



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 08:37 am BST

PDB ID : 1JN0  
Title : Crystal structure of the non-regulatory A4 isoform of spinach chloroplast glyceraldehyde-3-phosphate dehydrogenase complexed with NADP  
Authors : Fermani, S.; Ripamonti, A.; Sabatino, P.; Zanotti, G.; Scagliarini, S.; Sparla, F.; Trost, P.; Pupillo, P.  
Deposited on : 2001-07-21  
Resolution : 3.00 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

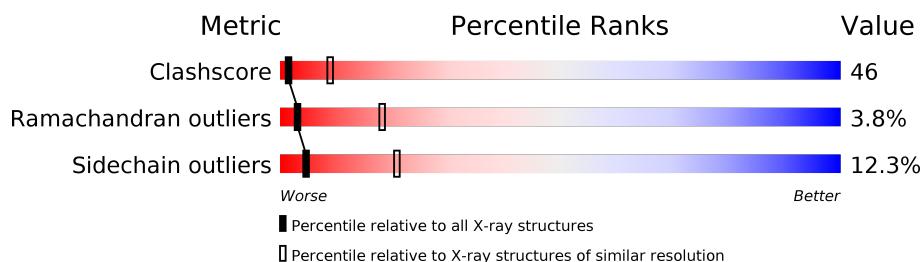
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	335	
1	B	335	
1	O	335	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7949 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 GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	334	Total	C	N	O	S	0	0	0
			2521	1589	439	482	11			
1	A	334	Total	C	N	O	S	0	0	0
			2521	1589	439	482	11			
1	B	334	Total	C	N	O	S	0	0	0
			2521	1589	439	482	11			

There are 6 discrepancies between the modelled and reference sequences:

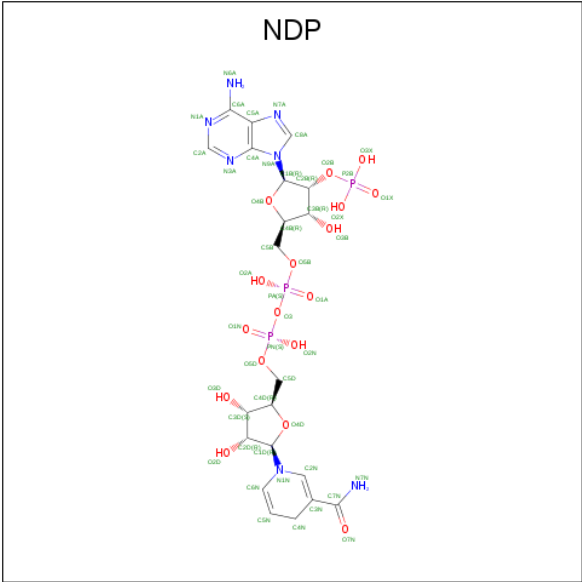
Chain	Residue	Modelled	Actual	Comment	Reference
O	?	-	ARG	DELETION	UNP P19866
O	?	-	ASP	DELETION	UNP P19866
A	?	-	ARG	DELETION	UNP P19866
A	?	-	ASP	DELETION	UNP P19866
B	?	-	ARG	DELETION	UNP P19866
B	?	-	ASP	DELETION	UNP P19866

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



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

- Molecule 4 is water.

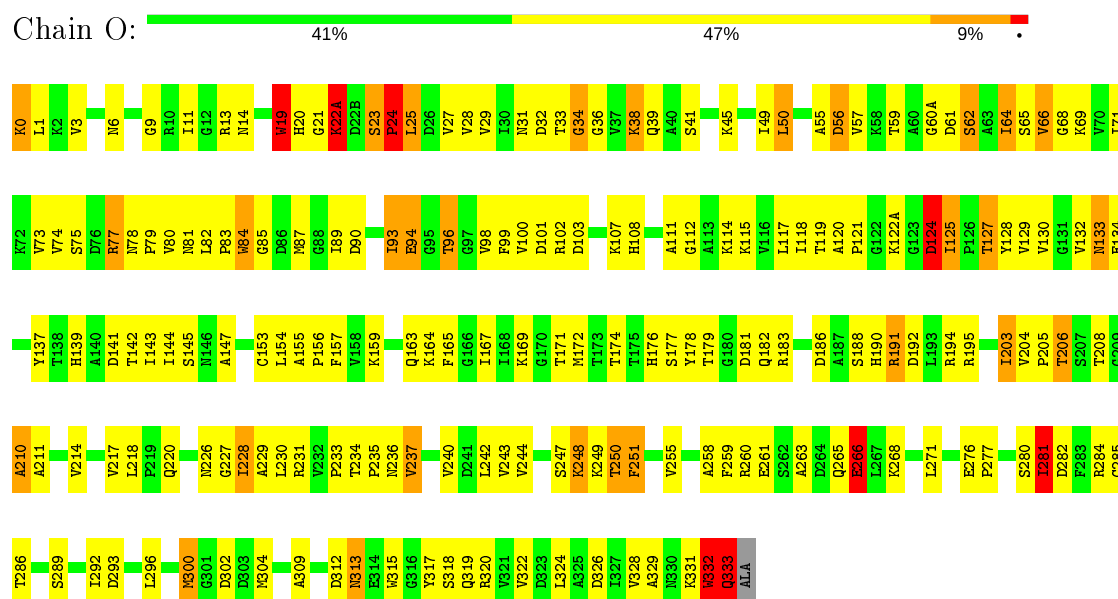
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	87	Total	O	0	0
			87	87		
4	A	65	Total	O	0	0
			65	65		
4	B	60	Total	O	0	0
			60	60		

### 3 Residue-property plots

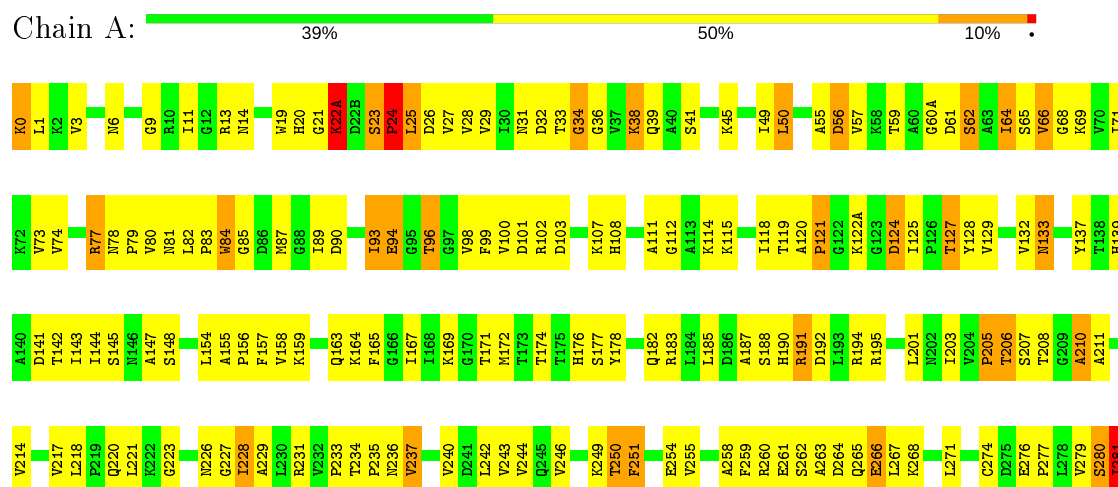
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

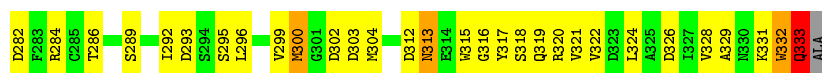
Note EDS was not executed.

#### • Molecule 1: GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE A



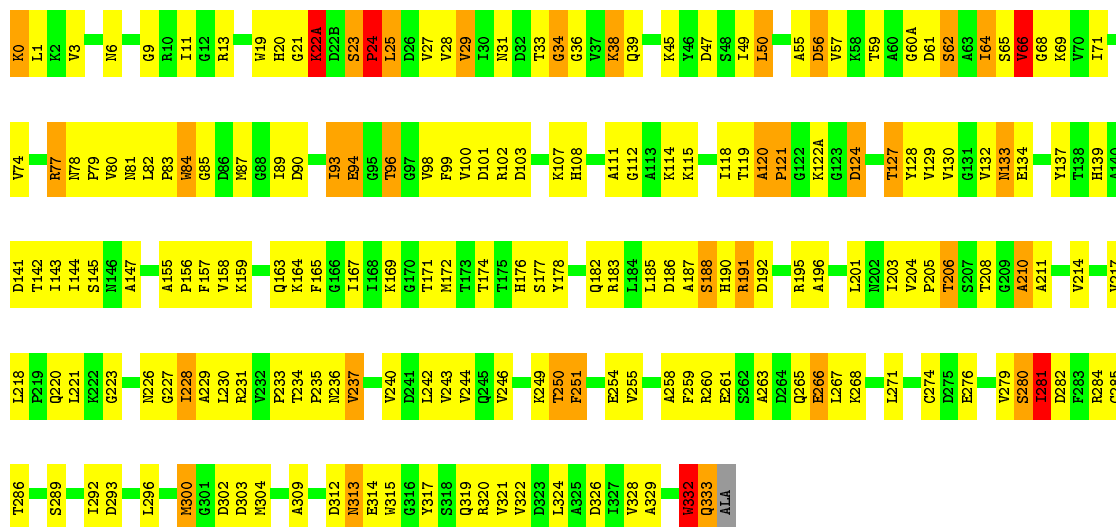
#### • Molecule 1: GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE A





• Molecule 1: GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE A

Chain B: 42% 47% 10%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.25Å 182.18Å 106.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.58 – 3.00	Depositor
% Data completeness (in resolution range)	93.0 (49.58-3.00)	Depositor
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.13	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.213 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7949	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.58	3/2562 (0.1%)	0.76	2/3479 (0.1%)
1	B	0.52	2/2562 (0.1%)	0.75	5/3479 (0.1%)
1	O	0.65	4/2562 (0.2%)	0.84	8/3479 (0.2%)
All	All	0.58	9/7686 (0.1%)	0.78	15/10437 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	266	GLU	CD-OE1	-11.03	1.13	1.25
1	O	333	GLN	CD-OE1	-7.77	1.06	1.24
1	A	333	GLN	CD-OE1	-6.64	1.09	1.24
1	A	333	GLN	C-O	-6.21	1.11	1.23
1	B	333	GLN	CD-OE1	-5.85	1.11	1.24
1	A	266	GLU	CD-OE1	-5.43	1.19	1.25
1	B	266	GLU	CD-OE1	-5.27	1.19	1.25
1	O	19	TRP	CB-CG	-5.26	1.40	1.50
1	O	19	TRP	CG-CD1	-5.01	1.29	1.36

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	19	TRP	CA-CB-CG	12.31	137.08	113.70
1	O	19	TRP	CB-CG-CD1	-9.65	114.45	127.00
1	O	19	TRP	CB-CG-CD2	8.50	137.65	126.60
1	O	333	GLN	CB-CA-C	-6.22	97.96	110.40
1	B	121	PRO	CA-N-CD	-5.99	103.11	111.50
1	A	24	PRO	N-CA-C	5.57	126.57	112.10
1	B	332	TRP	N-CA-C	5.47	125.77	111.00
1	O	24	PRO	N-CA-C	5.44	126.24	112.10
1	B	203	ILE	N-CA-C	-5.40	96.42	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	333	GLN	CB-CA-C	5.36	121.12	110.40
1	O	19	TRP	N-CA-CB	-5.30	101.05	110.60
1	O	124	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	B	24	PRO	N-CA-C	5.11	125.38	112.10
1	A	203	ILE	N-CA-C	-5.08	97.28	111.00
1	O	203	ILE	N-CA-C	-5.07	97.31	111.00

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	A	2521	0	2558	256	0
1	B	2521	0	2561	232	0
1	O	2521	0	2562	240	0
2	A	10	0	0	1	0
2	B	10	0	0	0	0
2	O	10	0	0	0	0
3	A	48	0	26	5	0
3	B	48	0	26	5	0
3	O	48	0	26	7	0
4	A	65	0	0	8	0
4	B	60	0	0	9	0
4	O	87	0	0	11	0
All	All	7949	0	7759	718	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 46.

