



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:24 am BST

PDB ID : 2Q46  
Title : Ensemble refinement of the protein crystal structure of gene product from Arabidopsis thaliana At5g02240  
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)  
Deposited on : 2007-05-31  
Resolution : 1.80 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 : 2.11  
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) : 2.11

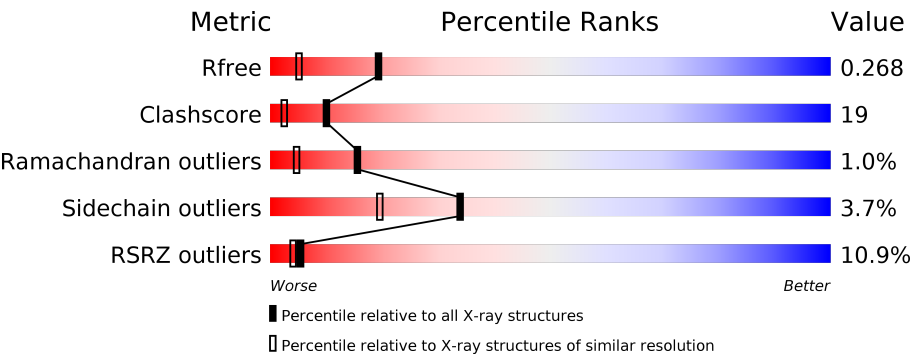
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	1-A	253	
1	1-B	253	
1	2-A	253	
1	2-B	253	
1	3-A	253	
1	3-B	253	

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Mol	Chain	Length	Quality of chain
1	4-A	253	
1	4-B	253	
1	5-A	253	
1	5-B	253	
1	6-A	253	
1	6-B	253	
1	7-A	253	
1	7-B	253	
1	8-A	253	
1	8-B	253	

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	1-A	800	X	-	-	-
2	NAP	1-B	801	X	-	-	-
2	NAP	2-A	800	X	-	-	-
2	NAP	2-B	801	X	-	-	-
2	NAP	3-A	800	X	-	-	-
2	NAP	3-B	801	X	-	-	-
2	NAP	4-B	801	X	-	-	-
2	NAP	5-A	800	X	-	-	-
2	NAP	5-B	801	X	-	-	-
2	NAP	6-A	800	X	-	-	-
2	NAP	6-B	801	X	-	-	-
2	NAP	7-A	800	X	-	-	-
2	NAP	7-B	801	X	-	-	-
2	NAP	8-A	800	X	-	-	-
2	NAP	8-B	801	X	-	-	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34496 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.

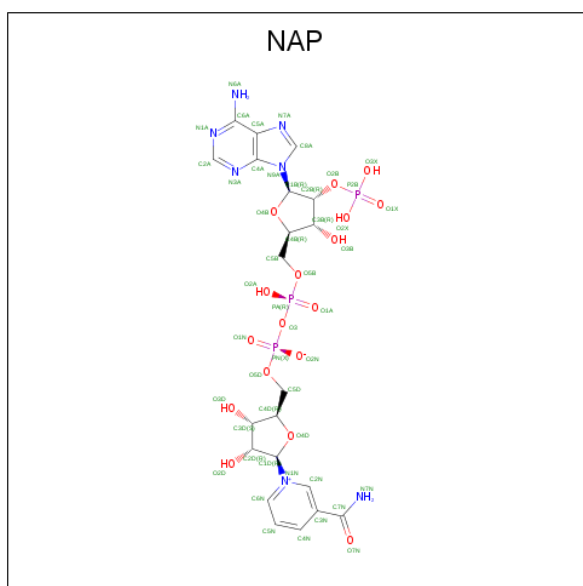
- Molecule 1 is a protein called Protein At5g02240.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0
1	2-A	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0
1	3-A	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0
1	4-A	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0
1	5-A	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0
1	6-A	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0
1	7-A	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0
1	8-A	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0
1	1-B	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0
1	2-B	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0
1	3-B	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0
1	4-B	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0
1	5-B	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0
1	6-B	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0
1	7-B	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0
1	8-B	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	EXPRESSION TAG	UNP Q94EG6
B	1	SER	-	EXPRESSION TAG	UNP Q94EG6

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	1-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	2-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	3-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	4-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	5-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	6-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	7-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	8-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	1-B	1	Total 48	C 21	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	2-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	3-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	4-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	5-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	6-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	7-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	8-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-A	204	Total	O	0	0
			204	204		
3	2-A	205	Total	O	0	0
			205	205		
3	3-A	205	Total	O	0	0
			205	205		
3	4-A	205	Total	O	0	0
			205	205		
3	5-A	205	Total	O	0	0
			205	205		
3	6-A	205	Total	O	0	0
			205	205		
3	7-A	205	Total	O	0	0
			205	205		
3	8-A	204	Total	O	0	0
			204	204		
3	1-B	196	Total	O	0	0
			196	196		
3	2-B	195	Total	O	0	0
			195	195		
3	3-B	195	Total	O	0	0
			195	195		
3	4-B	195	Total	O	0	0
			195	195		

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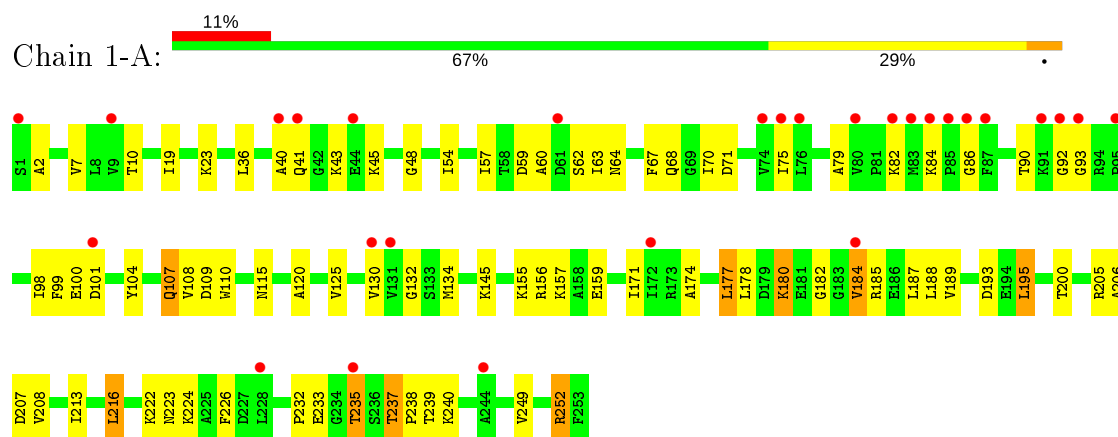
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	5-B	195	Total 195	O 195	0	0
3	6-B	195	Total 195	O 195	0	0
3	7-B	195	Total 195	O 195	0	0
3	8-B	196	Total 196	O 196	0	0

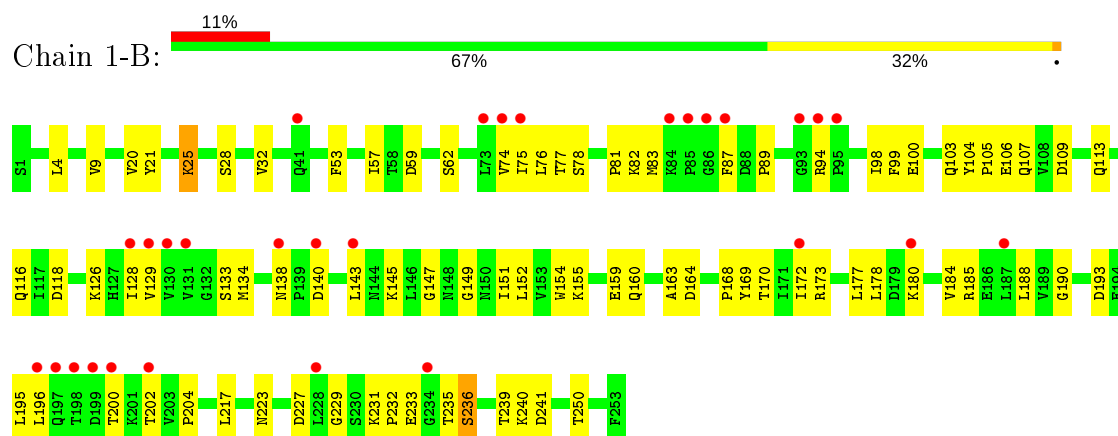
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

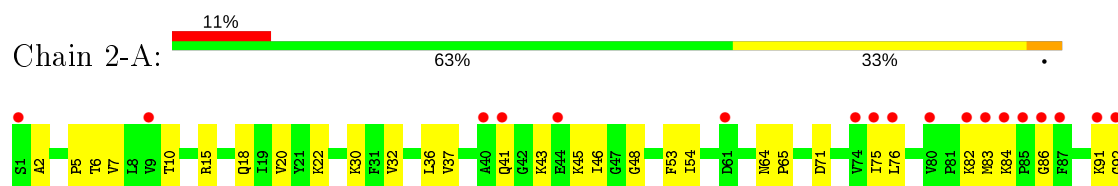
#### • Molecule 1: Protein At5g02240



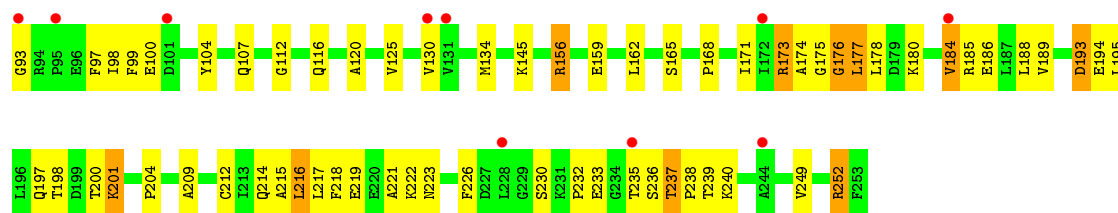
#### • Molecule 1: Protein At5g02240



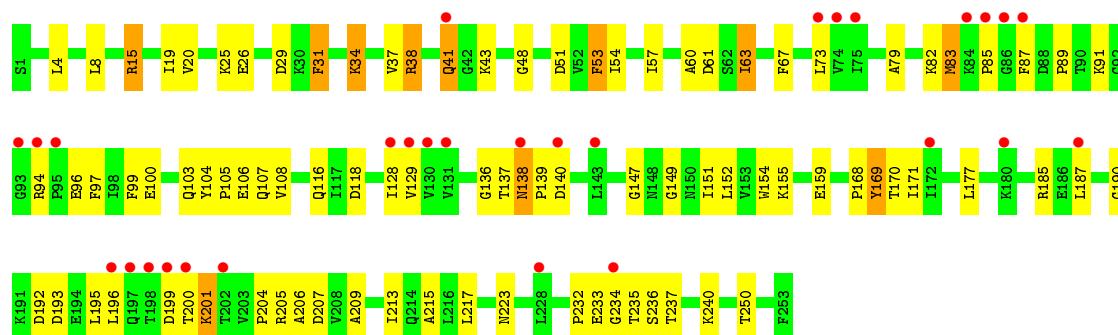
#### • Molecule 1: Protein At5g02240



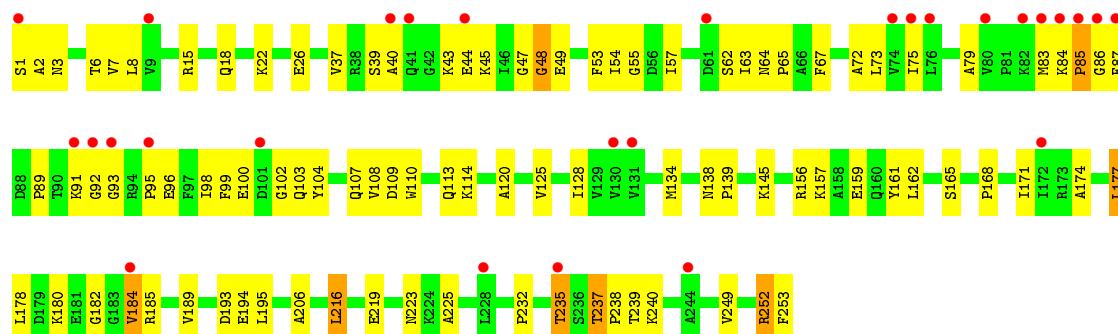




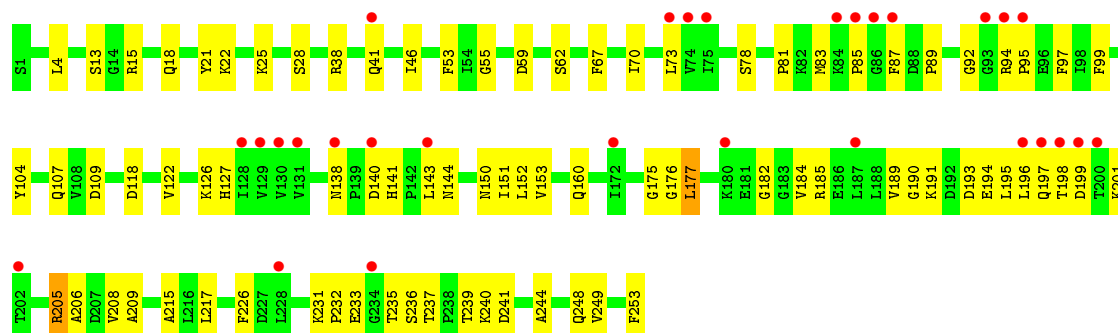
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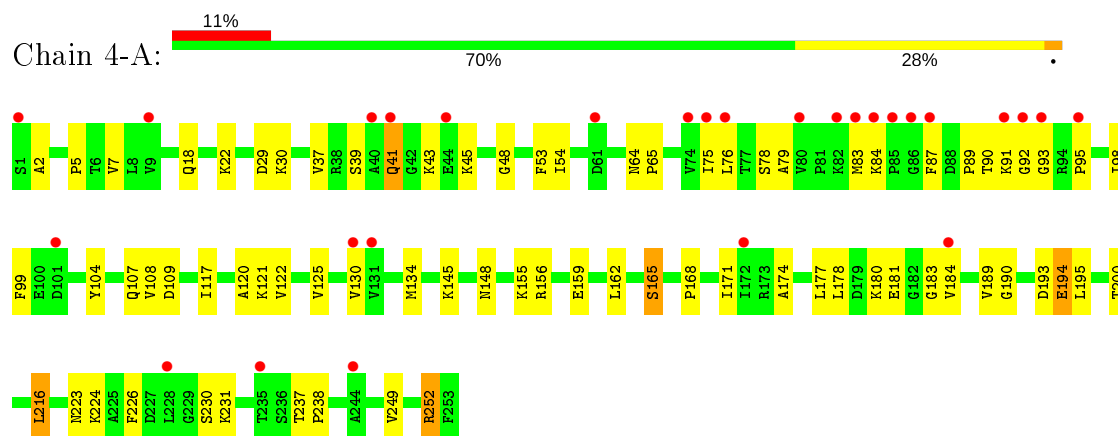
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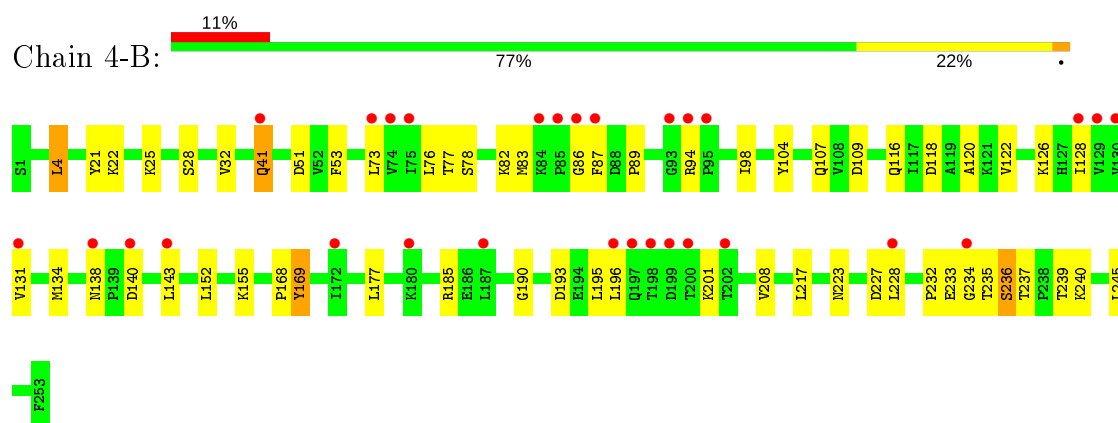
• Molecule 1: Protein At5g02240



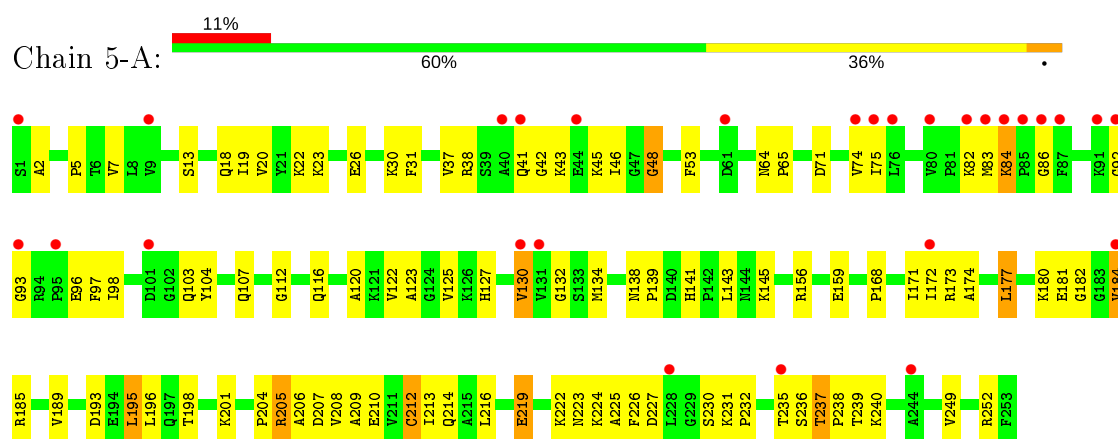
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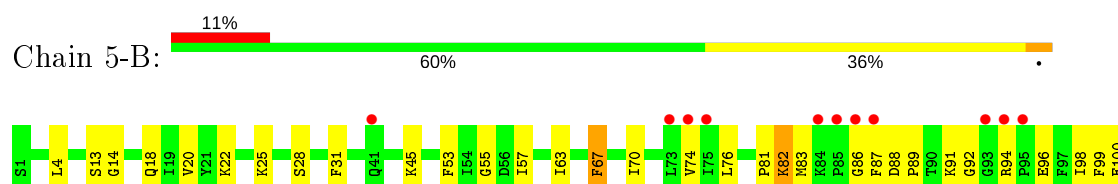
• Molecule 1: Protein At5g02240

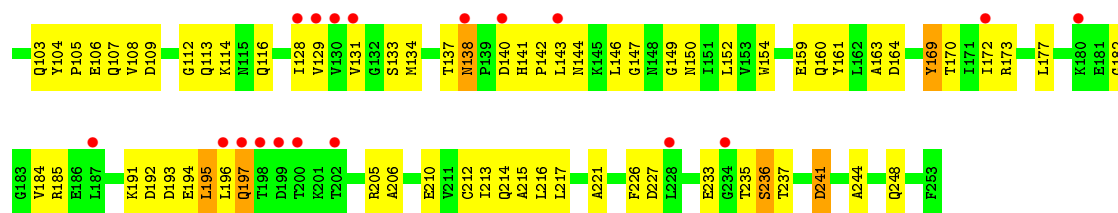


• Molecule 1: Protein At5g02240

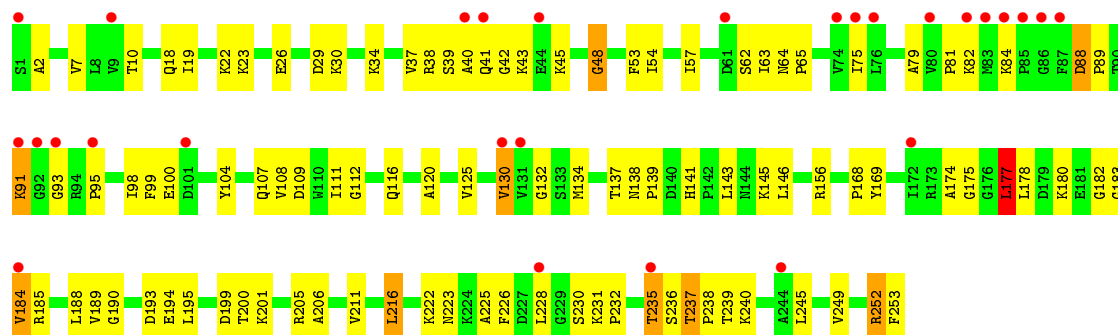


• Molecule 1: Protein At5g02240

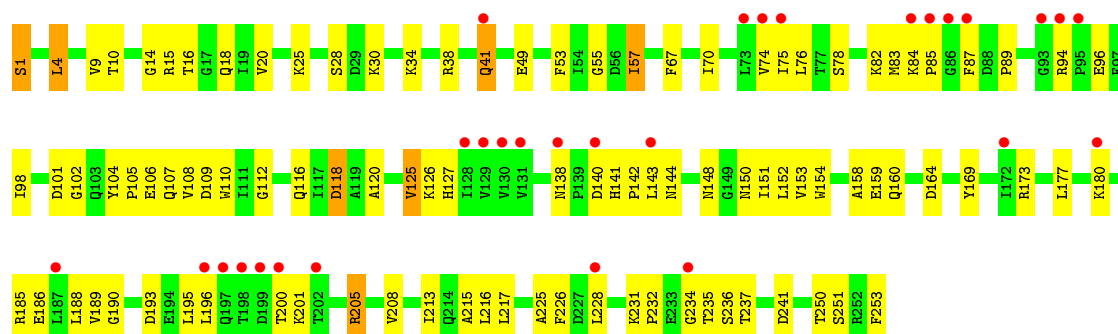




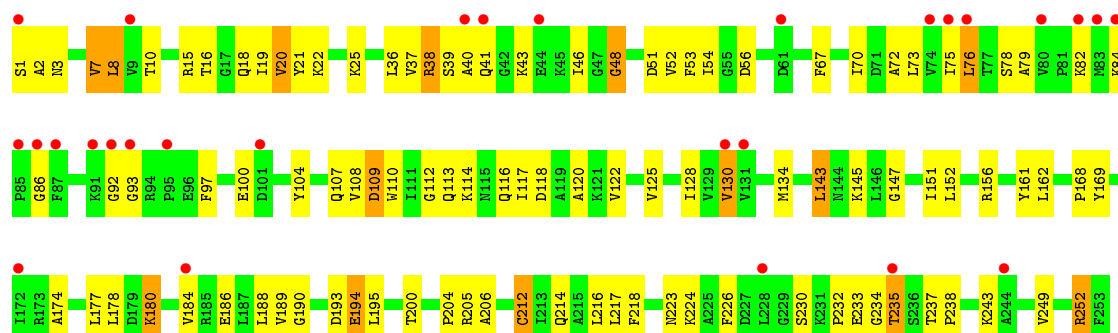
• Molecule 1: Protein At5g02240



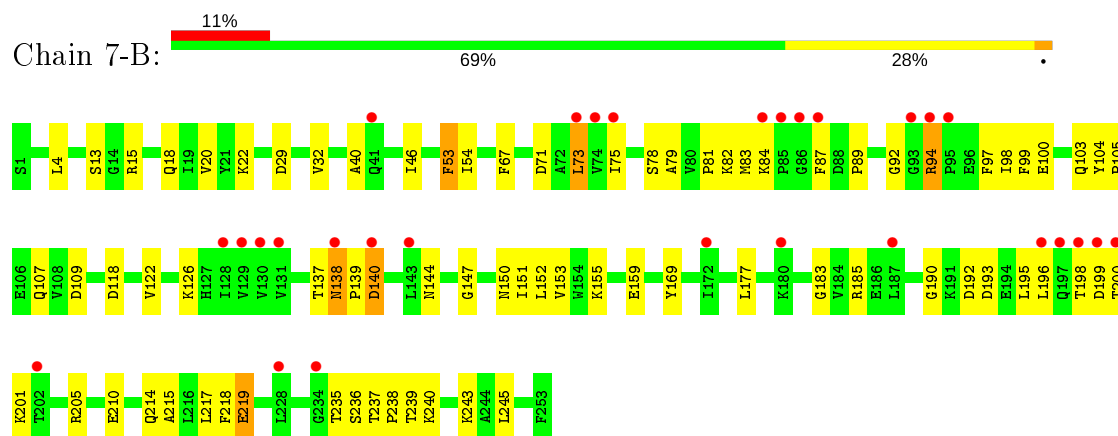
• Molecule 1: Protein At5g02240



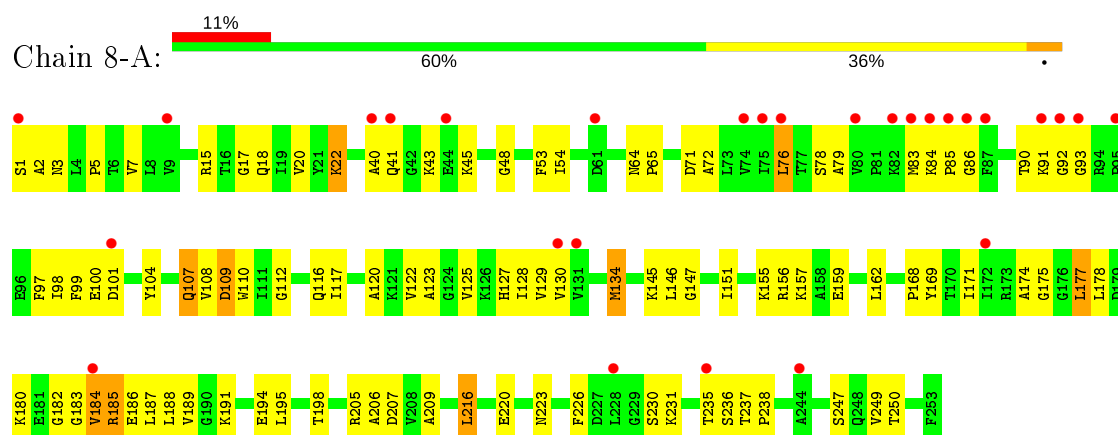
• Molecule 1: Protein At5g02240



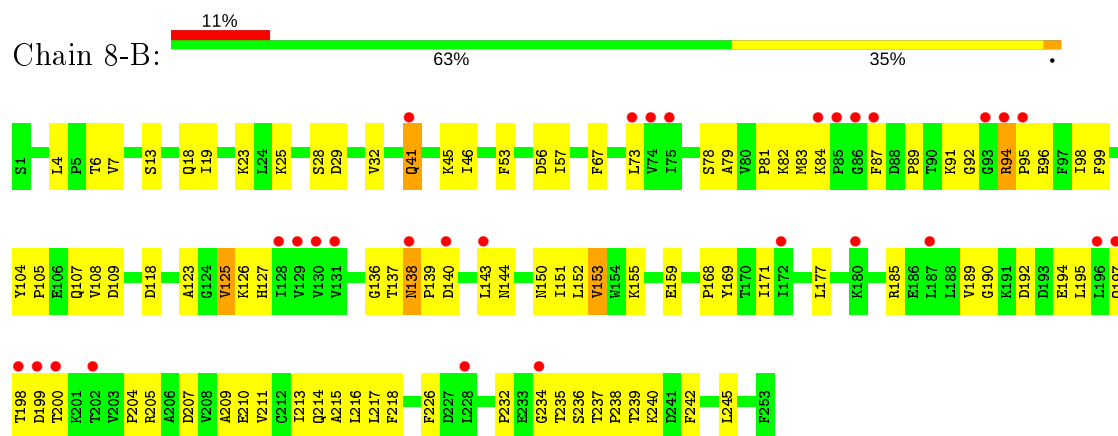
- Molecule 1: Protein At5g02240



- Molecule 1: Protein At5g02240



- Molecule 1: Protein At5g02240



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.75Å 69.80Å 83.83Å 90.00° 96.01° 90.00°	Depositor
Resolution (Å)	23.57 – 1.80 23.57 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.0 (23.57-1.80) 95.2 (23.57-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.53 (at 1.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.209 , 0.267 0.210 , 0.268	Depositor DCC
$R_{free}$ test set	2445 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.7	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 53.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	34496	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% 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	1-A	1.07	1/1941 (0.1%)	1.03	4/2621 (0.2%)
1	1-B	1.03	2/1941 (0.1%)	1.02	1/2621 (0.0%)
1	2-A	1.07	1/1941 (0.1%)	1.07	8/2621 (0.3%)
1	2-B	1.04	4/1941 (0.2%)	1.02	1/2621 (0.0%)
1	3-A	1.08	3/1941 (0.2%)	1.04	3/2621 (0.1%)
1	3-B	1.02	1/1941 (0.1%)	1.04	3/2621 (0.1%)
1	4-A	1.09	3/1941 (0.2%)	1.02	4/2621 (0.2%)
1	4-B	1.03	2/1941 (0.1%)	1.01	1/2621 (0.0%)
1	5-A	1.20	6/1941 (0.3%)	1.08	6/2621 (0.2%)
1	5-B	1.10	4/1941 (0.2%)	1.05	4/2621 (0.2%)
1	6-A	1.15	3/1941 (0.2%)	1.08	6/2621 (0.2%)
1	6-B	1.12	4/1941 (0.2%)	1.08	3/2621 (0.1%)
1	7-A	1.18	5/1941 (0.3%)	1.08	4/2621 (0.2%)
1	7-B	1.13	6/1941 (0.3%)	1.07	3/2621 (0.1%)
1	8-A	1.18	6/1941 (0.3%)	1.09	8/2621 (0.3%)
1	8-B	1.15	8/1941 (0.4%)	1.09	2/2621 (0.1%)
All	All	1.10	59/31056 (0.2%)	1.05	61/41936 (0.1%)

