



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2017 – 08:58 PM EDT

PDB ID : 2PKR  
Title : Crystal structure of (A+CTE)4 chimeric form of photosynthetic glyceraldehyde-3-phosphate dehydrogenase, complexed with NADP  
Authors : Fermani, S.; Falini, G.; Ripamonti, A.  
Deposited on : unknown  
Resolution : 2.40 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

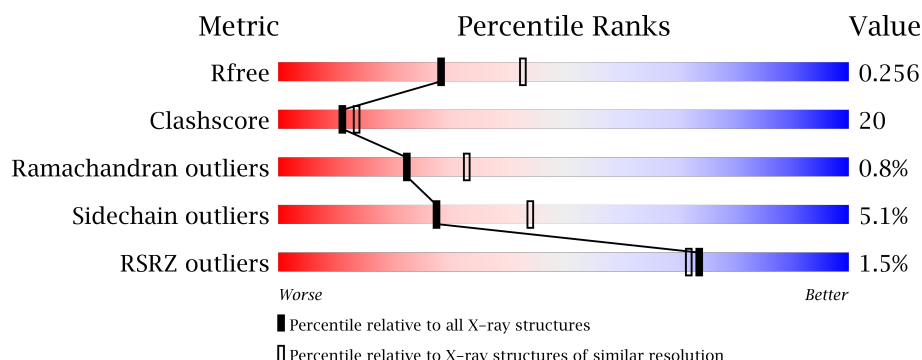
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	365	<div> <div>3%</div> <div>67% 19% 5% 8%</div> </div>
1	B	365	<div> <div>63% 24% 8%</div> </div>
1	C	365	<div> <div>68% 22% 8%</div> </div>
1	D	365	<div> <div>3%</div> <div>69% 20% 8%</div> </div>
1	H	365	<div> <div>2%</div> <div>68% 19% 8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	I	365	
1	L	365	
1	M	365	
1	O	365	
1	P	365	
1	Q	365	
1	R	365	

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	SO4	B	364	-	-	X	-
2	SO4	B	377	-	-	-	X
2	SO4	D	364	-	-	X	-
2	SO4	H	364	-	-	X	X
2	SO4	I	366	-	-	X	X
2	SO4	I	379	-	-	-	X
2	SO4	M	370	-	-	X	X
2	SO4	M	380	-	-	-	X
2	SO4	O	364	-	-	X	-
2	SO4	O	371	-	-	X	X
2	SO4	P	364	-	-	X	-
2	SO4	Q	373	-	-	-	X
2	SO4	Q	374	-	-	-	X
2	SO4	R	376	-	-	X	-
3	NDP	A	376	X	-	-	-
3	NDP	B	378	X	-	-	-
3	NDP	C	365	X	-	-	-
3	NDP	D	365	X	-	-	-
3	NDP	H	379	X	-	-	-
3	NDP	I	380	X	-	-	-
3	NDP	L	369	X	-	-	-
3	NDP	M	381	X	-	-	-
3	NDP	O	372	X	-	-	-
3	NDP	P	373	X	-	-	-
3	NDP	Q	375	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NDP	R	377	X	-	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31248 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 Aor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	337	Total	C	N	O	S	0	0	0
			2542	1599	445	487	11			
1	R	337	Total	C	N	O	S	0	0	0
			2542	1599	445	487	11			
1	P	337	Total	C	N	O	S	0	0	0
			2542	1599	445	487	11			
1	Q	337	Total	C	N	O	S	0	0	0
			2542	1599	445	487	11			
1	A	337	Total	C	N	O	S	0	0	0
			2542	1599	445	487	11			
1	B	337	Total	C	N	O	S	0	0	0
			2542	1599	445	487	11			
1	C	337	Total	C	N	O	S	0	0	0
			2542	1599	445	487	11			
1	D	336	Total	C	N	O	S	0	0	0
			2538	1597	444	486	11			
1	H	336	Total	C	N	O	S	0	0	0
			2538	1597	444	486	11			
1	I	337	Total	C	N	O	S	0	0	0
			2542	1599	445	487	11			
1	L	336	Total	C	N	O	S	0	0	0
			2538	1597	444	486	11			
1	M	337	Total	C	N	O	S	0	0	0
			2542	1599	445	487	11			

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



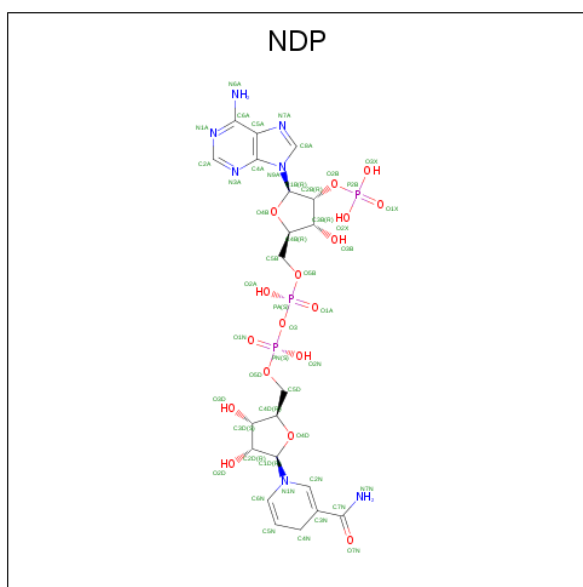
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	O	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	M	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 48	C 21	N 7	O 17	P 3	0	0
3	R	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	P	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	Q	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	D	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	H	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	I	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	L	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	M	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 4 is water.

