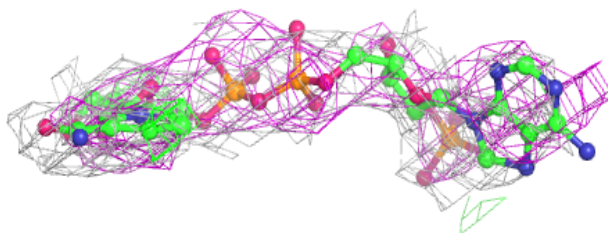
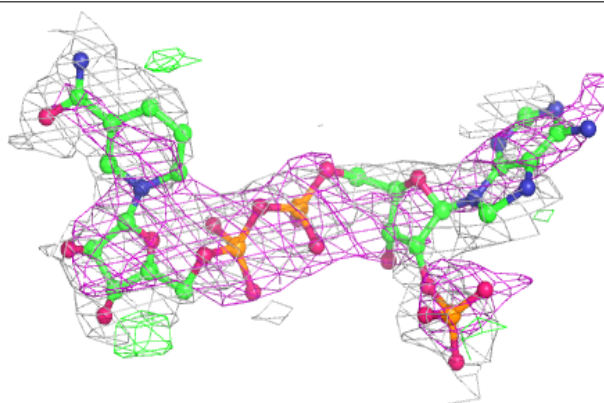
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAP C 3300:**

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

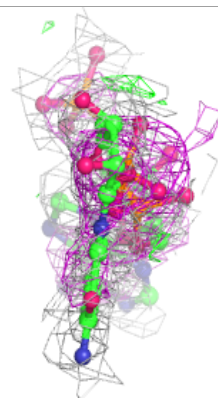
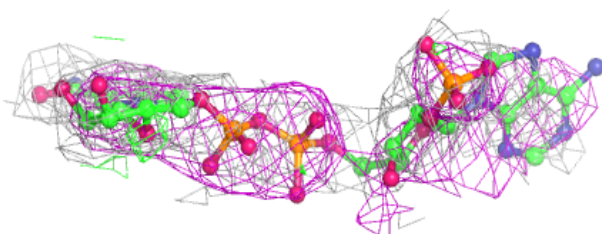
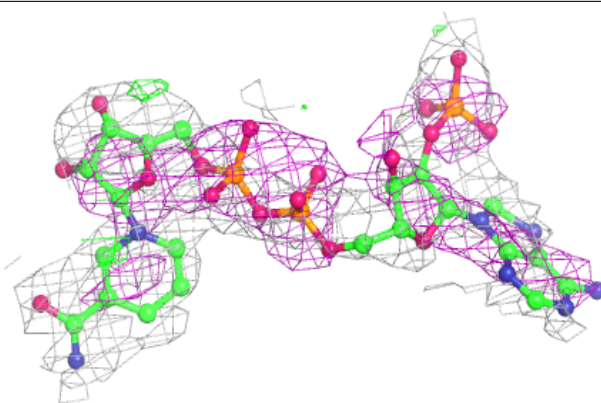
**Electron density around NAP D 4300:**

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

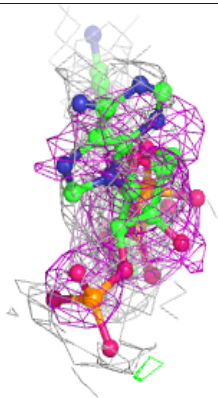
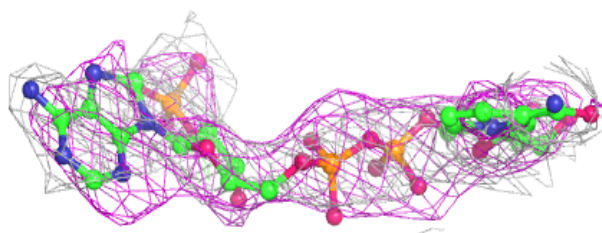
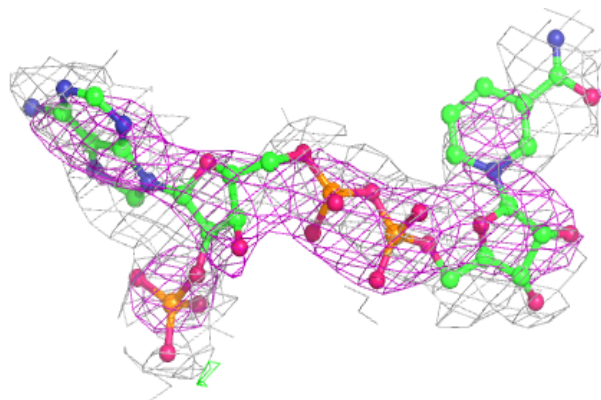