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5-A	212	CYS	CB-SG	-11.67	1.62	1.82
1	5-B	20	VAL	CB-CG1	8.21	1.70	1.52
1	8-A	134	MET	CG-SD	7.89	2.01	1.81
1	7-A	20	VAL	CB-CG2	7.38	1.68	1.52
1	8-B	123	ALA	CA-CB	6.94	1.67	1.52
1	7-B	215	ALA	CA-CB	6.85	1.66	1.52
1	6-B	20	VAL	CB-CG1	6.76	1.67	1.52
1	6-B	53	PHE	CE1-CZ	6.28	1.49	1.37
1	8-B	215	ALA	CA-CB	6.21	1.65	1.52
1	2-B	20	VAL	CB-CG1	6.20	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8-B	53	PHE	CE1-CZ	6.15	1.49	1.37
1	7-B	53	PHE	CE1-CZ	6.12	1.49	1.37
1	5-A	174	ALA	CA-CB	6.07	1.65	1.52
1	2-B	53	PHE	CE1-CZ	5.99	1.48	1.37
1	7-A	194	GLU	CD-OE1	5.98	1.32	1.25
1	1-B	53	PHE	CE1-CZ	5.92	1.48	1.37
1	5-B	53	PHE	CE1-CZ	5.87	1.48	1.37
1	3-B	53	PHE	CE1-CZ	5.87	1.48	1.37
1	2-A	194	GLU	CD-OE1	5.86	1.32	1.25
1	4-B	53	PHE	CE1-CZ	5.85	1.48	1.37
1	1-A	174	ALA	CA-CB	5.76	1.64	1.52
1	8-B	169	TYR	CD1-CE1	5.75	1.48	1.39
1	4-A	174	ALA	CA-CB	5.67	1.64	1.52
1	7-B	169	TYR	CD1-CE1	5.62	1.47	1.39
1	5-A	123	ALA	CA-CB	5.62	1.64	1.52
1	3-A	194	GLU	CD-OE1	5.56	1.31	1.25
1	8-A	174	ALA	CA-CB	5.54	1.64	1.52
1	7-B	20	VAL	CB-CG1	5.50	1.64	1.52
1	5-A	20	VAL	CB-CG2	5.46	1.64	1.52
1	4-A	194	GLU	CD-OE1	5.44	1.31	1.25
1	2-B	215	ALA	CA-CB	5.43	1.63	1.52
1	6-A	184	VAL	CB-CG2	-5.40	1.41	1.52
1	7-A	7	VAL	CB-CG1	5.40	1.64	1.52
1	8-A	130	VAL	CB-CG1	5.39	1.64	1.52
1	8-A	123	ALA	CA-CB	5.39	1.63	1.52
1	8-B	153	VAL	CB-CG1	5.38	1.64	1.52
1	5-A	184	VAL	CB-CG2	-5.35	1.41	1.52
1	7-A	174	ALA	CA-CB	5.33	1.63	1.52
1	8-A	184	VAL	CB-CG2	-5.33	1.41	1.52
1	5-A	130	VAL	CB-CG1	5.33	1.64	1.52
1	4-A	165	SER	CB-OG	5.26	1.49	1.42
1	7-A	130	VAL	CB-CG1	5.26	1.64	1.52
1	6-A	174	ALA	CA-CB	5.25	1.63	1.52
1	3-A	184	VAL	CB-CG2	-5.23	1.41	1.52
1	1-B	20	VAL	CB-CG1	5.22	1.63	1.52
1	5-B	169	TYR	CD1-CE1	5.20	1.47	1.39
1	6-B	67	PHE	CD2-CE2	5.19	1.49	1.39
1	3-A	174	ALA	CA-CB	5.18	1.63	1.52
1	8-B	226	PHE	CE2-CZ	5.18	1.47	1.37
1	8-B	67	PHE	CD2-CE2	5.15	1.49	1.39
1	6-B	169	TYR	CD1-CE1	5.14	1.47	1.39
1	4-B	169	TYR	CD1-CE1	5.13	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-B	169	TYR	CD1-CE1	5.11	1.47	1.39
1	6-A	130	VAL	CB-CG1	5.10	1.63	1.52
1	8-B	53	PHE	CD2-CE2	5.09	1.49	1.39
1	7-B	67	PHE	CD2-CE2	5.08	1.49	1.39
1	7-B	53	PHE	CD2-CE2	5.07	1.49	1.39
1	5-B	67	PHE	CD2-CE2	5.06	1.49	1.39
1	8-A	129	VAL	CB-CG1	5.02	1.63	1.52