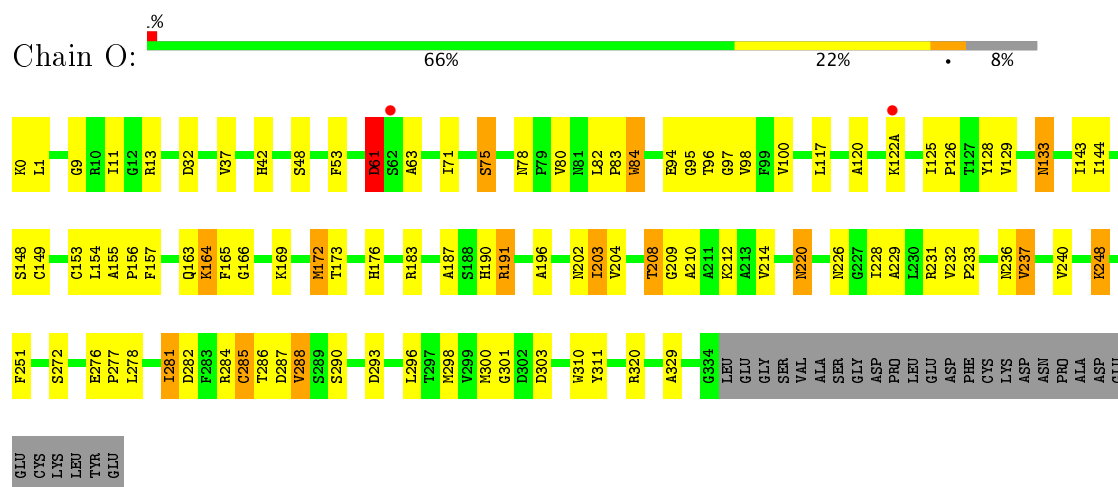


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	1	Total 1	O 1	0	0
4	H	2	Total 2	O 2	0	0
4	I	1	Total 1	O 1	0	0
4	L	4	Total 4	O 4	0	0
4	M	2	Total 2	O 2	0	0

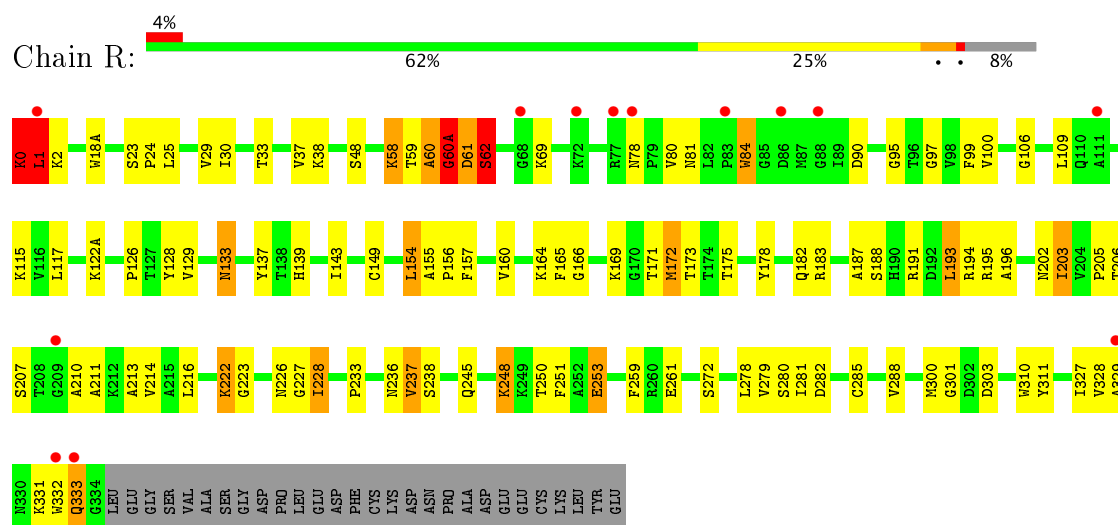
### 3 Residue-property plots

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 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: Glyceraldehyde-3-phosphate dehydrogenase Aor