All (718) 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:O:56:ASP:H	1:O:66:VAL:CG1	1.21	1.50
1:A:56:ASP:H	1:A:66:VAL:CG1	1.25	1.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ASP:N	1:B:66:VAL:HG12	1.45	1.31
1:B:56:ASP:H	1:B:66:VAL:CG1	1.46	1.28
1:O:56:ASP:N	1:O:66:VAL:CG1	2.04	1.19
1:A:56:ASP:N	1:A:66:VAL:CG1	2.09	1.15
1:A:0:LYS:HB3	4:A:1387:HOH:O	1.47	1.13
1:A:333:GLN:O	1:A:333:GLN:NE2	1.82	1.12
1:A:183:ARG:HD2	1:A:187:ALA:HB3	1.26	1.11
1:A:56:ASP:H	1:A:66:VAL:HG12	1.01	1.10
1:O:56:ASP:H	1:O:66:VAL:HG12	0.92	1.09
1:A:333:GLN:O	1:A:333:GLN:CD	1.92	1.08
1:A:332:TRP:CE3	1:A:333:GLN:CB	2.37	1.08
1:B:260:ARG:NH2	4:B:2365:HOH:O	1.89	1.05
1:A:19:TRP:HE1	1:A:27:VAL:HG21	1.17	1.05
1:A:38:LYS:H	1:A:38:LYS:HD3	1.17	1.05
1:B:38:LYS:H	1:B:38:LYS:HD3	1.19	1.05
1:O:38:LYS:HD3	1:O:38:LYS:H	1.20	1.04
1:O:56:ASP:N	1:O:66:VAL:HG12	1.68	1.03
1:B:24:PRO:HG3	4:B:2339:HOH:O	1.60	1.01
1:A:332:TRP:CE3	1:A:333:GLN:HB2	1.93	1.01
1:O:19:TRP:NE1	1:O:27:VAL:HG23	1.76	1.00
1:O:19:TRP:HE1	1:O:27:VAL:CG2	1.75	1.00
1:B:24:PRO:HB3	1:B:25:LEU:HD12	1.44	1.00
1:O:19:TRP:HE1	1:O:27:VAL:HG23	1.26	0.99
1:B:19:TRP:HE1	1:B:27:VAL:HG21	1.28	0.98
1:A:332:TRP:CE3	1:A:333:GLN:HB3	1.98	0.98
1:A:56:ASP:HB2	1:A:66:VAL:HG12	1.46	0.97
1:A:56:ASP:H	1:A:66:VAL:HG13	1.24	0.97
1:O:24:PRO:HB3	1:O:25:LEU:HD12	1.48	0.95
1:A:56:ASP:N	1:A:66:VAL:HG12	1.77	0.95
1:O:56:ASP:H	1:O:66:VAL:HG13	1.32	0.94
1:B:333:GLN:NE2	1:B:333:GLN:O	2.01	0.93
1:O:56:ASP:HB2	1:O:66:VAL:HG12	1.50	0.93
1:A:96:THR:OG1	1:A:98:VAL:HG22	1.69	0.93
1:A:19:TRP:HE1	1:A:27:VAL:CG2	1.82	0.93
1:B:183:ARG:HD2	1:B:187:ALA:HB3	1.48	0.92
1:A:24:PRO:HB3	1:A:25:LEU:HD12	1.52	0.92
1:A:332:TRP:CZ3	1:A:333:GLN:CB	2.53	0.91
1:B:129:VAL:H	1:B:133:ASN:HD21	1.18	0.91
1:A:124:ASP:HB3	4:A:1361:HOH:O	1.70	0.91
1:O:56:ASP:N	1:O:66:VAL:HG13	1.85	0.90
1:O:19:TRP:NE1	1:O:27:VAL:CG2	2.35	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ASP:N	1:A:66:VAL:HG13	1.81	0.89
1:B:55:ALA:HB1	1:B:66:VAL:HG13	1.53	0.89
2:A:1336:SO4:O2	4:A:1343:HOH:O	1.91	0.88
1:A:129:VAL:H	1:A:133:ASN:HD21	1.21	0.88
1:A:25:LEU:H	1:A:25:LEU:HD12	1.39	0.87
1:O:96:THR:OG1	1:O:98:VAL:HG22	1.74	0.87
1:O:79:PRO:HB2	1:O:107:LYS:HB3	1.56	0.87
1:B:96:THR:OG1	1:B:98:VAL:HG22	1.73	0.87
1:O:25:LEU:HD12	1:O:25:LEU:H	1.40	0.86
1:O:129:VAL:H	1:O:133:ASN:HD21	1.22	0.86
1:A:24:PRO:HG3	4:A:1388:HOH:O	1.75	0.86
1:O:19:TRP:CE2	1:O:27:VAL:HG23	2.10	0.86
1:B:79:PRO:HB2	1:B:107:LYS:HB3	1.58	0.85
1:A:79:PRO:HB2	1:A:107:LYS:HB3	1.58	0.85
1:A:119:THR:O	1:A:119:THR:HG22	1.77	0.84
1:B:25:LEU:HD12	1:B:25:LEU:H	1.43	0.83
1:A:121:PRO:HD3	1:A:147:ALA:C	1.99	0.83
1:O:65:SER:O	1:O:68:GLY:N	2.10	0.83
1:O:56:ASP:CB	1:O:66:VAL:HG12	2.08	0.83
1:O:19:TRP:CZ2	1:O:27:VAL:HG23	2.14	0.82
1:A:22(A):LYS:HE3	1:A:322:VAL:HG11	1.58	0.82
1:A:142:THR:HG23	1:A:143:ILE:HG13	1.61	0.82
1:O:121:PRO:HD3	1:O:147:ALA:C	2.00	0.82
1:A:261:GLU:O	1:A:265:GLN:HG2	1.79	0.82
1:A:56:ASP:CB	1:A:66:VAL:HG12	2.10	0.81
1:A:65:SER:O	1:A:68:GLY:N	2.12	0.81
1:A:129:VAL:H	1:A:133:ASN:ND2	1.77	0.81
1:A:332:TRP:CZ3	1:A:333:GLN:HB2	2.14	0.81
1:O:25:LEU:HA	4:O:6340:HOH:O	1.80	0.81
1:O:64:ILE:C	1:O:64:ILE:HD12	2.02	0.80
1:B:129:VAL:H	1:B:133:ASN:ND2	1.79	0.80
1:B:56:ASP:H	1:B:66:VAL:HG12	0.67	0.80
1:O:38:LYS:CD	1:O:38:LYS:H	1.95	0.80
1:A:90:ASP:HB3	1:A:333:GLN:OE1	1.81	0.80
1:O:119:THR:O	1:O:119:THR:HG22	1.80	0.80
1:A:19:TRP:NE1	1:A:27:VAL:CG2	2.45	0.80
1:B:167:ILE:HG12	1:B:244:VAL:HG21	1.62	0.80
1:B:90:ASP:HB3	1:B:333:GLN:HE22	1.46	0.80
1:A:19:TRP:NE1	1:A:27:VAL:HG21	1.96	0.80
1:O:236:ASN:OD1	1:O:313:ASN:ND2	2.14	0.80
1:B:77:ARG:H	1:B:77:ARG:HD3	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:228:ILE:HD13	1:O:228:ILE:H	1.46	0.79
1:A:332:TRP:HE3	1:A:333:GLN:HB3	1.44	0.79
1:B:228:ILE:HD13	1:B:228:ILE:H	1.45	0.79
1:O:183:ARG:NH1	1:O:190:HIS:HD2	1.81	0.79
1:A:167:ILE:HG12	1:A:244:VAL:HG21	1.63	0.79
1:O:129:VAL:H	1:O:133:ASN:ND2	1.80	0.79
1:O:77:ARG:HD3	1:O:77:ARG:H	1.47	0.79
1:O:183:ARG:NH1	1:O:190:HIS:CD2	2.50	0.78
1:A:228:ILE:HD13	1:A:228:ILE:H	1.45	0.78
1:B:100:VAL:HG23	1:B:122(A):LYS:HG2	1.65	0.78
1:B:142:THR:HG23	1:B:143:ILE:HG13	1.64	0.78
1:B:101:ASP:HA	1:B:122(A):LYS:HB2	1.67	0.77
1:B:19:TRP:HE1	1:B:27:VAL:CG2	1.96	0.77
1:B:65:SER:O	1:B:68:GLY:N	2.17	0.77
1:B:56:ASP:N	1:B:66:VAL:CG1	2.22	0.76
1:O:22(A):LYS:HE3	1:O:322:VAL:HG11	1.65	0.76
1:O:62:SER:HB2	1:O:71:ILE:O	1.85	0.76
1:B:19:TRP:NE1	1:B:27:VAL:HG21	1.99	0.76
1:B:155:ALA:HB3	1:B:156:PRO:HD3	1.65	0.76
1:B:78:ASN:OD1	1:B:80:VAL:HG22	1.86	0.76
1:B:22(A):LYS:HE3	1:B:322:VAL:HG11	1.66	0.76
1:A:38:LYS:CD	1:A:38:LYS:H	1.93	0.76
1:O:167:ILE:HG12	1:O:244:VAL:HG21	1.67	0.76
1:A:100:VAL:HG23	1:A:122(A):LYS:HG2	1.67	0.76
1:O:19:TRP:HZ2	1:O:27:VAL:H	1.34	0.76
1:A:77:ARG:HD3	1:A:77:ARG:H	1.49	0.75
1:O:142:THR:HG23	1:O:143:ILE:HG13	1.66	0.75
1:O:155:ALA:HB3	1:O:156:PRO:HD3	1.66	0.75
1:B:66:VAL:O	1:B:66:VAL:HG23	1.86	0.75
1:A:236:ASN:OD1	1:A:313:ASN:ND2	2.20	0.75
1:B:23:SER:N	1:B:24:PRO:HD3	2.02	0.75
1:A:83:PRO:HB2	1:A:87:MET:HE3	1.70	0.73
1:A:332:TRP:CZ3	1:A:333:GLN:HB3	2.21	0.73
1:B:62:SER:HB2	1:B:71:ILE:O	1.88	0.73
1:O:124:ASP:OD2	4:O:6363:HOH:O	2.06	0.73
1:A:332:TRP:HE3	1:A:333:GLN:CB	1.96	0.73
1:B:121:PRO:HD3	1:B:147:ALA:C	2.08	0.73
1:B:19:TRP:NE1	1:B:27:VAL:CG2	2.52	0.73
1:O:78:ASN:OD1	1:O:80:VAL:HG22	1.88	0.72
1:O:159:LYS:HG2	1:O:163:GLN:HE21	1.54	0.72
1:A:23:SER:N	1:A:24:PRO:HD3	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:23:SER:N	1:O:24:PRO:HD3	2.04	0.72
1:O:19:TRP:HA	1:O:22(A):LYS:HB2	1.72	0.72
1:O:100:VAL:HG23	1:O:122(A):LYS:HG2	1.70	0.72
1:A:155:ALA:HB3	1:A:156:PRO:HD3	1.71	0.72
1:O:101:ASP:HA	1:O:122(A):LYS:HB2	1.72	0.72
1:O:114:LYS:HD3	1:O:333:GLN:CD	2.10	0.71
1:A:159:LYS:HG2	1:A:163:GLN:HE21	1.55	0.71
1:A:78:ASN:OD1	1:A:80:VAL:HG22	1.90	0.71
1:B:250:THR:HG23	1:B:251:PHE:N	2.06	0.70
1:B:236:ASN:OD1	1:B:313:ASN:ND2	2.24	0.70
1:A:28:VAL:HG23	1:A:29:VAL:HG23	1.72	0.70
1:B:119:THR:O	1:B:119:THR:HG22	1.90	0.70
1:O:28:VAL:HG23	1:O:29:VAL:HG23	1.73	0.70
1:A:101:ASP:HA	1:A:122(A):LYS:HB2	1.74	0.70
1:B:100:VAL:HG23	1:B:122(A):LYS:CG	2.22	0.70
1:O:11:ILE:HD11	3:O:6335:NDP:C3N	2.22	0.70
1:A:19:TRP:HA	1:A:22(A):LYS:HB2	1.74	0.69
1:A:207:SER:N	4:A:1399:HOH:O	2.25	0.69
1:A:62:SER:HB2	1:A:71:ILE:O	1.91	0.69
1:A:64:ILE:O	1:A:64:ILE:HG13	1.91	0.69
1:B:28:VAL:HG23	1:B:29:VAL:HG23	1.73	0.69
1:A:333:GLN:C	1:A:333:GLN:NE2	2.46	0.68
1:B:24:PRO:CB	1:B:25:LEU:HD12	2.23	0.68
1:O:83:PRO:HB2	1:O:87:MET:HE3	1.74	0.68
1:B:249:LYS:HA	1:B:302:ASP:O	1.94	0.68
1:B:165:PHE:HE2	1:B:250:THR:HG1	1.37	0.68
1:A:100:VAL:HG23	1:A:122(A):LYS:CG	2.24	0.68
1:O:100:VAL:HG23	1:O:122(A):LYS:CG	2.24	0.68
1:O:191:ARG:HG2	1:O:191:ARG:HH11	1.58	0.68
1:B:83:PRO:HB2	1:B:87:MET:HE3	1.75	0.68
1:A:33:THR:HG23	3:A:1335:NDP:C2A	2.24	0.67
1:B:159:LYS:HG2	1:B:163:GLN:HE21	1.60	0.67
1:A:139:HIS:HB2	1:A:331:LYS:O	1.93	0.67
1:A:11:ILE:HD11	3:A:1335:NDP:C3N	2.26	0.66
1:B:19:TRP:HA	1:B:22(A):LYS:HB2	1.78	0.66
1:A:22(A):LYS:HE3	1:A:322:VAL:CG1	2.26	0.65
1:B:24:PRO:HB3	1:B:25:LEU:CD1	2.21	0.65
1:O:56:ASP:CA	1:O:66:VAL:HG12	2.26	0.65
1:B:228:ILE:N	1:B:228:ILE:HD13	2.11	0.65
1:B:271:LEU:HD11	1:B:292:ILE:HG12	1.78	0.65
1:O:129:VAL:N	1:O:133:ASN:HD21	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:ILE:HG13	1:B:64:ILE:O	1.96	0.65
1:A:177:SER:HB3	1:A:234:THR:O	1.97	0.65
1:O:177:SER:HB3	1:O:234:THR:O	1.96	0.65
1:B:129:VAL:N	1:B:133:ASN:HD21	1.92	0.64
1:A:191:ARG:HH11	1:A:191:ARG:HG2	1.62	0.64
1:O:228:ILE:N	1:O:228:ILE:HD13	2.13	0.64
1:O:24:PRO:HB3	1:O:25:LEU:CD1	2.25	0.64
1:A:326:ASP:O	1:A:329:ALA:HB3	1.98	0.63
1:B:211:ALA:HB1	1:B:226:ASN:HA	1.80	0.63
1:O:183:ARG:HH12	1:O:190:HIS:CD2	2.16	0.63
1:A:228:ILE:HD13	1:A:228:ILE:N	2.13	0.63
1:B:59:THR:HG22	1:B:60(A):GLY:H	1.64	0.63
1:B:6:ASN:HD22	1:B:96:THR:HG21	1.63	0.62