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2-A	173	ARG	NE-CZ-NH1	-9.84	115.38	120.30
1	6-A	156	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	8-A	156	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	5-A	156	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	2-A	156	ARG	NE-CZ-NH1	7.27	123.93	120.30
1	1-A	156	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	3-A	156	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	2-A	193	ASP	CB-CG-OD1	6.70	124.33	118.30
1	6-A	156	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	1-A	93	GLY	N-CA-C	-6.51	96.82	113.10
1	7-A	93	GLY	N-CA-C	-6.40	97.11	113.10
1	8-A	93	GLY	N-CA-C	-6.34	97.26	113.10
1	3-A	93	GLY	N-CA-C	-6.34	97.26	113.10
1	5-A	93	GLY	N-CA-C	-6.27	97.42	113.10
1	4-A	93	GLY	N-CA-C	-6.25	97.46	113.10
1	3-B	241	ASP	CB-CG-OD1	6.22	123.90	118.30
1	5-A	156	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	8-A	156	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	4-A	2	ALA	N-CA-C	-6.18	94.32	111.00
1	1-B	241	ASP	CB-CG-OD1	6.16	123.84	118.30
1	6-B	118	ASP	CB-CG-OD1	-6.11	112.81	118.30
1	3-A	2	ALA	N-CA-C	-6.00	94.79	111.00
1	2-A	156	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	8-A	2	ALA	N-CA-C	-5.94	94.97	111.00
1	5-A	2	ALA	N-CA-C	-5.91	95.05	111.00
1	4-A	156	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	7-A	2	ALA	N-CA-C	-5.84	95.22	111.00
1	6-A	91	LYS	N-CA-C	-5.83	95.27	111.00
1	2-A	2	ALA	N-CA-C	-5.74	95.51	111.00
1	1-A	2	ALA	N-CA-C	-5.71	95.59	111.00
1	8-B	56	ASP	CB-CG-OD2	5.67	123.41	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8-A	134	MET	CG-SD-CE	-5.66	91.15	100.20
1	6-A	2	ALA	N-CA-C	-5.65	95.75	111.00
1	6-A	93	GLY	N-CA-C	-5.61	99.09	113.10
1	2-A	212	CYS	CA-CB-SG	5.53	123.95	114.00
1	5-B	216	LEU	CB-CG-CD2	-5.51	101.64	111.00
1	6-B	241	ASP	CB-CG-OD1	5.43	123.18	118.30
1	8-A	185	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	7-A	122	VAL	CG1-CB-CG2	-5.40	102.26	110.90
1	2-A	173	ARG	NE-CZ-NH2	5.39	123.00	120.30
1	7-A	109	ASP	CB-CG-OD1	5.39	123.15	118.30
1	8-A	122	VAL	CG1-CB-CG2	-5.38	102.29	110.90
1	5-B	241	ASP	CB-CG-OD1	5.35	123.11	118.30
1	1-A	156	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	8-A	109	ASP	CB-CG-OD1	5.32	123.09	118.30
1	3-B	205	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	5-A	122	VAL	CG1-CB-CG2	-5.27	102.46	110.90
1	7-B	200	THR	N-CA-C	-5.24	96.84	111.00
1	3-B	92	GLY	N-CA-C	5.17	126.01	113.10
1	5-B	216	LEU	CA-CB-CG	5.16	127.17	115.30
1	7-B	71	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	8-B	200	THR	N-CA-C	-5.12	97.17	111.00
1	5-B	92	GLY	N-CA-C	5.06	125.75	113.10
1	2-B	200	THR	N-CA-C	-5.04	97.38	111.00
1	2-A	93	GLY	N-CA-C	-5.04	100.50	113.10
1	6-A	177	LEU	CB-CG-CD1	5.03	119.55	111.00
1	4-B	86	GLY	N-CA-C	5.03	125.67	113.10
1	4-A	122	VAL	CG1-CB-CG2	-5.03	102.86	110.90
1	5-A	205	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	6-B	205	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	7-B	71	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	1-A	1908	0	1935	67	0
1	1-B	1908	0	1935	70	0
1	2-A	1908	0	1935	65	0
1	2-B	1908	0	1935	79	0
1	3-A	1908	0	1935	70	0
1	3-B	1908	0	1935	68	0
1	4-A	1908	0	1935	56	0
1	4-B	1908	0	1935	59	0
1	5-A	1908	0	1935	73	0
1	5-B	1908	0	1935	82	0
1	6-A	1908	0	1935	85	0
1	6-B	1908	0	1935	84	0
1	7-A	1908	0	1935	90	0
1	7-B	1908	0	1935	63	0
1	8-A	1908	0	1935	85	0
1	8-B	1908	0	1935	83	0
2	1-A	48	0	24	5	0
2	1-B	48	0	24	4	0
2	2-A	48	0	24	4	0
2	2-B	48	0	23	1	0
2	3-A	48	0	24	2	0
2	3-B	48	0	23	3	0
2	4-A	48	0	23	9	0
2	4-B	48	0	24	2	0
2	5-A	48	0	24	2	0
2	5-B	48	0	23	1	0
2	6-A	48	0	24	3	0
2	6-B	48	0	23	8	0
2	7-A	48	0	24	2	0
2	7-B	48	0	23	3	0
2	8-A	48	0	23	4	0
2	8-B	48	0	23	2	0
3	1-A	204	0	0	4	0
3	1-B	196	0	0	7	0
3	2-A	205	0	0	7	0
3	2-B	195	0	0	9	0
3	3-A	205	0	0	7	0
3	3-B	195	0	0	13	0
3	4-A	205	0	0	7	0
3	4-B	195	0	0	9	0
3	5-A	205	0	0	10	0
3	5-B	195	0	0	15	0
3	6-A	205	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	6-B	195	0	0	10	0
3	7-A	205	0	0	3	0
3	7-B	195	0	0	12	0
3	8-A	204	0	0	9	0
3	8-B	196	0	0	13	0
All	All	34496	0	31336	1188	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (1188) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:MET:CG	1:A:134:MET:SD	2.01	1.46
2:A:800:NAP:C3B	2:A:800:NAP:O3B	1.69	1.39
2:A:800:NAP:O4B	2:A:800:NAP:C5B	1.98	1.11
2:A:800:NAP:O3B	2:A:800:NAP:C4B	2.07	1.02
1:A:79:ALA:HB2	1:A:108:VAL:HG21	1.43	1.01
2:A:800:NAP:O4B	2:A:800:NAP:C4B	1.99	1.00
1:A:188:LEU:HD21	1:A:231:LYS:HE3	1.44	0.97
1:A:230:SER:O	3:A:998:HOH:O	1.83	0.95
1:A:230:SER:O	3:A:998:HOH:O	1.88	0.90
1:A:79:ALA:HB2	1:A:108:VAL:CG2	2.02	0.89
1:B:195:LEU:HD12	1:B:195:LEU:H	1.38	0.89
1:A:79:ALA:HB2	1:A:108:VAL:CG2	2.02	0.88
2:A:800:NAP:O4B	2:A:800:NAP:H51A	1.71	0.88
1:A:79:ALA:HB2	1:A:108:VAL:HG21	1.55	0.88
1:B:138:ASN:HD21	1:B:140:ASP:HB2	1.38	0.88
1:B:138:ASN:HD21	1:B:140:ASP:HB2	1.38	0.87
1:A:79:ALA:HB2	1:A:108:VAL:CG2	2.04	0.87
1:B:126:LYS:NZ	3:B:956:HOH:O	2.08	0.85
1:A:18:GLN:O	1:A:22:LYS:HD3	1.73	0.85
1:B:233:GLU:HG2	3:B:976:HOH:O	1.74	0.85
1:B:190:GLY:HA3	1:B:195:LEU:HD11	1.57	0.85
1:A:60:ALA:HB2	1:A:115:ASN:HD21	1.38	0.85
1:A:75:ILE:HG21	1:A:113:GLN:OE1	1.75	0.84
1:A:18:GLN:O	1:A:22:LYS:HD3	1.77	0.83
1:A:210:GLU:O	1:A:214:GLN:HG2	1.78	0.83
1:B:83:MET:O	3:B:882:HOH:O	1.95	0.83
1:B:195:LEU:HD12	1:B:195:LEU:N	1.94	0.83
1:A:18:GLN:O	1:A:22:LYS:HD3	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:LEU:N	1:B:195:LEU:HD12	1.93	0.82
1:B:100:GLU:OE1	1:B:103:GLN:HG3	1.79	0.82
1:A:137:THR:HG23	3:A:995:HOH:O	1.79	0.82
1:B:195:LEU:HD12	1:B:195:LEU:H	1.43	0.81
1:B:126:LYS:NZ	3:B:956:HOH:O	2.10	0.81
1:A:209:ALA:O	1:A:212:CYS:HB3	1.79	0.81
1:B:126:LYS:NZ	3:B:956:HOH:O	2.10	0.81
1:A:79:ALA:HB2	1:A:108:VAL:HG21	1.61	0.80
1:B:78:SER:HB2	2:B:801:NAP:H3D	1.63	0.80
1:A:18:GLN:O	1:A:22:LYS:HD3	1.80	0.80
1:A:162:LEU:HD21	1:A:169:TYR:HB2	1.62	0.79
1:B:126:LYS:NZ	3:B:956:HOH:O	2.13	0.79
1:B:118:ASP:OD2	3:B:886:HOH:O	1.99	0.79
1:A:189:VAL:HG11	1:A:249:VAL:HG22	1.64	0.78
1:A:143:LEU:HD22	1:A:151:ILE:HG21	1.65	0.78
1:B:126:LYS:NZ	3:B:957:HOH:O	2.16	0.78
1:A:189:VAL:HG11	1:A:249:VAL:HG22	1.65	0.78
1:B:152:LEU:HD12	1:B:152:LEU:H	1.48	0.77
1:A:222:LYS:HE3	3:A:954:HOH:O	1.84	0.77
1:B:195:LEU:HD12	1:B:195:LEU:N	2.00	0.76
1:B:177:LEU:HD23	1:B:205:ARG:HE	1.51	0.76
1:A:102:GLY:HA2	1:A:107:GLN:NE2	1.99	0.76
1:A:79:ALA:HA	1:A:108:VAL:HG21	1.68	0.76
1:B:138:ASN:HD21	1:B:140:ASP:HB2	1.50	0.76
1:B:4:LEU:HD21	1:B:32:VAL:HG23	1.68	0.76
1:A:86:GLY:HA3	3:A:874:HOH:O	1.87	0.75
1:B:195:LEU:N	1:B:195:LEU:HD12	2.01	0.75
1:A:84:LYS:HE3	3:A:874:HOH:O	1.84	0.75
1:A:143:LEU:HD22	1:A:151:ILE:CG2	2.16	0.75
1:B:195:LEU:HD12	1:B:195:LEU:H	1.51	0.75
1:A:43:LYS:HG2	1:A:48:GLY:HA2	1.68	0.75
1:B:81:PRO:HG3	1:B:99:PHE:CZ	2.22	0.75
1:A:84:LYS:HE3	3:A:874:HOH:O	1.86	0.75
1:B:126:LYS:NZ	3:B:957:HOH:O	1.93	0.75
1:B:82:LYS:HE3	1:B:98:ILE:HG13	1.69	0.75
1:B:195:LEU:HD12	1:B:195:LEU:N	2.02	0.74
1:A:102:GLY:HA2	1:A:107:GLN:HE22	1.53	0.74
1:A:175:GLY:HA3	1:A:201:LYS:O	1.88	0.73
1:B:4:LEU:HD21	1:B:32:VAL:HG23	1.69	0.73
1:B:195:LEU:H	1:B:195:LEU:HD12	1.52	0.73
1:B:195:LEU:N	1:B:195:LEU:HD12	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ALA:CB	1:A:108:VAL:HG21	2.17	0.73
1:B:138:ASN:HD21	1:B:140:ASP:HB2	1.53	0.73
1:B:100:GLU:HB2	1:B:103:GLN:HB2	1.71	0.73
1:A:230:SER:O	3:A:997:HOH:O	2.06	0.73
1:A:120:ALA:HB1	1:A:125:VAL:HG11	1.70	0.73
1:A:134:MET:HE2	1:A:193:ASP:HA	1.71	0.73
1:A:162:LEU:HD11	1:A:169:TYR:HB3	1.70	0.73
1:B:1:SER:N	1:B:4:LEU:O	2.21	0.72
1:A:64:ASN:HB3	1:A:65:PRO:HD3	1.68	0.72
1:B:13:SER:HB2	1:B:45:LYS:HD2	1.70	0.72
1:A:37:VAL:HG12	1:A:39:SER:H	1.55	0.72
1:B:81:PRO:HG3	1:B:99:PHE:CE1	2.24	0.72
1:A:134:MET:HE2	1:A:193:ASP:HA	1.71	0.72
1:B:240:LYS:HE2	1:B:240:LYS:HA	1.71	0.72
1:B:159:GLU:HB3	1:B:171:ILE:HD13	1.72	0.72
1:A:1:SER:HB2	1:A:3:ASN:HB2	1.72	0.72
1:A:189:VAL:HG11	1:A:249:VAL:HG22	1.70	0.71
1:B:82:LYS:O	1:B:83:MET:HB2	1.89	0.71
1:A:134:MET:HE2	1:A:193:ASP:HA	1.73	0.71
1:B:190:GLY:HA3	1:B:195:LEU:HD11	1.72	0.71
1:A:134:MET:HE2	1:A:193:ASP:HA	1.72	0.71
1:A:230:SER:O	3:A:998:HOH:O	2.07	0.71
1:B:201:LYS:H	1:B:201:LYS:HD3	1.55	0.71
1:B:138:ASN:HD21	1:B:140:ASP:HB2	1.55	0.70
1:B:159:GLU:HB3	1:B:171:ILE:HD13	1.71	0.70
1:B:195:LEU:CD1	1:B:195:LEU:H	2.03	0.70
1:B:82:LYS:HE3	1:B:98:ILE:HD11	1.74	0.70
1:B:240:LYS:HE2	1:B:240:LYS:HA	1.72	0.70
1:A:86:GLY:HA3	3:A:874:HOH:O	1.92	0.70
1:A:60:ALA:HB2	1:A:115:ASN:ND2	2.07	0.70
1:B:82:LYS:HE3	1:B:98:ILE:HD11	1.73	0.70
1:A:134:MET:HE2	1:A:193:ASP:HA	1.74	0.70
1:B:118:ASP:OD2	3:B:887:HOH:O	2.08	0.70
1:B:240:LYS:HA	1:B:240:LYS:HE2	1.72	0.70
1:B:87:PHE:CZ	1:B:89:PRO:HA	2.26	0.70
1:A:175:GLY:O	1:A:177:LEU:HD13	1.92	0.69
1:B:21:TYR:OH	1:B:25:LYS:HE2	1.91	0.69
1:A:86:GLY:HA3	3:A:874:HOH:O	1.91	0.69
1:B:191:LYS:O	1:B:194:GLU:HG3	1.92	0.69
1:B:18:GLN:O	1:B:22:LYS:HG3	1.91	0.69
1:B:137:THR:O	1:B:139:PRO:HD3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:THR:O	1:A:240:LYS:HD3	1.92	0.69
1:B:195:LEU:HD12	1:B:195:LEU:N	2.05	0.69
1:A:83:MET:HG3	1:A:97:PHE:CE2	2.27	0.69
1:B:195:LEU:N	1:B:195:LEU:HD12	2.08	0.69
1:A:83:MET:SD	3:A:972:HOH:O	2.50	0.69
1:B:57:ILE:HG12	2:B:801:NAP:N6A	2.07	0.69
1:B:213:ILE:O	1:B:217:LEU:HD13	1.92	0.69
1:A:103:GLN:OE1	3:A:958:HOH:O	2.11	0.69
1:A:189:VAL:HG11	1:A:249:VAL:HG22	1.75	0.69
1:B:193:ASP:O	1:B:196:LEU:HB2	1.93	0.68
1:B:184:VAL:HG22	3:B:921:HOH:O	1.93	0.68
1:A:120:ALA:HB1	1:A:125:VAL:HG11	1.74	0.68
1:B:195:LEU:CD1	1:B:195:LEU:H	2.06	0.68
1:A:43:LYS:HG2	1:A:48:GLY:HA2	1.76	0.68
1:A:168:PRO:HA	1:A:223:ASN:HD21	1.57	0.68
1:A:1:SER:HB2	1:A:3:ASN:HB2	1.76	0.68
1:A:57:ILE:HA	1:A:63:ILE:HD13	1.75	0.68
1:B:83:MET:O	3:B:882:HOH:O	2.11	0.68
1:A:41:GLN:HG3	1:A:45:LYS:HE2	1.76	0.68
1:B:28:SER:O	3:B:928:HOH:O	2.12	0.68
1:B:97:PHE:O	1:B:147:GLY:HA2	1.94	0.68
1:A:180:LYS:HD3	1:A:185:ARG:HH11	1.58	0.68
1:B:104:TYR:HB2	1:B:107:GLN:HE22	1.59	0.68
1:A:239:THR:O	1:A:240:LYS:HD3	1.94	0.67
1:A:79:ALA:CB	1:A:108:VAL:HG21	2.24	0.67
1:A:43:LYS:HG2	1:A:48:GLY:HA2	1.74	0.67
1:A:79:ALA:HB2	1:A:108:VAL:CG2	2.24	0.67
1:B:13:SER:O	1:B:45:LYS:HE3	1.93	0.67
1:A:134:MET:CE	1:A:195:LEU:HB2	2.25	0.67
1:B:118:ASP:OD2	3:B:886:HOH:O	2.11	0.67
1:A:79:ALA:HA	1:A:108:VAL:HG21	1.76	0.67
1:B:185:ARG:HA	3:B:982:HOH:O	1.94	0.67
1:B:22:LYS:HE3	3:B:843:HOH:O	1.93	0.67
1:A:188:LEU:HD11	1:A:231:LYS:HG3	1.76	0.67
1:A:177:LEU:HG	1:A:205:ARG:HG2	1.75	0.67
1:A:189:VAL:HG11	1:A:249:VAL:HG22	1.77	0.67
1:A:239:THR:O	1:A:240:LYS:HD3	1.95	0.67
1:B:118:ASP:OD1	3:B:877:HOH:O	2.11	0.67
1:B:152:LEU:HD12	1:B:152:LEU:N	2.09	0.67
1:A:168:PRO:HA	1:A:223:ASN:ND2	2.10	0.67
1:B:138:ASN:ND2	1:B:140:ASP:HB2	2.11	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ASN:HB3	1:B:150:ASN:OD1	1.95	0.67
1:B:129:VAL:HG22	1:B:170:THR:HB	1.76	0.67
1:A:1:SER:HB2	1:A:3:ASN:HB2	1.77	0.67
1:A:134:MET:CE	1:A:195:LEU:HB2	2.25	0.66
1:B:195:LEU:H	1:B:195:LEU:HD12	1.59	0.66
1:A:120:ALA:HB1	1:A:125:VAL:HG11	1.77	0.66
1:B:184:VAL:HG22	3:B:922:HOH:O	1.96	0.66
1:B:118:ASP:OD2	3:B:886:HOH:O	2.13	0.66
1:A:180:LYS:HE3	1:A:180:LYS:HA	1.77	0.66
1:B:104:TYR:H	1:B:107:GLN:NE2	1.93	0.66
1:A:180:LYS:HA	1:A:180:LYS:HE3	1.77	0.66
1:B:94:ARG:HD3	1:B:94:ARG:H	1.60	0.66
1:A:86:GLY:HA3	3:A:874:HOH:O	1.95	0.66
1:B:232:PRO:HG2	1:B:235:THR:HG21	1.78	0.66
1:A:84:LYS:HE3	3:A:874:HOH:O	1.96	0.66
1:A:134:MET:HE2	1:A:193:ASP:HA	1.78	0.66
1:B:34:LYS:HD2	1:B:53:PHE:HE1	1.60	0.65
1:A:168:PRO:HA	1:A:223:ASN:HD21	1.59	0.65
1:B:190:GLY:HA3	1:B:195:LEU:HD11	1.77	0.65
1:A:79:ALA:CB	1:A:108:VAL:HG21	2.25	0.65
1:B:105:PRO:HD2	3:B:937:HOH:O	1.94	0.65
1:A:168:PRO:HA	1:A:223:ASN:ND2	2.11	0.65
1:A:120:ALA:HB1	1:A:125:VAL:HG11	1.78	0.65
1:A:84:LYS:HE3	3:A:874:HOH:O	1.95	0.65
1:B:177:LEU:HD23	1:B:205:ARG:NE	2.10	0.65
1:A:41:GLN:HG3	1:A:45:LYS:HE2	1.77	0.65
1:B:236:SER:OG	1:B:237:THR:N	2.29	0.65
1:B:104:TYR:HB3	3:B:937:HOH:O	1.95	0.65
1:B:28:SER:O	3:B:928:HOH:O	2.14	0.65
1:B:129:VAL:HG22	1:B:170:THR:HB	1.78	0.65
1:B:195:LEU:HD12	1:B:195:LEU:H	1.62	0.65
1:B:150:ASN:HD22	1:B:153:VAL:HG21	1.62	0.65
1:B:101:ASP:OD2	3:B:936:HOH:O	2.14	0.65
1:A:168:PRO:HA	1:A:223:ASN:HD21	1.61	0.65
1:A:64:ASN:HB3	1:A:65:PRO:HD3	1.79	0.65
1:A:127:HIS:ND1	1:A:216:LEU:HD12	2.12	0.65
1:B:195:LEU:H	1:B:195:LEU:CD1	2.10	0.65
1:B:78:SER:HB2	2:B:801:NAP:H3D	1.78	0.64
1:A:120:ALA:HB1	1:A:125:VAL:HG11	1.79	0.64
1:B:4:LEU:HD22	1:B:32:VAL:HG23	1.79	0.64
1:B:193:ASP:O	1:B:196:LEU:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:VAL:HG11	1:B:249:VAL:HG22	1.77	0.64
1:B:143:LEU:HD12	1:B:152:LEU:HD11	1.80	0.64
1:A:168:PRO:HA	1:A:223:ASN:ND2	2.13	0.64
1:B:21:TYR:OH	1:B:25:LYS:HE2	1.98	0.64
1:B:195:LEU:CD1	1:B:195:LEU:H	2.11	0.64
1:A:232:PRO:HG2	1:A:235:THR:HG21	1.79	0.64
1:B:34:LYS:HD2	1:B:70:ILE:HG22	1.80	0.64
1:B:82:LYS:HE3	1:B:98:ILE:HD11	1.80	0.63
1:A:145:LYS:HE3	3:A:977:HOH:O	1.98	0.63
1:A:104:TYR:H	1:A:107:GLN:NE2	1.96	0.63
1:A:145:LYS:HE3	3:A:978:HOH:O	1.98	0.63
1:B:138:ASN:ND2	1:B:140:ASP:H	1.96	0.63
1:B:82:LYS:HE3	1:B:98:ILE:CD1	2.27	0.63
1:B:191:LYS:HG3	3:B:947:HOH:O	1.99	0.63
1:B:137:THR:O	1:B:139:PRO:HD3	1.98	0.63
1:B:14:GLY:O	1:B:18:GLN:HG2	1.98	0.63
1:A:218:PHE:CD2	1:A:243:LYS:HG3	2.33	0.62
1:B:87:PHE:CG	1:B:95:PRO:HG3	2.33	0.62
1:B:104:TYR:H	1:B:107:GLN:NE2	1.97	0.62
1:A:39:SER:OG	1:A:41:GLN:HB3	1.99	0.62
1:B:144:ASN:OD1	1:B:153:VAL:HG23	1.99	0.62
1:B:81:PRO:HG3	1:B:99:PHE:CE1	2.33	0.62
1:A:168:PRO:HA	1:A:223:ASN:HD21	1.63	0.62
1:B:82:LYS:HE3	1:B:98:ILE:CD1	2.29	0.62
1:B:233:GLU:HG2	3:B:976:HOH:O	1.99	0.62
1:A:79:ALA:CA	1:A:108:VAL:HG21	2.30	0.62
1:A:168:PRO:HA	1:A:223:ASN:HD21	1.65	0.62
1:A:41:GLN:HG3	1:A:45:LYS:HE2	1.81	0.61
1:B:177:LEU:HD23	1:B:205:ARG:NE	2.14	0.61
1:B:195:LEU:CD1	1:B:195:LEU:H	2.12	0.61
1:A:104:TYR:H	1:A:107:GLN:NE2	1.97	0.61
1:A:210:GLU:OE1	1:A:214:GLN:NE2	2.33	0.61
2:A:800:NAP:O3B	2:A:800:NAP:C2B	2.39	0.61
1:A:252:ARG:CZ	1:A:252:ARG:HB2	2.30	0.61
1:A:104:TYR:H	1:A:107:GLN:NE2	1.98	0.61
1:B:104:TYR:HB2	1:B:107:GLN:HE22	1.65	0.61
1:B:31:PHE:HZ	1:B:217:LEU:HD11	1.65	0.61
1:B:104:TYR:HB2	1:B:107:GLN:HE22	1.65	0.61
1:A:252:ARG:HB2	1:A:252:ARG:NH1	2.15	0.61
1:B:15:ARG:HB3	1:B:205:ARG:CD	2.30	0.61
1:A:168:PRO:HA	1:A:223:ASN:ND2	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:THR:HB	3:B:887:HOH:O	2.00	0.61
1:B:25:LYS:HD3	1:B:25:LYS:C	2.21	0.61
1:A:19:ILE:O	1:A:23:LYS:HG3	2.00	0.61
1:B:138:ASN:ND2	1:B:140:ASP:H	1.98	0.61
1:B:240:LYS:HA	1:B:240:LYS:HE2	1.82	0.61
1:B:232:PRO:HG2	1:B:235:THR:HG22	1.83	0.61
1:B:49:GLU:OE2	1:B:49:GLU:N	2.34	0.61
1:B:144:ASN:HB3	1:B:150:ASN:OD1	2.01	0.60
1:B:57:ILE:N	2:B:801:NAP:H62A	1.99	0.60
1:A:213:ILE:O	1:A:216:LEU:HB2	2.02	0.60
1:A:41:GLN:O	1:A:45:LYS:HG3	2.02	0.60
1:B:199:ASP:OD1	1:B:201:LYS:HE3	2.00	0.60
1:B:15:ARG:HB3	1:B:205:ARG:HD3	1.84	0.60
1:A:134:MET:HE2	1:A:193:ASP:HA	1.84	0.60
1:B:237:THR:HG23	3:B:946:HOH:O	2.01	0.60
1:A:84:LYS:HD3	1:A:86:GLY:H	1.65	0.60
1:A:177:LEU:HD22	2:A:800:NAP:C2N	2.31	0.60
1:A:117:ILE:HG12	1:A:162:LEU:HD13	1.83	0.60
1:A:42:GLY:HA2	1:A:45:LYS:HD3	1.82	0.60
1:B:146:LEU:HB3	3:B:970:HOH:O	2.02	0.60
1:B:28:SER:O	3:B:928:HOH:O	2.16	0.60
1:A:104:TYR:HB2	1:A:107:GLN:NE2	2.17	0.60
1:B:82:LYS:HE3	1:B:98:ILE:CD1	2.31	0.60
1:A:151:ILE:HG12	1:A:155:LYS:HE2	1.84	0.60
1:B:177:LEU:HD23	1:B:205:ARG:NE	2.17	0.59
1:A:29:ASP:OD1	1:A:30:LYS:HG2	2.02	0.59
1:A:232:PRO:HG2	1:A:235:THR:HG21	1.83	0.59
1:B:40:ALA:HA	1:B:54:ILE:HD13	1.84	0.59
1:B:104:TYR:H	1:B:107:GLN:NE2	2.01	0.59
1:A:189:VAL:HG13	1:A:226:PHE:HB2	1.83	0.59
1:A:19:ILE:HG22	1:A:23:LYS:HE2	1.84	0.59
1:B:94:ARG:H	1:B:94:ARG:HD3	1.68	0.59
1:B:193:ASP:HB3	1:B:196:LEU:HD12	1.84	0.59
1:A:189:VAL:HG11	1:A:249:VAL:CG2	2.32	0.59
1:A:185:ARG:HD3	1:A:231:LYS:O	2.03	0.59
1:B:77:THR:HG21	1:B:116:GLN:NE2	2.18	0.59
1:B:105:PRO:HD2	3:B:937:HOH:O	2.02	0.59
1:B:81:PRO:HG3	1:B:99:PHE:CZ	2.37	0.59
1:A:185:ARG:C	1:A:238:PRO:HA	2.23	0.59
1:B:77:THR:HG21	1:B:116:GLN:NE2	2.18	0.58
1:A:175:GLY:O	1:A:176:GLY:C	2.41	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:VAL:HG22	1:B:228:LEU:HD23	1.85	0.58
1:A:232:PRO:HG2	1:A:235:THR:HG21	1.84	0.58
1:A:168:PRO:HA	1:A:223:ASN:ND2	2.18	0.58
1:A:104:TYR:H	1:A:107:GLN:NE2	2.01	0.58
1:A:43:LYS:HD2	1:A:54:ILE:HD11	1.84	0.58
1:B:79:ALA:HB2	1:B:105:PRO:HA	1.84	0.58
1:A:180:LYS:HD3	1:A:185:ARG:NH1	2.18	0.58
1:B:18:GLN:HB2	3:B:990:HOH:O	2.02	0.58
1:A:49:GLU:HG3	3:A:938:HOH:O	2.04	0.58
1:B:55:GLY:HA3	1:B:63:ILE:HG22	1.84	0.58
1:B:57:ILE:HD12	1:B:116:GLN:HE21	1.69	0.58
1:A:232:PRO:HG2	1:A:235:THR:CG2	2.33	0.58
1:B:240:LYS:O	3:B:984:HOH:O	2.17	0.58
1:A:15:ARG:N	2:A:800:NAP:O2A	2.37	0.58
1:A:182:GLY:HA3	1:A:206:ALA:HB3	1.85	0.58
1:B:185:ARG:HG3	3:B:921:HOH:O	2.04	0.58
1:A:189:VAL:HG11	1:A:249:VAL:HG22	1.86	0.58
1:B:104:TYR:HB2	1:B:107:GLN:HE22	1.68	0.58
1:B:4:LEU:CD2	1:B:32:VAL:HG23	2.33	0.58
1:B:78:SER:HA	1:B:109:ASP:OD2	2.04	0.58
1:B:155:LYS:O	1:B:159:GLU:HG3	2.03	0.58
1:A:104:TYR:HB2	1:A:107:GLN:OE1	2.04	0.58
1:A:189:VAL:CG2	1:A:245:LEU:HD11	2.34	0.58
1:A:82:LYS:HD3	1:A:100:GLU:OE2	2.04	0.58
1:B:195:LEU:HD12	1:B:195:LEU:H	1.68	0.58
1:A:67:PHE:O	1:A:70:ILE:HG12	2.03	0.58
1:B:73:LEU:HD22	1:B:120:ALA:HB2	1.86	0.58
1:A:41:GLN:OE1	1:A:45:LYS:HG3	2.04	0.58
1:A:114:LYS:HG3	1:A:161:TYR:CE1	2.39	0.58
1:A:37:VAL:HG11	1:A:43:LYS:N	2.19	0.57
1:B:87:PHE:CE2	1:B:89:PRO:HA	2.39	0.57
1:A:5:PRO:HA	1:A:71:ASP:OD1	2.04	0.57
1:B:155:LYS:O	1:B:159:GLU:HG3	2.04	0.57
1:B:138:ASN:HD22	1:B:140:ASP:H	1.51	0.57
1:B:151:ILE:HG23	1:B:152:LEU:HD12	1.85	0.57
1:B:143:LEU:HD12	1:B:152:LEU:HD11	1.86	0.57
1:B:31:PHE:HZ	1:B:217:LEU:HD11	1.68	0.57
1:A:120:ALA:HB1	1:A:125:VAL:HG11	1.86	0.57
1:A:134:MET:CE	1:A:134:MET:CG	2.82	0.57
1:A:79:ALA:CA	1:A:108:VAL:HG21	2.35	0.57
1:B:87:PHE:CE2	1:B:89:PRO:HA	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:ASP:O	1:B:196:LEU:HB2	2.05	0.57
1:A:177:LEU:HG	1:A:205:ARG:HG2	1.87	0.57
1:B:195:LEU:CD1	1:B:195:LEU:N	2.66	0.57
1:B:185:ARG:HA	3:B:983:HOH:O	2.04	0.57
1:B:100:GLU:HG2	3:B:935:HOH:O	2.04	0.57
1:B:195:LEU:N	1:B:195:LEU:CD1	2.66	0.57
1:B:201:LYS:N	1:B:201:LYS:HD3	2.18	0.57
1:B:18:GLN:HB2	3:B:989:HOH:O	2.04	0.57
1:B:185:ARG:HG3	3:B:921:HOH:O	2.04	0.57
1:B:78:SER:HA	1:B:109:ASP:OD2	2.04	0.57
1:A:189:VAL:HG13	1:A:226:PHE:HB2	1.87	0.57
1:B:136:GLY:HA3	3:B:942:HOH:O	2.04	0.57
1:B:152:LEU:CD1	1:B:152:LEU:H	2.16	0.57
1:B:150:ASN:ND2	1:B:153:VAL:HG21	2.19	0.57
1:A:104:TYR:HB2	1:A:107:GLN:HE22	1.69	0.57
1:A:5:PRO:HD2	1:A:30:LYS:O	2.05	0.57
1:B:190:GLY:HA3	1:B:195:LEU:HD11	1.86	0.57
1:B:195:LEU:N	1:B:195:LEU:CD1	2.66	0.56
1:A:107:GLN:O	1:A:111:ILE:HB	2.05	0.56
1:A:224:LYS:HE2	1:A:252:ARG:HH12	1.70	0.56
1:A:189:VAL:HG11	1:A:249:VAL:HG22	1.87	0.56
1:B:114:LYS:HG3	1:B:161:TYR:CE1	2.40	0.56
1:A:184:VAL:O	1:A:233:GLU:HG3	2.04	0.56
1:A:79:ALA:CA	1:A:108:VAL:HG21	2.35	0.56
1:A:177:LEU:HD22	2:A:800:NAP:C2N	2.35	0.56
1:A:15:ARG:N	2:A:800:NAP:O2A	2.38	0.56
1:A:194:GLU:HG3	1:A:195:LEU:HD12	1.88	0.56
1:B:144:ASN:OD1	1:B:153:VAL:HG23	2.05	0.56
1:A:37:VAL:HG12	1:A:39:SER:H	1.70	0.56
1:B:185:ARG:HG3	3:B:921:HOH:O	2.04	0.56
1:A:134:MET:HE3	1:A:195:LEU:HB2	1.86	0.56
1:B:134:MET:HB3	1:B:196:LEU:HD21	1.88	0.56
1:B:195:LEU:CD1	1:B:195:LEU:N	2.68	0.56
1:A:117:ILE:HD13	1:A:162:LEU:HB2	1.87	0.56
1:B:82:LYS:HG3	1:B:98:ILE:HG13	1.87	0.56
1:B:100:GLU:HG3	3:B:935:HOH:O	2.05	0.56
1:B:241:ASP:OD2	1:B:244:ALA:CB	2.53	0.56
1:A:104:TYR:O	1:A:108:VAL:HG22	2.05	0.56
1:A:197:GLN:HA	1:A:197:GLN:HE21	1.71	0.56
1:A:41:GLN:O	1:A:45:LYS:HG3	2.05	0.56
1:A:15:ARG:N	2:A:800:NAP:O2A	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:GLN:OE1	1:A:218:PHE:HE1	1.88	0.56
1:A:83:MET:SD	1:A:95:PRO:HB3	2.46	0.56
1:B:155:LYS:O	1:B:159:GLU:HG3	2.06	0.56
1:B:177:LEU:HD11	1:B:208:VAL:HG21	1.86	0.55
1:B:195:LEU:CD1	1:B:195:LEU:H	2.18	0.55
1:B:22:LYS:HG3	3:B:989:HOH:O	2.05	0.55
1:B:195:LEU:N	1:B:195:LEU:CD1	2.69	0.55
1:B:128:ILE:O	1:B:169:TYR:HA	2.06	0.55
1:A:232:PRO:HG2	1:A:235:THR:HG21	1.89	0.55
1:A:5:PRO:HA	1:A:71:ASP:OD1	2.06	0.55
1:A:137:THR:O	1:A:137:THR:HG22	2.06	0.55
1:B:180:LYS:O	1:B:204:PRO:HB3	2.07	0.55
1:B:185:ARG:HG3	3:B:921:HOH:O	2.06	0.55
1:B:104:TYR:HB2	1:B:107:GLN:HE22	1.71	0.55
1:B:233:GLU:HG2	3:B:976:HOH:O	2.06	0.55
1:A:112:GLY:O	1:A:116:GLN:HG3	2.06	0.55
1:A:22:LYS:O	1:A:26:GLU:HG3	2.07	0.55
1:B:106:GLU:HB2	1:B:154:TRP:CE2	2.42	0.55
1:A:7:VAL:HG22	1:A:72:ALA:HB3	1.88	0.55
1:B:83:MET:O	3:B:883:HOH:O	2.18	0.55
1:B:83:MET:HA	1:B:96:GLU:O	2.06	0.55
1:A:37:VAL:HG12	1:A:39:SER:H	1.71	0.55
1:A:189:VAL:HG11	1:A:249:VAL:CG2	2.36	0.55
1:B:235:THR:OG1	1:B:236:SER:N	2.40	0.55
1:B:57:ILE:HD11	1:B:108:VAL:O	2.07	0.55
1:B:22:LYS:HG3	3:B:989:HOH:O	2.06	0.55
1:B:232:PRO:HG2	1:B:235:THR:CG2	2.37	0.55
1:B:67:PHE:O	1:B:70:ILE:HG12	2.07	0.55
1:A:159:GLU:HB3	1:A:171:ILE:HD13	1.89	0.55
1:B:213:ILE:O	1:B:217:LEU:HD13	2.06	0.55
1:A:132:GLY:O	2:A:800:NAP:H6N	2.06	0.55
1:A:143:LEU:HD23	1:A:143:LEU:O	2.06	0.54
1:A:223:ASN:O	1:A:252:ARG:NE	2.40	0.54
1:A:239:THR:O	1:A:240:LYS:HD3	2.07	0.54
1:A:31:PHE:CE1	1:A:213:ILE:HG23	2.41	0.54
1:A:101:ASP:HA	1:A:104:TYR:HE2	1.72	0.54
1:A:98:ILE:HG13	1:A:99:PHE:N	2.23	0.54
1:B:28:SER:O	3:B:929:HOH:O	2.18	0.54
1:B:67:PHE:O	1:B:70:ILE:HG23	2.07	0.54
1:B:87:PHE:CD2	1:B:89:PRO:HD3	2.42	0.54
1:A:10:THR:HG22	1:A:36:LEU:HD23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ALA:O	1:B:213:ILE:HG12	2.07	0.54
1:B:195:LEU:HD12	1:B:195:LEU:H	1.71	0.54
1:B:240:LYS:HE2	1:B:240:LYS:HA	1.88	0.54
1:B:194:GLU:OE1	3:B:888:HOH:O	2.18	0.54
1:A:34:LYS:HE3	1:A:53:PHE:CE1	2.42	0.54
1:A:97:PHE:O	1:A:147:GLY:HA2	2.06	0.54
1:A:182:GLY:HA3	1:A:206:ALA:HB3	1.90	0.54
1:A:86:GLY:HA3	3:A:874:HOH:O	2.06	0.54
1:B:155:LYS:HE3	2:B:801:NAP:O2D	2.08	0.54
1:A:134:MET:HE3	1:A:195:LEU:HB2	1.90	0.54
1:A:19:ILE:CG2	1:A:23:LYS:HE2	2.38	0.54
1:A:232:PRO:HG2	1:A:235:THR:CG2	2.37	0.54
1:B:195:LEU:CD1	1:B:195:LEU:H	2.20	0.54
1:A:8:LEU:O	1:A:73:LEU:HA	2.08	0.54
1:B:94:ARG:HG2	1:B:94:ARG:HH21	1.72	0.54
1:B:143:LEU:HD12	1:B:152:LEU:HD11	1.90	0.54
1:B:143:LEU:CB	1:B:152:LEU:HD11	2.37	0.54
1:B:191:LYS:HG2	1:B:192:ASP:OD1	2.08	0.54
1:B:81:PRO:HG3	1:B:99:PHE:CZ	2.43	0.54
1:A:197:GLN:CA	1:A:197:GLN:HE21	2.21	0.54
1:A:10:THR:HG22	1:A:36:LEU:HD23	1.89	0.54
1:A:84:LYS:NZ	3:A:874:HOH:O	2.35	0.54
1:B:128:ILE:O	1:B:169:TYR:HA	2.08	0.53
1:A:184:VAL:HG13	1:A:233:GLU:HB2	1.89	0.53
2:A:800:NAP:HO3A	2:A:800:NAP:C3B	2.12	0.53
1:B:94:ARG:HH21	1:B:94:ARG:HG2	1.73	0.53
1:A:57:ILE:HG12	2:A:800:NAP:N1A	2.22	0.53
1:B:138:ASN:ND2	1:B:140:ASP:H	2.06	0.53
1:B:185:ARG:HG3	3:B:922:HOH:O	2.07	0.53
1:B:240:LYS:HA	1:B:240:LYS:HE2	1.89	0.53
1:B:109:ASP:HB3	1:B:155:LYS:HG2	1.89	0.53
1:A:137:THR:CG2	1:A:137:THR:O	2.56	0.53
1:A:169:TYR:HH	1:A:252:ARG:HG3	1.72	0.53
1:B:78:SER:O	2:B:801:NAP:H8A	2.09	0.53
1:B:38:ARG:C	1:B:38:ARG:HD3	2.28	0.53
1:B:82:LYS:O	1:B:83:MET:CB	2.56	0.53
1:B:74:VAL:HG13	1:B:212:CYS:SG	2.48	0.53
1:B:241:ASP:OD2	1:B:244:ALA:HB2	2.09	0.53
1:B:82:LYS:HG3	1:B:98:ILE:HG13	1.90	0.53
1:B:168:PRO:HA	1:B:223:ASN:HD21	1.73	0.53
1:A:252:ARG:CB	1:A:252:ARG:NH1	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:GLN:OE1	1:B:218:PHE:HE1	1.90	0.53
1:B:94:ARG:HG3	3:B:850:HOH:O	2.07	0.53
1:A:57:ILE:HA	1:A:63:ILE:HG21	1.90	0.53
1:A:120:ALA:HB1	1:A:125:VAL:HG11	1.91	0.53
1:B:194:GLU:HA	1:B:197:GLN:NE2	2.23	0.53
1:A:177:LEU:HG	1:A:205:ARG:HG2	1.91	0.53
1:B:127:HIS:HE1	1:B:215:ALA:O	1.91	0.53
1:A:82:LYS:HD3	1:A:100:GLU:OE2	2.08	0.53
1:A:83:MET:SD	1:A:95:PRO:HB3	2.48	0.53
1:B:128:ILE:O	1:B:169:TYR:HA	2.09	0.53
1:B:170:THR:HG22	1:B:172:ILE:HG13	1.91	0.53
1:A:117:ILE:CD1	1:A:162:LEU:HB2	2.39	0.53
1:B:82:LYS:HG3	1:B:98:ILE:HG13	1.91	0.53
1:B:82:LYS:HD3	1:B:100:GLU:CD	2.29	0.53
1:A:20:VAL:HG13	1:A:212:CYS:SG	2.48	0.53
1:B:209:ALA:O	1:B:213:ILE:HG12	2.08	0.52
1:B:189:VAL:HG11	1:B:249:VAL:CG2	2.40	0.52
1:B:87:PHE:CE2	1:B:95:PRO:HG3	2.44	0.52
1:A:198:THR:O	1:A:201:LYS:HE2	2.08	0.52
1:B:182:GLY:HA3	1:B:206:ALA:HB3	1.92	0.52
1:B:73:LEU:HD21	1:B:75:ILE:HD11	1.91	0.52
1:A:41:GLN:O	1:A:45:LYS:HG3	2.09	0.52
1:B:190:GLY:HA3	1:B:195:LEU:HD11	1.91	0.52
1:A:98:ILE:HD11	1:A:104:TYR:OH	2.08	0.52
1:A:18:GLN:HG3	1:A:19:ILE:N	2.25	0.52
1:A:194:GLU:HG3	1:A:195:LEU:HD22	1.90	0.52
1:B:94:ARG:HG2	1:B:94:ARG:HH21	1.73	0.52
1:A:178:LEU:HB3	1:A:180:LYS:HG3	1.92	0.52
1:B:193:ASP:HB3	1:B:196:LEU:HG	1.90	0.52
1:A:232:PRO:HG2	1:A:235:THR:HG21	1.91	0.52
1:A:82:LYS:HD3	1:A:100:GLU:OE2	2.08	0.52
1:B:15:ARG:N	2:B:801:NAP:O2A	2.36	0.52
1:B:196:LEU:N	1:B:196:LEU:HD23	2.24	0.52
1:B:144:ASN:HB3	1:B:150:ASN:OD1	2.10	0.52
1:A:178:LEU:HB3	1:A:180:LYS:HG3	1.92	0.52
1:B:137:THR:O	1:B:139:PRO:HD3	2.08	0.52
1:A:177:LEU:HD22	2:A:800:NAP:C2N	2.40	0.52
1:A:200:THR:HG21	1:A:231:LYS:HG2	1.91	0.52
1:A:84:LYS:CD	1:A:86:GLY:H	2.21	0.52
1:B:138:ASN:C	1:B:138:ASN:HD22	2.13	0.52
1:B:77:THR:HG21	1:B:116:GLN:HE22	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:LYS:HE3	1:B:98:ILE:HD11	1.90	0.52
1:B:151:ILE:HG23	1:B:152:LEU:N	2.23	0.52
1:A:37:VAL:O	1:A:54:ILE:HA	2.10	0.52
1:B:237:THR:HG23	3:B:946:HOH:O	2.10	0.52
1:A:98:ILE:HG13	1:A:99:PHE:N	2.25	0.52
1:A:159:GLU:HB3	1:A:171:ILE:HD13	1.92	0.52
1:B:200:THR:HG22	1:B:231:LYS:HA	1.90	0.52
1:B:239:THR:O	1:B:240:LYS:HE2	2.09	0.52
1:A:112:GLY:O	1:A:116:GLN:HG3	2.09	0.52
1:A:134:MET:HE3	1:A:195:LEU:HB2	1.91	0.52
1:A:109:ASP:CG	1:A:155:LYS:HZ3	2.13	0.52
1:B:100:GLU:HB2	1:B:103:GLN:HB2	1.91	0.52
1:A:84:LYS:HE3	3:A:874:HOH:O	2.10	0.52
1:B:177:LEU:HD22	2:B:801:NAP:C2N	2.40	0.51
1:A:186:GLU:O	1:A:230:SER:HB2	2.10	0.51
1:B:193:ASP:HB3	1:B:196:LEU:HD12	1.91	0.51
1:A:184:VAL:HG12	3:A:808:HOH:O	2.09	0.51
1:B:193:ASP:O	1:B:196:LEU:HB2	2.11	0.51
1:A:177:LEU:HG	1:A:205:ARG:HG2	1.92	0.51
1:B:235:THR:OG1	1:B:236:SER:N	2.44	0.51
1:B:138:ASN:ND2	1:B:140:ASP:HB2	2.24	0.51
1:B:109:ASP:O	1:B:113:GLN:HB2	2.10	0.51
1:B:25:LYS:HD3	1:B:26:GLU:N	2.25	0.51
1:B:94:ARG:HD2	3:B:850:HOH:O	2.09	0.51
1:A:159:GLU:HB3	1:A:171:ILE:HD13	1.92	0.51
1:A:188:LEU:HD12	1:A:200:THR:HB	1.92	0.51
1:A:22:LYS:HZ2	1:A:46:ILE:HB	1.75	0.51
1:B:144:ASN:OD1	1:B:153:VAL:HG23	2.10	0.51
1:B:208:VAL:HG22	1:B:228:LEU:HD23	1.92	0.51
1:A:15:ARG:HB3	1:A:205:ARG:CD	2.41	0.51
1:B:77:THR:HG21	1:B:116:GLN:HE22	1.75	0.51
1:B:38:ARG:O	1:B:38:ARG:HD3	2.11	0.51
1:B:104:TYR:HB3	3:B:937:HOH:O	2.10	0.51
1:B:186:GLU:OE1	1:B:231:LYS:HD2	2.10	0.51
1:B:94:ARG:HH21	1:B:94:ARG:HG2	1.74	0.51
1:B:198:THR:HB	3:B:887:HOH:O	2.11	0.51
1:A:183:GLY:CA	3:A:927:HOH:O	2.58	0.51
1:A:223:ASN:O	1:A:252:ARG:NE	2.43	0.51
1:B:83:MET:O	3:B:882:HOH:O	2.19	0.51
1:B:30:LYS:HD3	1:B:217:LEU:HD11	1.93	0.51
1:A:79:ALA:HB2	1:A:108:VAL:CG2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ARG:HH21	1:B:94:ARG:HG2	1.76	0.51
1:B:239:THR:O	1:B:240:LYS:HE2	2.10	0.51
1:B:76:LEU:HD21	1:B:131:VAL:HG21	1.93	0.51
1:B:57:ILE:HA	1:B:63:ILE:HD13	1.92	0.51
1:B:237:THR:HG23	3:B:946:HOH:O	2.11	0.51
1:A:134:MET:CE	1:A:195:LEU:HB2	2.41	0.51
1:B:136:GLY:HA3	3:B:941:HOH:O	2.10	0.50
1:B:38:ARG:HH11	1:B:38:ARG:HG3	1.76	0.50
1:B:118:ASP:OD2	3:B:886:HOH:O	2.20	0.50
1:B:240:LYS:O	3:B:983:HOH:O	2.20	0.50
1:B:239:THR:HG21	1:B:245:LEU:HD22	1.93	0.50
1:A:198:THR:O	1:A:201:LYS:HD3	2.10	0.50
1:A:232:PRO:HG2	1:A:235:THR:HG21	1.94	0.50
1:B:83:MET:HA	1:B:96:GLU:O	2.11	0.50
1:B:57:ILE:HG13	1:B:112:GLY:HA3	1.93	0.50
1:A:56:ASP:OD2	2:A:800:NAP:N6A	2.42	0.50
1:A:8:LEU:HG	1:A:8:LEU:O	2.11	0.50
1:B:178:LEU:HD11	1:B:202:THR:OG1	2.11	0.50
1:A:178:LEU:HB3	1:A:180:LYS:HG3	1.94	0.50
1:B:138:ASN:ND2	1:B:140:ASP:H	2.09	0.50
1:A:184:VAL:HG12	3:A:808:HOH:O	2.09	0.50
1:B:128:ILE:O	1:B:169:TYR:HA	2.11	0.50
1:A:108:VAL:HG23	1:A:109:ASP:N	2.25	0.50
1:A:177:LEU:HD22	2:A:800:NAP:C2N	2.42	0.50
1:A:134:MET:HE3	1:A:195:LEU:HB2	1.93	0.50
1:A:38:ARG:O	1:A:54:ILE:HG23	2.12	0.50
1:A:21:TYR:CD1	1:A:46:ILE:HB	2.45	0.50
1:A:108:VAL:HG23	1:A:109:ASP:N	2.26	0.50
1:B:185:ARG:O	1:B:238:PRO:HA	2.12	0.50
1:B:190:GLY:HA3	1:B:195:LEU:HD11	1.94	0.50
1:B:182:GLY:HA3	1:B:206:ALA:HB3	1.93	0.50
1:A:206:ALA:O	1:A:209:ALA:HB3	2.11	0.50
1:B:213:ILE:N	1:B:213:ILE:HD13	2.27	0.50
1:B:104:TYR:H	1:B:107:GLN:NE2	2.10	0.50