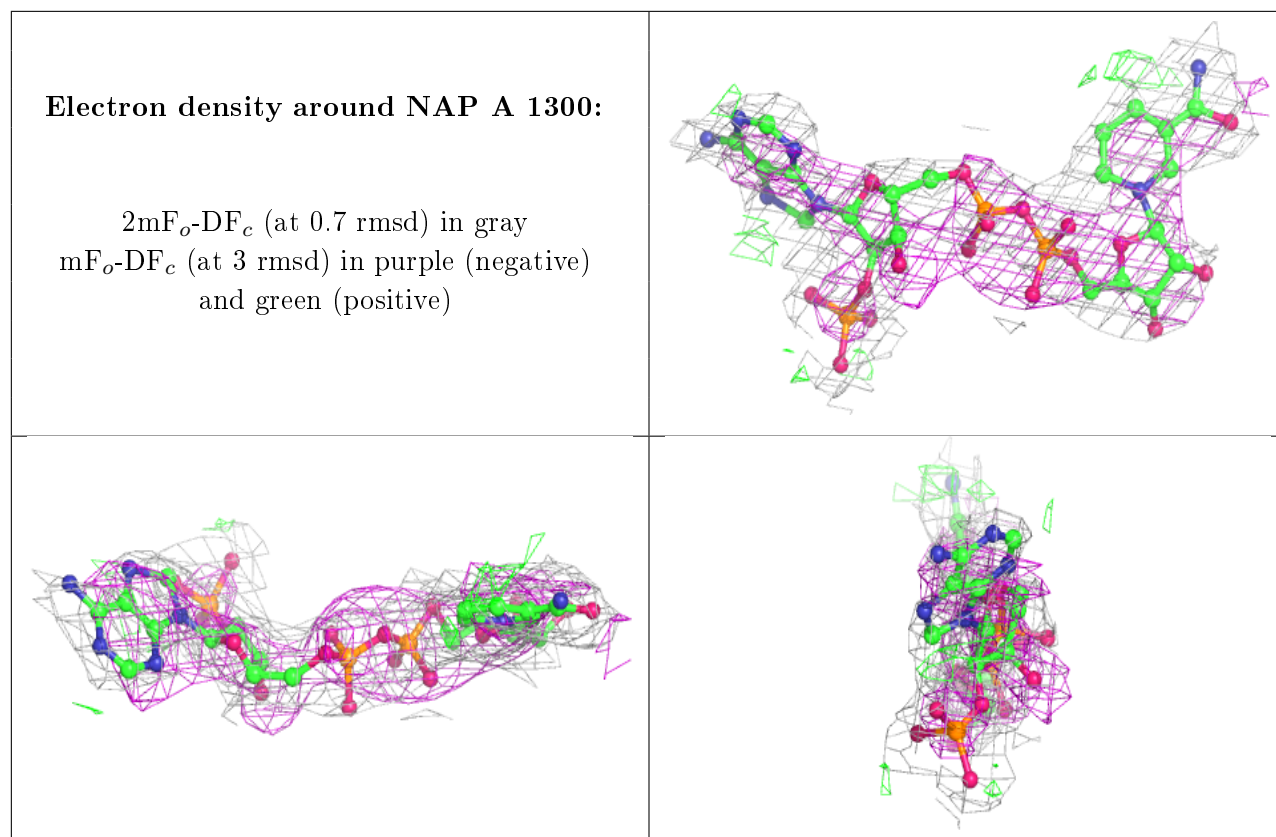
**Electron density around NAP E 5300:**

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

**Electron density around NAP B 2300:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.