1:O:211:ALA:HB1	1:O:226:ASN:HA	1.81	0.62
1:O:284:ARG:HD2	4:O:6370:HOH:O	1.99	0.62
1:B:19:TRP:O	1:B:20:HIS:C	2.37	0.62
1:A:144:ILE:HG21	1:A:324:LEU:HD21	1.82	0.62
1:B:64:ILE:HD12	1:B:65:SER:O	1.98	0.62
1:B:6:ASN:ND2	1:B:96:THR:HG21	2.13	0.62
1:O:6:ASN:ND2	1:O:96:THR:HG21	2.14	0.62
1:A:19:TRP:NE1	1:A:27:VAL:HG23	2.13	0.62
1:B:55:ALA:HA	1:B:66:VAL:HG11	1.81	0.62
1:A:59:THR:HG22	1:A:60(A):GLY:H	1.65	0.62
1:B:38:LYS:CD	1:B:38:LYS:H	1.95	0.62
1:A:24:PRO:CB	1:A:25:LEU:HD12	2.30	0.61
1:B:144:ILE:HG21	1:B:324:LEU:HD21	1.81	0.61
1:O:55:ALA:HB1	1:O:66:VAL:HG13	1.81	0.61
1:B:191:ARG:HG2	1:B:191:ARG:HH11	1.65	0.61
1:B:332:TRP:CE3	1:B:333:GLN:HB3	2.35	0.61
1:B:177:SER:HB3	1:B:234:THR:O	2.01	0.61
1:O:28:VAL:HG23	1:O:29:VAL:CG2	2.31	0.61
1:B:129:VAL:HG23	1:B:217:VAL:HG11	1.82	0.61
1:A:137:TYR:CE1	1:A:144:ILE:HD11	2.36	0.61
1:A:19:TRP:O	1:A:20:HIS:C	2.37	0.61
1:O:24:PRO:HA	4:O:6356:HOH:O	2.00	0.61
1:O:64:ILE:HD12	1:O:65:SER:O	2.01	0.61
1:A:129:VAL:N	1:A:133:ASN:HD21	1.94	0.61
1:B:66:VAL:O	1:B:66:VAL:CG2	2.48	0.61
1:A:326:ASP:OD1	4:A:1388:HOH:O	2.16	0.60
1:O:24:PRO:HG3	4:O:6360:HOH:O	2.00	0.60
1:A:300:MET:HA	1:A:300:MET:HE3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:33:THR:HG23	3:O:6335:NDP:C2A	2.31	0.60
1:B:28:VAL:HG23	1:B:29:VAL:CG2	2.30	0.60
1:O:144:ILE:HG21	1:O:324:LEU:HD21	1.82	0.60
1:A:28:VAL:HG23	1:A:29:VAL:CG2	2.31	0.60
1:A:82:LEU:HD13	1:A:84:TRP:CZ2	2.36	0.60
1:B:11:ILE:HG21	1:B:119:THR:HG21	1.83	0.60
1:O:19:TRP:O	1:O:20:HIS:C	2.39	0.60
1:A:172:MET:O	1:A:227:GLY:HA3	2.02	0.60
1:B:182:GLN:HG2	4:B:2338:HOH:O	2.00	0.60
1:B:132:VAL:HG13	1:B:218:LEU:HD21	1.82	0.60
1:A:185:LEU:CD2	1:B:49:ILE:HD11	2.32	0.60
1:A:324:LEU:O	1:A:328:VAL:HG23	2.02	0.60
1:A:24:PRO:HB3	1:A:25:LEU:CD1	2.27	0.59
1:A:6:ASN:HD22	1:A:96:THR:HG21	1.67	0.59
1:O:271:LEU:HD11	1:O:292:ILE:HG12	1.84	0.59
1:O:83:PRO:HB2	1:O:87:MET:CE	2.32	0.59
1:A:185:LEU:HD21	1:B:49:ILE:HD11	1.83	0.59
1:O:19:TRP:CZ2	1:O:27:VAL:CG2	2.85	0.59
1:O:249:LYS:HA	1:O:302:ASP:O	2.03	0.59
1:B:77:ARG:HH11	1:B:77:ARG:HG3	1.66	0.59
1:A:206:THR:HG22	1:A:229:ALA:HB3	1.85	0.59
1:O:19:TRP:CE2	1:O:27:VAL:CG2	2.82	0.59
1:O:6:ASN:HD22	1:O:96:THR:HG21	1.67	0.59
1:A:271:LEU:HD11	1:A:292:ILE:HG12	1.84	0.59
1:O:59:THR:HG22	1:O:60(A):GLY:H	1.68	0.59
1:A:19:TRP:CE2	1:A:27:VAL:HG23	2.38	0.59
1:B:49:ILE:HA	1:B:284:ARG:NH2	2.18	0.59
1:O:129:VAL:HG23	1:O:217:VAL:HG11	1.85	0.59
1:A:211:ALA:HB1	1:A:226:ASN:HA	1.84	0.58
1:O:242:LEU:HD12	1:O:243:VAL:N	2.18	0.58
1:A:249:LYS:HA	1:A:302:ASP:O	2.02	0.58
1:B:144:ILE:HG22	1:B:145:SER:N	2.18	0.58
1:O:181:ASP:O	1:O:183:ARG:NH1	2.35	0.58
1:B:172:MET:O	1:B:227:GLY:HA3	2.04	0.58
1:O:82:LEU:HD13	1:O:84:TRP:CZ2	2.38	0.58
1:A:144:ILE:HG22	1:A:145:SER:N	2.18	0.58
1:O:22(A):LYS:HE3	1:O:322:VAL:CG1	2.33	0.58
1:O:64:ILE:HA	1:O:69:LYS:O	2.03	0.58
1:O:121:PRO:HD3	1:O:147:ALA:O	2.02	0.58
1:A:192:ASP:HB3	1:A:195:ARG:HB2	1.86	0.58
1:B:90:ASP:CB	1:B:333:GLN:HE22	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ASP:HB3	1:B:333:GLN:NE2	2.17	0.57
1:O:24:PRO:CB	1:O:25:LEU:HD12	2.28	0.57
1:O:139:HIS:CG	1:O:139:HIS:O	2.58	0.57
1:O:144:ILE:HG22	1:O:145:SER:N	2.19	0.57
1:A:64:ILE:HA	1:A:69:LYS:O	2.05	0.57
1:A:83:PRO:HB2	1:A:87:MET:CE	2.33	0.57
1:A:64:ILE:HD12	1:A:65:SER:O	2.04	0.57
1:O:132:VAL:HG13	1:O:218:LEU:HD21	1.87	0.57
1:A:121:PRO:HD3	1:A:147:ALA:O	2.03	0.57
1:A:210:ALA:O	1:A:214:VAL:HG23	2.05	0.57
1:A:49:ILE:HA	1:A:284:ARG:NH2	2.20	0.57
1:B:127:THR:HB	1:B:145:SER:HB3	1.87	0.57
1:O:115:LYS:HD3	1:O:141:ASP:O	2.04	0.57
1:O:49:ILE:HA	1:O:284:ARG:NH2	2.20	0.57
1:O:324:LEU:O	1:O:328:VAL:HG23	2.04	0.56
1:B:210:ALA:O	1:B:214:VAL:HG23	2.05	0.56
1:B:22(A):LYS:HE3	1:B:322:VAL:CG1	2.34	0.56
1:B:31:ASN:HA	1:B:74:VAL:O	2.05	0.56
1:B:326:ASP:O	1:B:329:ALA:HB3	2.06	0.56
1:O:172:MET:O	1:O:227:GLY:HA3	2.06	0.56
1:B:11:ILE:HG21	1:B:119:THR:CG2	2.35	0.56
1:B:137:TYR:CE1	1:B:144:ILE:HD11	2.41	0.56
1:O:66:VAL:HG23	1:O:66:VAL:O	2.05	0.56
1:A:129:VAL:HG23	1:A:217:VAL:HG11	1.86	0.56
1:A:223:GLY:N	4:A:1365:HOH:O	2.29	0.56
1:A:56:ASP:CA	1:A:66:VAL:HG12	2.36	0.56
1:A:77:ARG:HG3	1:A:77:ARG:HH11	1.70	0.56
1:A:6:ASN:ND2	1:A:96:THR:HG21	2.19	0.56
1:A:38:LYS:HG2	1:A:39:GLN:H	1.70	0.56
1:O:284:ARG:NH1	4:O:6370:HOH:O	2.38	0.56
1:O:45:LYS:HG2	1:O:57:VAL:HB	1.88	0.56
1:A:139:HIS:O	1:A:139:HIS:CG	2.59	0.56
1:O:210:ALA:O	1:O:214:VAL:HG23	2.05	0.56
1:O:38:LYS:HG2	1:O:39:GLN:H	1.71	0.56
1:A:132:VAL:HG13	1:A:218:LEU:HD21	1.87	0.55
1:O:137:TYR:CE1	1:O:144:ILE:HD11	2.41	0.55
1:A:31:ASN:HA	1:A:74:VAL:O	2.06	0.55
1:B:324:LEU:O	1:B:328:VAL:HG23	2.05	0.55
1:O:64:ILE:HD12	1:O:65:SER:N	2.21	0.55
1:O:300:MET:HB3	4:O:6416:HOH:O	2.05	0.55
1:B:192:ASP:HB3	1:B:195:ARG:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:ILE:HD11	1:B:284:ARG:HH11	1.72	0.55
1:A:96:THR:HG1	1:A:98:VAL:HG22	1.69	0.55
1:B:77:ARG:N	1:B:77:ARG:HD3	2.20	0.55
1:O:100:VAL:HA	1:O:118:ILE:HD13	1.89	0.55
1:A:25:LEU:HD12	1:A:25:LEU:N	2.17	0.55
1:B:100:VAL:HA	1:B:118:ILE:HD13	1.89	0.55
1:B:102:ARG:HH12	1:B:142:THR:CG2	2.20	0.55
1:O:191:ARG:NH1	1:O:191:ARG:HG2	2.22	0.55
1:O:192:ASP:HB3	1:O:195:ARG:HB2	1.89	0.55
1:A:66:VAL:HG23	1:A:66:VAL:O	2.07	0.54
1:B:19:TRP:CE2	1:B:27:VAL:HG23	2.42	0.54
1:B:82:LEU:HD13	1:B:84:TRP:CZ2	2.42	0.54
1:A:119:THR:CG2	1:A:119:THR:O	2.50	0.54
1:O:127:THR:HB	1:O:145:SER:HB3	1.89	0.54
1:B:23:SER:N	1:B:24:PRO:CD	2.70	0.54
1:O:77:ARG:HH11	1:O:77:ARG:HG3	1.71	0.54
1:B:176:HIS:O	1:B:231:ARG:HA	2.06	0.54
1:B:79:PRO:HA	1:B:82:LEU:CD1	2.37	0.54
1:O:159:LYS:HB2	1:O:218:LEU:HD11	1.90	0.54
1:O:79:PRO:HA	1:O:82:LEU:CD1	2.37	0.54
1:B:300:MET:HA	1:B:300:MET:HE3	1.90	0.54
1:O:77:ARG:HD3	1:O:77:ARG:N	2.21	0.54
1:A:176:HIS:O	1:A:231:ARG:HA	2.07	0.54
1:B:55:ALA:CA	1:B:66:VAL:CG1	2.86	0.54
1:A:157:PHE:HB2	1:A:259:PHE:CE1	2.43	0.54
1:B:22(A):LYS:HE2	1:B:319:GLN:OE1	2.07	0.54
1:B:64:ILE:HA	1:B:69:LYS:O	2.08	0.54
1:O:64:ILE:O	1:O:64:ILE:HG13	2.07	0.54
1:A:33:THR:HG23	3:A:1335:NDP:N3A	2.23	0.54
1:B:45:LYS:HG2	1:B:57:VAL:HB	1.90	0.54
1:B:6:ASN:HD22	1:B:96:THR:CG2	2.20	0.54
1:B:38:LYS:HG2	1:B:39:GLN:H	1.73	0.53
1:O:31:ASN:HA	1:O:74:VAL:O	2.08	0.53
1:A:39:GLN:NE2	1:B:190:HIS:H	2.04	0.53
1:B:80:VAL:CG1	1:B:107:LYS:HG3	2.37	0.53
1:A:251:PHE:CD1	1:A:251:PHE:N	2.76	0.53
1:A:77:ARG:N	1:A:77:ARG:HD3	2.21	0.53
1:A:79:PRO:HA	1:A:82:LEU:CD1	2.39	0.53
1:B:157:PHE:HB2	1:B:259:PHE:CE1	2.44	0.53
1:B:211:ALA:CB	1:B:226:ASN:HA	2.37	0.53
1:O:211:ALA:CB	1:O:226:ASN:HA	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:TRP:HZ3	1:A:333:GLN:HG3	1.72	0.53
1:B:242:LEU:HD12	1:B:243:VAL:N	2.23	0.53
1:B:29:VAL:HG21	1:B:87:MET:HE1	1.91	0.53
1:O:179:THR:HB	4:O:6341:HOH:O	2.08	0.53
1:B:83:PRO:HB2	1:B:87:MET:CE	2.37	0.53
1:A:242:LEU:HD12	1:A:243:VAL:N	2.24	0.53
1:B:33:THR:HG23	3:B:2335:NDP:C2A	2.38	0.53
1:A:159:LYS:HB2	1:A:218:LEU:HD11	1.91	0.53
1:O:1:LEU:HD22	1:O:329:ALA:HA	1.91	0.53
1:O:80:VAL:CG1	1:O:107:LYS:HG3	2.39	0.53
1:A:80:VAL:CG1	1:A:107:LYS:HG3	2.40	0.52
1:A:319:GLN:OE1	1:A:319:GLN:HA	2.08	0.52
1:A:36:GLY:HA3	1:A:38:LYS:HE2	1.91	0.52
1:A:55:ALA:HB1	1:A:66:VAL:HG13	1.90	0.52
1:A:94:GLU:OE2	1:A:96:THR:HG23	2.09	0.52
1:B:159:LYS:HB2	1:B:218:LEU:HD11	1.92	0.52
1:B:82:LEU:HD11	4:B:2380:HOH:O	2.09	0.52
1:A:11:ILE:HD11	3:A:1335:NDP:H42N	1.91	0.52
1:A:102:ARG:HH12	1:A:142:THR:CG2	2.22	0.52
1:B:115:LYS:HD3	1:B:141:ASP:O	2.10	0.52
1:O:55:ALA:HA	1:O:66:VAL:HG11	1.90	0.52
1:O:84:TRP:HA	1:O:89:ILE:HG12	1.91	0.52
1:A:128:TYR:HA	1:A:133:ASN:HD21	1.74	0.52
1:A:38:LYS:HD3	1:A:38:LYS:N	2.03	0.52
1:B:19:TRP:NE1	1:B:27:VAL:HG23	2.24	0.52
1:B:33:THR:HG23	3:B:2335:NDP:N3A	2.24	0.52
1:B:289:SER:OG	1:B:320:ARG:HD2	2.08	0.52
1:O:183:ARG:CZ	1:O:190:HIS:CD2	2.92	0.52
1:B:11:ILE:HD11	3:B:2335:NDP:C3N	2.40	0.52
1:O:102:ARG:HH12	1:O:142:THR:CG2	2.23	0.52
1:O:206:THR:HG22	1:O:229:ALA:HB3	1.92	0.52