1:B:57:ILE:H	2:B:801:NAP:C6A	2.24	0.50
1:B:214:GLN:OE1	1:B:218:PHE:HE1	1.95	0.50
1:B:143:LEU:HD12	1:B:152:LEU:HD11	1.91	0.50
1:B:177:LEU:HD13	2:B:801:NAP:C3N	2.42	0.50
1:B:143:LEU:CD1	1:B:152:LEU:HD11	2.42	0.50
1:B:177:LEU:HD13	2:B:801:NAP:C3N	2.42	0.50
1:A:22:LYS:O	1:A:26:GLU:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:VAL:HG13	1:B:226:PHE:CD2	2.47	0.50
1:B:82:LYS:HG3	1:B:98:ILE:HG13	1.94	0.50
1:A:79:ALA:CB	1:A:108:VAL:HG21	2.42	0.50
1:B:170:THR:HG22	1:B:172:ILE:HG13	1.94	0.50
1:A:177:LEU:HD22	2:A:800:NAP:C2N	2.41	0.50
1:B:195:LEU:HD23	1:B:229:GLY:HA3	1.93	0.50
1:A:75:ILE:HB	1:A:130:VAL:HG23	1.93	0.50
1:B:76:LEU:HD21	1:B:131:VAL:CG2	2.42	0.50
1:A:235:THR:HG22	3:A:993:HOH:O	2.12	0.49
1:A:110:TRP:CH2	1:A:114:LYS:HD2	2.47	0.49
1:B:235:THR:OG1	1:B:236:SER:N	2.45	0.49
1:B:138:ASN:ND2	1:B:140:ASP:H	2.10	0.49
1:A:19:ILE:HG21	1:A:206:ALA:HA	1.94	0.49
1:A:5:PRO:HA	1:A:71:ASP:OD1	2.12	0.49
1:A:177:LEU:HB2	2:A:800:NAP:O7N	2.12	0.49
1:B:160:GLN:HA	1:B:253:PHE:CE2	2.46	0.49
1:B:133:SER:O	3:B:941:HOH:O	2.20	0.49
1:A:7:VAL:HG11	1:A:216:LEU:HD21	1.93	0.49
1:B:195:LEU:O	1:B:201:LYS:HB3	2.13	0.49
1:B:94:ARG:HG2	1:B:94:ARG:HH21	1.77	0.49
1:B:57:ILE:HG13	1:B:112:GLY:CA	2.42	0.49
1:A:195:LEU:N	1:A:195:LEU:HD22	2.27	0.49
1:A:79:ALA:HB2	1:A:108:VAL:CG2	2.43	0.49
1:B:13:SER:HA	1:B:46:ILE:HG21	1.93	0.49
1:A:169:TYR:CE2	1:A:223:ASN:HA	2.47	0.49
1:B:104:TYR:HB2	1:B:107:GLN:NE2	2.26	0.49
1:A:220:GLU:HG2	1:A:247:SER:OG	2.12	0.49
1:A:78:SER:HB2	2:A:800:NAP:H3D	1.95	0.49
1:A:7:VAL:HG11	1:A:216:LEU:HD21	1.95	0.49
1:A:98:ILE:HG13	1:A:99:PHE:N	2.27	0.49
1:B:244:ALA:O	1:B:248:GLN:HG3	2.12	0.49
1:A:178:LEU:HB3	1:A:180:LYS:HG3	1.95	0.49
1:A:84:LYS:HD3	1:A:84:LYS:C	2.32	0.49
1:B:79:ALA:HB2	1:B:105:PRO:HA	1.92	0.49
1:A:156:ARG:HA	1:A:159:GLU:OE2	2.12	0.49
1:B:43:LYS:HG2	1:B:48:GLY:HA2	1.95	0.49
1:B:160:GLN:HA	1:B:253:PHE:HE2	1.77	0.49
1:A:37:VAL:HG22	1:A:53:PHE:O	2.11	0.49
1:B:233:GLU:HG2	3:B:976:HOH:O	2.13	0.49
1:A:55:GLY:HA2	1:A:62:SER:HB2	1.95	0.49
1:A:162:LEU:HD11	1:A:169:TYR:CB	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:LEU:HD22	2:A:800:NAP:C2N	2.43	0.49
1:B:138:ASN:ND2	1:B:140:ASP:H	2.11	0.49
1:A:169:TYR:OH	1:A:252:ARG:HG3	2.12	0.49
1:A:178:LEU:HD12	1:A:204:PRO:HD3	1.95	0.49
1:A:21:TYR:OH	1:A:52:VAL:CG2	2.61	0.49
1:B:15:ARG:N	2:B:801:NAP:O2A	2.40	0.49
1:B:129:VAL:HG11	1:B:212:CYS:SG	2.53	0.49
1:B:120:ALA:HB1	1:B:125:VAL:HG11	1.94	0.49
1:A:40:ALA:HA	1:A:54:ILE:HD11	1.95	0.49
1:A:8:LEU:O	1:A:73:LEU:HD12	2.13	0.49
1:A:104:TYR:HB2	1:A:107:GLN:NE2	2.28	0.49
1:A:224:LYS:HE2	1:A:252:ARG:NH1	2.28	0.49
1:A:40:ALA:HB2	3:A:921:HOH:O	2.11	0.49
1:A:117:ILE:HG12	1:A:128:ILE:HD13	1.95	0.49
1:B:138:ASN:ND2	1:B:140:ASP:H	2.10	0.48
1:A:178:LEU:HB3	1:A:180:LYS:HG3	1.95	0.48
1:B:195:LEU:O	1:B:201:LYS:HB3	2.13	0.48
1:B:94:ARG:NH2	1:B:94:ARG:HG2	2.27	0.48
1:A:108:VAL:HG23	1:A:109:ASP:N	2.27	0.48
1:A:214:GLN:HA	1:A:217:LEU:HD12	1.95	0.48
1:B:143:LEU:HB3	1:B:152:LEU:HD11	1.95	0.48
1:B:74:VAL:HA	1:B:129:VAL:O	2.13	0.48
1:A:19:ILE:O	1:A:23:LYS:HG3	2.12	0.48
1:A:43:LYS:HE3	1:A:52:VAL:HB	1.94	0.48
1:B:81:PRO:HG3	1:B:99:PHE:CE1	2.48	0.48
1:B:237:THR:HG23	3:B:947:HOH:O	2.11	0.48
1:B:215:ALA:HA	1:B:221:ALA:CB	2.43	0.48
1:A:184:VAL:HG12	3:A:808:HOH:O	2.12	0.48
1:B:190:GLY:HA3	1:B:195:LEU:HD11	1.96	0.48
1:A:19:ILE:HD13	1:A:206:ALA:HA	1.95	0.48
1:A:134:MET:HE1	1:A:195:LEU:HB2	1.95	0.48
1:B:144:ASN:HA	1:B:150:ASN:HA	1.94	0.48
1:A:239:THR:O	1:A:240:LYS:HD3	2.13	0.48
1:A:189:VAL:HG13	1:A:226:PHE:HB2	1.94	0.48
1:A:53:PHE:N	1:A:53:PHE:CD1	2.82	0.48
1:A:184:VAL:HG23	3:A:982:HOH:O	2.13	0.48
1:A:79:ALA:CA	1:A:108:VAL:HG21	2.44	0.48
1:B:4:LEU:CD2	1:B:32:VAL:HG23	2.43	0.48
1:A:141:HIS:CE1	1:A:143:LEU:HD12	2.49	0.48
1:B:84:LYS:NZ	1:B:84:LYS:HB3	2.28	0.48
1:A:7:VAL:HG11	1:A:216:LEU:HD21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:GLY:HA3	1:A:195:LEU:HD21	1.96	0.48
1:A:184:VAL:HG22	1:A:233:GLU:HG3	1.94	0.48
1:B:28:SER:O	3:B:929:HOH:O	2.19	0.48
1:B:13:SER:HA	1:B:46:ILE:HG21	1.96	0.48
1:A:41:GLN:NE2	1:B:250:THR:HG21	2.29	0.48
1:B:57:ILE:HA	1:B:63:ILE:HG21	1.94	0.48
1:B:87:PHE:CZ	1:B:95:PRO:HG3	2.48	0.48
1:A:155:LYS:HE3	2:A:800:NAP:O2D	2.14	0.48
1:A:223:ASN:ND2	3:A:951:HOH:O	2.47	0.48
1:B:188:LEU:HD12	1:B:200:THR:HB	1.96	0.48
1:B:232:PRO:HG2	1:B:235:THR:CG2	2.44	0.48
1:A:185:ARG:O	1:A:238:PRO:HA	2.13	0.48
1:B:239:THR:HG21	1:B:245:LEU:HD22	1.96	0.48
1:A:108:VAL:HG23	1:A:109:ASP:N	2.29	0.48
1:B:163:ALA:HA	1:B:169:TYR:CE2	2.49	0.48
1:B:94:ARG:NH2	1:B:94:ARG:HG2	2.28	0.48
1:A:223:ASN:O	1:A:252:ARG:NE	2.46	0.48
1:B:236:SER:OG	1:B:237:THR:N	2.47	0.48
1:A:189:VAL:HG11	1:A:249:VAL:CG2	2.43	0.48
1:B:94:ARG:N	1:B:94:ARG:HD3	2.26	0.48
1:A:189:VAL:HG11	1:A:249:VAL:HG22	1.94	0.48
1:A:59:ASP:OD1	1:A:62:SER:HB3	2.13	0.48
1:A:162:LEU:O	1:A:165:SER:HB2	2.14	0.48
1:A:182:GLY:HA3	1:A:206:ALA:HB3	1.96	0.48
1:A:183:GLY:CA	3:A:928:HOH:O	2.61	0.48
1:B:147:GLY:C	1:B:149:GLY:N	2.68	0.48
1:A:18:GLN:O	1:A:22:LYS:HD3	2.14	0.48
1:B:104:TYR:HB2	1:B:107:GLN:NE2	2.27	0.48
1:B:138:ASN:ND2	1:B:140:ASP:HB2	2.19	0.48
1:B:84:LYS:HG3	1:B:96:GLU:HB2	1.96	0.48
1:A:151:ILE:HG23	1:A:152:LEU:N	2.28	0.48
1:A:79:ALA:CB	1:A:108:VAL:HG21	2.44	0.48
1:B:232:PRO:HG2	1:B:235:THR:CG2	2.44	0.47
1:B:94:ARG:NH2	1:B:94:ARG:HG2	2.27	0.47
1:B:78:SER:HA	1:B:109:ASP:OD2	2.14	0.47
1:A:7:VAL:HG11	1:A:216:LEU:HD21	1.96	0.47
1:B:134:MET:SD	1:B:227:ASP:HB3	2.54	0.47
1:A:20:VAL:HG21	1:A:76:LEU:CD1	2.44	0.47
1:A:178:LEU:C	1:A:180:LYS:H	2.17	0.47
1:A:7:VAL:HG11	1:A:216:LEU:HD21	1.96	0.47
1:A:22:LYS:HD2	1:A:22:LYS:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:PRO:HG3	1:B:99:PHE:CZ	2.50	0.47
1:A:197:GLN:HA	1:A:197:GLN:NE2	2.28	0.47
1:B:57:ILE:HD12	1:B:116:GLN:HE21	1.79	0.47
1:B:138:ASN:C	1:B:138:ASN:HD22	2.16	0.47
1:A:84:LYS:HD3	1:A:84:LYS:C	2.34	0.47
1:B:21:TYR:HH	1:B:25:LYS:HE2	1.77	0.47
1:B:159:GLU:OE1	1:B:173:ARG:NE	2.42	0.47
1:B:232:PRO:HG2	1:B:235:THR:HG22	1.95	0.47
1:A:190:GLY:HA3	1:A:195:LEU:CD2	2.44	0.47
1:A:187:LEU:HD21	1:A:207:ASP:CG	2.35	0.47
1:A:74:VAL:HG11	1:A:212:CYS:SG	2.55	0.47
1:A:184:VAL:HG13	1:A:233:GLU:HB2	1.97	0.47
1:B:233:GLU:HG2	3:B:977:HOH:O	2.14	0.47
1:B:9:VAL:HG23	1:B:76:LEU:HD12	1.97	0.47
1:A:224:LYS:HE2	1:A:252:ARG:HH12	1.80	0.47
1:A:31:PHE:CE1	1:A:213:ILE:CG2	2.98	0.47
1:B:88:ASP:OD2	1:B:91:LYS:HB2	2.15	0.47
1:B:235:THR:OG1	1:B:236:SER:N	2.46	0.47
1:B:151:ILE:HG23	1:B:152:LEU:CD1	2.44	0.47
1:A:120:ALA:HB1	1:A:125:VAL:HG11	1.97	0.47
1:B:87:PHE:CD2	1:B:95:PRO:HG3	2.50	0.47
1:A:222:LYS:HE3	3:A:910:HOH:O	2.15	0.47
1:A:30:LYS:HD3	1:A:217:LEU:HD22	1.97	0.47
1:A:98:ILE:HG13	1:A:99:PHE:N	2.30	0.47
1:B:94:ARG:NH2	1:B:94:ARG:HG2	2.30	0.47
1:B:159:GLU:OE1	1:B:173:ARG:NH1	2.44	0.47
1:A:182:GLY:HA3	1:A:206:ALA:HB3	1.97	0.47
1:A:225:ALA:HB3	1:A:253:PHE:HA	1.97	0.47
1:A:113:GLN:HA	1:A:116:GLN:OE1	2.15	0.47
1:A:104:TYR:H	1:A:107:GLN:NE2	2.13	0.47
1:A:19:ILE:O	1:A:23:LYS:HG3	2.15	0.47
1:B:76:LEU:CD2	1:B:131:VAL:HB	2.45	0.47
1:A:22:LYS:NZ	1:A:46:ILE:HB	2.29	0.47
1:A:83:MET:HG3	1:A:97:PHE:CZ	2.50	0.47
1:B:177:LEU:HD23	1:B:205:ARG:NE	2.29	0.47
1:A:219:GLU:HG2	3:A:913:HOH:O	2.15	0.47
1:B:129:VAL:HG22	1:B:170:THR:HB	1.96	0.47
1:B:41:GLN:HB3	3:B:963:HOH:O	2.15	0.47
1:B:76:LEU:HD21	1:B:131:VAL:HG21	1.96	0.47
1:A:112:GLY:O	1:A:116:GLN:HG3	2.14	0.47
1:A:79:ALA:HB2	1:A:108:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:GLU:HB2	1:B:237:THR:O	2.15	0.47
1:B:9:VAL:HG23	1:B:74:VAL:HB	1.97	0.47
1:A:175:GLY:H	2:A:800:NAP:H5N	1.78	0.47
1:A:159:GLU:HB3	1:A:171:ILE:HD13	1.97	0.47
1:B:151:ILE:CG2	1:B:152:LEU:HD12	2.45	0.47
1:B:31:PHE:CZ	1:B:217:LEU:HD11	2.46	0.46
1:A:78:SER:HB2	2:A:800:NAP:H3D	1.97	0.46
1:B:82:LYS:HG3	1:B:98:ILE:HG13	1.98	0.46
2:B:801:NAP:H3B	2:B:801:NAP:O2X	2.15	0.46
1:A:191:LYS:HG3	3:A:925:HOH:O	2.14	0.46
1:A:195:LEU:HA	1:A:198:THR:HG23	1.97	0.46
1:A:98:ILE:HG13	1:A:99:PHE:N	2.29	0.46
2:B:801:NAP:O2X	2:B:801:NAP:H3B	2.15	0.46
1:B:239:THR:O	1:B:240:LYS:CE	2.63	0.46
1:A:184:VAL:HG12	3:A:808:HOH:O	2.16	0.46
1:A:171:ILE:O	1:A:225:ALA:HA	2.15	0.46
1:A:233:GLU:HG2	1:A:234:GLY:N	2.30	0.46
1:B:183:GLY:O	1:B:238:PRO:HB3	2.15	0.46
1:B:8:LEU:HD23	1:B:73:LEU:CD1	2.45	0.46
1:A:237:THR:HA	1:A:238:PRO:HD3	1.71	0.46
1:A:108:VAL:HG23	1:A:109:ASP:N	2.31	0.46
1:B:104:TYR:HB2	1:B:107:GLN:NE2	2.29	0.46
1:A:21:TYR:O	1:A:25:LYS:HG2	2.15	0.46
1:B:235:THR:OG1	1:B:236:SER:N	2.48	0.46
1:B:94:ARG:N	1:B:94:ARG:HD3	2.30	0.46
1:A:41:GLN:NE2	1:B:250:THR:HG21	2.30	0.46
1:A:43:LYS:HD2	1:A:54:ILE:CD1	2.46	0.46
1:A:190:GLY:HA3	1:A:195:LEU:CD1	2.45	0.46
1:B:22:LYS:HE2	3:B:989:HOH:O	2.16	0.46
1:B:239:THR:O	1:B:240:LYS:HE2	2.15	0.46
1:B:82:LYS:O	1:B:98:ILE:N	2.36	0.46
1:B:100:GLU:HB3	1:B:103:GLN:HB2	1.96	0.46
1:B:105:PRO:HB3	1:B:151:ILE:HG13	1.97	0.46
1:A:223:ASN:HB2	1:A:252:ARG:NH2	2.31	0.46
1:B:134:MET:SD	1:B:227:ASP:HB3	2.55	0.46
1:A:132:GLY:O	2:A:800:NAP:H6N	2.15	0.46
1:A:189:VAL:HG11	1:A:249:VAL:CG2	2.39	0.46
1:A:53:PHE:N	1:A:53:PHE:CD1	2.83	0.46
1:B:195:LEU:O	1:B:201:LYS:HB3	2.15	0.46
1:B:78:SER:HA	1:B:109:ASP:OD2	2.16	0.46
1:B:144:ASN:CA	1:B:150:ASN:HA	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:PRO:O	1:B:205:ARG:C	2.54	0.46
1:B:94:ARG:HG2	1:B:94:ARG:NH2	2.31	0.46
1:A:22:LYS:O	1:A:26:GLU:HG3	2.16	0.46
1:A:45:LYS:NZ	1:A:45:LYS:HB3	2.30	0.46
1:B:137:THR:HG23	1:B:193:ASP:OD2	2.15	0.46
1:A:78:SER:HB2	2:A:800:NAP:H3D	1.97	0.46
1:A:175:GLY:O	1:A:177:LEU:CD1	2.63	0.46
1:B:201:LYS:N	1:B:201:LYS:CD	2.78	0.46
1:A:194:GLU:HG3	1:A:195:LEU:HD12	1.97	0.46
1:B:151:ILE:HG23	1:B:152:LEU:HD12	1.98	0.46
1:A:84:LYS:NZ	1:A:85:PRO:HD2	2.31	0.46
1:A:87:PHE:O	1:A:89:PRO:HD3	2.16	0.46
1:B:87:PHE:CD2	1:B:89:PRO:HD3	2.50	0.46
1:A:25:LYS:NZ	1:A:51:ASP:OD2	2.48	0.46
1:A:40:ALA:HA	1:A:54:ILE:HD11	1.98	0.46
1:A:188:LEU:HD12	1:A:230:SER:HA	1.96	0.46
1:A:237:THR:HA	1:A:238:PRO:HD3	1.69	0.46
1:B:104:TYR:HB2	1:B:107:GLN:HE22	1.81	0.46
1:B:87:PHE:CZ	1:B:89:PRO:HA	2.51	0.46
1:A:181:GLU:OE2	1:A:184:VAL:HB	2.16	0.46
1:B:57:ILE:HD12	1:B:116:GLN:HE21	1.80	0.46
1:B:233:GLU:HG3	1:B:233:GLU:O	2.16	0.46
1:B:82:LYS:N	1:B:82:LYS:HD3	2.30	0.46
1:A:40:ALA:N	3:A:921:HOH:O	2.49	0.46
1:A:16:THR:HB	1:A:76:LEU:HD22	1.97	0.46
1:B:207:ASP:O	1:B:211:VAL:HG23	2.16	0.46
1:B:239:THR:O	1:B:240:LYS:CE	2.64	0.45
1:A:91:LYS:HD2	1:A:91:LYS:HA	1.88	0.45
1:B:78:SER:N	2:B:801:NAP:H51A	2.31	0.45
1:A:20:VAL:CG2	1:A:209:ALA:HA	2.46	0.45
1:B:138:ASN:ND2	1:B:140:ASP:H	2.15	0.45
1:A:223:ASN:O	1:A:252:ARG:NE	2.49	0.45
1:B:83:MET:O	3:B:882:HOH:O	2.21	0.45
1:A:134:MET:SD	1:A:175:GLY:HA2	2.56	0.45
1:B:143:LEU:HB2	1:B:152:LEU:HD11	1.97	0.45
1:A:224:LYS:HD2	1:A:249:VAL:HB	1.96	0.45
1:A:43:LYS:HG2	1:A:48:GLY:HA2	1.98	0.45
1:B:180:LYS:HG3	1:B:185:ARG:NH1	2.32	0.45
1:A:41:GLN:NE2	1:B:250:THR:HG21	2.32	0.45
1:B:100:GLU:HB3	1:B:103:GLN:HB2	1.99	0.45
1:B:237:THR:HG23	3:B:946:HOH:O	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:GLU:OE1	1:A:171:ILE:CG2	2.64	0.45
1:B:34:LYS:HD3	1:B:51:ASP:O	2.17	0.45
1:B:63:ILE:HG13	1:B:67:PHE:CE2	2.51	0.45
1:B:99:PHE:CE2	1:B:149:GLY:HA3	2.51	0.45
1:A:6:THR:HG22	1:A:6:THR:O	2.14	0.45
1:A:84:LYS:HE3	3:A:874:HOH:O	2.16	0.45
1:B:143:LEU:HD12	1:B:152:LEU:HD11	1.98	0.45
1:A:189:VAL:HG13	1:A:226:PHE:HB2	1.98	0.45
1:B:239:THR:O	1:B:240:LYS:HE2	2.16	0.45
1:B:84:LYS:HG3	1:B:96:GLU:O	2.17	0.45
1:A:59:ASP:HB3	1:A:62:SER:OG	2.16	0.45
1:B:106:GLU:HG3	1:B:154:TRP:CE2	2.52	0.45
1:B:59:ASP:HB3	1:B:62:SER:OG	2.16	0.45
1:A:75:ILE:HB	1:A:130:VAL:HG23	1.98	0.45
1:A:223:ASN:ND2	3:A:951:HOH:O	2.50	0.45
1:B:193:ASP:O	1:B:196:LEU:HB2	2.17	0.45
1:A:183:GLY:HA2	3:A:927:HOH:O	2.16	0.45
1:B:195:LEU:CD1	1:B:195:LEU:N	2.73	0.45
1:A:107:GLN:HE21	1:A:107:GLN:HB2	1.67	0.45
1:A:75:ILE:HB	1:A:130:VAL:HG23	1.98	0.45
1:B:76:LEU:HD21	1:B:131:VAL:CG2	2.46	0.45
1:B:143:LEU:HB2	1:B:152:LEU:HD22	1.99	0.45
1:A:118:ASP:OD1	1:A:161:TYR:HE1	1.99	0.45
1:A:128:ILE:O	1:A:169:TYR:HA	2.16	0.45
1:B:82:LYS:HE3	1:B:98:ILE:CD1	2.47	0.45
1:A:189:VAL:HG11	1:A:249:VAL:CG2	2.46	0.45
1:B:151:ILE:HG23	1:B:152:LEU:CD1	2.46	0.45
1:B:78:SER:HA	1:B:109:ASP:OD2	2.17	0.45
1:A:190:GLY:HA3	1:A:195:LEU:CD1	2.46	0.45
1:B:185:ARG:HA	3:B:982:HOH:O	2.16	0.45
1:A:159:GLU:HB3	1:A:171:ILE:HD13	1.98	0.45
1:A:223:ASN:ND2	3:A:950:HOH:O	2.50	0.45
1:A:97:PHE:O	1:A:147:GLY:HA2	2.16	0.45
1:B:232:PRO:HB2	3:B:857:HOH:O	2.15	0.45
1:B:206:ALA:O	1:B:209:ALA:HB3	2.16	0.45
1:A:172:ILE:HG12	1:A:226:PHE:CZ	2.51	0.45
1:B:106:GLU:O	1:B:110:TRP:HB3	2.17	0.45
1:B:4:LEU:CD2	1:B:32:VAL:HG23	2.42	0.45
1:A:134:MET:SD	1:A:134:MET:CB	2.96	0.45
1:A:182:GLY:HA2	3:A:808:HOH:O	2.16	0.45
1:B:232:PRO:O	1:B:235:THR:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:TYR:HB3	3:B:937:HOH:O	2.17	0.45
1:B:151:ILE:CG2	1:B:152:LEU:N	2.80	0.45
1:B:189:VAL:HG13	1:B:226:PHE:HB2	1.99	0.45
1:A:180:LYS:O	1:A:204:PRO:HB3	2.17	0.45
1:B:160:GLN:HE21	1:B:164:ASP:CG	2.19	0.45
1:B:57:ILE:N	2:B:801:NAP:N6A	2.63	0.45
1:A:75:ILE:HG23	1:A:116:GLN:HE22	1.82	0.45
1:A:146:LEU:HD13	1:A:146:LEU:C	2.37	0.45
1:A:1:SER:C	1:A:3:ASN:H	2.20	0.45
1:A:235:THR:O	1:A:236:SER:HB2	2.16	0.45
1:B:159:GLU:CD	1:B:173:ARG:HE	2.20	0.45
1:A:215:ALA:HA	1:A:221:ALA:CB	2.47	0.45
1:B:159:GLU:CD	1:B:173:ARG:HE	2.20	0.45
1:B:219:GLU:OE2	1:B:219:GLU:O	2.35	0.45
1:A:109:ASP:CG	1:A:155:LYS:NZ	2.70	0.45
1:A:189:VAL:HG13	1:A:226:PHE:CD2	2.52	0.44
1:A:222:LYS:HE3	3:A:953:HOH:O	2.17	0.44
1:B:79:ALA:HB2	1:B:108:VAL:HB	1.98	0.44
1:A:82:LYS:O	1:A:97:PHE:HA	2.16	0.44
1:A:237:THR:HA	1:A:238:PRO:HD3	1.71	0.44
1:A:59:ASP:CG	1:A:62:SER:HB3	2.37	0.44
1:B:105:PRO:HD2	3:B:937:HOH:O	2.17	0.44
1:B:192:ASP:N	1:B:192:ASP:OD2	2.48	0.44
1:B:175:GLY:HA3	1:B:201:LYS:O	2.17	0.44
1:B:41:GLN:HG2	3:B:963:HOH:O	2.17	0.44
1:A:184:VAL:O	1:A:238:PRO:HG3	2.17	0.44
1:B:13:SER:HA	1:B:46:ILE:HG21	1.99	0.44
2:B:801:NAP:O3B	3:B:955:HOH:O	2.21	0.44
1:A:57:ILE:HG12	2:A:800:NAP:C6A	2.48	0.44
1:B:145:LYS:O	1:B:147:GLY:N	2.50	0.44
1:B:106:GLU:HB2	1:B:154:TRP:CE2	2.53	0.44
1:A:7:VAL:HA	1:A:72:ALA:HB3	1.98	0.44
1:A:181:GLU:HG2	1:A:182:GLY:N	2.32	0.44
1:B:163:ALA:HA	1:B:169:TYR:CE2	2.53	0.44
1:B:22:LYS:CE	3:B:989:HOH:O	2.64	0.44
1:B:22:LYS:HG3	3:B:989:HOH:O	2.17	0.44
1:A:43:LYS:HG2	1:A:48:GLY:HA2	1.98	0.44
1:A:1:SER:HB2	1:A:3:ASN:CB	2.47	0.44
1:B:214:GLN:HG3	1:B:242:PHE:CD2	2.52	0.44
1:A:110:TRP:CD2	1:A:157:LYS:HD3	2.53	0.44
1:A:43:LYS:HG2	1:A:48:GLY:HA2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:LEU:HD13	2:B:801:NAP:C3N	2.47	0.44
1:B:138:ASN:C	1:B:138:ASN:ND2	2.71	0.44
1:B:236:SER:OG	1:B:237:THR:N	2.50	0.44
1:A:175:GLY:H	2:A:800:NAP:C5N	2.31	0.44
1:B:37:VAL:O	1:B:54:ILE:HA	2.18	0.44
1:B:82:LYS:HB2	1:B:83:MET:H	1.67	0.44
1:A:104:TYR:HB2	1:A:107:GLN:NE2	2.33	0.44
1:A:112:GLY:O	1:A:116:GLN:HG3	2.18	0.44
1:A:18:GLN:O	1:A:22:LYS:HD3	2.17	0.44
1:A:98:ILE:HG13	1:A:99:PHE:N	2.32	0.44
1:A:91:LYS:HD2	1:A:91:LYS:HA	1.94	0.44
1:B:177:LEU:HB3	1:B:205:ARG:NH1	2.33	0.44
1:A:127:HIS:HA	1:A:168:PRO:O	2.18	0.44
1:A:219:GLU:OE1	3:A:910:HOH:O	2.20	0.44
1:B:241:ASP:OD2	1:B:244:ALA:HB3	2.18	0.44
1:A:110:TRP:CH2	1:A:114:LYS:HD2	2.53	0.44
1:B:138:ASN:C	1:B:138:ASN:ND2	2.71	0.44
1:A:75:ILE:HB	1:A:130:VAL:HG23	1.99	0.44
1:A:7:VAL:HG11	1:A:216:LEU:HD21	2.00	0.44
1:B:134:MET:SD	1:B:227:ASP:HB3	2.58	0.44
1:A:225:ALA:CB	1:A:253:PHE:HA	2.48	0.44
1:A:57:ILE:HA	1:A:63:ILE:HD13	2.00	0.44
1:B:84:LYS:HG3	1:B:96:GLU:CB	2.48	0.44
1:A:184:VAL:HG11	1:A:233:GLU:OE1	2.18	0.44
1:B:41:GLN:HB2	1:B:41:GLN:HE21	1.50	0.44
1:A:134:MET:CE	1:A:195:LEU:HB2	2.47	0.43
1:A:189:VAL:HG13	1:A:226:PHE:HB2	2.00	0.43
1:B:138:ASN:C	1:B:138:ASN:ND2	2.70	0.43
1:B:168:PRO:HA	1:B:223:ASN:HD21	1.82	0.43
1:A:43:LYS:HE2	1:A:48:GLY:O	2.18	0.43
1:B:84:LYS:CD	1:B:96:GLU:HB2	2.48	0.43
1:A:100:GLU:HB2	1:A:103:GLN:HB2	2.01	0.43
1:A:161:TYR:O	1:A:165:SER:HB3	2.17	0.43
1:B:239:THR:O	1:B:240:LYS:HE2	2.18	0.43
1:A:237:THR:HA	1:A:238:PRO:HD3	1.79	0.43
1:A:132:GLY:O	2:A:800:NAP:H6N	2.18	0.43
1:A:84:LYS:HB3	1:A:96:GLU:HB2	2.00	0.43
1:A:184:VAL:HG12	3:A:808:HOH:O	2.18	0.43
1:A:134:MET:CE	1:A:195:LEU:HB2	2.48	0.43
1:A:7:VAL:HG11	1:A:216:LEU:HD21	2.00	0.43
1:A:189:VAL:HG11	1:A:249:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ASN:HB3	1:A:65:PRO:HD3	1.99	0.43
1:B:19:ILE:CG2	1:B:23:LYS:HE3	2.48	0.43
1:A:185:ARG:C	1:A:238:PRO:HA	2.39	0.43
1:B:28:SER:O	3:B:928:HOH:O	2.21	0.43
1:A:177:LEU:HD22	2:A:800:NAP:C3N	2.47	0.43
1:A:72:ALA:HA	1:A:125:VAL:CG2	2.49	0.43
1:B:184:VAL:HG22	3:B:921:HOH:O	2.18	0.43
1:A:75:ILE:HB	1:A:130:VAL:HG23	2.00	0.43
1:B:109:ASP:O	1:B:158:ALA:HB2	2.19	0.43
1:A:37:VAL:CG1	1:A:38:ARG:N	2.82	0.43
1:B:94:ARG:HG3	3:B:850:HOH:O	2.18	0.43
1:A:235:THR:HG22	3:A:994:HOH:O	2.18	0.43
1:B:176:GLY:HA2	2:B:801:NAP:H4N	2.00	0.43
1:A:235:THR:HG22	3:A:994:HOH:O	2.18	0.43
1:A:79:ALA:HB2	1:A:108:VAL:HG23	2.00	0.43
1:B:127:HIS:HA	1:B:168:PRO:O	2.18	0.43
1:A:180:LYS:HG3	1:A:185:ARG:NH1	2.34	0.43
1:B:38:ARG:HA	1:B:55:GLY:O	2.17	0.43
1:B:177:LEU:HD13	2:B:801:NAP:C3N	2.49	0.43
1:B:244:ALA:O	1:B:248:GLN:HG3	2.19	0.43
1:A:53:PHE:N	1:A:53:PHE:CD1	2.87	0.43
1:B:101:ASP:OD2	1:B:102:GLY:N	2.51	0.43
1:B:151:ILE:HG23	1:B:152:LEU:CD1	2.48	0.43
1:B:177:LEU:HD23	1:B:205:ARG:NE	2.33	0.43
1:A:214:GLN:OE1	1:A:218:PHE:HE1	2.02	0.43
1:A:67:PHE:O	1:A:70:ILE:HG12	2.19	0.43
1:A:186:GLU:OE2	1:A:231:LYS:HD2	2.19	0.43
1:A:17:GLY:HA2	1:A:76:LEU:HD13	2.00	0.43
1:B:197:GLN:N	1:B:197:GLN:OE1	2.51	0.43
1:A:219:GLU:HG2	3:A:892:HOH:O	2.19	0.43
1:A:75:ILE:HB	1:A:130:VAL:HG23	2.00	0.43
1:B:57:ILE:HG21	1:B:77:THR:HG21	2.01	0.43
1:B:21:TYR:CZ	1:B:25:LYS:HD2	2.54	0.43
1:B:196:LEU:HB2	1:B:197:GLN:OE1	2.19	0.43
1:A:84:LYS:HD3	1:A:85:PRO:CD	2.49	0.43
1:A:91:LYS:HA	1:A:91:LYS:HD2	1.85	0.43
1:B:81:PRO:HG3	1:B:99:PHE:CE1	2.54	0.43
1:A:5:PRO:HD2	1:A:30:LYS:O	2.19	0.43
1:A:47:GLY:O	1:A:48:GLY:C	2.56	0.43
1:A:90:THR:O	1:A:90:THR:HG22	2.18	0.43
1:B:232:PRO:HG2	1:B:235:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:VAL:HG23	3:A:982:HOH:O	2.19	0.43
1:B:104:TYR:HB2	1:B:107:GLN:HE22	1.84	0.43
1:B:16:THR:HB	1:B:76:LEU:HD22	2.01	0.43
1:A:39:SER:OG	1:A:41:GLN:HB3	2.19	0.43
1:B:232:PRO:HG2	1:B:235:THR:CG2	2.46	0.43
1:A:64:ASN:O	1:A:68:GLN:HG2	2.18	0.42
1:B:168:PRO:HA	1:B:223:ASN:ND2	2.34	0.42
1:A:64:ASN:HB3	1:A:65:PRO:HD3	2.00	0.42
1:B:15:ARG:HB3	1:B:205:ARG:NE	2.33	0.42
1:B:87:PHE:CD2	1:B:89:PRO:HD3	2.53	0.42
1:A:196:LEU:O	1:A:201:LYS:NZ	2.49	0.42
1:A:84:LYS:HB3	1:A:96:GLU:HB3	2.01	0.42
1:B:14:GLY:O	1:B:18:GLN:HG2	2.19	0.42
1:B:141:HIS:ND1	1:B:142:PRO:HD2	2.34	0.42
1:B:213:ILE:O	1:B:216:LEU:HB2	2.19	0.42
1:B:83:MET:O	1:B:84:LYS:C	2.56	0.42
1:A:8:LEU:HD11	1:A:36:LEU:HB2	2.01	0.42
1:A:43:LYS:HG2	1:A:48:GLY:HA2	2.00	0.42
1:A:188:LEU:HD12	1:A:200:THR:HB	2.01	0.42
1:A:44:GLU:O	1:A:45:LYS:C	2.55	0.42
1:A:29:ASP:OD1	1:A:30:LYS:HG3	2.18	0.42
1:B:239:THR:HG21	1:B:245:LEU:HD22	2.01	0.42
1:A:207:ASP:O	1:A:208:VAL:C	2.57	0.42
1:A:236:SER:OG	1:A:237:THR:N	2.48	0.42
1:A:189:VAL:CG1	1:A:249:VAL:HG22	2.45	0.42
1:A:64:ASN:HB3	1:A:65:PRO:HD3	2.00	0.42
1:A:185:ARG:C	1:A:238:PRO:HA	2.39	0.42
1:B:138:ASN:C	1:B:138:ASN:HD22	2.22	0.42
1:A:84:LYS:HD3	1:A:85:PRO:N	2.33	0.42
1:A:91:LYS:HD2	1:A:91:LYS:HA	1.86	0.42
1:A:237:THR:HA	1:A:238:PRO:HD3	1.75	0.42
1:A:41:GLN:CD	1:A:45:LYS:HE2	2.39	0.42
1:A:45:LYS:NZ	1:A:45:LYS:CB	2.82	0.42
1:B:141:HIS:HA	1:B:142:PRO:HD3	1.92	0.42
1:B:232:PRO:HG2	1:B:235:THR:CG2	2.48	0.42
1:B:6:THR:HA	1:B:32:VAL:O	2.20	0.42
1:B:77:THR:CG2	1:B:116:GLN:HE22	2.32	0.42
1:A:47:GLY:O	1:A:49:GLU:N	2.53	0.42
1:B:180:LYS:HG3	1:B:185:ARG:HH12	1.85	0.42
1:A:194:GLU:HG2	1:A:195:LEU:HD22	2.01	0.42
1:A:185:ARG:HB3	1:A:231:LYS:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:LYS:CD	1:A:165:SER:OG	2.68	0.42
1:A:183:GLY:HA2	3:A:928:HOH:O	2.18	0.42
1:A:236:SER:OG	1:A:237:THR:N	2.52	0.42
1:B:15:ARG:HA	1:B:18:GLN:HE21	1.85	0.42
1:B:210:GLU:HA	1:B:210:GLU:OE1	2.20	0.42
1:A:237:THR:HA	1:A:238:PRO:HD3	1.71	0.42
1:B:19:ILE:HG21	1:B:206:ALA:HA	2.01	0.42
1:B:59:ASP:HB3	1:B:62:SER:OG	2.19	0.42
1:A:181:GLU:OE2	1:A:184:VAL:HB	2.19	0.42
1:A:10:THR:HG21	1:A:116:GLN:NE2	2.35	0.42
1:A:86:GLY:HA3	3:A:874:HOH:O	2.19	0.42
1:B:87:PHE:HE2	1:B:89:PRO:HA	1.82	0.42
1:B:160:GLN:HE21	1:B:164:ASP:CG	2.23	0.42
1:B:180:LYS:HD2	1:B:233:GLU:OE2	2.18	0.42
1:A:235:THR:HG23	3:A:994:HOH:O	2.20	0.42
1:B:118:ASP:O	1:B:122:VAL:HG23	2.19	0.42
1:B:55:GLY:CA	1:B:63:ILE:HG22	2.48	0.42
1:A:194:GLU:CG	1:A:195:LEU:HD12	2.50	0.42
1:A:10:THR:HG22	1:A:36:LEU:HD23	2.01	0.42
1:B:147:GLY:C	1:B:149:GLY:N	2.73	0.42
1:B:155:LYS:HE3	2:B:801:NAP:O2D	2.20	0.42
1:A:134:MET:HE1	1:A:195:LEU:HB2	2.00	0.42
1:A:53:PHE:N	1:A:53:PHE:CD1	2.87	0.42
1:B:76:LEU:HD23	1:B:131:VAL:HB	2.02	0.42
1:A:81:PRO:HG3	1:A:146:LEU:HD21	2.02	0.42
1:B:38:ARG:HA	1:B:55:GLY:O	2.20	0.42
1:A:53:PHE:N	1:A:53:PHE:CD1	2.87	0.42
1:A:120:ALA:HB1	1:A:125:VAL:CG1	2.49	0.42
1:B:75:ILE:HG21	1:B:113:GLN:HG2	2.02	0.42
1:A:189:VAL:HG11	1:A:249:VAL:CG2	2.49	0.42
1:B:177:LEU:HD23	1:B:205:ARG:HE	1.85	0.42
1:B:25:LYS:HE2	1:B:51:ASP:OD2	2.20	0.42
1:B:57:ILE:HD11	1:B:108:VAL:HG13	2.02	0.42
1:A:237:THR:HA	1:A:238:PRO:HD3	1.71	0.42
1:B:177:LEU:HB3	1:B:205:ARG:NH1	2.33	0.42
2:B:801:NAP:O3B	3:B:954:HOH:O	2.21	0.42
1:A:155:LYS:O	1:A:159:GLU:HG3	2.20	0.42
1:B:97:PHE:O	1:B:147:GLY:HA2	2.20	0.42
1:B:81:PRO:HG3	1:B:99:PHE:CZ	2.54	0.42
1:A:138:ASN:HA	1:A:139:PRO:HD2	1.95	0.42
1:A:88:ASP:OD1	1:A:89:PRO:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:LYS:HD2	1:A:86:GLY:H	1.85	0.42
1:B:118:ASP:O	1:B:122:VAL:HG23	2.20	0.42
1:A:100:GLU:O	1:A:101:ASP:C	2.58	0.42
1:A:112:GLY:O	1:A:116:GLN:HG3	2.20	0.42
1:B:214:GLN:HG3	1:B:242:PHE:CG	2.54	0.42
1:A:71:ASP:C	1:A:125:VAL:HG23	2.41	0.41
1:B:60:ALA:HB1	3:B:806:HOH:O	2.20	0.41
1:A:104:TYR:H	1:A:107:GLN:HE21	1.67	0.41
1:B:77:THR:CG2	1:B:116:GLN:HE22	2.33	0.41
1:B:73:LEU:HD22	1:B:120:ALA:CB	2.50	0.41
1:B:106:GLU:HB2	1:B:154:TRP:CE2	2.55	0.41
1:A:183:GLY:CA	3:A:928:HOH:O	2.67	0.41
1:A:156:ARG:NH2	3:A:825:HOH:O	2.53	0.41
1:A:118:ASP:OD1	1:A:161:TYR:CE1	2.73	0.41
1:B:83:MET:O	1:B:84:LYS:C	2.59	0.41
1:A:84:LYS:HD3	1:A:85:PRO:HD2	2.01	0.41
1:B:89:PRO:C	1:B:91:LYS:H	2.24	0.41
1:B:141:HIS:CE1	1:B:143:LEU:HG	2.55	0.41
1:B:41:GLN:HB3	3:B:963:HOH:O	2.19	0.41
1:A:173:ARG:O	1:A:227:ASP:HA	2.20	0.41
1:A:41:GLN:O	1:A:45:LYS:HG3	2.20	0.41
1:B:191:LYS:HG3	3:B:947:HOH:O	2.19	0.41
1:A:108:VAL:HG23	1:A:109:ASP:N	2.35	0.41
1:A:199:ASP:C	1:A:200:THR:HG23	2.41	0.41
1:A:188:LEU:HD12	1:A:200:THR:HB	2.01	0.41
1:B:87:PHE:CE2	1:B:89:PRO:HB3	2.56	0.41
1:B:204:PRO:O	1:B:205:ARG:C	2.59	0.41
1:A:189:VAL:HG13	1:A:226:PHE:CD2	2.56	0.41
1:B:218:PHE:HD2	1:B:243:LYS:HG3	1.85	0.41
1:A:60:ALA:CB	1:A:115:ASN:ND2	2.79	0.41
1:A:83:MET:HE2	1:A:97:PHE:CE1	2.55	0.41
1:A:120:ALA:O	1:A:125:VAL:HG12	2.20	0.41
1:A:104:TYR:O	1:A:108:VAL:HG22	2.20	0.41
1:A:151:ILE:HG23	1:A:152:LEU:H	1.85	0.41
1:B:53:PHE:N	1:B:53:PHE:CD1	2.87	0.41
1:A:151:ILE:CG1	1:A:155:LYS:HE2	2.49	0.41
1:B:91:LYS:O	1:B:91:LYS:HG2	2.20	0.41
1:A:20:VAL:CG2	1:A:209:ALA:HA	2.50	0.41
1:A:110:TRP:CD2	1:A:157:LYS:HD3	2.55	0.41
1:A:43:LYS:O	1:A:48:GLY:N	2.52	0.41
1:B:83:MET:O	3:B:882:HOH:O	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ASN:ND2	3:A:951:HOH:O	2.53	0.41
1:A:37:VAL:HG22	1:A:38:ARG:H	1.85	0.41
1:B:144:ASN:HB3	1:B:150:ASN:OD1	2.21	0.41
1:B:172:ILE:HG12	1:B:226:PHE:CZ	2.55	0.41
1:A:81:PRO:CG	1:A:146:LEU:HD21	2.50	0.41
1:B:105:PRO:HB2	1:B:154:TRP:CD1	2.55	0.41
1:B:41:GLN:HB3	3:B:963:HOH:O	2.21	0.41
2:B:801:NAP:O2X	2:B:801:NAP:H3B	2.21	0.41
1:B:7:VAL:HG11	1:B:216:LEU:HD11	2.02	0.41
1:B:133:SER:HB2	2:B:801:NAP:C6N	2.51	0.41
1:A:53:PHE:N	1:A:53:PHE:CD1	2.88	0.41
1:A:1:SER:C	1:A:3:ASN:H	2.20	0.41
1:B:104:TYR:HB2	1:B:107:GLN:NE2	2.34	0.41
1:A:141:HIS:CE1	1:A:143:LEU:HD12	2.55	0.41
1:A:169:TYR:CZ	1:A:223:ASN:HA	2.55	0.41
1:A:45:LYS:HA	1:A:45:LYS:HD3	1.90	0.41
1:A:185:ARG:HD2	1:A:204:PRO:HG2	2.03	0.41
1:A:186:GLU:OE2	1:A:236:SER:HB3	2.20	0.41
1:A:182:GLY:HA2	3:A:808:HOH:O	2.20	0.41
1:A:104:TYR:O	1:A:108:VAL:HG22	2.20	0.41
1:A:177:LEU:HD11	1:A:208:VAL:HG21	2.02	0.41
1:A:128:ILE:HB	1:A:162:LEU:HD11	2.02	0.41
1:A:225:ALA:CB	1:A:253:PHE:HA	2.51	0.41
1:A:87:PHE:HE1	1:A:89:PRO:HB3	1.85	0.41
1:A:98:ILE:HG13	1:A:99:PHE:H	1.84	0.41
1:A:114:LYS:HG3	1:A:161:TYR:CZ	2.56	0.41
1:A:98:ILE:CG1	1:A:99:PHE:N	2.83	0.41
1:B:188:LEU:HD21	1:B:231:LYS:HE3	2.03	0.41
1:A:63:ILE:O	1:A:67:PHE:HD2	2.03	0.41
1:A:43:LYS:CG	1:A:48:GLY:HA2	2.45	0.41
1:B:127:HIS:HE1	1:B:215:ALA:O	2.03	0.41
1:B:210:GLU:O	1:B:214:GLN:HG2	2.20	0.41
1:A:13:SER:HB3	1:A:37:VAL:HG21	2.03	0.41
1:B:107:GLN:O	1:B:112:GLY:N	2.51	0.41
1:A:104:TYR:HB2	1:A:107:GLN:NE2	2.35	0.41
1:A:82:LYS:HD3	1:A:100:GLU:OE2	2.21	0.41
1:B:76:LEU:HD23	1:B:76:LEU:HA	1.82	0.41
1:A:107:GLN:HE21	1:A:107:GLN:HB2	1.66	0.41
1:A:7:VAL:HA	1:A:72:ALA:O	2.21	0.41
1:A:40:ALA:HA	1:A:54:ILE:HD11	2.02	0.41
1:A:117:ILE:HG12	1:A:162:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:MET:HG3	1:A:175:GLY:HA2	2.02	0.41
1:B:57:ILE:HD11	1:B:108:VAL:HG13	2.02	0.41
1:B:104:TYR:H	1:B:107:GLN:NE2	2.19	0.41
1:A:168:PRO:HA	1:A:223:ASN:HD21	1.85	0.41
1:B:199:ASP:HA	1:B:201:LYS:HD2	2.03	0.41
1:B:118:ASP:O	1:B:122:VAL:HG23	2.20	0.41
1:A:222:LYS:HE3	3:A:954:HOH:O	2.21	0.41
1:B:225:ALA:O	1:B:251:SER:HB2	2.21	0.41
1:A:104:TYR:O	1:A:108:VAL:HG22	2.20	0.41
1:B:192:ASP:OD2	1:B:192:ASP:N	2.51	0.41
1:B:82:LYS:HE3	1:B:98:ILE:HD11	2.03	0.41
1:A:110:TRP:CZ2	1:A:157:LYS:HE3	2.56	0.41
1:A:37:VAL:O	1:A:54:ILE:HA	2.22	0.40
1:B:104:TYR:H	1:B:107:GLN:HE21	1.69	0.40
1:B:143:LEU:CD1	1:B:152:LEU:HD11	2.51	0.40
1:B:231:LYS:HB3	1:B:235:THR:CG2	2.52	0.40
1:B:168:PRO:HA	1:B:223:ASN:ND2	2.36	0.40
1:A:211:VAL:HG21	1:A:228:LEU:HD21	2.03	0.40
1:B:210:GLU:OE1	1:B:210:GLU:HA	2.21	0.40
1:A:232:PRO:HG2	1:A:235:THR:CG2	2.51	0.40
1:A:40:ALA:HA	1:A:54:ILE:HD13	2.02	0.40
1:A:173:ARG:NH1	3:A:811:HOH:O	2.51	0.40
1:B:187:LEU:HD21	1:B:207:ASP:CG	2.42	0.40
1:B:34:LYS:HB2	1:B:34:LYS:HE3	1.83	0.40
1:A:5:PRO:HD2	1:A:30:LYS:O	2.21	0.40
1:B:109:ASP:HA	3:B:934:HOH:O	2.21	0.40
1:B:118:ASP:HA	3:B:877:HOH:O	2.21	0.40
1:B:231:LYS:HB3	1:B:235:THR:CG2	2.51	0.40
1:B:10:THR:OG1	1:B:75:ILE:HA	2.21	0.40
1:A:187:LEU:HD21	1:A:207:ASP:CG	2.41	0.40
1:B:193:ASP:O	1:B:196:LEU:HB2	2.22	0.40
1:B:206:ALA:O	1:B:209:ALA:N	2.54	0.40
1:B:83:MET:HG3	1:B:97:PHE:CZ	2.56	0.40
1:A:237:THR:HA	1:A:238:PRO:HD3	1.73	0.40
1:A:81:PRO:CB	1:A:146:LEU:HD21	2.51	0.40
1:A:224:LYS:HE2	1:A:252:ARG:HH12	1.87	0.40
1:B:82:LYS:N	1:B:98:ILE:O	2.43	0.40
1:A:177:LEU:HD22	2:A:800:NAP:C3N	2.50	0.40
1:A:6:THR:HA	1:A:32:VAL:HB	2.03	0.40
1:A:223:ASN:ND2	3:A:951:HOH:O	2.55	0.40
1:B:193:ASP:HB3	1:B:196:LEU:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ASN:HA	1:A:139:PRO:HD2	1.96	0.40
1:A:53:PHE:CD1	1:A:53:PHE:N	2.89	0.40
1:A:134:MET:HE1	1:A:195:LEU:HB2	2.00	0.40
1:B:160:GLN:HE21	1:B:164:ASP:CG	2.24	0.40
1:B:219:GLU:HB2	3:B:835:HOH:O	2.21	0.40
1:B:104:TYR:HB2	1:B:107:GLN:NE2	2.34	0.40
1:B:232:PRO:HG2	1:B:235:THR:HG22	2.03	0.40
1:A:138:ASN:HA	1:A:139:PRO:HD2	1.96	0.40
1:A:64:ASN:HB3	1:A:65:PRO:HD3	2.03	0.40
1:B:22:LYS:CE	3:B:843:HOH:O	2.61	0.40
1:B:160:GLN:HA	1:B:253:PHE:CE2	2.56	0.40
1:B:1:SER:H3	1:B:4:LEU:C	2.25	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	251/253 (99%)	238 (95%)	11 (4%)	2 (1%)	19	7
1	1-B	251/253 (99%)	234 (93%)	15 (6%)	2 (1%)	19	7
1	2-A	251/253 (99%)	237 (94%)	11 (4%)	3 (1%)	13	3
1	2-B	251/253 (99%)	228 (91%)	20 (8%)	3 (1%)	13	3
1	3-A	251/253 (99%)	232 (92%)	16 (6%)	3 (1%)	13	3
1	3-B	251/253 (99%)	233 (93%)	17 (7%)	1 (0%)	34	21
1	4-A	251/253 (99%)	241 (96%)	7 (3%)	3 (1%)	13	3
1	4-B	251/253 (99%)	235 (94%)	14 (6%)	2 (1%)	19	7
1	5-A	251/253 (99%)	236 (94%)	13 (5%)	2 (1%)	19	7
1	5-B	251/253 (99%)	233 (93%)	15 (6%)	3 (1%)	13	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	6-A	251/253 (99%)	236 (94%)	11 (4%)	4 (2%)	9	2
1	6-B	251/253 (99%)	233 (93%)	15 (6%)	3 (1%)	13	3
1	7-A	251/253 (99%)	237 (94%)	12 (5%)	2 (1%)	19	7
1	7-B	251/253 (99%)	233 (93%)	17 (7%)	1 (0%)	34	21
1	8-A	251/253 (99%)	240 (96%)	10 (4%)	1 (0%)	34	21
1	8-B	251/253 (99%)	236 (94%)	11 (4%)	4 (2%)	9	2
All	All	4016/4048 (99%)	3762 (94%)	215 (5%)	39 (1%)	15	5