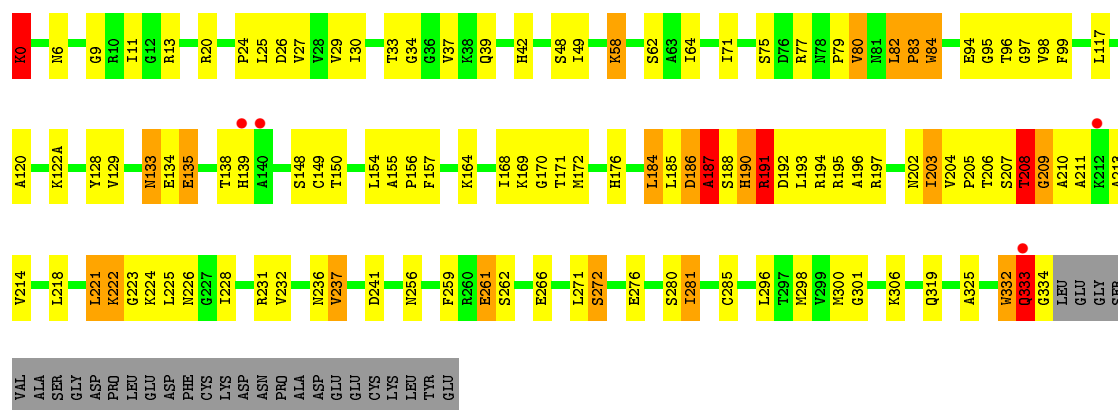


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase Aor



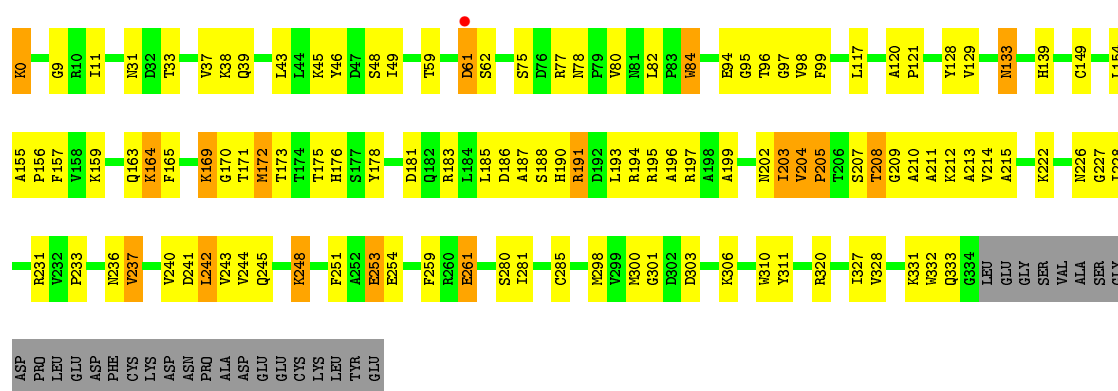
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase Aor





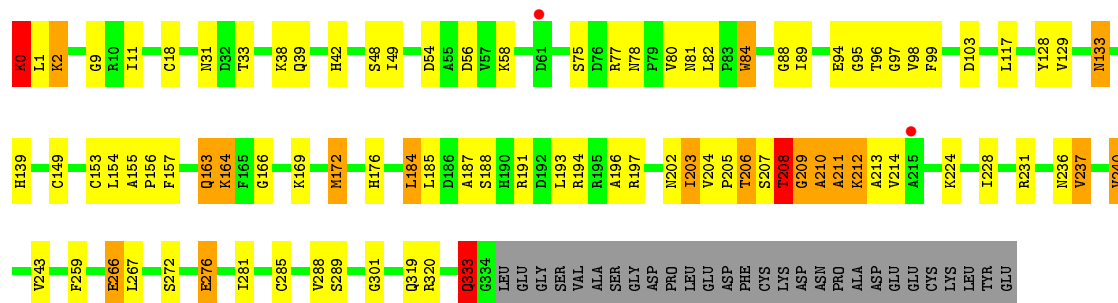
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase Aor

Chain Q: 61% 27% 5% 8%



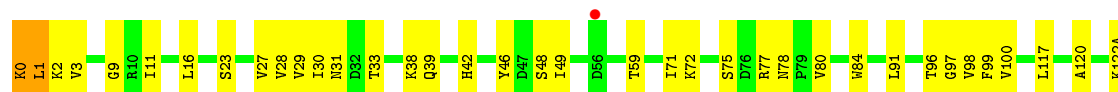
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase Aor