1:O:22(A):LYS:HE2	1:O:319:GLN:OE1	2.09	0.52
1:B:293:ASP:OD2	1:B:296:LEU:HG	2.10	0.52
1:A:84:TRP:HA	1:A:89:ILE:HG12	1.92	0.52
1:A:22(A):LYS:HE2	1:A:319:GLN:OE1	2.09	0.52
1:B:251:PHE:N	1:B:251:PHE:CD1	2.78	0.52
1:O:176:HIS:O	1:O:231:ARG:HA	2.10	0.52
1:A:11:ILE:HG21	1:A:119:THR:HG21	1.92	0.52
1:O:139:HIS:NE2	1:O:332:TRP:HE3	2.07	0.52
1:O:29:VAL:HG11	1:O:87:MET:HE1	1.92	0.52
1:A:23:SER:N	1:A:24:PRO:CD	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:62:SER:HA	1:O:73:VAL:HG23	1.92	0.51
1:A:211:ALA:CB	1:A:226:ASN:HA	2.40	0.51
1:A:250:THR:HG23	1:A:251:PHE:N	2.25	0.51
1:O:300:MET:HA	1:O:300:MET:HE3	1.92	0.51
1:A:266:GLU:HG2	1:A:267:LEU:HG	1.91	0.51
1:B:266:GLU:HG2	1:B:267:LEU:HG	1.92	0.51
1:O:167:ILE:HG23	1:O:244:VAL:CG2	2.41	0.51
1:O:23:SER:N	1:O:24:PRO:CD	2.73	0.51
1:B:139:HIS:O	1:B:139:HIS:CG	2.63	0.51
1:O:157:PHE:HB2	1:O:259:PHE:CE1	2.45	0.51
1:B:211:ALA:HB3	4:B:2357:HOH:O	2.10	0.51
1:O:312:ASP:OD1	1:O:315:TRP:N	2.42	0.51
1:O:25:LEU:HD12	1:O:25:LEU:N	2.18	0.51
1:O:260:ARG:HD3	4:O:6339:HOH:O	2.09	0.51
1:O:251:PHE:N	1:O:251:PHE:CD1	2.79	0.51
1:B:85:GLY:CA	1:B:112:GLY:HA3	2.41	0.51
1:O:250:THR:HG23	1:O:251:PHE:N	2.25	0.51
1:O:11:ILE:HG21	1:O:119:THR:HG21	1.93	0.50
1:A:1:LEU:HB3	1:A:25:LEU:HB3	1.92	0.50
1:O:19:TRP:HZ2	1:O:27:VAL:HG23	1.73	0.50
1:B:55:ALA:CB	1:B:66:VAL:HG13	2.33	0.50
1:B:34:GLY:HA3	1:B:39:GLN:OE1	2.11	0.50
1:B:36:GLY:HA3	1:B:38:LYS:HE2	1.94	0.50
1:B:55:ALA:HA	1:B:66:VAL:CG1	2.41	0.50
1:A:261:GLU:O	1:A:265:GLN:CG	2.58	0.50
1:B:121:PRO:HD3	1:B:147:ALA:O	2.10	0.50
1:B:165:PHE:HE2	1:B:250:THR:OG1	1.92	0.50
1:B:1:LEU:HB3	1:B:25:LEU:HB3	1.92	0.50
1:B:29:VAL:HG11	1:B:87:MET:HE1	1.92	0.50
1:B:56:ASP:CA	1:B:66:VAL:HG12	2.35	0.50
1:A:29:VAL:HG21	1:A:87:MET:HE1	1.94	0.50
1:A:85:GLY:CA	1:A:112:GLY:HA3	2.42	0.50
1:B:101:ASP:CA	1:B:122(A):LYS:HB2	2.38	0.50
1:O:128:TYR:HA	1:O:133:ASN:HD21	1.77	0.50
1:O:208:THR:HG22	1:O:228:ILE:HA	1.94	0.50
1:O:172:MET:HE1	1:O:240:VAL:HG23	1.94	0.50
1:O:45:LYS:HE2	1:O:55:ALA:O	2.11	0.50
1:B:45:LYS:HE2	1:B:55:ALA:O	2.12	0.50
1:B:84:TRP:CE3	1:B:89:ILE:HG13	2.47	0.50
1:O:84:TRP:CE3	1:O:89:ILE:HG13	2.47	0.50
1:A:100:VAL:HA	1:A:118:ILE:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLY:HA3	1:A:39:GLN:OE1	2.12	0.49
1:O:281:ILE:HD11	1:O:284:ARG:HH11	1.77	0.49
1:B:25:LEU:HD12	1:B:25:LEU:N	2.21	0.49
1:A:139:HIS:O	1:A:139:HIS:ND1	2.46	0.49
1:B:167:ILE:HG23	1:B:244:VAL:CG2	2.42	0.49
1:A:165:PHE:CE2	1:A:250:THR:OG1	2.65	0.49
1:A:191:ARG:NH1	1:A:191:ARG:HG2	2.24	0.49
1:O:21:GLY:O	1:O:22(A):LYS:C	2.50	0.49
1:A:61:ASP:O	1:A:62:SER:HB3	2.13	0.49
1:O:85:GLY:CA	1:O:112:GLY:HA3	2.43	0.49
1:O:6:ASN:HD22	1:O:96:THR:CG2	2.24	0.49
1:A:167:ILE:HG23	1:A:244:VAL:CG2	2.42	0.49
1:A:84:TRP:CE3	1:A:89:ILE:HG13	2.48	0.49
1:O:319:GLN:OE1	1:O:319:GLN:HA	2.12	0.49
1:A:6:ASN:HD22	1:A:96:THR:CG2	2.24	0.49
1:B:172:MET:HE1	1:B:240:VAL:HG23	1.95	0.49
1:A:332:TRP:CZ3	1:A:333:GLN:HG3	2.47	0.49
1:A:80:VAL:HG23	1:A:81:ASN:ND2	2.27	0.49
1:B:129:VAL:CG2	1:B:217:VAL:HG11	2.42	0.49
1:A:172:MET:HE1	1:A:240:VAL:HG23	1.95	0.49
1:A:235:PRO:CG	1:B:201:LEU:HD21	2.42	0.49
1:O:119:THR:O	1:O:119:THR:CG2	2.53	0.49
1:B:79:PRO:HB2	1:B:107:LYS:CB	2.37	0.49
1:O:293:ASP:OD2	1:O:296:LEU:HG	2.12	0.49
1:A:300:MET:O	1:A:304:MET:HB3	2.13	0.48
1:A:11:ILE:HG21	1:A:119:THR:CG2	2.44	0.48
1:A:165:PHE:HE2	1:A:250:THR:OG1	1.96	0.48
1:B:80:VAL:HG23	1:B:81:ASN:ND2	2.28	0.48
1:A:21:GLY:O	1:A:22(A):LYS:C	2.51	0.48
1:A:263:ALA:O	1:A:268:LYS:HA	2.13	0.48
1:A:77:ARG:O	1:A:79:PRO:HD3	2.13	0.48
1:B:319:GLN:HA	1:B:319:GLN:OE1	2.12	0.48
1:B:84:TRP:HA	1:B:89:ILE:HG12	1.95	0.48
1:O:119:THR:HG23	1:O:317:TYR:HE2	1.78	0.48
1:O:139:HIS:NE2	1:O:332:TRP:CE3	2.81	0.48
1:B:171:THR:HA	1:B:226:ASN:O	2.12	0.48
1:O:101:ASP:CA	1:O:122(A):LYS:HB2	2.42	0.48
1:A:115:LYS:HD3	1:A:141:ASP:O	2.13	0.48
1:A:174:THR:HG23	1:A:174:THR:O	2.12	0.48
1:B:133:ASN:HD22	1:B:133:ASN:H	1.60	0.48
1:B:47:ASP:OD2	4:B:2378:HOH:O	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:84:TRP:HA	1:O:89:ILE:CG1	2.43	0.48
1:A:281:ILE:HD11	1:A:284:ARG:HH11	1.78	0.48
1:A:289:SER:OG	1:A:320:ARG:HD2	2.12	0.48
1:B:98:VAL:HG23	1:B:99:PHE:CD2	2.48	0.48
1:O:172:MET:CE	1:O:240:VAL:HG23	2.43	0.48
1:O:33:THR:HG23	3:O:6335:NDP:N3A	2.28	0.48
1:O:94:GLU:OE2	1:O:96:THR:HG23	2.13	0.48
1:B:191:ARG:HG2	1:B:191:ARG:NH1	2.28	0.48
1:O:98:VAL:HG23	1:O:99:PHE:CD2	2.49	0.48
1:A:19:TRP:CZ2	1:A:27:VAL:HG23	2.49	0.48
1:A:332:TRP:CZ3	1:A:333:GLN:CG	2.97	0.48
1:B:90:ASP:O	1:B:114:LYS:HB2	2.14	0.48
1:A:45:LYS:HG2	1:A:57:VAL:HB	1.96	0.47
1:A:208:THR:HG22	1:A:228:ILE:HA	1.96	0.47
1:B:263:ALA:O	1:B:268:LYS:HA	2.14	0.47
1:O:36:GLY:HA3	1:O:38:LYS:HE2	1.95	0.47
1:O:80:VAL:HG23	1:O:81:ASN:ND2	2.29	0.47
1:O:82:LEU:HA	1:O:83:PRO:HD3	1.63	0.47
1:B:21:GLY:O	1:B:22(A):LYS:C	2.50	0.47
1:A:127:THR:HB	1:A:145:SER:HB3	1.97	0.47
1:B:261:GLU:O	1:B:265:GLN:HG2	2.15	0.47
1:A:9:GLY:O	1:A:13:ARG:HG3	2.15	0.47
1:O:19:TRP:NE1	1:O:27:VAL:HG21	2.23	0.47
1:O:326:ASP:O	1:O:329:ALA:HB3	2.15	0.47
1:A:55:ALA:HA	1:A:66:VAL:HG11	1.96	0.47
1:A:49:ILE:HD11	1:B:185:LEU:HD21	1.97	0.47
1:B:312:ASP:OD1	1:B:315:TRP:N	2.46	0.47
1:O:90:ASP:O	1:O:114:LYS:HB2	2.15	0.47
1:O:128:TYR:CE2	1:O:137:TYR:HA	2.50	0.47
1:A:281:ILE:HG22	1:A:282:ASP:N	2.30	0.47
1:A:65:SER:O	1:A:66:VAL:C	2.54	0.47
1:O:64:ILE:O	1:O:64:ILE:CG1	2.62	0.47
1:A:119:THR:HG23	1:A:317:TYR:HE2	1.80	0.47
1:A:171:THR:HA	1:A:226:ASN:O	2.14	0.47
1:A:22(A):LYS:HB3	1:A:24:PRO:HG2	1.97	0.47
1:O:11:ILE:HG21	1:O:119:THR:CG2	2.45	0.47
1:O:1:LEU:HB3	1:O:25:LEU:HB3	1.97	0.47
1:B:128:TYR:CE2	1:B:137:TYR:HA	2.49	0.47
1:B:1:LEU:HD22	1:B:329:ALA:HA	1.97	0.47
1:O:137:TYR:OH	1:O:328:VAL:HG13	2.14	0.47
1:A:262:SER:HA	1:A:266:GLU:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:118:ILE:HG22	1:O:120:ALA:H	1.79	0.46
1:O:263:ALA:O	1:O:268:LYS:HA	2.16	0.46
1:O:79:PRO:HA	1:O:82:LEU:HD12	1.96	0.46
1:A:124:ASP:N	1:A:124:ASP:OD1	2.45	0.46
1:A:137:TYR:OH	1:A:328:VAL:HG13	2.16	0.46
1:O:157:PHE:CE2	1:O:242:LEU:HD23	2.51	0.46
1:O:332:TRP:CZ3	1:O:333:GLN:HB3	2.51	0.46
1:A:293:ASP:OD2	1:A:296:LEU:HG	2.14	0.46
1:B:144:ILE:CG2	1:B:145:SER:N	2.78	0.46
1:O:11:ILE:HD11	3:O:6335:NDP:H42N	1.96	0.46
1:O:172:MET:SD	1:O:172:MET:C	2.94	0.46
1:O:174:THR:HG23	1:O:174:THR:O	2.16	0.46
1:B:172:MET:SD	1:B:172:MET:C	2.94	0.46
1:A:45:LYS:HE2	1:A:55:ALA:O	2.16	0.46
1:B:94:GLU:OE2	1:B:96:THR:HG23	2.15	0.46
1:O:144:ILE:CG2	1:O:145:SER:N	2.79	0.46
1:A:195:ARG:HH22	1:A:231:ARG:NH2	2.13	0.46
1:A:235:PRO:HG2	1:B:201:LEU:HD21	1.98	0.46
1:B:77:ARG:HG3	1:B:77:ARG:NH1	2.30	0.46
1:O:171:THR:HA	1:O:226:ASN:O	2.15	0.46
1:O:165:PHE:O	1:O:247:SER:HB3	2.16	0.46
1:B:274:CYS:SG	1:B:276:GLU:HB2	2.56	0.45
1:B:82:LEU:HA	1:B:83:PRO:HD3	1.63	0.45
1:O:139:HIS:O	1:O:139:HIS:ND1	2.49	0.45
1:O:129:VAL:CG2	1:O:217:VAL:HG11	2.47	0.45
1:A:22(A):LYS:HB3	1:A:24:PRO:CG	2.47	0.45
1:A:139:HIS:CD2	1:A:332:TRP:HB3	2.51	0.45
1:B:137:TYR:OH	1:B:328:VAL:HG13	2.16	0.45
1:B:133:ASN:HD22	1:B:133:ASN:N	2.13	0.45
1:B:139:HIS:NE2	1:B:332:TRP:HE3	2.14	0.45
1:B:246:VAL:HG22	1:B:303:ASP:O	2.17	0.45
1:O:281:ILE:HG22	1:O:282:ASP:N	2.31	0.45
1:A:228:ILE:N	1:A:228:ILE:CD1	2.80	0.45
1:B:228:ILE:CD1	1:B:228:ILE:N	2.78	0.45
1:A:118:ILE:HG22	1:A:120:ALA:H	1.81	0.45
1:A:11:ILE:HD11	3:A:1335:NDP:C4N	2.46	0.45
1:B:218:LEU:HB2	1:B:221:LEU:HD12	1.98	0.45
1:O:19:TRP:O	1:O:22(A):LYS:N	2.50	0.45
1:O:34:GLY:HA3	1:O:39:GLN:OE1	2.16	0.45
1:O:292:ILE:HD13	1:O:309:ALA:HB2	1.98	0.45
1:O:38:LYS:N	1:O:38:LYS:HD3	2.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ILE:CG2	1:A:145:SER:N	2.78	0.45
1:A:129:VAL:CG2	1:A:217:VAL:HG11	2.46	0.45
1:O:125:ILE:O	1:O:127:THR:HG22	2.17	0.45
1:O:55:ALA:CA	1:O:66:VAL:HG13	2.47	0.45
1:O:55:ALA:CA	1:O:66:VAL:CG1	2.95	0.45
1:O:9:GLY:O	1:O:13:ARG:HG3	2.16	0.45
1:A:90:ASP:O	1:A:114:LYS:HB2	2.16	0.45