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2-A	92	GLY
1	2-A	174	ALA
1	2-B	83	MET
1	3-A	48	GLY
1	4-A	92	GLY
1	5-A	92	GLY
1	8-A	92	GLY
1	1-A	92	GLY
1	1-B	236	SER
1	3-A	92	GLY
1	4-A	41	GLN
1	5-B	86	GLY
1	6-A	95	PRO
1	7-A	92	GLY
1	8-B	92	GLY
1	2-B	234	GLY
1	5-B	25	LYS
1	5-B	236	SER
1	6-A	39	SER
1	6-A	42	GLY
1	1-A	90	THR
1	4-B	236	SER
1	7-A	48	GLY
1	2-A	176	GLY
1	4-A	48	GLY
1	6-B	25	LYS
1	1-B	25	LYS
1	8-B	192	ASP
1	3-B	85	PRO

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Mol	Chain	Res	Type
1	6-B	85	PRO
1	8-B	234	GLY
1	2-B	85	PRO
1	5-A	48	GLY
1	4-B	234	GLY
1	6-A	48	GLY
1	7-B	92	GLY
1	8-B	125	VAL
1	3-A	85	PRO
1	6-B	234	GLY

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	203/203 (100%)	193 (95%)	10 (5%)	25	11
1	1-B	203/203 (100%)	202 (100%)	1 (0%)	88	87
1	2-A	203/203 (100%)	194 (96%)	9 (4%)	28	14
1	2-B	203/203 (100%)	190 (94%)	13 (6%)	17	6
1	3-A	203/203 (100%)	196 (97%)	7 (3%)	37	22
1	3-B	203/203 (100%)	196 (97%)	7 (3%)	37	22
1	4-A	203/203 (100%)	197 (97%)	6 (3%)	41	27
1	4-B	203/203 (100%)	200 (98%)	3 (2%)	65	56
1	5-A	203/203 (100%)	196 (97%)	7 (3%)	37	22
1	5-B	203/203 (100%)	198 (98%)	5 (2%)	47	34
1	6-A	203/203 (100%)	195 (96%)	8 (4%)	32	17
1	6-B	203/203 (100%)	197 (97%)	6 (3%)	41	27
1	7-A	203/203 (100%)	192 (95%)	11 (5%)	22	9
1	7-B	203/203 (100%)	195 (96%)	8 (4%)	32	17
1	8-A	203/203 (100%)	196 (97%)	7 (3%)	37	22
1	8-B	203/203 (100%)	192 (95%)	11 (5%)	22	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3248/3248 (100%)	3129 (96%)	119 (4%)	34	19

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	107	GLN
1	1-A	145	LYS
1	1-A	177	LEU
1	1-A	180	LYS
1	1-A	184	VAL
1	1-A	195	LEU
1	1-A	216	LEU
1	1-A	235	THR
1	1-A	237	THR
1	1-A	252	ARG
1	1-B	217	LEU
1	2-A	76	LEU
1	2-A	145	LYS
1	2-A	177	LEU
1	2-A	184	VAL
1	2-A	195	LEU
1	2-A	201	LYS
1	2-A	216	LEU
1	2-A	237	THR
1	2-A	252	ARG
1	2-B	4	LEU
1	2-B	15	ARG
1	2-B	29	ASP
1	2-B	31	PHE
1	2-B	34	LYS
1	2-B	38	ARG
1	2-B	41	GLN
1	2-B	61	ASP
1	2-B	63	ILE
1	2-B	87	PHE
1	2-B	94	ARG
1	2-B	138	ASN
1	2-B	201	LYS
1	3-A	145	LYS
1	3-A	177	LEU
1	3-A	195	LEU
1	3-A	216	LEU