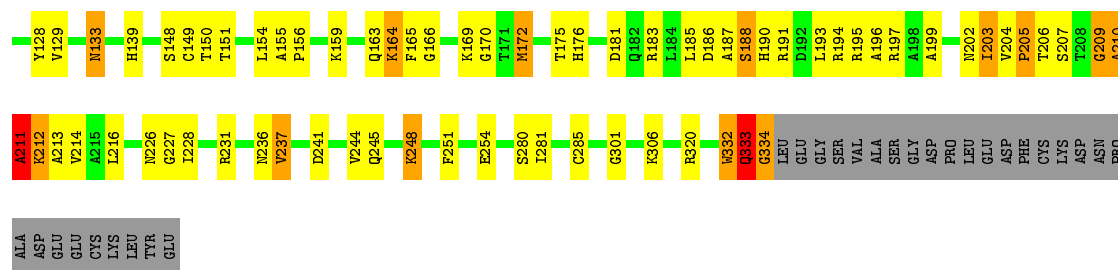
Chain A: 67% 19% 5% 8%



• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase Aor

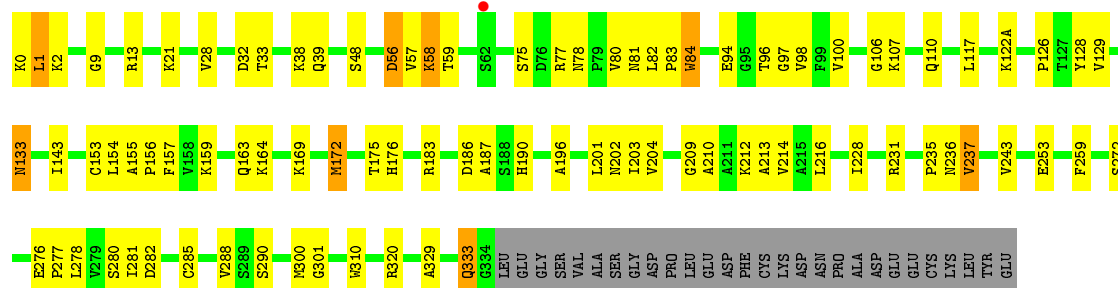
Chain B: 63% 24% 8%





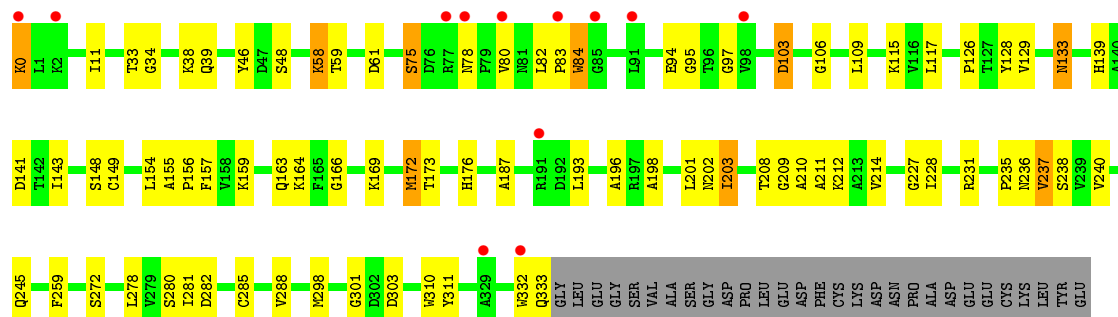
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase Aor

Chain C: 68% 22% 8%



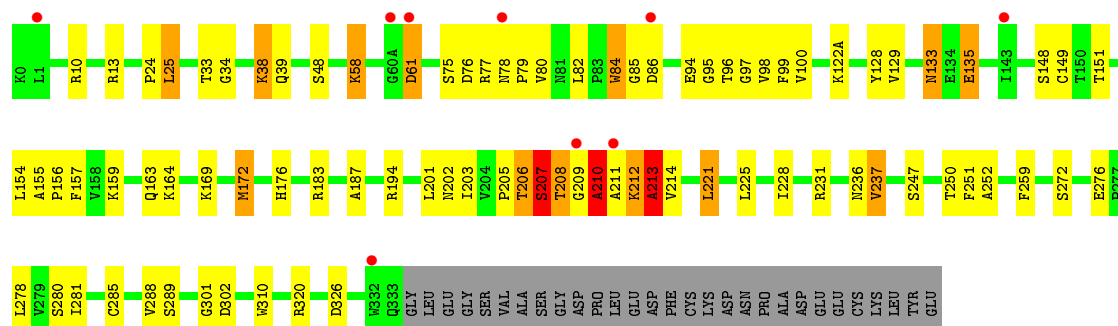
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase Aor