1:A:84:TRP:HA	1:A:89:ILE:CG1	2.46	0.45
1:A:94:GLU:HG2	1:A:108:HIS:CD2	2.52	0.45
1:A:167:ILE:HG23	1:A:244:VAL:HG23	1.99	0.45
1:B:101:ASP:OD2	1:B:103:ASP:HB2	2.17	0.45
1:B:139:HIS:O	1:B:139:HIS:ND1	2.50	0.45
1:B:178:TYR:HA	1:B:182:GLN:OE1	2.17	0.45
1:B:206:THR:HG22	1:B:229:ALA:HB3	1.99	0.45
1:A:82:LEU:HA	1:A:83:PRO:HD3	1.64	0.45
1:B:100:VAL:HG23	1:B:122(A):LYS:HG3	1.99	0.45
1:A:101:ASP:CA	1:A:122(A):LYS:HB2	2.43	0.44
1:B:164:LYS:HD2	1:B:258:ALA:HB1	1.98	0.44
1:O:114:LYS:HE2	1:O:333:GLN:NE2	2.32	0.44
1:O:115:LYS:HZ2	1:O:137:TYR:HH	1.55	0.44
1:O:178:TYR:HA	1:O:182:GLN:OE1	2.16	0.44
1:B:172:MET:CE	1:B:240:VAL:HG23	2.47	0.44
1:A:114:LYS:HD2	1:A:333:GLN:OE1	2.18	0.44
1:A:133:ASN:HD22	1:A:133:ASN:H	1.66	0.44
1:A:172:MET:SD	1:A:172:MET:C	2.96	0.44
1:B:208:THR:HG22	1:B:228:ILE:HA	1.99	0.44
1:O:29:VAL:HG21	1:O:87:MET:HE1	1.99	0.44
1:O:79:PRO:HB2	1:O:107:LYS:CB	2.37	0.44
1:B:250:THR:CG2	1:B:251:PHE:N	2.74	0.44
1:B:167:ILE:HG23	1:B:244:VAL:HG23	1.99	0.44
1:B:119:THR:O	1:B:119:THR:CG2	2.62	0.44
1:B:3:VAL:HG13	1:B:93:ILE:HD13	2.00	0.44
1:A:172:MET:CE	1:A:240:VAL:HG23	2.48	0.44
1:B:167:ILE:CG1	1:B:244:VAL:HG21	2.42	0.44
1:O:100:VAL:HG23	1:O:122(A):LYS:HG3	1.99	0.44
1:O:261:GLU:O	1:O:265:GLN:HG2	2.16	0.44
1:O:55:ALA:HA	1:O:66:VAL:CG1	2.48	0.44
1:A:101:ASP:OD2	1:A:103:ASP:HB2	2.18	0.44
1:A:167:ILE:CG1	1:A:244:VAL:HG21	2.43	0.44
1:A:274:CYS:SG	1:A:276:GLU:HB2	2.58	0.44
1:A:32:ASP:O	1:A:33:THR:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:LEU:HA	1:A:50:LEU:HD12	1.83	0.44
1:O:289:SER:OG	1:O:320:ARG:HD2	2.18	0.44
1:A:26:ASP:O	1:A:28:VAL:HG13	2.17	0.43
1:O:236:ASN:O	1:O:237:VAL:HB	2.18	0.43
1:O:164:LYS:HD2	1:O:258:ALA:HB1	2.00	0.43
1:O:266:GLU:HG3	1:O:266:GLU:H	1.12	0.43
1:A:194:ARG:NH1	1:A:205:PRO:HB2	2.33	0.43
1:A:332:TRP:HZ3	1:A:333:GLN:CB	2.25	0.43
1:B:9:GLY:O	1:B:13:ARG:HG3	2.18	0.43
1:O:77:ARG:O	1:O:79:PRO:HD3	2.18	0.43
1:O:133:ASN:HD22	1:O:133:ASN:H	1.65	0.43
1:B:118:ILE:HG22	1:B:120:ALA:H	1.83	0.43
1:O:94:GLU:HG2	1:O:108:HIS:CD2	2.54	0.43
1:B:77:ARG:O	1:B:79:PRO:HD3	2.19	0.43
1:O:228:ILE:N	1:O:228:ILE:CD1	2.79	0.43
1:A:29:VAL:HG11	1:A:87:MET:HE1	2.00	0.43
1:B:128:TYR:CZ	1:B:137:TYR:HA	2.54	0.43
1:O:11:ILE:HD11	3:O:6335:NDP:C4N	2.48	0.43
1:A:164:LYS:HD2	1:A:258:ALA:HB1	2.00	0.43
1:A:77:ARG:HG3	1:A:77:ARG:NH1	2.34	0.43
1:A:1:LEU:HD22	1:A:329:ALA:HA	2.00	0.43
1:A:98:VAL:HG23	1:A:99:PHE:CD2	2.53	0.43
1:O:25:LEU:N	1:O:25:LEU:CD1	2.81	0.43
1:B:250:THR:OG1	1:B:254:GLU:OE1	2.37	0.43
1:B:84:TRP:HA	1:B:89:ILE:CG1	2.48	0.43
1:A:14:ASN:HB3	1:A:318:SER:OG	2.19	0.43
1:A:62:SER:HA	1:A:73:VAL:HG23	1.99	0.43
1:B:50:LEU:HD13	4:B:2346:HOH:O	2.19	0.43
1:B:61:ASP:O	1:B:62:SER:HB3	2.19	0.43
1:O:0:LYS:HD2	4:O:6411:HOH:O	2.19	0.43
1:O:55:ALA:CB	1:O:66:VAL:HG13	2.48	0.43
1:O:77:ARG:H	1:O:77:ARG:CD	2.25	0.43
1:B:82:LEU:O	1:B:111:ALA:HB1	2.19	0.42
1:B:11:ILE:HD11	3:B:2335:NDP:H42N	2.00	0.42
1:B:19:TRP:CZ2	1:B:27:VAL:HG23	2.53	0.42
1:O:101:ASP:OD2	1:O:103:ASP:HB2	2.18	0.42
1:O:205:PRO:HA	1:O:230:LEU:HD23	2.01	0.42
1:A:125:ILE:O	1:A:127:THR:HG22	2.19	0.42
1:A:201:LEU:HD21	1:B:235:PRO:CG	2.48	0.42
1:A:55:ALA:CA	1:A:66:VAL:HG13	2.49	0.42
1:A:94:GLU:CD	1:A:96:THR:HG23	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:GLY:HA2	4:B:2384:HOH:O	2.19	0.42
1:B:22(A):LYS:HB3	1:B:24:PRO:CG	2.49	0.42
1:O:62:SER:HA	1:O:73:VAL:CG2	2.48	0.42
1:A:0:LYS:HB2	1:A:0:LYS:HE3	1.28	0.42
1:A:178:TYR:HA	1:A:182:GLN:OE1	2.19	0.42
1:B:38:LYS:N	1:B:38:LYS:HD3	2.05	0.42
1:O:248:LYS:HB3	1:O:248:LYS:NZ	2.28	0.42
1:B:205:PRO:HA	1:B:230:LEU:HD23	2.02	0.42
1:O:3:VAL:HG13	1:O:93:ILE:HD13	2.01	0.42
1:A:32:ASP:C	1:A:34:GLY:N	2.72	0.42
1:A:3:VAL:HG13	1:A:93:ILE:HD13	2.02	0.42
1:B:128:TYR:HA	1:B:133:ASN:HD21	1.83	0.42
1:O:281:ILE:CG2	1:O:282:ASP:N	2.82	0.42
1:O:64:ILE:CD1	1:O:65:SER:O	2.65	0.42
1:O:74:VAL:HG12	1:O:75:SER:N	2.35	0.42
1:A:82:LEU:O	1:A:111:ALA:HB1	2.19	0.42
1:B:139:HIS:NE2	1:B:332:TRP:CE3	2.88	0.42
1:B:174:THR:O	1:B:174:THR:HG23	2.18	0.42
1:B:281:ILE:HG22	1:B:282:ASP:N	2.34	0.42
1:A:121:PRO:HD3	1:A:148:SER:N	2.34	0.42
1:O:14:ASN:HB3	1:O:318:SER:OG	2.20	0.42
1:O:234:THR:HA	1:O:235:PRO:HD3	1.85	0.42
1:A:255:VAL:HG12	1:A:259:PHE:CE2	2.54	0.42
1:A:22(A):LYS:CE	1:A:322:VAL:HG11	2.41	0.42
1:B:183:ARG:CD	1:B:187:ALA:HB3	2.34	0.42
1:B:94:GLU:HG2	1:B:108:HIS:CD2	2.55	0.42
1:O:203:ILE:O	1:O:205:PRO:HD3	2.20	0.42
1:A:316:GLY:O	1:A:319:GLN:HB2	2.20	0.42
1:A:32:ASP:O	1:A:34:GLY:N	2.53	0.42
1:B:79:PRO:HA	1:B:82:LEU:HD12	2.00	0.42
1:O:22(A):LYS:HB3	1:O:24:PRO:CG	2.49	0.42
1:A:128:TYR:CE2	1:A:137:TYR:HA	2.54	0.42
1:B:317:TYR:O	1:B:321:VAL:HG23	2.19	0.42
1:B:55:ALA:HB1	1:B:66:VAL:CG1	2.37	0.42
1:A:128:TYR:CA	1:A:133:ASN:HD21	2.31	0.41
1:B:300:MET:O	1:B:304:MET:HB3	2.20	0.41
1:O:82:LEU:O	1:O:111:ALA:HB1	2.19	0.41
1:O:32:ASP:O	1:O:33:THR:C	2.58	0.41
1:A:317:TYR:O	1:A:321:VAL:HG23	2.19	0.41
1:A:154:LEU:HA	1:A:157:PHE:CE1	2.55	0.41
1:A:158:VAL:HG11	1:A:221:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:PHE:CZ	1:A:254:GLU:HB2	2.56	0.41
1:O:154:LEU:HA	1:O:157:PHE:CE1	2.55	0.41
1:O:167:ILE:CG1	1:O:244:VAL:HG21	2.45	0.41
1:O:77:ARG:NH1	1:O:77:ARG:HG3	2.34	0.41
1:A:50:LEU:HD13	4:A:1340:HOH:O	2.20	0.41
1:A:94:GLU:OE1	1:A:96:THR:HG23	2.20	0.41
1:O:130:VAL:HA	1:O:134:GLU:HB3	2.02	0.41
1:A:100:VAL:HG23	1:A:122(A):LYS:HG3	2.01	0.41
1:A:194:ARG:HH11	1:A:205:PRO:HB2	1.86	0.41
1:A:281:ILE:CG2	1:A:282:ASP:N	2.81	0.41
1:A:312:ASP:OD1	1:A:315:TRP:N	2.46	0.41
1:B:124:ASP:HA	4:B:2386:HOH:O	2.19	0.41
1:B:236:ASN:O	1:B:237:VAL:HB	2.20	0.41
1:O:128:TYR:CA	1:O:133:ASN:HD21	2.33	0.41
1:O:61:ASP:O	1:O:62:SER:HB3	2.20	0.41
1:A:137:TYR:HE1	1:A:144:ILE:HD11	1.83	0.41
1:B:211:ALA:HB1	1:B:226:ASN:CA	2.48	0.41
1:B:204:VAL:HB	1:B:231:ARG:HB2	2.02	0.41
1:O:11:ILE:HD11	3:O:6335:NDP:C7N	2.51	0.41
1:O:255:VAL:HG12	1:O:259:PHE:CE2	2.56	0.41
1:O:276:GLU:HA	1:O:277:PRO:HD3	1.72	0.41
1:B:31:ASN:ND2	3:B:2335:NDP:H2A	2.35	0.41
1:B:29:VAL:HG11	1:B:87:MET:CE	2.51	0.41
1:O:167:ILE:HG23	1:O:244:VAL:HG23	2.02	0.41
1:O:300:MET:O	1:O:304:MET:HB3	2.20	0.41
1:A:190:HIS:H	1:B:39:GLN:NE2	2.17	0.41
1:B:255:VAL:HG12	1:B:259:PHE:CE2	2.56	0.41
1:A:55:ALA:HA	1:A:66:VAL:CG1	2.51	0.41
1:B:23:SER:H	1:B:24:PRO:HD3	1.81	0.41
1:O:194:ARG:NH1	1:O:205:PRO:HG2	2.36	0.41
1:A:176:HIS:HB3	1:A:231:ARG:HD3	2.03	0.40
1:A:236:ASN:O	1:A:237:VAL:HB	2.22	0.40
1:B:190:HIS:HB3	1:B:196:ALA:HB2	2.02	0.40
1:B:281:ILE:HD12	1:B:284:ARG:HD2	2.03	0.40
1:B:292:ILE:HD13	1:B:309:ALA:HB2	2.04	0.40
1:O:204:VAL:HB	1:O:231:ARG:HB2	2.02	0.40
1:O:22(A):LYS:HG3	4:O:6360:HOH:O	2.21	0.40
1:O:137:TYR:CD2	1:O:331:LYS:HG3	2.56	0.40
1:A:246:VAL:HG22	1:A:303:ASP:O	2.22	0.40
1:B:130:VAL:HA	1:B:134:GLU:HB3	2.03	0.40
1:B:195:ARG:HH22	1:B:231:ARG:NH2	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:PRO:HG3	1:B:201:LEU:HD21	2.03	0.40
1:B:281:ILE:CG2	1:B:282:ASP:N	2.84	0.40
1:O:64:ILE:CD1	1:O:64:ILE:C	2.70	0.40
1:A:19:TRP:O	1:A:22(A):LYS:N	2.55	0.40
1:B:0:LYS:HB2	1:B:0:LYS:HE3	1.22	0.40
1:O:50:LEU:HA	1:O:50:LEU:HD12	1.87	0.40
1:A:115:LYS:NZ	1:A:328:VAL:HG13	2.36	0.40
1:A:250:THR:O	1:A:299:VAL:HG11	2.22	0.40
1:A:39:GLN:OE1	1:B:188:SER:HB3	2.21	0.40
1:B:236:ASN:OD1	1:B:314:GLU:HG3	2.22	0.40
1:O:165:PHE:CE2	1:O:250:THR:OG1	2.75	0.40
1:A:260:ARG:O	1:A:264:ASP:OD2	2.40	0.40
1:A:276:GLU:HA	1:A:277:PRO:HD3	1.74	0.40
1:A:279:VAL:O	1:A:280:SER:C	2.60	0.40
1:A:49:ILE:HD11	1:B:185:LEU:CD2	2.52	0.40
1:B:158:VAL:HG11	1:B:221:LEU:HD13	2.03	0.40
1:B:279:VAL:O	1:B:280:SER:C	2.60	0.40
1:B:119:THR:HG23	1:B:317:TYR:HE2	1.86	0.40
1:O:317:TYR:CG	3:O:6335:NDP:H5N	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/335 (99%)	284 (86%)	36 (11%)	12 (4%)	3	19
1	B	332/335 (99%)	281 (85%)	38 (11%)	13 (4%)	3	17
1	O	332/335 (99%)	281 (85%)	38 (11%)	13 (4%)	3	17
All	All	996/1005 (99%)	846 (85%)	112 (11%)	38 (4%)	3	18