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Mol	Chain	Res	Type
1	3-A	235	THR
1	3-A	237	THR
1	3-A	252	ARG
1	3-B	4	LEU
1	3-B	73	LEU
1	3-B	177	LEU
1	3-B	197	GLN
1	3-B	198	THR
1	3-B	199	ASP
1	3-B	217	LEU
1	4-A	76	LEU
1	4-A	145	LYS
1	4-A	148	ASN
1	4-A	177	LEU
1	4-A	216	LEU
1	4-A	252	ARG
1	4-B	4	LEU
1	4-B	41	GLN
1	4-B	217	LEU
1	5-A	84	LYS
1	5-A	145	LYS
1	5-A	177	LEU
1	5-A	195	LEU
1	5-A	219	GLU
1	5-A	237	THR
1	5-A	252	ARG
1	5-B	4	LEU
1	5-B	82	LYS
1	5-B	138	ASN
1	5-B	195	LEU
1	5-B	197	GLN
1	6-A	62	SER
1	6-A	88	ASP
1	6-A	91	LYS
1	6-A	177	LEU
1	6-A	216	LEU
1	6-A	235	THR
1	6-A	237	THR
1	6-A	252	ARG
1	6-B	1	SER
1	6-B	4	LEU
1	6-B	41	GLN

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Mol	Chain	Res	Type
1	6-B	57	ILE
1	6-B	125	VAL
1	6-B	148	ASN
1	7-A	8	LEU
1	7-A	38	ARG
1	7-A	76	LEU
1	7-A	143	LEU
1	7-A	145	LYS
1	7-A	177	LEU
1	7-A	180	LYS
1	7-A	212	CYS
1	7-A	216	LEU
1	7-A	235	THR
1	7-A	252	ARG
1	7-B	29	ASP
1	7-B	73	LEU
1	7-B	94	ARG
1	7-B	138	ASN
1	7-B	140	ASP
1	7-B	199	ASP
1	7-B	217	LEU
1	7-B	219	GLU
1	8-A	22	LYS
1	8-A	76	LEU
1	8-A	90	THR
1	8-A	107	GLN
1	8-A	177	LEU
1	8-A	216	LEU
1	8-A	250	THR
1	8-B	4	LEU
1	8-B	25	LYS
1	8-B	29	ASP
1	8-B	41	GLN
1	8-B	73	LEU
1	8-B	94	ARG
1	8-B	125	VAL
1	8-B	138	ASN
1	8-B	189	VAL
1	8-B	199	ASP
1	8-B	217	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	18	GLN
1	1-A	107	GLN
1	1-A	115	ASN
1	1-A	148	ASN
1	1-A	197	GLN
1	1-A	223	ASN
1	1-B	41	GLN
1	1-B	107	GLN
1	1-B	127	HIS
1	1-B	138	ASN
1	1-B	148	ASN
1	1-B	223	ASN
1	2-A	107	GLN
1	2-A	116	GLN
1	2-A	197	GLN
1	2-A	223	ASN
1	2-B	68	GLN
1	2-B	107	GLN
1	2-B	138	ASN
1	2-B	223	ASN
1	3-A	116	GLN
1	3-A	148	ASN
1	3-A	160	GLN
1	3-A	223	ASN
1	3-B	18	GLN
1	3-B	41	GLN
1	3-B	107	GLN
1	3-B	138	ASN
1	3-B	148	ASN
1	3-B	223	ASN
1	4-A	107	GLN
1	4-A	116	GLN
1	4-A	148	ASN
1	4-A	223	ASN
1	4-B	41	GLN
1	4-B	107	GLN
1	4-B	138	ASN
1	4-B	148	ASN
1	4-B	223	ASN
1	5-A	107	GLN
1	5-A	148	ASN
1	5-A	214	GLN
1	5-B	107	GLN

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Mol	Chain	Res	Type
1	5-B	138	ASN
1	5-B	148	ASN
1	5-B	160	GLN
1	5-B	223	ASN
1	6-A	107	GLN
1	6-A	116	GLN
1	6-A	148	ASN
1	6-A	223	ASN
1	6-B	18	GLN
1	6-B	107	GLN
1	6-B	138	ASN
1	6-B	148	ASN
1	6-B	223	ASN
1	7-A	103	GLN
1	7-A	107	GLN
1	7-A	116	GLN
1	7-A	160	GLN
1	7-A	223	ASN
1	7-B	107	GLN
1	7-B	115	ASN
1	7-B	138	ASN
1	7-B	223	ASN
1	8-A	107	GLN
1	8-A	116	GLN
1	8-A	223	ASN
1	8-B	18	GLN
1	8-B	41	GLN
1	8-B	107	GLN
1	8-B	138	ASN
1	8-B	148	ASN
1	8-B	150	ASN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAP	4-A	800	-	45,52,52	5.11	18 (40%)	56,80,80	4.61	15 (26%)
2	NAP	7-B	801	-	45,52,52	2.52	21 (46%)	56,80,80	2.38	10 (17%)
2	NAP	2-B	801	-	45,52,52	2.21	18 (40%)	56,80,80	2.81	9 (16%)
2	NAP	2-A	800	-	45,52,52	2.43	10 (22%)	56,80,80	3.17	12 (21%)
2	NAP	3-B	801	-	45,52,52	2.34	14 (31%)	56,80,80	2.89	10 (17%)
2	NAP	5-A	800	-	45,52,52	2.31	13 (28%)	56,80,80	2.97	12 (21%)
2	NAP	6-B	801	-	45,52,52	2.37	16 (35%)	56,80,80	2.05	11 (19%)
2	NAP	5-B	801	-	45,52,52	2.03	16 (35%)	56,80,80	2.85	12 (21%)
2	NAP	1-A	800	-	45,52,52	2.58	13 (28%)	56,80,80	3.25	12 (21%)
2	NAP	1-B	801	-	45,52,52	2.14	16 (35%)	56,80,80	2.85	11 (19%)
2	NAP	6-A	800	-	45,52,52	2.45	13 (28%)	56,80,80	3.11	13 (23%)
2	NAP	7-A	800	-	45,52,52	2.40	13 (28%)	56,80,80	3.10	10 (17%)
2	NAP	4-B	801	-	45,52,52	2.14	16 (35%)	56,80,80	2.88	11 (19%)
2	NAP	3-A	800	-	45,52,52	2.43	13 (28%)	56,80,80	3.18	15 (26%)
2	NAP	8-A	800	-	45,52,52	2.51	13 (28%)	56,80,80	3.24	14 (25%)
2	NAP	8-B	801	-	45,52,52	2.52	19 (42%)	56,80,80	2.47	11 (19%)

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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	2-B	801	-	1/1/12/12	7/31/67/67	0/5/5/5
2	NAP	7-B	801	-	1/1/12/12	10/31/67/67	0/5/5/5
2	NAP	2-A	800	-	1/1/12/12	13/31/67/67	0/5/5/5
2	NAP	3-B	801	-	1/1/12/12	10/31/67/67	0/5/5/5
2	NAP	5-A	800	-	1/1/12/12	10/31/67/67	0/5/5/5
2	NAP	6-B	801	-	1/1/12/12	8/31/67/67	0/5/5/5
2	NAP	5-B	801	-	1/1/12/12	10/31/67/67	0/5/5/5
2	NAP	1-A	800	-	1/1/12/12	10/31/67/67	0/5/5/5
2	NAP	1-B	801	-	1/1/12/12	10/31/67/67	0/5/5/5
2	NAP	6-A	800	-	1/1/12/12	10/31/67/67	0/5/5/5
2	NAP	7-A	800	-	1/1/12/12	10/31/67/67	0/5/5/5
2	NAP	4-B	801	-	1/1/12/12	13/31/67/67	0/5/5/5
2	NAP	4-A	800	-	-	10/31/67/67	0/5/5/5
2	NAP	3-A	800	-	1/1/12/12	11/31/67/67	0/5/5/5
2	NAP	8-A	800	-	1/1/12/12	14/31/67/67	0/5/5/5
2	NAP	8-B	801	-	1/1/12/12	10/31/67/67	0/5/5/5

All (242) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	4-A	800	NAP	O4B-C4B	24.24	1.99	1.45
2	4-A	800	NAP	C3B-C2B	-15.39	1.18	1.52
2	4-A	800	NAP	O3B-C3B	11.18	1.69	1.43
2	8-A	800	NAP	O4B-C1B	10.99	1.56	1.41
2	2-A	800	NAP	O4B-C1B	10.09	1.55	1.41
2	3-A	800	NAP	O4B-C1B	9.90	1.54	1.41
2	6-A	800	NAP	O4B-C1B	9.57	1.54	1.41
2	1-A	800	NAP	O4B-C1B	9.13	1.53	1.41
2	5-A	800	NAP	O4B-C1B	8.49	1.52	1.41
2	1-A	800	NAP	O4B-C4B	7.94	1.62	1.45
2	7-A	800	NAP	O4B-C1B	7.85	1.52	1.41
2	8-A	800	NAP	P2B-O2B	7.29	1.73	1.59
2	2-A	800	NAP	P2B-O2B	7.02	1.72	1.59
2	3-A	800	NAP	P2B-O2B	7.00	1.72	1.59
2	6-A	800	NAP	P2B-O2B	6.54	1.71	1.59
2	1-A	800	NAP	P2B-O2B	6.50	1.71	1.59
2	6-B	801	NAP	O4B-C4B	-6.48	1.30	1.45
2	7-A	800	NAP	O4B-C4B	6.12	1.58	1.45
2	8-B	801	NAP	P2B-O2B	6.11	1.70	1.59
2	3-B	801	NAP	O4B-C1B	6.09	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5-A	800	NAP	P2B-O2B	5.88	1.70	1.59
2	7-B	801	NAP	P2B-O2B	5.86	1.70	1.59
2	7-B	801	NAP	C4A-N3A	5.66	1.43	1.35
2	8-B	801	NAP	C2A-N3A	5.61	1.41	1.32
2	7-B	801	NAP	C2A-N3A	5.59	1.41	1.32
2	7-B	801	NAP	O4B-C4B	-5.53	1.32	1.45
2	8-B	801	NAP	C4A-N3A	5.51	1.43	1.35
2	8-B	801	NAP	O4B-C4B	-5.42	1.32	1.45
2	3-B	801	NAP	C2A-N3A	5.41	1.40	1.32
2	6-B	801	NAP	O5B-C5B	-5.41	1.24	1.44
2	4-B	801	NAP	O4B-C1B	5.36	1.48	1.41
2	7-A	800	NAP	C2N-N1N	5.34	1.41	1.35
2	5-B	801	NAP	C4A-N3A	5.23	1.42	1.35
2	1-B	801	NAP	C4A-N3A	5.19	1.42	1.35
2	3-B	801	NAP	C4A-N3A	5.12	1.42	1.35
2	2-B	801	NAP	C4A-N3A	5.09	1.42	1.35
2	1-B	801	NAP	O4B-C1B	5.03	1.48	1.41
2	2-B	801	NAP	C2A-N3A	4.99	1.40	1.32
2	4-B	801	NAP	C4A-N3A	4.98	1.42	1.35
2	4-A	800	NAP	C3B-C4B	4.97	1.65	1.53
2	3-B	801	NAP	P2B-O2B	4.91	1.68	1.59
2	4-A	800	NAP	C4A-N3A	4.88	1.42	1.35
2	8-B	801	NAP	O4B-C1B	4.86	1.47	1.41
2	6-B	801	NAP	C2A-N3A	4.73	1.39	1.32
2	4-A	800	NAP	C5B-C4B	4.69	1.66	1.51
2	2-A	800	NAP	C2N-N1N	4.64	1.40	1.35
2	1-B	801	NAP	C2A-N3A	4.59	1.39	1.32
2	2-B	801	NAP	O4B-C1B	4.57	1.47	1.41
2	7-A	800	NAP	P2B-O2B	4.54	1.67	1.59
2	7-A	800	NAP	PA-O1A	-4.51	1.34	1.50
2	8-B	801	NAP	C2N-N1N	4.50	1.40	1.35
2	4-A	800	NAP	PA-O1A	-4.48	1.35	1.50
2	2-B	801	NAP	C2N-N1N	4.47	1.40	1.35
2	7-B	801	NAP	O4B-C1B	4.44	1.47	1.41
2	4-B	801	NAP	C2A-N3A	4.43	1.39	1.32
2	5-B	801	NAP	O4B-C1B	4.41	1.47	1.41
2	5-B	801	NAP	C2A-N3A	4.38	1.39	1.32
2	6-A	800	NAP	O4B-C4B	4.35	1.54	1.45
2	7-B	801	NAP	C2N-N1N	4.33	1.40	1.35
2	3-B	801	NAP	C2N-N1N	4.33	1.40	1.35
2	4-A	800	NAP	C2A-N3A	4.28	1.39	1.32
2	6-B	801	NAP	C4N-C3N	4.07	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	6-B	801	NAP	C2N-N1N	4.03	1.39	1.35
2	6-B	801	NAP	C4A-N3A	4.02	1.41	1.35
2	1-B	801	NAP	C4N-C3N	3.99	1.46	1.39
2	4-A	800	NAP	O4B-C1B	3.91	1.46	1.41
2	4-A	800	NAP	C2N-N1N	3.82	1.39	1.35
2	6-B	801	NAP	P2B-O2B	3.81	1.66	1.59
2	8-A	800	NAP	C2A-N3A	3.78	1.38	1.32
2	4-B	801	NAP	C2N-N1N	3.74	1.39	1.35
2	6-A	800	NAP	O4D-C1D	-3.71	1.35	1.41
2	2-A	800	NAP	C2A-N3A	3.66	1.38	1.32
2	6-A	800	NAP	C4N-C3N	3.65	1.45	1.39
2	3-A	800	NAP	C2A-N3A	3.59	1.37	1.32
2	5-B	801	NAP	O5B-C5B	-3.54	1.31	1.44
2	8-B	801	NAP	C3N-C7N	3.52	1.55	1.50
2	5-A	800	NAP	O4B-C4B	3.51	1.52	1.45
2	6-A	800	NAP	C2A-N3A	3.51	1.37	1.32
2	2-B	801	NAP	C3N-C7N	3.49	1.55	1.50
2	7-B	801	NAP	C3N-C7N	3.49	1.55	1.50
2	3-B	801	NAP	C6N-N1N	3.48	1.43	1.35
2	7-A	800	NAP	C2A-N3A	3.47	1.37	1.32
2	3-B	801	NAP	C3N-C7N	3.46	1.55	1.50
2	1-A	800	NAP	C2A-N3A	3.45	1.37	1.32
2	1-A	800	NAP	C4N-C3N	3.44	1.45	1.39
2	5-A	800	NAP	C2N-N1N	3.43	1.39	1.35
2	4-B	801	NAP	C6N-N1N	3.42	1.43	1.35
2	5-A	800	NAP	C4N-C3N	3.42	1.45	1.39
2	5-A	800	NAP	C2A-N3A	3.40	1.37	1.32
2	7-B	801	NAP	C6N-N1N	3.39	1.43	1.35
2	6-A	800	NAP	C6N-N1N	3.37	1.43	1.35
2	6-B	801	NAP	C3B-C4B	3.35	1.61	1.53
2	3-A	800	NAP	C4N-C3N	3.34	1.45	1.39
2	6-B	801	NAP	C6N-N1N	3.33	1.43	1.35
2	8-B	801	NAP	C6N-N1N	3.33	1.43	1.35
2	8-A	800	NAP	C2D-C1D	-3.33	1.48	1.53
2	3-B	801	NAP	C4N-C3N	3.31	1.45	1.39
2	1-B	801	NAP	C2N-N1N	3.30	1.39	1.35
2	2-B	801	NAP	C4N-C3N	3.28	1.44	1.39
2	4-A	800	NAP	C4N-C3N	3.28	1.44	1.39
2	2-B	801	NAP	C6N-N1N	3.25	1.43	1.35
2	1-A	800	NAP	O4D-C1D	-3.24	1.36	1.41
2	1-B	801	NAP	P2B-O2B	3.24	1.65	1.59
2	4-B	801	NAP	P2B-O2B	3.24	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1-A	800	NAP	C6N-N1N	3.22	1.43	1.35
2	4-B	801	NAP	C4N-C3N	3.20	1.44	1.39
2	2-B	801	NAP	P2B-O2B	3.20	1.65	1.59
2	7-B	801	NAP	C4N-C3N	3.17	1.44	1.39
2	3-A	800	NAP	C2N-N1N	3.15	1.38	1.35
2	7-A	800	NAP	C4N-C3N	3.13	1.44	1.39
2	4-B	801	NAP	C2N-C3N	3.11	1.43	1.39
2	2-B	801	NAP	O4B-C4B	3.11	1.51	1.45
2	5-A	800	NAP	C3B-C4B	-3.10	1.45	1.53
2	8-A	800	NAP	C3B-C4B	-3.09	1.45	1.53
2	6-B	801	NAP	C3N-C7N	3.09	1.55	1.50
2	7-B	801	NAP	O5B-C5B	-3.08	1.32	1.44
2	3-A	800	NAP	C3B-C4B	-3.06	1.45	1.53
2	8-B	801	NAP	C4N-C3N	3.06	1.44	1.39
2	3-A	800	NAP	C6N-N1N	3.05	1.42	1.35
2	2-A	800	NAP	C3B-C4B	-3.04	1.45	1.53
2	6-B	801	NAP	C7N-N7N	3.04	1.38	1.33
2	8-A	800	NAP	C4A-N3A	3.00	1.39	1.35
2	5-B	801	NAP	C2N-N1N	3.00	1.38	1.35
2	2-A	800	NAP	C4A-N3A	2.95	1.39	1.35
2	3-A	800	NAP	C4A-N3A	2.94	1.39	1.35
2	5-A	800	NAP	C6N-N1N	2.92	1.42	1.35
2	4-B	801	NAP	C3N-C7N	2.92	1.55	1.50
2	6-A	800	NAP	C3B-C4B	-2.91	1.45	1.53
2	7-B	801	NAP	C3D-C4D	2.88	1.60	1.53
2	3-A	800	NAP	O4D-C1D	-2.87	1.37	1.41
2	8-B	801	NAP	C3D-C4D	2.86	1.60	1.53
2	6-A	800	NAP	C4A-N3A	2.85	1.39	1.35
2	8-A	800	NAP	C6N-N1N	2.85	1.42	1.35
2	4-A	800	NAP	C2A-N1A	2.85	1.39	1.33
2	1-B	801	NAP	C6N-N1N	2.84	1.42	1.35
2	8-B	801	NAP	O5B-C5B	-2.83	1.33	1.44
2	5-B	801	NAP	C4N-C3N	2.81	1.44	1.39
2	5-B	801	NAP	O4B-C4B	2.81	1.51	1.45
2	4-A	800	NAP	P2B-O2B	2.81	1.64	1.59
2	1-B	801	NAP	C2N-C3N	2.80	1.43	1.39
2	1-A	800	NAP	C3B-C4B	-2.78	1.45	1.53
2	7-A	800	NAP	PN-O1N	-2.77	1.41	1.50
2	1-A	800	NAP	C2N-N1N	2.77	1.38	1.35
2	4-B	801	NAP	O4B-C4B	2.75	1.51	1.45
2	3-B	801	NAP	C3B-C4B	-2.75	1.46	1.53
2	1-B	801	NAP	O4B-C4B	2.73	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5-A	800	NAP	C3D-C4D	2.73	1.60	1.53
2	4-A	800	NAP	PN-O1N	-2.72	1.41	1.50
2	2-A	800	NAP	C4N-C3N	2.72	1.44	1.39
2	3-B	801	NAP	C3D-C4D	2.72	1.59	1.53
2	8-A	800	NAP	O3D-C3D	-2.71	1.36	1.43
2	2-B	801	NAP	C3D-C4D	2.70	1.59	1.53
2	8-B	801	NAP	C5D-C4D	-2.70	1.43	1.51
2	5-B	801	NAP	O3D-C3D	-2.67	1.36	1.43
2	7-A	800	NAP	C3D-C4D	2.66	1.59	1.53
2	5-B	801	NAP	C2N-C3N	2.66	1.43	1.39
2	5-A	800	NAP	PA-O1A	-2.66	1.41	1.50
2	6-A	800	NAP	C3D-C4D	2.65	1.59	1.53
2	7-B	801	NAP	C5D-C4D	-2.65	1.43	1.51
2	1-B	801	NAP	C3N-C7N	2.65	1.54	1.50
2	1-A	800	NAP	C4A-N3A	2.64	1.39	1.35
2	4-A	800	NAP	C6N-N1N	2.64	1.41	1.35
2	8-A	800	NAP	C4N-C3N	2.63	1.43	1.39
2	1-B	801	NAP	PA-O2A	-2.63	1.43	1.55
2	7-A	800	NAP	C3B-C4B	-2.62	1.46	1.53
2	7-A	800	NAP	C6N-N1N	2.58	1.41	1.35
2	5-B	801	NAP	P2B-O2B	2.58	1.64	1.59
2	2-A	800	NAP	C6N-N1N	2.58	1.41	1.35
2	2-A	800	NAP	C3D-C4D	2.58	1.59	1.53
2	3-A	800	NAP	O4B-C4B	2.56	1.50	1.45
2	1-B	801	NAP	O4D-C4D	2.56	1.50	1.45
2	2-B	801	NAP	O5B-C5B	-2.55	1.34	1.44
2	6-B	801	NAP	PA-O1A	-2.55	1.41	1.50
2	5-A	800	NAP	C4A-N3A	2.54	1.39	1.35
2	1-A	800	NAP	C3D-C4D	2.53	1.59	1.53
2	6-A	800	NAP	O4D-C4D	2.53	1.50	1.45
2	5-A	800	NAP	O4D-C4D	2.52	1.50	1.45
2	3-A	800	NAP	C3D-C4D	2.52	1.59	1.53
2	4-A	800	NAP	C3D-C4D	2.50	1.59	1.53
2	6-A	800	NAP	C2N-N1N	2.50	1.38	1.35
2	4-B	801	NAP	C2D-C1D	-2.50	1.50	1.53
2	1-B	801	NAP	O5B-C5B	-2.49	1.35	1.44
2	1-B	801	NAP	O3D-C3D	-2.49	1.37	1.43
2	1-B	801	NAP	C3B-C4B	-2.49	1.46	1.53
2	7-A	800	NAP	C4A-N3A	2.48	1.39	1.35
2	5-B	801	NAP	C6N-N1N	2.48	1.41	1.35
2	5-B	801	NAP	O4D-C4D	2.48	1.50	1.45
2	3-B	801	NAP	C5D-C4D	-2.48	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	4-B	801	NAP	O5B-C5B	-2.46	1.35	1.44
2	5-A	800	NAP	O4D-C1D	-2.46	1.37	1.41
2	2-B	801	NAP	C5D-C4D	-2.43	1.44	1.51
2	4-B	801	NAP	O4D-C4D	2.37	1.50	1.45
2	4-B	801	NAP	C3B-C4B	-2.34	1.47	1.53
2	2-B	801	NAP	PA-O2A	-2.32	1.44	1.55
2	2-B	801	NAP	C3B-C4B	-2.32	1.47	1.53
2	8-A	800	NAP	C3D-C4D	2.31	1.58	1.53
2	2-A	800	NAP	O4B-C4B	2.30	1.50	1.45
2	8-B	801	NAP	C2A-N1A	2.30	1.38	1.33
2	4-A	800	NAP	O3D-C3D	-2.30	1.37	1.43
2	8-B	801	NAP	PA-O1A	-2.28	1.42	1.50
2	6-B	801	NAP	O4D-C4D	2.27	1.50	1.45
2	2-B	801	NAP	O3B-C3B	2.27	1.48	1.43
2	6-B	801	NAP	C3D-C4D	2.27	1.58	1.53
2	5-B	801	NAP	PA-O2A	-2.26	1.44	1.55
2	8-B	801	NAP	C5N-C4N	2.26	1.43	1.38
2	8-B	801	NAP	O2B-C2B	-2.25	1.35	1.44
2	7-B	801	NAP	C5N-C4N	2.25	1.43	1.38
2	7-B	801	NAP	C8A-N7A	2.24	1.38	1.34
2	1-A	800	NAP	O4D-C4D	2.23	1.50	1.45
2	5-B	801	NAP	C8A-N7A	2.22	1.38	1.34
2	2-B	801	NAP	C8A-N7A	2.21	1.38	1.34
2	4-B	801	NAP	PA-O2A	-2.21	1.45	1.55
2	7-B	801	NAP	C2A-N1A	2.20	1.38	1.33
2	7-B	801	NAP	PA-O1A	-2.20	1.43	1.50
2	1-B	801	NAP	C5A-C4A	2.19	1.46	1.40
2	8-B	801	NAP	P2B-O2X	2.18	1.63	1.54
2	3-B	801	NAP	C5N-C4N	2.16	1.43	1.38
2	5-B	801	NAP	C5A-C4A	2.16	1.46	1.40
2	8-A	800	NAP	O4B-C4B	2.16	1.49	1.45
2	3-B	801	NAP	C2A-N1A	2.15	1.37	1.33
2	7-B	801	NAP	C5A-C4A	2.15	1.46	1.40
2	7-B	801	NAP	O2B-C2B	-2.14	1.36	1.44
2	8-B	801	NAP	C5A-C4A	2.13	1.46	1.40
2	8-A	800	NAP	C5B-C4B	-2.12	1.45	1.51
2	3-B	801	NAP	C5A-C4A	2.12	1.46	1.40
2	7-B	801	NAP	PA-O2A	-2.11	1.45	1.55
2	6-B	801	NAP	O2B-C2B	-2.11	1.36	1.44
2	6-B	801	NAP	C5D-C4D	-2.10	1.45	1.51
2	7-B	801	NAP	PN-O2N	-2.10	1.45	1.55
2	3-A	800	NAP	O4D-C4D	2.10	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	6-A	800	NAP	C5B-C4B	-2.08	1.45	1.51
2	8-B	801	NAP	PN-O2N	-2.08	1.45	1.55
2	7-B	801	NAP	P2B-O2X	2.08	1.62	1.54
2	8-A	800	NAP	C3B-C2B	2.07	1.57	1.52
2	4-B	801	NAP	C5A-C4A	2.06	1.46	1.40
2	5-B	801	NAP	C5N-C4N	2.05	1.43	1.38
2	1-A	800	NAP	C3B-C2B	-2.03	1.48	1.52
2	3-A	800	NAP	O3D-C3D	-2.03	1.38	1.43
2	7-A	800	NAP	O3D-C3D	-2.01	1.38	1.43
2	2-B	801	NAP	C5N-C4N	2.01	1.43	1.38
2	2-B	801	NAP	C5A-C4A	2.01	1.46	1.40
2	4-A	800	NAP	PA-O2A	-2.01	1.45	1.55