Chain D: 3% 69% 20% 8%

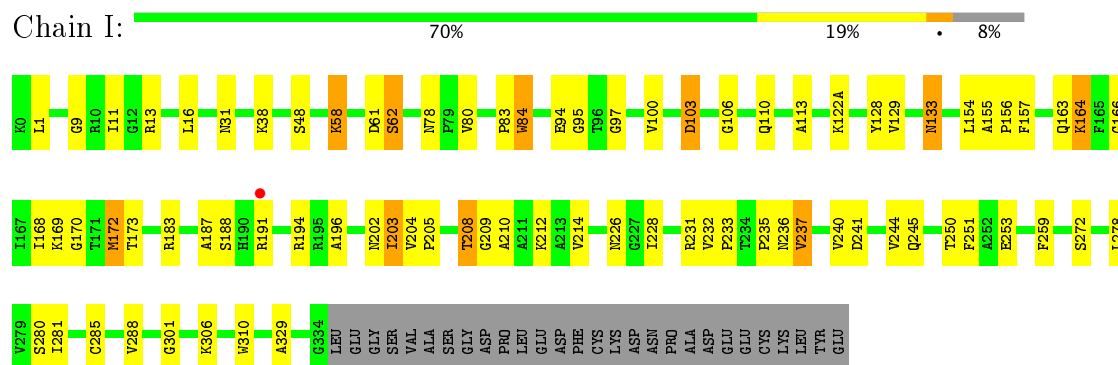


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase Aor

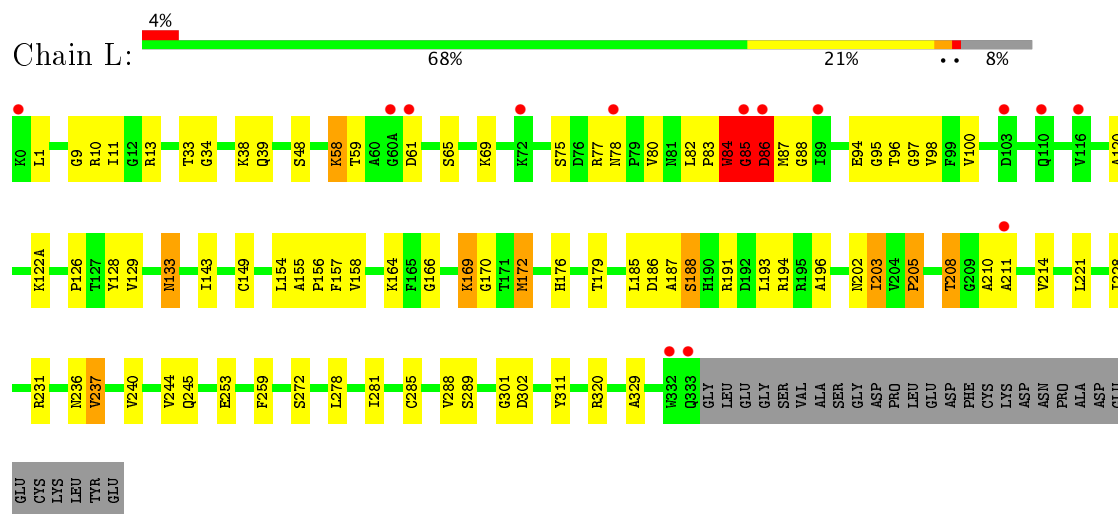
Chain H: 2% 68% 19% 8%



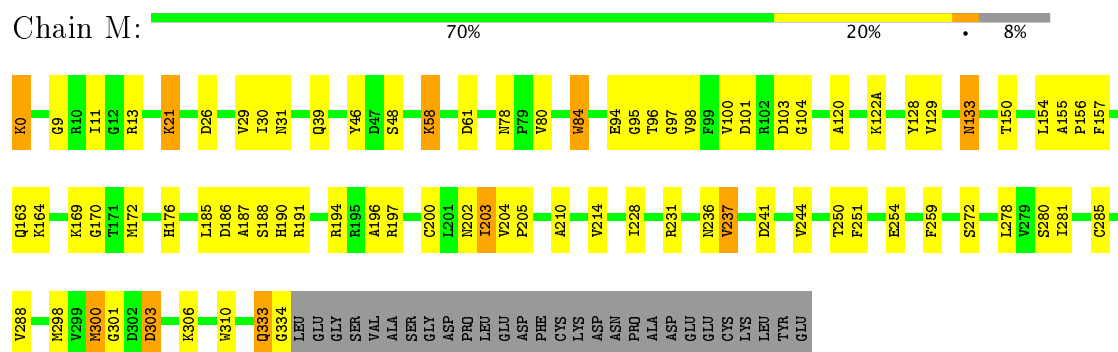
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase Aor



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase Aor



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase Aor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.38Å 217.71Å 114.79Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	63.22 – 2.40 73.14 – 2.40	Depositor EDS
% Data completeness (in resolution range)	76.5 (63.22-2.40) 76.5 (73.14-2.40)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.249 , 0.258 0.248 , 0.256	Depositor DCC
$R_{free}$ test set	7785 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , -6.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.478 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	31248	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.39 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.7836e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: 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	0.65	3/2583 (0.1%)	0.96	9/3507 (0.3%)
1	B	0.74	4/2583 (0.2%)	0.95	11/3507 (0.3%)
1	C	0.60	0/2583	0.86	4/3507 (0.1%)
1	D	0.59	0/2579	0.82	3/3502 (0.1%)
1	H	0.66	3/2579 (0.1%)	0.97	12/3502 (0.3%)
1	I	0.57	0/2583	0.81	1/3507 (0.0%)
1	L	0.61	1/2579 (0.0%)	0.92	13/3502 (0.4%)
1	M	0.57	1/2583 (0.0%)	0.82	3/3507 (0.1%)
1	O	0.61	0/2583	0.88	4/3507 (0.1%)
1	P	0.66	1/2583 (0.0%)	1.04	16/3507 (0.5%)
1	Q	0.59	1/2583 (0.0%)	0.90	8/3507 (0.2%)
1	R	0.64	2/2583 (0.1%)	0.99	12/3507 (0.3%)
All	All	0.63	16/30984 (0.1%)	0.91	96/42069 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	7
1	B	0	3
1	C	0	1
1	H	1	5
1	I	0	1
1	L	0	2
1	M	0	2
1	O	0	2
1	P	1	7
1	Q	0	6
1	R	0	8