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	24	PRO
1	O	66	VAL
1	A	24	PRO
1	A	66	VAL
1	A	332	TRP
1	B	24	PRO
1	B	66	VAL
1	B	280	SER
1	O	34	GLY
1	O	124	ASP
1	O	280	SER
1	A	34	GLY
1	A	280	SER
1	B	34	GLY
1	O	233	PRO
1	A	124	ASP
1	A	210	ALA
1	A	233	PRO
1	B	124	ASP
1	O	22(A)	LYS
1	O	62	SER
1	O	210	ALA
1	O	237	VAL
1	O	332	TRP
1	A	62	SER
1	A	237	VAL
1	B	22(A)	LYS
1	B	62	SER
1	B	210	ALA
1	B	233	PRO
1	B	237	VAL
1	O	186	ASP
1	A	22(A)	LYS
1	A	281	ILE
1	B	186	ASP
1	O	281	ILE
1	B	281	ILE
1	B	120	ALA

### 5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	277/277 (100%)	244 (88%)	33 (12%)	5	22
1	B	277/277 (100%)	246 (89%)	31 (11%)	6	24
1	O	277/277 (100%)	239 (86%)	38 (14%)	3	17
All	All	831/831 (100%)	729 (88%)	102 (12%)	4	21

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	0	LYS
1	O	19	TRP
1	O	22(A)	LYS
1	O	23	SER
1	O	24	PRO
1	O	25	LEU
1	O	38	LYS
1	O	41	SER
1	O	50	LEU
1	O	56	ASP
1	O	64	ILE
1	O	77	ARG
1	O	84	TRP
1	O	93	ILE
1	O	94	GLU
1	O	96	THR
1	O	117	LEU
1	O	125	ILE
1	O	127	THR
1	O	133	ASN
1	O	153	CYS
1	O	169	LYS
1	O	188	SER
1	O	191	ARG
1	O	206	THR
1	O	220	GLN
1	O	228	ILE
1	O	248	LYS
1	O	250	THR
1	O	251	PHE