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4-A	800	NAP	C2B-C3B-C4B	18.26	141.66	101.99
2	4-A	800	NAP	O4B-C4B-C3B	-17.71	70.07	105.11
2	2-A	800	NAP	C5B-C4B-C3B	15.62	173.71	115.18
2	8-A	800	NAP	C5B-C4B-C3B	15.60	173.66	115.18
2	4-B	801	NAP	C5B-C4B-C3B	15.58	173.57	115.18
2	3-A	800	NAP	C5B-C4B-C3B	15.57	173.53	115.18
2	1-B	801	NAP	C5B-C4B-C3B	15.52	173.33	115.18
2	3-B	801	NAP	C5B-C4B-C3B	15.43	173.01	115.18
2	5-B	801	NAP	C5B-C4B-C3B	15.39	172.85	115.18
2	7-A	800	NAP	C5B-C4B-C3B	15.21	172.20	115.18
2	2-B	801	NAP	C5B-C4B-C3B	15.20	172.16	115.18
2	5-A	800	NAP	C5B-C4B-C3B	15.10	171.76	115.18
2	6-A	800	NAP	C5B-C4B-C3B	14.38	169.07	115.18
2	4-A	800	NAP	O4B-C4B-C5B	-13.46	65.09	109.37
2	1-A	800	NAP	C5B-C4B-C3B	13.36	165.24	115.18
2	4-A	800	NAP	O3B-C3B-C4B	-11.99	76.39	111.05
2	8-B	801	NAP	C5B-C4B-C3B	10.87	155.91	115.18
2	4-A	800	NAP	O5B-C5B-C4B	-10.15	74.06	108.99
2	7-B	801	NAP	C5B-C4B-C3B	10.02	152.74	115.18
2	1-A	800	NAP	O4B-C4B-C5B	-9.64	77.64	109.37
2	1-A	800	NAP	O5B-C5B-C4B	-8.87	78.47	108.99
2	6-A	800	NAP	O4B-C4B-C5B	-8.55	81.25	109.37
2	7-A	800	NAP	O5B-C5B-C4B	-8.48	79.81	108.99
2	8-A	800	NAP	O4B-C4B-C5B	-8.38	81.81	109.37
2	3-A	800	NAP	O4B-C4B-C5B	-8.30	82.07	109.37
2	2-A	800	NAP	O4B-C4B-C5B	-8.29	82.10	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7-A	800	NAP	O4B-C4B-C5B	-8.27	82.18	109.37
2	6-A	800	NAP	O5B-C5B-C4B	-8.13	81.03	108.99
2	6-B	801	NAP	C5B-C4B-C3B	7.99	145.11	115.18
2	1-A	800	NAP	O4B-C4B-C3B	-7.84	89.60	105.11
2	8-A	800	NAP	O5B-C5B-C4B	-7.58	82.90	108.99
2	5-A	800	NAP	O4B-C4B-C5B	-7.52	84.64	109.37
2	5-A	800	NAP	O5B-C5B-C4B	-7.47	83.27	108.99
2	3-A	800	NAP	O5B-C5B-C4B	-7.27	83.95	108.99
2	2-A	800	NAP	O5B-C5B-C4B	-7.21	84.18	108.99
2	8-A	800	NAP	O2A-PA-O1A	-7.05	77.38	112.24
2	3-B	801	NAP	O4B-C4B-C5B	-6.66	87.47	109.37
2	5-B	801	NAP	O4B-C4B-C5B	-6.62	87.59	109.37
2	8-B	801	NAP	O2A-PA-O1A	-6.62	79.53	112.24
2	4-B	801	NAP	O4B-C4B-C5B	-6.60	87.66	109.37
2	1-B	801	NAP	O4B-C4B-C5B	-6.58	87.74	109.37
2	2-B	801	NAP	O4B-C4B-C5B	-6.55	87.81	109.37
2	2-A	800	NAP	O2A-PA-O1A	-6.48	80.19	112.24
2	7-B	801	NAP	O2A-PA-O1A	-6.33	80.96	112.24
2	3-A	800	NAP	O2A-PA-O1A	-6.31	81.03	112.24
2	3-A	800	NAP	O4B-C1B-C2B	-6.23	95.78	106.59
2	2-A	800	NAP	O4B-C1B-C2B	-6.14	95.94	106.59
2	2-B	801	NAP	O4B-C1B-C2B	-6.13	95.95	106.59
2	8-A	800	NAP	O4B-C1B-C2B	-6.10	96.00	106.59
2	1-B	801	NAP	O4B-C1B-C2B	-5.99	96.20	106.59
2	6-A	800	NAP	O2A-PA-O1A	-5.98	82.67	112.24
2	3-B	801	NAP	O4B-C1B-C2B	-5.92	96.32	106.59
2	4-B	801	NAP	O4B-C1B-C2B	-5.84	96.47	106.59
2	8-B	801	NAP	O4B-C4B-C5B	-5.82	90.22	109.37
2	6-A	800	NAP	O4B-C4B-C3B	-5.77	93.69	105.11
2	1-A	800	NAP	C2B-C3B-C4B	5.76	114.50	101.99
2	6-B	801	NAP	C2B-C3B-C4B	-5.68	89.66	101.99
2	7-B	801	NAP	O4B-C4B-C5B	-5.66	90.74	109.37
2	6-A	800	NAP	O4B-C1B-C2B	-5.63	96.82	106.59
2	7-B	801	NAP	O4B-C1B-C2B	-5.62	96.85	106.59
2	8-B	801	NAP	O4B-C1B-C2B	-5.58	96.91	106.59
2	5-B	801	NAP	O4B-C1B-C2B	-5.58	96.92	106.59
2	1-A	800	NAP	O2A-PA-O1A	-5.55	84.78	112.24
2	1-A	800	NAP	O4B-C1B-C2B	-5.55	96.96	106.59
2	5-A	800	NAP	O4B-C1B-C2B	-5.48	97.08	106.59
2	3-B	801	NAP	O5B-C5B-C4B	-5.48	90.14	108.99
2	7-A	800	NAP	O4B-C4B-C3B	-5.46	94.32	105.11
2	5-B	801	NAP	O5B-C5B-C4B	-5.38	90.46	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7-A	800	NAP	O4B-C1B-C2B	-5.37	97.27	106.59
2	8-B	801	NAP	O5B-C5B-C4B	-5.33	90.65	108.99
2	1-B	801	NAP	O5B-C5B-C4B	-5.20	91.10	108.99
2	4-B	801	NAP	O5B-C5B-C4B	-5.18	91.15	108.99
2	8-A	800	NAP	O4B-C4B-C3B	-5.16	94.90	105.11
2	7-B	801	NAP	O5B-C5B-C4B	-5.11	91.39	108.99
2	2-B	801	NAP	O5B-C5B-C4B	-5.10	91.42	108.99
2	3-A	800	NAP	O4B-C4B-C3B	-5.05	95.13	105.11
2	2-A	800	NAP	O4B-C4B-C3B	-4.87	95.48	105.11
2	3-B	801	NAP	O2A-PA-O1A	-4.83	88.35	112.24
2	6-B	801	NAP	O4B-C1B-C2B	-4.60	98.61	106.59
2	4-A	800	NAP	O4B-C1B-C2B	-4.46	98.85	106.59
2	4-B	801	NAP	O3B-C3B-C4B	-4.25	98.77	111.05
2	5-A	800	NAP	O2A-PA-O1A	-4.17	91.61	112.24
2	6-B	801	NAP	O5B-C5B-C4B	-4.13	94.79	108.99
2	5-A	800	NAP	O4B-C4B-C3B	-3.97	97.26	105.11
2	1-B	801	NAP	O3B-C3B-C4B	-3.97	99.58	111.05
2	6-B	801	NAP	O4B-C4B-C5B	-3.96	96.33	109.37
2	2-B	801	NAP	PA-O5B-C5B	3.88	144.46	121.68
2	3-B	801	NAP	PA-O5B-C5B	3.83	144.14	121.68
2	1-B	801	NAP	PA-O5B-C5B	3.83	144.13	121.68
2	4-B	801	NAP	PA-O5B-C5B	3.74	143.59	121.68
2	2-B	801	NAP	O3B-C3B-C4B	-3.73	100.25	111.05
2	7-A	800	NAP	O2A-PA-O1A	-3.71	93.90	112.24
2	3-A	800	NAP	PA-O5B-C5B	3.67	143.21	121.68
2	6-B	801	NAP	O2A-PA-O1A	-3.65	94.19	112.24
2	2-B	801	NAP	O2A-PA-O1A	-3.65	94.20	112.24
2	1-A	800	NAP	PA-O5B-C5B	3.65	143.07	121.68
2	2-A	800	NAP	PA-O5B-C5B	3.64	143.02	121.68
2	5-B	801	NAP	PA-O5B-C5B	3.52	142.30	121.68
2	6-A	800	NAP	C2B-C3B-C4B	3.50	109.60	101.99
2	5-B	801	NAP	O3B-C3B-C4B	-3.49	100.95	111.05
2	7-B	801	NAP	C3B-C2B-C1B	-3.43	96.44	102.89
2	8-B	801	NAP	C3B-C2B-C1B	-3.40	96.51	102.89
2	7-A	800	NAP	C2B-C3B-C4B	3.38	109.33	101.99
2	6-A	800	NAP	PA-O5B-C5B	3.36	141.41	121.68
2	7-B	801	NAP	PA-O5B-C5B	3.31	141.09	121.68
2	8-A	800	NAP	PA-O5B-C5B	3.26	140.80	121.68
2	4-B	801	NAP	O4B-C4B-C3B	-3.23	98.72	105.11
2	1-B	801	NAP	O4B-C4B-C3B	-3.18	98.83	105.11
2	8-B	801	NAP	PA-O5B-C5B	3.18	140.31	121.68
2	3-B	801	NAP	O3B-C3B-C4B	-3.15	101.95	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5-A	800	NAP	PA-O5B-C5B	3.05	139.58	121.68
2	7-A	800	NAP	PA-O5B-C5B	2.95	138.96	121.68
2	3-B	801	NAP	O4B-C4B-C3B	-2.94	99.31	105.11
2	3-B	801	NAP	O5B-PA-O1A	2.93	120.51	109.07
2	3-A	800	NAP	O5B-PA-O1A	2.88	120.34	109.07
2	5-B	801	NAP	O4B-C4B-C3B	-2.84	99.50	105.11
2	7-B	801	NAP	C2B-C3B-C4B	-2.84	95.83	101.99
2	8-B	801	NAP	O5B-PA-O1A	2.82	120.08	109.07
2	2-A	800	NAP	O5B-PA-O1A	2.79	119.97	109.07
2	5-B	801	NAP	C3N-C7N-N7N	-2.76	114.44	117.75
2	4-A	800	NAP	C5B-C4B-C3B	2.73	125.41	115.18
2	7-B	801	NAP	O5B-PA-O1A	2.73	119.72	109.07
2	5-B	801	NAP	C2A-N1A-C6A	2.67	123.32	118.75
2	8-A	800	NAP	O5B-PA-O1A	2.66	119.44	109.07
2	7-A	800	NAP	O5B-PA-O1A	2.58	119.13	109.07
2	4-B	801	NAP	C2A-N1A-C6A	2.57	123.16	118.75
2	2-B	801	NAP	O4B-C4B-C3B	-2.57	100.03	105.11
2	6-B	801	NAP	PA-O5B-C5B	2.54	136.57	121.68
2	8-A	800	NAP	C3B-C2B-C1B	-2.54	98.12	102.89
2	4-A	800	NAP	O2A-PA-O1A	-2.54	99.70	112.24
2	4-A	800	NAP	PA-O5B-C5B	2.51	136.42	121.68
2	4-B	801	NAP	C3N-C7N-N7N	-2.51	114.74	117.75
2	5-A	800	NAP	O7N-C7N-N7N	2.46	126.08	122.58
2	1-B	801	NAP	C2A-N1A-C6A	2.45	122.94	118.75
2	4-B	801	NAP	C5A-C6A-N6A	2.43	124.04	120.35
2	6-A	800	NAP	C3N-C7N-N7N	-2.42	114.84	117.75
2	5-A	800	NAP	C2B-C3B-C4B	2.42	107.26	101.99
2	4-A	800	NAP	C2A-N1A-C6A	2.42	122.89	118.75
2	8-A	800	NAP	O7N-C7N-N7N	2.41	126.00	122.58
2	6-A	800	NAP	O7N-C7N-N7N	2.40	125.99	122.58
2	3-A	800	NAP	O7N-C7N-N7N	2.38	125.95	122.58
2	6-B	801	NAP	C3B-C2B-C1B	-2.36	98.45	102.89
2	1-A	800	NAP	O7N-C7N-N7N	2.35	125.91	122.58
2	1-A	800	NAP	C3N-C7N-N7N	-2.32	114.97	117.75
2	5-B	801	NAP	O2A-PA-O1A	-2.31	100.81	112.24
2	8-B	801	NAP	O4B-C4B-C3B	-2.31	100.54	105.11
2	6-B	801	NAP	O4D-C1D-C2D	2.30	110.28	106.93
2	4-A	800	NAP	N3A-C2A-N1A	-2.30	125.09	128.68
2	3-A	800	NAP	C3N-C7N-N7N	-2.28	115.02	117.75
2	6-B	801	NAP	O2B-C2B-C3B	-2.27	103.44	111.68
2	7-B	801	NAP	O4D-C1D-C2D	2.27	110.24	106.93
2	2-B	801	NAP	O4D-C1D-C2D	2.26	110.23	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	6-B	801	NAP	C2A-N1A-C6A	2.26	122.62	118.75
2	8-A	800	NAP	C3N-C7N-N7N	-2.25	115.05	117.75
2	5-B	801	NAP	C6N-N1N-C2N	-2.23	119.94	121.97
2	4-A	800	NAP	O7N-C7N-N7N	2.22	125.73	122.58
2	7-A	800	NAP	C5A-C6A-N1A	-2.22	115.33	120.35
2	8-A	800	NAP	O2B-C2B-C3B	-2.20	103.72	111.68
2	3-A	800	NAP	O2B-C2B-C1B	2.19	117.98	110.10
2	5-A	800	NAP	O2B-C2B-C3B	-2.19	103.75	111.68
2	8-B	801	NAP	O4D-C1D-C2D	2.18	110.11	106.93
2	2-A	800	NAP	O2B-C2B-C3B	-2.18	103.78	111.68
2	4-A	800	NAP	O5B-PA-O1A	2.18	117.57	109.07
2	6-A	800	NAP	O2B-C2B-C3B	-2.17	103.80	111.68
2	4-B	801	NAP	C5A-C6A-N1A	-2.17	115.43	120.35
2	5-A	800	NAP	C5A-C6A-N1A	-2.17	115.44	120.35
2	1-A	800	NAP	C5A-C6A-N1A	-2.15	115.49	120.35
2	3-B	801	NAP	O4D-C1D-C2D	2.14	110.06	106.93
2	2-A	800	NAP	O2B-C2B-C1B	2.14	117.80	110.10
2	8-A	800	NAP	C5A-C6A-N1A	-2.14	115.51	120.35
2	4-A	800	NAP	C3N-C7N-N7N	-2.13	115.20	117.75
2	8-A	800	NAP	O2B-C2B-C1B	2.13	117.76	110.10
2	3-A	800	NAP	O2B-C2B-C3B	-2.11	104.02	111.68
2	4-A	800	NAP	C5A-C6A-N1A	-2.11	115.56	120.35
2	5-A	800	NAP	C3N-C7N-N7N	-2.10	115.23	117.75
2	2-A	800	NAP	C5A-C6A-N1A	-2.10	115.59	120.35
2	1-B	801	NAP	C5A-C6A-N6A	2.09	123.52	120.35
2	6-A	800	NAP	C5A-C6A-N1A	-2.08	115.63	120.35
2	3-A	800	NAP	C5A-C6A-N1A	-2.08	115.63	120.35
2	3-A	800	NAP	C3B-C2B-C1B	-2.07	98.99	102.89
2	5-B	801	NAP	C5A-C6A-N1A	-2.07	115.66	120.35
2	1-A	800	NAP	O2B-C2B-C3B	-2.07	104.18	111.68
2	1-B	801	NAP	C5A-C6A-N1A	-2.04	115.72	120.35
2	3-A	800	NAP	C2B-C3B-C4B	2.02	106.39	101.99
2	2-A	800	NAP	C2B-C3B-C4B	2.01	106.37	101.99
2	6-A	800	NAP	O4D-C4D-C3D	-2.01	101.14	105.11
2	8-B	801	NAP	C2B-C3B-C4B	-2.01	97.64	101.99
2	1-B	801	NAP	O2A-PA-O1A	-2.00	102.33	112.24

All (15) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	7-B	801	NAP	C4B
2	2-B	801	NAP	C4B

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Mol	Chain	Res	Type	Atom
2	2-A	800	NAP	C4B
2	3-B	801	NAP	C4B
2	5-A	800	NAP	C4B
2	6-B	801	NAP	C4B
2	5-B	801	NAP	C4B
2	1-A	800	NAP	C4B
2	1-B	801	NAP	C4B
2	6-A	800	NAP	C4B
2	7-A	800	NAP	C4B
2	4-B	801	NAP	C4B
2	3-A	800	NAP	C4B
2	8-A	800	NAP	C4B
2	8-B	801	NAP	C4B

All (166) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	4-A	800	NAP	C5B-O5B-PA-O2A
2	4-A	800	NAP	C5B-O5B-PA-O3
2	4-A	800	NAP	O4D-C1D-N1N-C2N
2	4-A	800	NAP	O4D-C1D-N1N-C6N
2	4-A	800	NAP	C2D-C1D-N1N-C2N
2	4-A	800	NAP	C2D-C1D-N1N-C6N
2	7-B	801	NAP	C5B-O5B-PA-O3
2	7-B	801	NAP	C3B-C2B-O2B-P2B
2	7-B	801	NAP	O4D-C1D-N1N-C2N
2	7-B	801	NAP	O4D-C1D-N1N-C6N
2	7-B	801	NAP	C2D-C1D-N1N-C2N
2	7-B	801	NAP	C2D-C1D-N1N-C6N
2	2-B	801	NAP	C5B-O5B-PA-O2A
2	2-B	801	NAP	C5B-O5B-PA-O3
2	2-B	801	NAP	O4D-C1D-N1N-C2N
2	2-B	801	NAP	O4D-C1D-N1N-C6N
2	2-B	801	NAP	C2D-C1D-N1N-C2N
2	2-B	801	NAP	C2D-C1D-N1N-C6N
2	2-A	800	NAP	C5B-O5B-PA-O2A
2	2-A	800	NAP	C5B-O5B-PA-O3
2	2-A	800	NAP	C3B-C4B-C5B-O5B
2	2-A	800	NAP	O4D-C1D-N1N-C2N
2	2-A	800	NAP	O4D-C1D-N1N-C6N
2	2-A	800	NAP	C2D-C1D-N1N-C2N
2	2-A	800	NAP	C2D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
2	3-B	801	NAP	C5B-O5B-PA-O2A
2	3-B	801	NAP	C5B-O5B-PA-O3
2	3-B	801	NAP	O4D-C1D-N1N-C2N
2	3-B	801	NAP	O4D-C1D-N1N-C6N
2	3-B	801	NAP	C2D-C1D-N1N-C2N
2	3-B	801	NAP	C2D-C1D-N1N-C6N
2	5-A	800	NAP	C5B-O5B-PA-O2A
2	5-A	800	NAP	C5B-O5B-PA-O3
2	5-A	800	NAP	O4B-C4B-C5B-O5B
2	5-A	800	NAP	O4D-C1D-N1N-C2N
2	5-A	800	NAP	O4D-C1D-N1N-C6N
2	5-A	800	NAP	C2D-C1D-N1N-C2N
2	5-A	800	NAP	C2D-C1D-N1N-C6N
2	6-B	801	NAP	C5B-O5B-PA-O3
2	6-B	801	NAP	O4D-C1D-N1N-C2N
2	6-B	801	NAP	O4D-C1D-N1N-C6N
2	6-B	801	NAP	C2D-C1D-N1N-C2N
2	6-B	801	NAP	C2D-C1D-N1N-C6N
2	5-B	801	NAP	C5B-O5B-PA-O3
2	5-B	801	NAP	O4B-C4B-C5B-O5B
2	5-B	801	NAP	C2B-O2B-P2B-O2X
2	5-B	801	NAP	O4D-C1D-N1N-C2N
2	5-B	801	NAP	O4D-C1D-N1N-C6N
2	5-B	801	NAP	C2D-C1D-N1N-C2N
2	5-B	801	NAP	C2D-C1D-N1N-C6N
2	1-A	800	NAP	C5B-O5B-PA-O2A
2	1-A	800	NAP	C5B-O5B-PA-O3
2	1-A	800	NAP	O4B-C4B-C5B-O5B
2	1-A	800	NAP	C3B-C2B-O2B-P2B
2	1-A	800	NAP	O4D-C1D-N1N-C2N
2	1-A	800	NAP	O4D-C1D-N1N-C6N
2	1-A	800	NAP	C2D-C1D-N1N-C2N
2	1-A	800	NAP	C2D-C1D-N1N-C6N
2	1-B	801	NAP	C5B-O5B-PA-O3
2	1-B	801	NAP	O4B-C4B-C5B-O5B
2	1-B	801	NAP	C2B-O2B-P2B-O2X
2	1-B	801	NAP	O4D-C1D-N1N-C2N
2	1-B	801	NAP	O4D-C1D-N1N-C6N
2	1-B	801	NAP	C2D-C1D-N1N-C2N
2	1-B	801	NAP	C2D-C1D-N1N-C6N
2	6-A	800	NAP	C5B-O5B-PA-O2A
2	6-A	800	NAP	C5B-O5B-PA-O3

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Mol	Chain	Res	Type	Atoms
2	6-A	800	NAP	O4B-C4B-C5B-O5B
2	6-A	800	NAP	C3B-C4B-C5B-O5B
2	6-A	800	NAP	O4D-C1D-N1N-C2N
2	6-A	800	NAP	O4D-C1D-N1N-C6N
2	6-A	800	NAP	C2D-C1D-N1N-C2N
2	6-A	800	NAP	C2D-C1D-N1N-C6N
2	7-A	800	NAP	C5B-O5B-PA-O3
2	7-A	800	NAP	C3B-C4B-C5B-O5B
2	7-A	800	NAP	O4D-C1D-N1N-C2N
2	7-A	800	NAP	O4D-C1D-N1N-C6N
2	7-A	800	NAP	C2D-C1D-N1N-C2N
2	7-A	800	NAP	C2D-C1D-N1N-C6N
2	4-B	801	NAP	C5B-O5B-PA-O3
2	4-B	801	NAP	O4B-C4B-C5B-O5B
2	4-B	801	NAP	C2B-O2B-P2B-O2X
2	4-B	801	NAP	O4D-C1D-N1N-C2N
2	4-B	801	NAP	O4D-C1D-N1N-C6N
2	3-A	800	NAP	C5B-O5B-PA-O2A
2	3-A	800	NAP	C5B-O5B-PA-O3
2	3-A	800	NAP	C3B-C4B-C5B-O5B
2	3-A	800	NAP	O4D-C1D-N1N-C2N
2	3-A	800	NAP	O4D-C1D-N1N-C6N
2	3-A	800	NAP	C2D-C1D-N1N-C2N
2	3-A	800	NAP	C2D-C1D-N1N-C6N
2	8-A	800	NAP	C5B-O5B-PA-O2A
2	8-A	800	NAP	C5B-O5B-PA-O3
2	8-A	800	NAP	C3B-C4B-C5B-O5B
2	8-A	800	NAP	O4D-C1D-N1N-C2N
2	8-A	800	NAP	O4D-C1D-N1N-C6N
2	8-A	800	NAP	C2D-C1D-N1N-C6N
2	8-B	801	NAP	C5B-O5B-PA-O3
2	8-B	801	NAP	C3B-C2B-O2B-P2B
2	8-B	801	NAP	O4D-C1D-N1N-C2N
2	8-B	801	NAP	O4D-C1D-N1N-C6N
2	8-B	801	NAP	C2D-C1D-N1N-C2N
2	8-B	801	NAP	C2D-C1D-N1N-C6N
2	4-A	800	NAP	O4B-C4B-C5B-O5B
2	4-A	800	NAP	C3B-C4B-C5B-O5B
2	2-B	801	NAP	O4B-C4B-C5B-O5B
2	3-B	801	NAP	O4B-C4B-C5B-O5B
2	5-A	800	NAP	C3B-C4B-C5B-O5B
2	6-B	801	NAP	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	7-A	800	NAP	O4B-C4B-C5B-O5B
2	8-B	801	NAP	O4B-C4B-C5B-O5B
2	3-B	801	NAP	C3B-C2B-O2B-P2B
2	5-B	801	NAP	C3B-C2B-O2B-P2B
2	7-B	801	NAP	O4B-C4B-C5B-O5B
2	4-A	800	NAP	C3B-C2B-O2B-P2B
2	2-A	800	NAP	C3B-C2B-O2B-P2B
2	5-A	800	NAP	C3B-C2B-O2B-P2B
2	1-B	801	NAP	C3B-C2B-O2B-P2B
2	6-A	800	NAP	C3B-C2B-O2B-P2B
2	4-B	801	NAP	C3B-C2B-O2B-P2B
2	3-A	800	NAP	C3B-C2B-O2B-P2B
2	8-A	800	NAP	C3B-C2B-O2B-P2B
2	8-A	800	NAP	C2N-C3N-C7N-O7N
2	4-A	800	NAP	C1B-C2B-O2B-P2B
2	5-A	800	NAP	C1B-C2B-O2B-P2B
2	6-B	801	NAP	C1B-C2B-O2B-P2B
2	1-B	801	NAP	C1B-C2B-O2B-P2B
2	6-A	800	NAP	C1B-C2B-O2B-P2B
2	4-B	801	NAP	C1B-C2B-O2B-P2B
2	7-B	801	NAP	C3B-C4B-C5B-O5B
2	8-B	801	NAP	C3B-C4B-C5B-O5B
2	8-A	800	NAP	C4N-C3N-C7N-O7N
2	2-A	800	NAP	C1B-C2B-O2B-P2B
2	3-A	800	NAP	C1B-C2B-O2B-P2B
2	8-A	800	NAP	C1B-C2B-O2B-P2B
2	8-A	800	NAP	C2N-C3N-C7N-N7N
2	2-A	800	NAP	O4B-C4B-C5B-O5B
2	3-A	800	NAP	O4B-C4B-C5B-O5B
2	8-A	800	NAP	C4N-C3N-C7N-N7N
2	2-A	800	NAP	C2N-C3N-C7N-O7N
2	4-B	801	NAP	C4N-C3N-C7N-O7N
2	7-B	801	NAP	C2B-O2B-P2B-O2X
2	3-B	801	NAP	C2B-O2B-P2B-O2X
2	8-B	801	NAP	C2B-O2B-P2B-O2X
2	8-A	800	NAP	O4B-C4B-C5B-O5B
2	2-A	800	NAP	PN-O3-PA-O1A
2	3-A	800	NAP	PN-O3-PA-O1A
2	7-B	801	NAP	C5B-O5B-PA-O2A
2	5-B	801	NAP	C5B-O5B-PA-O2A
2	7-A	800	NAP	C5B-O5B-PA-O2A
2	8-B	801	NAP	C5B-O5B-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	1-A	800	NAP	C1B-C2B-O2B-P2B
2	2-A	800	NAP	C4N-C3N-C7N-O7N
2	4-B	801	NAP	C4N-C3N-C7N-N7N
2	4-B	801	NAP	C2N-C3N-C7N-O7N
2	6-B	801	NAP	C3B-C2B-O2B-P2B
2	7-A	800	NAP	C3B-C2B-O2B-P2B
2	3-B	801	NAP	C1B-C2B-O2B-P2B
2	5-B	801	NAP	C1B-C2B-O2B-P2B
2	7-A	800	NAP	C1B-C2B-O2B-P2B
2	8-A	800	NAP	PN-O3-PA-O1A
2	1-A	800	NAP	C2B-O2B-P2B-O2X
2	4-B	801	NAP	C2D-C1D-N1N-C2N
2	4-B	801	NAP	C2D-C1D-N1N-C6N
2	4-B	801	NAP	C2N-C3N-C7N-N7N
2	1-B	801	NAP	C5B-O5B-PA-O2A

There are no ring outliers.