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	3	44

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	210	ALA	C-N	14.89	1.68	1.34
1	B	333	GLN	C-N	-11.20	1.12	1.33
1	A	0	LYS	C-O	10.76	1.43	1.23
1	B	205	PRO	C-N	9.79	1.56	1.34
1	L	205	PRO	C-N	-7.87	1.16	1.34
1	H	210	ALA	C-N	7.45	1.51	1.34
1	A	206	THR	C-N	-6.90	1.18	1.34
1	P	82	LEU	C-N	6.82	1.47	1.34
1	R	62	SER	C-N	6.75	1.49	1.34
1	R	0	LYS	N-CA	6.60	1.59	1.46
1	M	334	GLY	N-CA	-6.25	1.36	1.46
1	H	205	PRO	C-N	-5.31	1.21	1.34
1	B	334	GLY	C-O	5.21	1.31	1.23
1	A	0	LYS	C-N	-5.19	1.22	1.34
1	Q	0	LYS	C-N	5.17	1.46	1.34
1	H	61	ASP	CB-CG	5.02	1.62	1.51

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	62	SER	O-C-N	-19.79	91.04	122.70
1	A	0	LYS	CA-C-O	-14.38	89.89	120.10
1	C	333	GLN	C-N-CA	13.54	150.73	122.30
1	H	206	THR	C-N-CA	12.83	153.76	121.70
1	A	206	THR	C-N-CA	11.39	150.18	121.70
1	Q	0	LYS	O-C-N	-11.07	104.98	122.70
1	L	208	THR	C-N-CA	10.75	144.88	122.30
1	B	333	GLN	C-N-CA	10.72	144.82	122.30
1	A	0	LYS	CA-C-N	10.69	140.72	117.20
1	P	0	LYS	O-C-N	10.61	139.68	122.70
1	Q	204	VAL	C-N-CD	10.56	150.57	128.40
1	R	60(A)	GLY	C-N-CA	10.27	147.38	121.70
1	B	211	ALA	C-N-CA	9.87	146.37	121.70
1	B	334	GLY	CA-C-O	-9.50	103.50	120.60
1	M	303	ASP	CB-CG-OD1	9.30	126.67	118.30
1	H	61	ASP	CB-CG-OD1	9.26	126.64	118.30
1	H	210	ALA	O-C-N	-8.64	108.88	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	206	THR	C-N-CA	8.62	143.25	121.70
1	P	0	LYS	CA-C-N	-8.56	98.36	117.20
1	L	61	ASP	CB-CG-OD1	8.44	125.90	118.30
1	P	83	PRO	O-C-N	-8.40	109.26	122.70
1	H	61	ASP	CB-CA-C	-8.36	93.69	110.40
1	D	0	LYS	O-C-N	-8.21	109.57	122.70
1	P	186	ASP	CB-CG-OD1	8.18	125.66	118.30
1	L	61	ASP	CB-CA-C	-8.06	94.28	110.40
1	L	86	ASP	CB-CG-OD1	8.05	125.55	118.30
1	B	210	ALA	O-C-N	8.02	135.53	122.70
1	B	206	THR	C-N-CA	8.01	141.73	121.70
1	Q	205	PRO	CA-N-CD	-7.99	100.31	111.50
1	H	38	LYS	C-N-CA	7.80	141.21	121.70
1	R	1	LEU	CA-C-N	-7.73	100.19	117.20
1	Q	0	LYS	C-N-CA	7.68	140.89	121.70
1	H	205	PRO	C-N-CA	7.37	140.12	121.70
1	A	209	GLY	O-C-N	-7.35	110.94	122.70
1	H	86	ASP	CB-CG-OD1	7.14	124.73	118.30
1	P	192	ASP	CB-CG-OD1	7.10	124.69	118.30
1	H	213	ALA	O-C-N	-6.71	111.97	122.70
1	B	203	ILE	N-CA-C	-6.69	92.95	111.00
1	P	191	ARG	O-C-N	6.65	133.33	122.70