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Mol	Chain	Res	Type
1	O	266	GLU
1	O	281	ILE
1	O	285	CYS
1	O	286	THR
1	O	300	MET
1	O	313	ASN
1	O	332	TRP
1	O	333	GLN
1	A	0	LYS
1	A	22(A)	LYS
1	A	23	SER
1	A	24	PRO
1	A	25	LEU
1	A	38	LYS
1	A	41	SER
1	A	50	LEU
1	A	56	ASP
1	A	64	ILE
1	A	77	ARG
1	A	84	TRP
1	A	93	ILE
1	A	94	GLU
1	A	96	THR
1	A	121	PRO
1	A	127	THR
1	A	133	ASN
1	A	169	LYS
1	A	188	SER
1	A	191	ARG
1	A	205	PRO
1	A	206	THR
1	A	220	GLN
1	A	228	ILE
1	A	250	THR
1	A	251	PHE
1	A	281	ILE
1	A	286	THR
1	A	295	SER
1	A	300	MET
1	A	313	ASN
1	A	333	GLN
1	B	0	LYS

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Mol	Chain	Res	Type
1	B	22(A)	LYS
1	B	23	SER
1	B	25	LEU
1	B	29	VAL
1	B	38	LYS
1	B	50	LEU
1	B	56	ASP
1	B	64	ILE
1	B	66	VAL
1	B	77	ARG
1	B	84	TRP
1	B	93	ILE
1	B	94	GLU
1	B	96	THR
1	B	127	THR
1	B	133	ASN
1	B	169	LYS
1	B	188	SER
1	B	191	ARG
1	B	206	THR
1	B	220	GLN
1	B	228	ILE
1	B	250	THR
1	B	251	PHE
1	B	281	ILE
1	B	285	CYS
1	B	286	THR
1	B	300	MET
1	B	313	ASN
1	B	332	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	81	ASN
1	O	133	ASN
1	O	163	GLN
1	O	256	ASN
1	O	333	GLN
1	A	81	ASN
1	A	133	ASN
1	A	163	GLN

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Mol	Chain	Res	Type
1	A	256	ASN
1	B	81	ASN
1	B	133	ASN
1	B	163	GLN
1	B	256	ASN
1	B	333	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

9 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	SO4	A	1337	-	4,4,4	0.07	0	6,6,6	0.10	0
2	SO4	O	6336	-	4,4,4	0.32	0	6,6,6	0.09	0
2	SO4	O	6337	-	4,4,4	0.14	0	6,6,6	0.20	0
2	SO4	A	1336	3	4,4,4	0.23	0	6,6,6	0.08	0
3	NDP	A	1335	2	45,52,52	1.58	6 (13%)	53,80,80	1.59	10 (18%)
3	NDP	O	6335	-	45,52,52	1.58	6 (13%)	53,80,80	1.59	10 (18%)
2	SO4	B	2337	-	4,4,4	0.24	0	6,6,6	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NDP	B	2335	-	45,52,52	1.58	6 (13%)	53,80,80	1.59	10 (18%)
2	SO4	B	2336	-	4,4,4	0.25	0	6,6,6	0.11	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	O	6335	-	-	9/30/77/77	0/5/5/5
3	NDP	A	1335	2	-	9/30/77/77	0/5/5/5
3	NDP	B	2335	-	-	9/30/77/77	0/5/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2335	NDP	C4N-C3N	-5.46	1.39	1.49
3	A	1335	NDP	C4N-C3N	-5.45	1.39	1.49
3	O	6335	NDP	C4N-C3N	-5.43	1.39	1.49
3	A	1335	NDP	P2B-O1X	3.95	1.63	1.50
3	B	2335	NDP	P2B-O1X	3.94	1.63	1.50
3	O	6335	NDP	P2B-O1X	3.94	1.63	1.50
3	B	2335	NDP	C6N-C5N	3.84	1.40	1.33
3	A	1335	NDP	C6N-C5N	3.81	1.40	1.33
3	O	6335	NDP	C6N-C5N	3.80	1.40	1.33
3	A	1335	NDP	C4N-C5N	-3.55	1.39	1.48
3	O	6335	NDP	C4N-C5N	-3.55	1.39	1.48
3	B	2335	NDP	C4N-C5N	-3.52	1.39	1.48
3	A	1335	NDP	C7N-C3N	2.99	1.55	1.48
3	B	2335	NDP	C7N-C3N	2.98	1.55	1.48
3	O	6335	NDP	C7N-C3N	2.97	1.55	1.48
3	A	1335	NDP	C2N-C3N	2.32	1.41	1.34
3	O	6335	NDP	C2N-C3N	2.30	1.41	1.34
3	B	2335	NDP	C2N-C3N	2.29	1.41	1.34

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1335	NDP	C4A-C5A-N7A	4.36	113.94	109.40
3	B	2335	NDP	C4A-C5A-N7A	4.33	113.92	109.40
3	O	6335	NDP	C4A-C5A-N7A	4.33	113.91	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1335	NDP	N3A-C2A-N1A	-4.17	122.17	128.68
3	O	6335	NDP	N3A-C2A-N1A	-4.15	122.19	128.68
3	B	2335	NDP	N3A-C2A-N1A	-4.15	122.19	128.68
3	A	1335	NDP	O3X-P2B-O2X	3.72	121.85	107.64
3	O	6335	NDP	O3X-P2B-O2X	3.71	121.83	107.64
3	B	2335	NDP	O3X-P2B-O2X	3.71	121.81	107.64
3	O	6335	NDP	O3D-C3D-C4D	-2.88	102.72	111.05
3	B	2335	NDP	O3D-C3D-C4D	-2.87	102.74	111.05
3	A	1335	NDP	O3D-C3D-C4D	-2.86	102.77	111.05
3	B	2335	NDP	C1D-N1N-C6N	-2.33	115.81	120.83
3	O	6335	NDP	C1D-N1N-C6N	-2.33	115.81	120.83
3	A	1335	NDP	C1D-N1N-C6N	-2.32	115.83	120.83
3	B	2335	NDP	O5D-PN-O1N	-2.31	100.04	109.07
3	O	6335	NDP	O5D-PN-O1N	-2.30	100.08	109.07
3	B	2335	NDP	N6A-C6A-N1A	2.29	123.33	118.57
3	A	1335	NDP	O5D-PN-O1N	-2.29	100.12	109.07
3	A	1335	NDP	N6A-C6A-N1A	2.27	123.28	118.57
3	O	6335	NDP	N6A-C6A-N1A	2.26	123.26	118.57
3	A	1335	NDP	O2X-P2B-O1X	-2.17	102.20	110.68
3	O	6335	NDP	O2X-P2B-O1X	-2.16	102.23	110.68
3	B	2335	NDP	O2X-P2B-O1X	-2.16	102.23	110.68
3	A	1335	NDP	C3N-C2N-N1N	-2.14	120.04	123.10
3	B	2335	NDP	C3N-C2N-N1N	-2.10	120.10	123.10
3	O	6335	NDP	C3N-C2N-N1N	-2.08	120.13	123.10
3	B	2335	NDP	O4B-C1B-C2B	-2.06	103.02	106.59
3	A	1335	NDP	O4B-C1B-C2B	-2.05	103.03	106.59
3	O	6335	NDP	O4B-C1B-C2B	-2.04	103.04	106.59

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1335	NDP	C5B-O5B-PA-O1A
3	A	1335	NDP	PN-O3-PA-O5B
3	O	6335	NDP	C5B-O5B-PA-O1A
3	O	6335	NDP	PN-O3-PA-O5B
3	B	2335	NDP	C5B-O5B-PA-O1A
3	B	2335	NDP	PN-O3-PA-O5B
3	A	1335	NDP	C5B-O5B-PA-O3
3	O	6335	NDP	C5B-O5B-PA-O3
3	B	2335	NDP	C5B-O5B-PA-O3
3	A	1335	NDP	PA-O3-PN-O2N

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	O	6335	NDP	PA-O3-PN-O2N
3	B	2335	NDP	PA-O3-PN-O2N
3	A	1335	NDP	O4D-C1D-N1N-C6N
3	O	6335	NDP	O4D-C1D-N1N-C6N
3	B	2335	NDP	O4D-C1D-N1N-C6N
3	A	1335	NDP	O4B-C4B-C5B-O5B
3	O	6335	NDP	O4B-C4B-C5B-O5B
3	B	2335	NDP	O4B-C4B-C5B-O5B
3	A	1335	NDP	C2D-C1D-N1N-C6N
3	O	6335	NDP	C2D-C1D-N1N-C6N
3	B	2335	NDP	C2D-C1D-N1N-C6N
3	A	1335	NDP	O4D-C1D-N1N-C2N
3	B	2335	NDP	O4D-C1D-N1N-C2N
3	A	1335	NDP	PA-O3-PN-O1N
3	O	6335	NDP	PA-O3-PN-O1N
3	B	2335	NDP	PA-O3-PN-O1N
3	O	6335	NDP	O4D-C1D-N1N-C2N