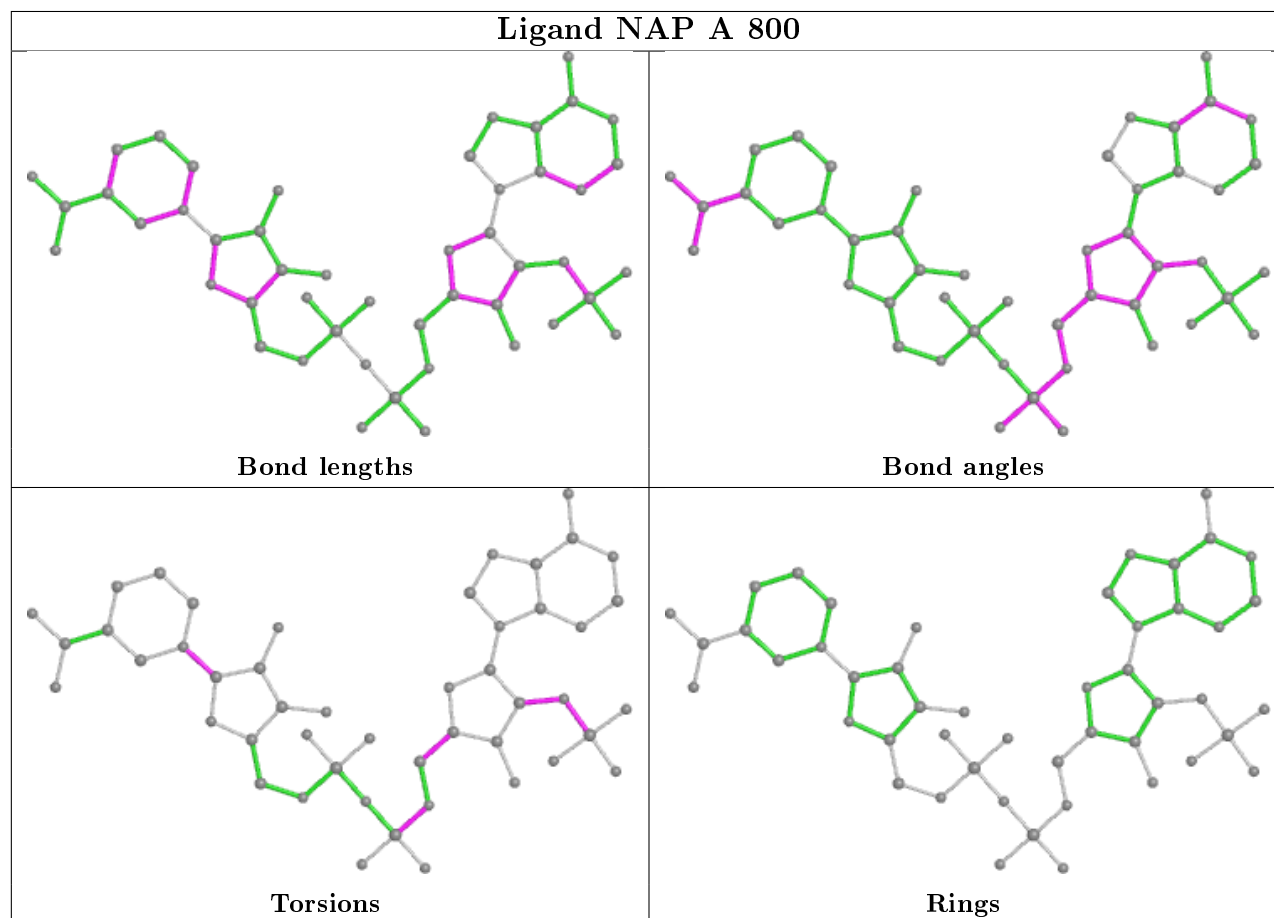
16 monomers are involved in 55 short contacts:

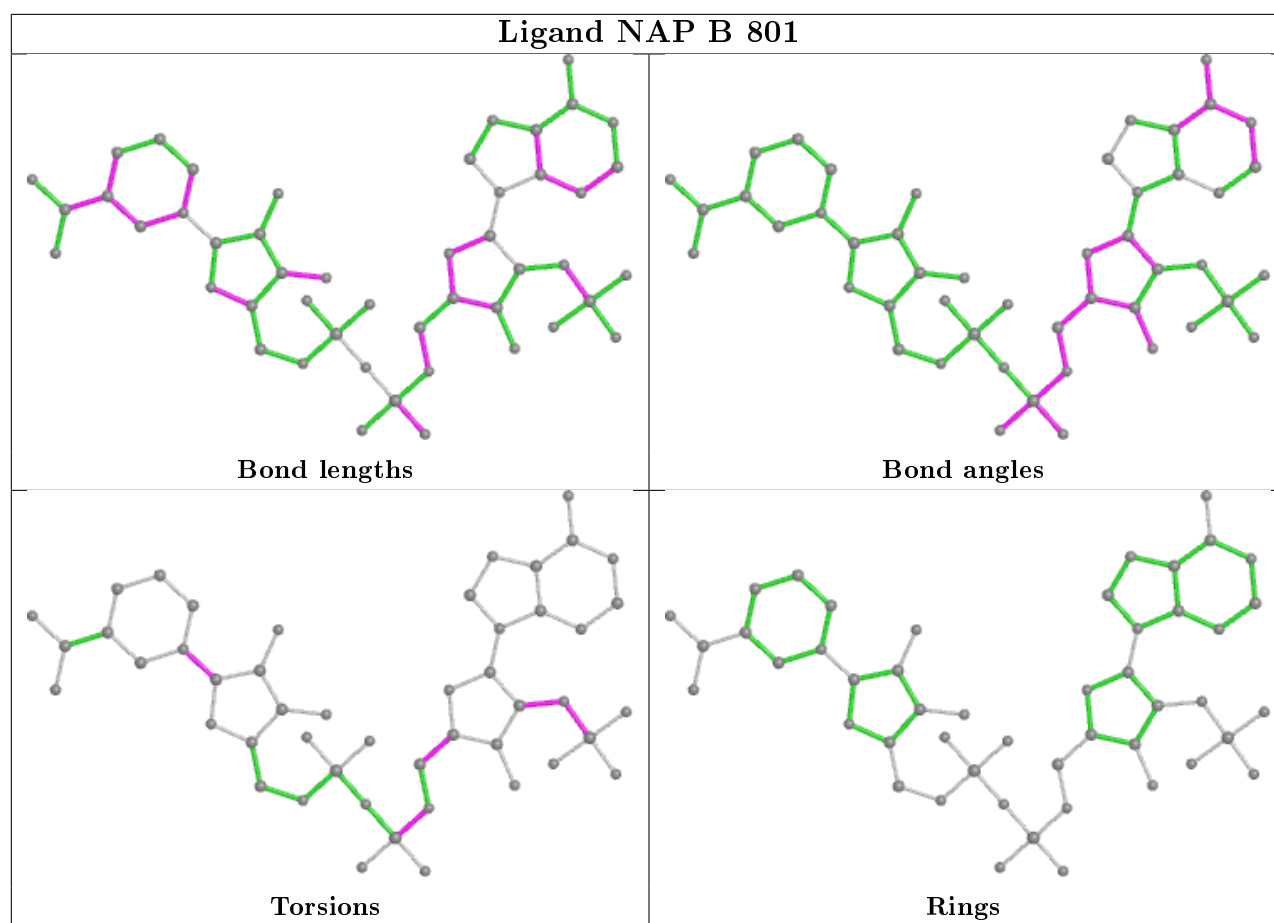
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	4-A	800	NAP	9	0
2	7-B	801	NAP	3	0
2	2-B	801	NAP	1	0
2	2-A	800	NAP	4	0
2	3-B	801	NAP	3	0
2	5-A	800	NAP	2	0
2	6-B	801	NAP	8	0
2	5-B	801	NAP	1	0
2	1-A	800	NAP	5	0
2	1-B	801	NAP	4	0
2	6-A	800	NAP	3	0
2	7-A	800	NAP	2	0
2	4-B	801	NAP	2	0
2	3-A	800	NAP	2	0
2	8-A	800	NAP	4	0
2	8-B	801	NAP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.



Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1-A	253/253 (100%)	0.67	28 (11%) 5 4	10, 21, 42, 58	253 (100%)
1	1-B	253/253 (100%)	0.71	29 (11%) 4 3	8, 21, 43, 62	253 (100%)
1	2-A	253/253 (100%)	0.67	28 (11%) 5 4	10, 21, 42, 58	253 (100%)
1	2-B	253/253 (100%)	0.71	29 (11%) 4 3	8, 21, 43, 62	253 (100%)
1	3-A	253/253 (100%)	0.67	28 (11%) 5 4	10, 21, 42, 58	253 (100%)
1	3-B	253/253 (100%)	0.71	29 (11%) 4 3	8, 21, 43, 62	253 (100%)
1	4-A	253/253 (100%)	0.67	28 (11%) 5 4	10, 21, 42, 58	253 (100%)
1	4-B	253/253 (100%)	0.71	29 (11%) 4 3	8, 21, 43, 62	253 (100%)
1	5-A	253/253 (100%)	0.67	28 (11%) 5 4	10, 21, 42, 58	253 (100%)
1	5-B	253/253 (100%)	0.71	29 (11%) 4 3	8, 21, 43, 62	253 (100%)
1	6-A	253/253 (100%)	0.67	28 (11%) 5 4	10, 21, 42, 58	253 (100%)
1	6-B	253/253 (100%)	0.71	29 (11%) 4 3	8, 21, 43, 62	253 (100%)
1	7-A	253/253 (100%)	0.67	28 (11%) 5 4	10, 21, 42, 58	253 (100%)
1	7-B	253/253 (100%)	0.71	29 (11%) 4 3	8, 21, 43, 62	253 (100%)
1	8-A	253/253 (100%)	0.67	28 (11%) 5 4	10, 21, 42, 58	253 (100%)
1	8-B	253/253 (100%)	0.71	29 (11%) 4 3	8, 21, 43, 62	253 (100%)
All	All	4048/4048 (100%)	0.69	456 (11%) 5 3	8, 21, 45, 62	4048 (100%)

All (456) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-B	86	GLY	6.9
1	2-B	86	GLY	6.9
1	3-B	86	GLY	6.9
1	4-B	86	GLY	6.9
1	5-B	86	GLY	6.9

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Mol	Chain	Res	Type	RSRZ
1	6-B	86	GLY	6.9
1	7-B	86	GLY	6.9
1	8-B	86	GLY	6.9
1	1-A	85	PRO	6.2
1	2-A	85	PRO	6.2
1	3-A	85	PRO	6.2
1	4-A	85	PRO	6.2
1	5-A	85	PRO	6.2
1	6-A	85	PRO	6.2
1	7-A	85	PRO	6.2
1	8-A	85	PRO	6.2
1	1-B	85	PRO	5.9
1	2-B	85	PRO	5.9
1	3-B	85	PRO	5.9
1	4-B	85	PRO	5.9
1	5-B	85	PRO	5.9
1	6-B	85	PRO	5.9
1	7-B	85	PRO	5.9
1	8-B	85	PRO	5.9
1	1-A	1	SER	5.4
1	2-A	1	SER	5.4
1	3-A	1	SER	5.4
1	4-A	1	SER	5.4
1	5-A	1	SER	5.4
1	6-A	1	SER	5.4
1	7-A	1	SER	5.4
1	8-A	1	SER	5.4
1	1-A	93	GLY	4.6
1	2-A	93	GLY	4.6
1	3-A	93	GLY	4.6
1	4-A	93	GLY	4.6
1	5-A	93	GLY	4.6
1	6-A	93	GLY	4.6
1	7-A	93	GLY	4.6
1	8-A	93	GLY	4.6
1	1-A	86	GLY	4.5
1	2-A	86	GLY	4.5
1	3-A	86	GLY	4.5
1	4-A	86	GLY	4.5
1	5-A	86	GLY	4.5
1	6-A	86	GLY	4.5
1	7-A	86	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	8-A	86	GLY	4.5
1	1-B	93	GLY	4.3
1	2-B	93	GLY	4.3
1	3-B	93	GLY	4.3
1	4-B	93	GLY	4.3
1	5-B	93	GLY	4.3
1	6-B	93	GLY	4.3
1	7-B	93	GLY	4.3
1	8-B	93	GLY	4.3
1	1-B	197	GLN	4.2
1	2-B	197	GLN	4.2
1	3-B	197	GLN	4.2
1	4-B	197	GLN	4.2
1	5-B	197	GLN	4.2
1	6-B	197	GLN	4.2
1	7-B	197	GLN	4.2
1	8-B	197	GLN	4.2
1	1-A	101	ASP	3.7
1	2-A	101	ASP	3.7
1	3-A	101	ASP	3.7
1	4-A	101	ASP	3.7
1	5-A	101	ASP	3.7
1	6-A	101	ASP	3.7
1	7-A	101	ASP	3.7
1	8-A	101	ASP	3.7
1	1-B	129	VAL	3.6
1	2-B	129	VAL	3.6
1	3-B	129	VAL	3.6
1	4-B	129	VAL	3.6
1	5-B	129	VAL	3.6
1	6-B	129	VAL	3.6
1	7-B	129	VAL	3.6
1	8-B	129	VAL	3.6
1	1-A	80	VAL	3.6
1	2-A	80	VAL	3.6
1	3-A	80	VAL	3.6
1	4-A	80	VAL	3.6
1	5-A	80	VAL	3.6
1	6-A	80	VAL	3.6
1	7-A	80	VAL	3.6
1	8-A	80	VAL	3.6
1	1-B	198	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	2-B	198	THR	3.5
1	3-B	198	THR	3.5
1	4-B	198	THR	3.5
1	5-B	198	THR	3.5
1	6-B	198	THR	3.5
1	7-B	198	THR	3.5
1	8-B	198	THR	3.5
1	1-B	143	LEU	3.5
1	2-B	143	LEU	3.5
1	3-B	143	LEU	3.5
1	4-B	143	LEU	3.5
1	5-B	143	LEU	3.5
1	6-B	143	LEU	3.5
1	7-B	143	LEU	3.5
1	8-B	143	LEU	3.5
1	1-A	40	ALA	3.4
1	2-A	40	ALA	3.4
1	3-A	40	ALA	3.4
1	4-A	40	ALA	3.4
1	5-A	40	ALA	3.4
1	6-A	40	ALA	3.4
1	7-A	40	ALA	3.4
1	8-A	40	ALA	3.4
1	1-B	131	VAL	3.4
1	2-B	131	VAL	3.4
1	3-B	131	VAL	3.4
1	4-B	131	VAL	3.4
1	5-B	131	VAL	3.4
1	6-B	131	VAL	3.4
1	7-B	131	VAL	3.4
1	8-B	131	VAL	3.4
1	1-B	87	PHE	3.4
1	2-B	87	PHE	3.4
1	3-B	87	PHE	3.4
1	4-B	87	PHE	3.4
1	5-B	87	PHE	3.4
1	6-B	87	PHE	3.4
1	7-B	87	PHE	3.4
1	8-B	87	PHE	3.4
1	1-B	94	ARG	3.3
1	2-B	94	ARG	3.3
1	3-B	94	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	4-B	94	ARG	3.3
1	5-B	94	ARG	3.3
1	6-B	94	ARG	3.3
1	7-B	94	ARG	3.3
1	8-B	94	ARG	3.3
1	1-B	234	GLY	3.1
1	2-B	234	GLY	3.1
1	3-B	234	GLY	3.1
1	4-B	234	GLY	3.1
1	5-B	234	GLY	3.1
1	6-B	234	GLY	3.1
1	7-B	234	GLY	3.1
1	8-B	234	GLY	3.1
1	1-B	172	ILE	3.1
1	2-B	172	ILE	3.1
1	3-B	172	ILE	3.1
1	4-B	172	ILE	3.1
1	5-B	172	ILE	3.1
1	6-B	172	ILE	3.1
1	7-B	172	ILE	3.1
1	8-B	172	ILE	3.1
1	1-A	74	VAL	3.1
1	2-A	74	VAL	3.1
1	3-A	74	VAL	3.1
1	4-A	74	VAL	3.1
1	5-A	74	VAL	3.1
1	6-A	74	VAL	3.1
1	7-A	74	VAL	3.1
1	8-A	74	VAL	3.1
1	1-A	92	GLY	3.0
1	2-A	92	GLY	3.0
1	3-A	92	GLY	3.0
1	4-A	92	GLY	3.0
1	5-A	92	GLY	3.0
1	6-A	92	GLY	3.0
1	7-A	92	GLY	3.0
1	8-A	92	GLY	3.0
1	1-A	91	LYS	3.0
1	2-A	91	LYS	3.0
1	3-A	91	LYS	3.0
1	4-A	91	LYS	3.0
1	5-A	91	LYS	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	6-A	91	LYS	3.0
1	7-A	91	LYS	3.0
1	8-A	91	LYS	3.0
1	1-A	76	LEU	3.0
1	2-A	76	LEU	3.0
1	3-A	76	LEU	3.0
1	4-A	76	LEU	3.0
1	5-A	76	LEU	3.0
1	6-A	76	LEU	3.0
1	7-A	76	LEU	3.0
1	8-A	76	LEU	3.0
1	1-B	200	THR	2.8
1	2-B	200	THR	2.8
1	3-B	200	THR	2.8
1	4-B	200	THR	2.8
1	5-B	200	THR	2.8
1	6-B	200	THR	2.8
1	7-B	200	THR	2.8
1	8-B	200	THR	2.8
1	1-B	138	ASN	2.7
1	2-B	138	ASN	2.7
1	3-B	138	ASN	2.7
1	4-B	138	ASN	2.7
1	5-B	138	ASN	2.7
1	6-B	138	ASN	2.7
1	7-B	138	ASN	2.7
1	8-B	138	ASN	2.7
1	1-A	172	ILE	2.7
1	2-A	172	ILE	2.7
1	3-A	172	ILE	2.7
1	4-A	172	ILE	2.7
1	5-A	172	ILE	2.7
1	6-A	172	ILE	2.7
1	7-A	172	ILE	2.7
1	8-A	172	ILE	2.7
1	1-A	87	PHE	2.7
1	2-A	87	PHE	2.7
1	3-A	87	PHE	2.7
1	4-A	87	PHE	2.7
1	5-A	87	PHE	2.7
1	6-A	87	PHE	2.7
1	7-A	87	PHE	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	8-A	87	PHE	2.7
1	1-A	130	VAL	2.6
1	2-A	130	VAL	2.6
1	3-A	130	VAL	2.6
1	4-A	130	VAL	2.6
1	5-A	130	VAL	2.6
1	6-A	130	VAL	2.6
1	7-A	130	VAL	2.6
1	8-A	130	VAL	2.6
1	1-A	9	VAL	2.6
1	1-B	130	VAL	2.6
1	2-A	9	VAL	2.6
1	2-B	130	VAL	2.6
1	3-A	9	VAL	2.6
1	3-B	130	VAL	2.6
1	4-A	9	VAL	2.6
1	4-B	130	VAL	2.6
1	5-A	9	VAL	2.6
1	5-B	130	VAL	2.6
1	6-A	9	VAL	2.6
1	6-B	130	VAL	2.6
1	7-A	9	VAL	2.6
1	7-B	130	VAL	2.6
1	8-A	9	VAL	2.6
1	8-B	130	VAL	2.6
1	1-B	199	ASP	2.6
1	2-B	199	ASP	2.6
1	3-B	199	ASP	2.6
1	4-B	199	ASP	2.6
1	5-B	199	ASP	2.6
1	6-B	199	ASP	2.6
1	7-B	199	ASP	2.6
1	8-B	199	ASP	2.6
1	1-A	84	LYS	2.6
1	2-A	84	LYS	2.6
1	3-A	84	LYS	2.6
1	4-A	84	LYS	2.6
1	5-A	84	LYS	2.6
1	6-A	84	LYS	2.6
1	7-A	84	LYS	2.6
1	8-A	84	LYS	2.6
1	1-A	235	THR	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	2-A	235	THR	2.6
1	3-A	235	THR	2.6
1	4-A	235	THR	2.6
1	5-A	235	THR	2.6
1	6-A	235	THR	2.6
1	7-A	235	THR	2.6
1	8-A	235	THR	2.6
1	1-B	75	ILE	2.5
1	2-B	75	ILE	2.5
1	3-B	75	ILE	2.5
1	4-B	75	ILE	2.5
1	5-B	75	ILE	2.5
1	6-B	75	ILE	2.5
1	7-B	75	ILE	2.5
1	8-B	75	ILE	2.5
1	1-B	228	LEU	2.5
1	2-B	228	LEU	2.5
1	3-B	228	LEU	2.5
1	4-B	228	LEU	2.5
1	5-B	228	LEU	2.5
1	6-B	228	LEU	2.5
1	7-B	228	LEU	2.5
1	8-B	228	LEU	2.5
1	1-B	202	THR	2.5
1	2-B	202	THR	2.5
1	3-B	202	THR	2.5
1	4-B	202	THR	2.5
1	5-B	202	THR	2.5
1	6-B	202	THR	2.5
1	7-B	202	THR	2.5
1	8-B	202	THR	2.5
1	1-B	140	ASP	2.5
1	2-B	140	ASP	2.5
1	3-B	140	ASP	2.5
1	4-B	140	ASP	2.5
1	5-B	140	ASP	2.5
1	6-B	140	ASP	2.5
1	7-B	140	ASP	2.5
1	8-B	140	ASP	2.5
1	1-A	83	MET	2.4
1	2-A	83	MET	2.4
1	3-A	83	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	4-A	83	MET	2.4
1	5-A	83	MET	2.4
1	6-A	83	MET	2.4
1	7-A	83	MET	2.4
1	8-A	83	MET	2.4
1	1-A	131	VAL	2.4
1	2-A	131	VAL	2.4
1	3-A	131	VAL	2.4
1	4-A	131	VAL	2.4
1	5-A	131	VAL	2.4
1	6-A	131	VAL	2.4
1	7-A	131	VAL	2.4
1	8-A	131	VAL	2.4
1	1-A	244	ALA	2.4
1	2-A	244	ALA	2.4
1	3-A	244	ALA	2.4
1	4-A	244	ALA	2.4
1	5-A	244	ALA	2.4
1	6-A	244	ALA	2.4
1	7-A	244	ALA	2.4
1	8-A	244	ALA	2.4
1	1-B	74	VAL	2.4
1	2-B	74	VAL	2.4
1	3-B	74	VAL	2.4
1	4-B	74	VAL	2.4
1	5-B	74	VAL	2.4
1	6-B	74	VAL	2.4
1	7-B	74	VAL	2.4
1	8-B	74	VAL	2.4
1	1-A	228	LEU	2.3
1	2-A	228	LEU	2.3
1	3-A	228	LEU	2.3
1	4-A	228	LEU	2.3
1	5-A	228	LEU	2.3
1	6-A	228	LEU	2.3
1	7-A	228	LEU	2.3
1	8-A	228	LEU	2.3
1	1-A	61	ASP	2.3
1	2-A	61	ASP	2.3
1	3-A	61	ASP	2.3
1	4-A	61	ASP	2.3
1	5-A	61	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	6-A	61	ASP	2.3
1	7-A	61	ASP	2.3
1	8-A	61	ASP	2.3
1	1-B	180	LYS	2.3
1	2-B	180	LYS	2.3
1	3-B	180	LYS	2.3
1	4-B	180	LYS	2.3
1	5-B	180	LYS	2.3
1	6-B	180	LYS	2.3
1	7-B	180	LYS	2.3
1	8-B	180	LYS	2.3
1	1-A	95	PRO	2.3
1	1-B	95	PRO	2.3
1	2-A	95	PRO	2.3
1	2-B	95	PRO	2.3
1	3-A	95	PRO	2.3
1	3-B	95	PRO	2.3
1	4-A	95	PRO	2.3
1	4-B	95	PRO	2.3
1	5-A	95	PRO	2.3
1	5-B	95	PRO	2.3
1	6-A	95	PRO	2.3
1	6-B	95	PRO	2.3
1	7-A	95	PRO	2.3
1	7-B	95	PRO	2.3
1	8-A	95	PRO	2.3
1	8-B	95	PRO	2.3
1	1-A	41	GLN	2.2
1	2-A	41	GLN	2.2
1	3-A	41	GLN	2.2
1	4-A	41	GLN	2.2
1	5-A	41	GLN	2.2
1	6-A	41	GLN	2.2
1	7-A	41	GLN	2.2
1	8-A	41	GLN	2.2
1	1-A	82	LYS	2.2
1	2-A	82	LYS	2.2
1	3-A	82	LYS	2.2
1	4-A	82	LYS	2.2
1	5-A	82	LYS	2.2
1	6-A	82	LYS	2.2
1	7-A	82	LYS	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	8-A	82	LYS	2.2
1	1-A	184	VAL	2.2
1	2-A	184	VAL	2.2
1	3-A	184	VAL	2.2
1	4-A	184	VAL	2.2
1	5-A	184	VAL	2.2
1	6-A	184	VAL	2.2
1	7-A	184	VAL	2.2
1	8-A	184	VAL	2.2
1	1-B	73	LEU	2.2
1	2-B	73	LEU	2.2
1	3-B	73	LEU	2.2
1	4-B	73	LEU	2.2
1	5-B	73	LEU	2.2
1	6-B	73	LEU	2.2
1	7-B	73	LEU	2.2
1	8-B	73	LEU	2.2
1	1-A	44	GLU	2.2
1	2-A	44	GLU	2.2
1	3-A	44	GLU	2.2
1	4-A	44	GLU	2.2
1	5-A	44	GLU	2.2
1	6-A	44	GLU	2.2
1	7-A	44	GLU	2.2
1	8-A	44	GLU	2.2
1	1-B	196	LEU	2.1
1	2-B	196	LEU	2.1
1	3-B	196	LEU	2.1
1	4-B	196	LEU	2.1
1	5-B	196	LEU	2.1
1	6-B	196	LEU	2.1
1	7-B	196	LEU	2.1
1	8-B	196	LEU	2.1
1	1-B	41	GLN	2.1
1	2-B	41	GLN	2.1
1	3-B	41	GLN	2.1
1	4-B	41	GLN	2.1
1	5-B	41	GLN	2.1
1	6-B	41	GLN	2.1
1	7-B	41	GLN	2.1
1	8-B	41	GLN	2.1
1	1-A	75	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	2-A	75	ILE	2.1
1	3-A	75	ILE	2.1
1	4-A	75	ILE	2.1
1	5-A	75	ILE	2.1
1	6-A	75	ILE	2.1
1	7-A	75	ILE	2.1
1	8-A	75	ILE	2.1
1	1-B	84	LYS	2.1
1	2-B	84	LYS	2.1
1	3-B	84	LYS	2.1
1	4-B	84	LYS	2.1
1	5-B	84	LYS	2.1
1	6-B	84	LYS	2.1
1	7-B	84	LYS	2.1
1	8-B	84	LYS	2.1
1	1-B	128	ILE	2.1
1	2-B	128	ILE	2.1
1	3-B	128	ILE	2.1
1	4-B	128	ILE	2.1
1	5-B	128	ILE	2.1
1	6-B	128	ILE	2.1
1	7-B	128	ILE	2.1
1	8-B	128	ILE	2.1
1	1-B	187	LEU	2.0
1	2-B	187	LEU	2.0
1	3-B	187	LEU	2.0
1	4-B	187	LEU	2.0
1	5-B	187	LEU	2.0
1	6-B	187	LEU	2.0
1	7-B	187	LEU	2.0
1	8-B	187	LEU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

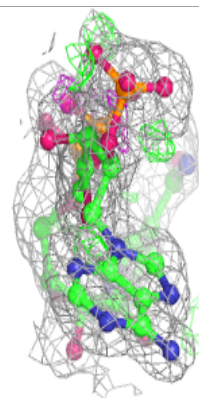
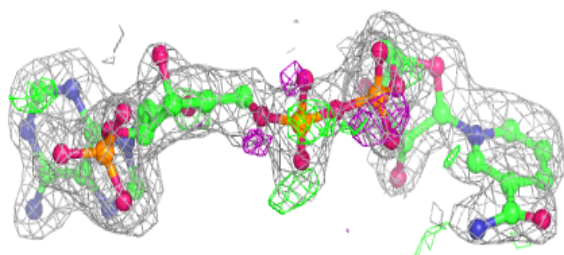
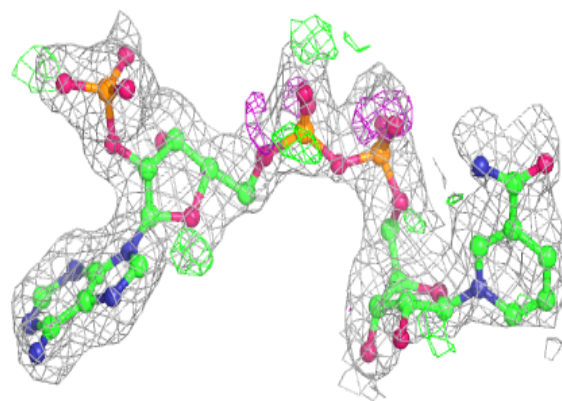
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAP	7-B	801	48/48	0.91	0.15	15,24,29,30	48
2	NAP	2-B	801	48/48	0.91	0.15	18,25,29,29	48
2	NAP	3-B	801	48/48	0.91	0.15	17,24,29,30	48
2	NAP	6-B	801	48/48	0.91	0.15	19,24,29,31	48
2	NAP	5-B	801	48/48	0.91	0.15	18,24,28,30	48
2	NAP	1-B	801	48/48	0.91	0.15	20,25,30,31	48
2	NAP	4-B	801	48/48	0.91	0.15	19,25,30,32	48
2	NAP	8-B	801	48/48	0.91	0.15	14,24,28,30	48
2	NAP	1-A	800	48/48	0.93	0.12	17,23,30,33	48
2	NAP	5-A	800	48/48	0.93	0.12	18,23,28,30	48
2	NAP	6-A	800	48/48	0.93	0.12	16,22,30,32	48
2	NAP	7-A	800	48/48	0.93	0.12	17,23,29,30	48
2	NAP	2-A	800	48/48	0.93	0.12	17,22,29,32	48
2	NAP	3-A	800	48/48	0.93	0.12	15,22,29,31	48
2	NAP	8-A	800	48/48	0.93	0.12	13,23,29,31	48
2	NAP	4-A	800	48/48	0.93	0.12	17,23,28,30	48

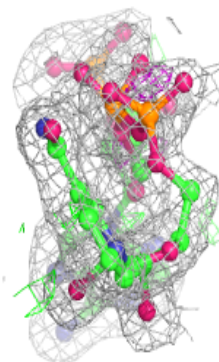
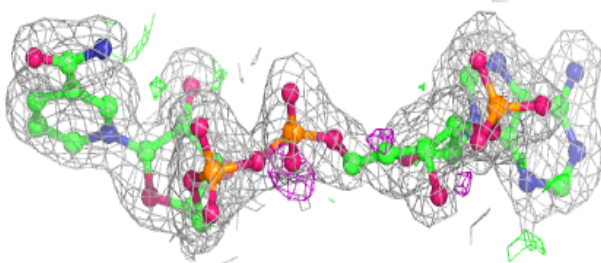
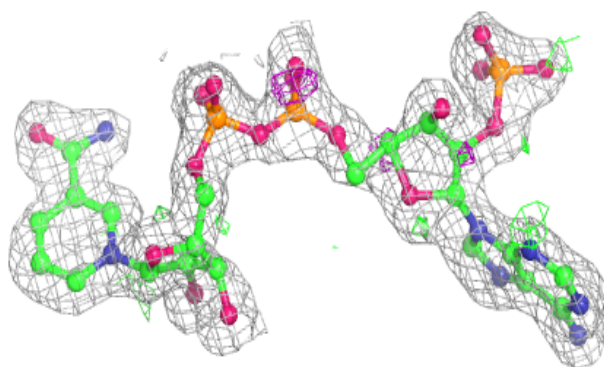
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAP B 801:**

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

**Electron density around NAP A 800:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.