1	Q	203	ILE	N-CA-C	-6.58	93.22	111.00
1	L	88	GLY	O-C-N	6.57	133.21	122.70
1	L	84	TRP	CA-C-O	6.40	133.53	120.10
1	D	203	ILE	N-CA-C	-6.34	93.89	111.00
1	P	333	GLN	C-N-CA	6.29	135.51	122.30
1	L	88	GLY	CA-C-N	-6.28	103.39	117.20
1	C	203	ILE	N-CA-C	-6.26	94.10	111.00
1	L	85	GLY	CA-C-N	-6.26	103.43	117.20
1	R	203	ILE	N-CA-C	-6.23	94.19	111.00
1	B	209	GLY	O-C-N	-6.22	112.74	122.70
1	A	203	ILE	N-CA-C	-6.21	94.23	111.00
1	Q	208	THR	CA-C-N	-6.21	103.78	116.20
1	P	332	TRP	C-N-CA	6.17	137.13	121.70
1	O	287	ASP	CB-CG-OD1	6.16	123.85	118.30
1	L	203	ILE	N-CA-C	-6.10	94.53	111.00
1	M	333	GLN	C-N-CA	6.01	134.92	122.30
1	Q	0	LYS	CA-C-N	5.95	130.30	117.20
1	I	203	ILE	N-CA-C	-5.89	95.11	111.00
1	O	288	VAL	O-C-N	-5.85	113.34	122.70
1	P	208	THR	C-N-CA	5.79	134.47	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	333	GLN	C-N-CA	5.77	134.42	122.30
1	P	26	ASP	CB-CG-OD1	5.76	123.49	118.30
1	R	0	LYS	C-N-CA	5.74	136.04	121.70
1	R	207	SER	CA-C-N	-5.70	104.67	117.20
1	P	26	ASP	O-C-N	-5.68	113.61	122.70
1	Q	175	THR	N-CA-C	-5.65	95.74	111.00
1	R	61	ASP	CA-C-O	5.64	131.95	120.10
1	P	6	ASN	O-C-N	-5.64	113.61	123.20
1	O	203	ILE	N-CA-C	-5.62	95.83	111.00
1	A	208	THR	N-CA-CB	5.62	120.97	110.30
1	H	203	ILE	N-CA-C	-5.61	95.85	111.00
1	H	61	ASP	N-CA-CB	5.61	120.70	110.60
1	H	38	LYS	CA-C-N	-5.61	104.86	117.20
1	R	60	ALA	CB-CA-C	5.56	118.44	110.10
1	P	80	VAL	O-C-N	-5.54	113.83	122.70
1	P	122(A)	LYS	C-N-CA	-5.45	110.85	122.30
1	B	175	THR	N-CA-C	-5.38	96.47	111.00
1	C	1	LEU	O-C-N	-5.37	114.11	122.70
1	P	187	ALA	CA-C-N	-5.33	105.48	117.20
1	L	84	TRP	C-N-CA	-5.33	111.11	122.30
1	B	210	ALA	C-N-CA	-5.31	108.43	121.70
1	L	245	GLN	N-CA-C	-5.29	96.72	111.00
1	R	60(A)	GLY	CA-C-O	-5.28	111.10	120.60
1	H	212	LYS	N-CA-CB	5.28	120.10	110.60
1	M	203	ILE	N-CA-C	-5.24	96.87	111.00
1	R	175	THR	N-CA-C	-5.19	96.99	111.00
1	A	333	GLN	N-CA-CB	5.12	119.81	110.60
1	R	61	ASP	N-CA-CB	5.11	119.79	110.60
1	B	332	TRP	C-N-CA	5.11	134.47	121.70
1	A	206	THR	O-C-N	5.09	130.84	122.70
1	B	210	ALA	CA-C-N	-5.08	106.02	117.20
1	L	84	TRP	CA-C-N	-5.08	106.05	116.20
1	C	175	THR	N-CA-C	-5.07	97.31	111.00
1	R	61	ASP	C-N-CA	-5.06	109.04	121.70
1	O	61	ASP	CB-CG-OD2	5.04	122.84	118.30
1	D	0	LYS	CA-C-N	5.04	128.29	117.20
1	L	61	ASP	N-CA-CB	5.02	119.63	110.60