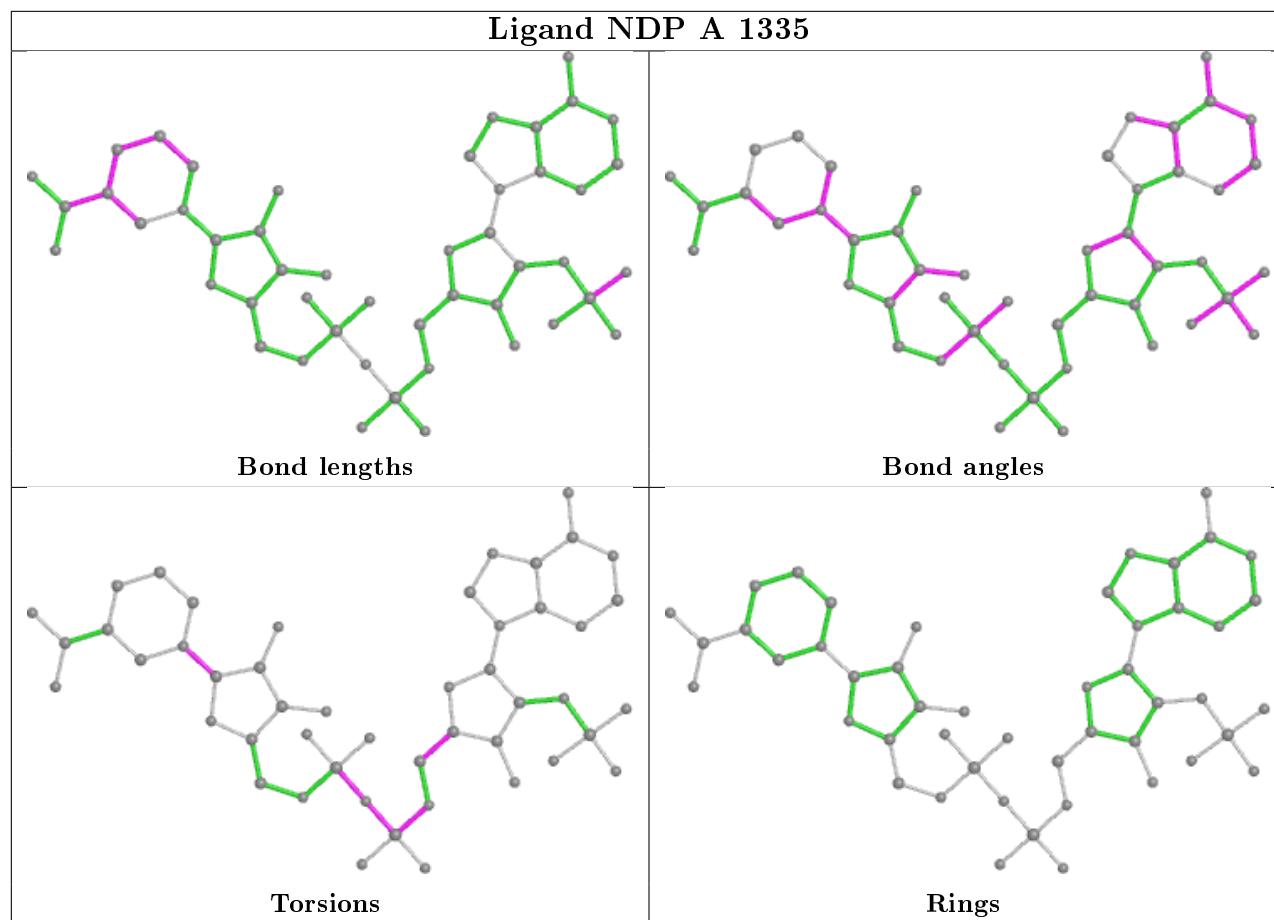
There are no ring outliers.

4 monomers are involved in 18 short contacts:

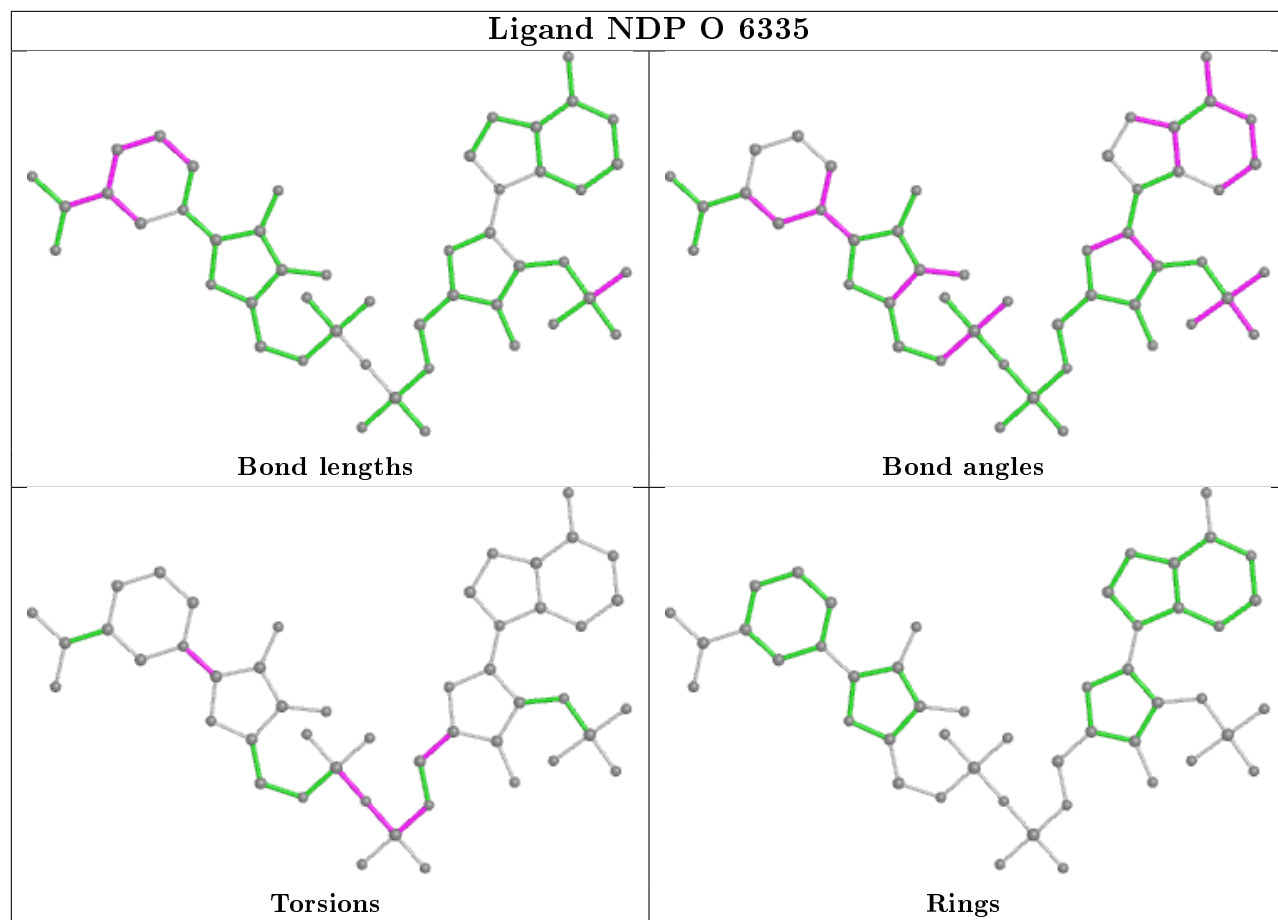
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1336	SO4	1	0
3	A	1335	NDP	5	0
3	O	6335	NDP	7	0
3	B	2335	NDP	5	0

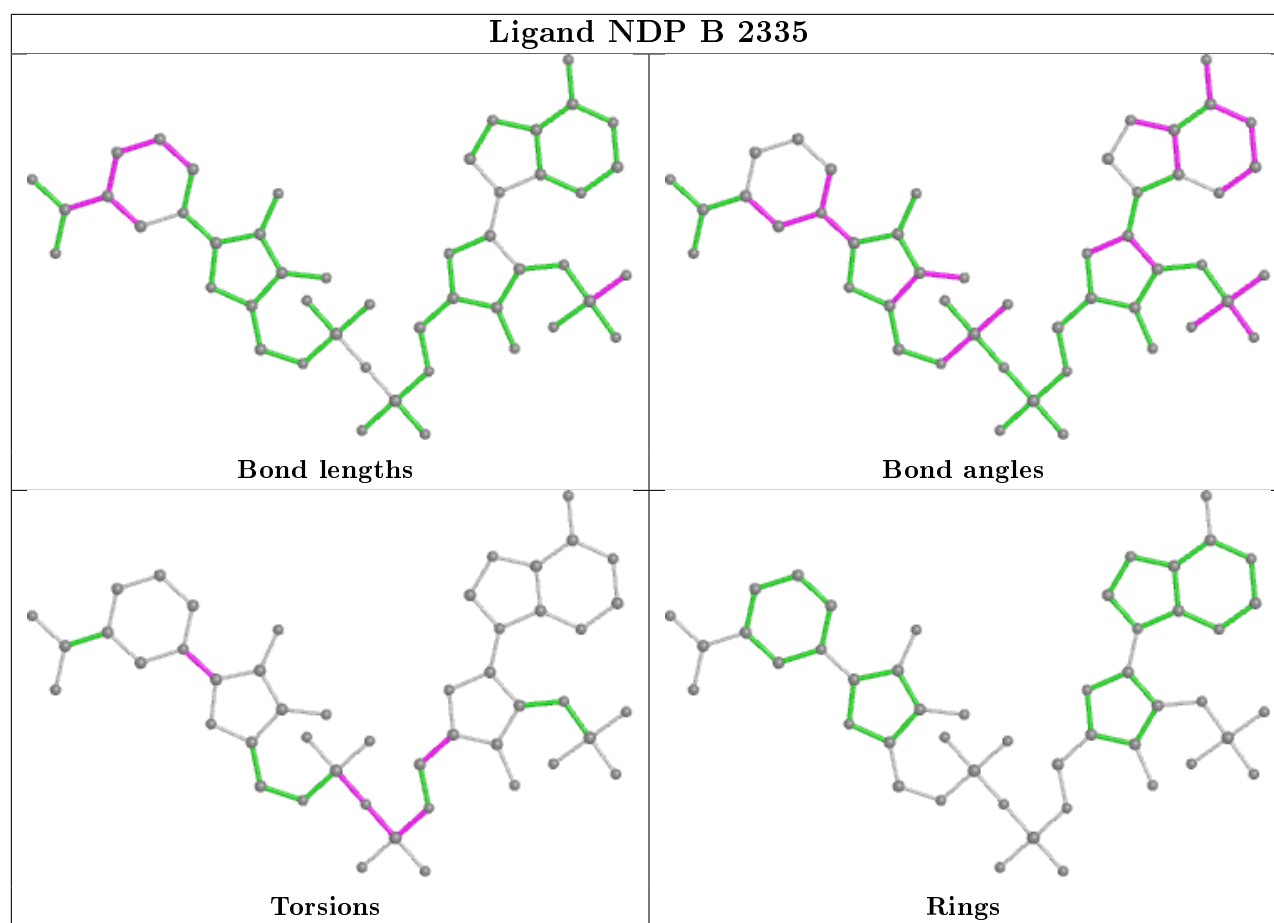
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

## Ligand NDP A 1335



## Ligand NDP O 6335





## 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.