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	P	208	THR	CA

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Mol	Chain	Res	Type	Atom
1	A	208	THR	CA
1	H	212	LYS	CA

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	0	LYS	Mainchain,Peptide
1	A	206	THR	Peptide
1	A	208	THR	Peptide
1	A	210	ALA	Mainchain
1	A	211	ALA	Mainchain
1	A	212	LYS	Mainchain
1	B	211	ALA	Peptide
1	B	333	GLN	Mainchain,Peptide
1	C	333	GLN	Peptide
1	H	207	SER	Peptide
1	H	210	ALA	Mainchain
1	H	213	ALA	Mainchain
1	H	38	LYS	Mainchain
1	H	85	GLY	Mainchain
1	I	62	SER	Mainchain
1	L	208	THR	Mainchain
1	L	85	GLY	Mainchain
1	M	300	MET	Mainchain
1	M	333	GLN	Mainchain
1	O	285	CYS	Mainchain
1	O	61	ASP	Mainchain
1	P	187	ALA	Mainchain
1	P	203	ILE	Mainchain
1	P	207	SER	Mainchain
1	P	208	THR	Mainchain,Peptide
1	P	80	VAL	Mainchain
1	P	83	PRO	Mainchain
1	Q	0	LYS	Mainchain
1	Q	204	VAL	Mainchain
1	Q	207	SER	Mainchain,Peptide
1	Q	208	THR	Mainchain
1	Q	213	ALA	Mainchain
1	R	0	LYS	Mainchain,Peptide
1	R	206	THR	Mainchain
1	R	333	GLN	Mainchain,Peptide
1	R	60(A)	GLY	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
1	R	62	SER	Mainchain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2542	0	2573	123	0
1	B	2542	0	2573	132	0
1	C	2542	0	2576	117	0
1	D	2538	0	2574	86	0
1	H	2538	0	2571	96	0
1	I	2542	0	2577	112	0
1	L	2538	0	2572	82	1
1	M	2542	0	2577	94	0
1	O	2542	0	2577	154	0
1	P	2542	0	2575	151	0
1	Q	2542	0	2577	167	1
1	R	2542	0	2575	154	0
2	A	15	0	0	0	0
2	B	15	0	0	2	0
2	C	10	0	0	0	0
2	D	10	0	0	2	0
2	H	15	0	0	4	0
2	I	15	0	0	6	0
2	L	10	0	0	1	0
2	M	15	0	0	3	0
2	O	15	0	0	4	0
2	P	15	0	0	6	0
2	Q	20	0	0	1	0
2	R	15	0	0	3	0
3	A	48	0	20	19	0
3	B	48	0	21	13	0
3	C	48	0	20	16	0
3	D	48	0	19	6	0
3	H	48	0	20	14	0
3	I	48	0	20	10	0
3	L	48	0	20	14	0
3	M	48	0	20	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	48	0	21	15	0
3	P	48	0	21	11	0
3	Q	48	0	21	16	0
3	R	48	0	20	5	0
4	H	2	0	0	0	0
4	I	1	0	0	0	0
4	L	4	0	0	0	0
4	M	2	0	0	1	0
4	O	1	0	0	0	0
All	All	31248	0	31140	1242	1

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 20.

All (1242) 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)
3:D:365:NDP:C3D	3:D:365:NDP:C2D	1.76	1.64
3:M:381:NDP:C1D	3:M:381:NDP:C2D	1.76	1.62
3:I:380:NDP:C1D	3:I:380:NDP:C2D	1.77	1.61
3:C:365:NDP:C2D	3:C:365:NDP:C1D	1.79	1.59
3:B:378:NDP:C1D	3:B:378:NDP:C2D	1.78	1.55
3:P:373:NDP:C1D	3:P:373:NDP:C2D	1.80	1.52
3:Q:375:NDP:C1D	3:Q:375:NDP:C2D	1.82	1.52
3:L:369:NDP:C2D	3:L:369:NDP:C1D	1.85	1.50
3:C:365:NDP:O4B	3:C:365:NDP:C4B	1.64	1.46
3:A:376:NDP:C4B	3:A:376:NDP:O4B	1.63	1.45
3:B:378:NDP:C4B	3:B:378:NDP:O4B	1.65	1.44
3:O:372:NDP:O4B	3:O:372:NDP:C4B	1.65	1.44
3:P:373:NDP:C4B	3:P:373:NDP:O4B	1.64	1.44
3:R:377:NDP:O4B	3:R:377:NDP:C4B	1.65	1.44
1:O:163:GLN:NE2	1:O:164:LYS:HZ2	1.14	1.43
1:B:210:ALA:C	1:B:211:ALA:N	1.68	1.43
3:O:372:NDP:C1D	3:O:372:NDP:C2D	1.96	1.43
3:Q:375:NDP:C4B	3:Q:375:NDP:O4B	1.64	1.43
3:D:365:NDP:O4B	3:D:365:NDP:C4B	1.65	1.43
1:Q:154:LEU:HD11	1:Q:242:LEU:CD2	1.47	1.43
3:I:380:NDP:C4B	3:I:380:NDP:O4B	1.64	1.42
1:R:165:PHE:HA	1:R:248:LYS:CD	1.47	1.42
3:A:376:NDP:C1D	3:A:376:NDP:O4D	1.67	1.41
3:M:381:NDP:C4B	3:M:381:NDP:O4B	1.65	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:GLN:NE2	1:A:164:LYS:NZ	1.64	1.39
1:Q:191:ARG:H	1:Q:191:ARG:CD	1.10	1.37
3:L:369:NDP:O4B	3:L:369:NDP:C4B	1.64	1.36
1:Q:154:LEU:CD1	1:Q:242:LEU:HD23	1.53	1.36
3:H:379:NDP:C4B	3:H:379:NDP:O4B	1.65	1.35
3:A:376:NDP:C1D	3:A:376:NDP:C2D	2.04	1.34
1:B:165:PHE:HA	1:B:248:LYS:CD	1.57	1.33
1:O:163:GLN:HE22	1:O:164:LYS:NZ	1.25	1.30
1:I:163:GLN:NE2	1:I:164:LYS:HZ2	1.30	1.27
1:O:163:GLN:NE2	1:O:164:LYS:NZ	1.78	1.27
1:R:60:ALA:O	1:R:60(A):GLY:O	1.55	1.22
1:O:251:PHE:HB2	2:O:371:SO4:O2	1.42	1.19
1:O:165:PHE:HD1	1:O:248:LYS:HD3	1.06	1.18
1:Q:191:ARG:N	1:Q:191:ARG:HD2	1.18	1.18
1:H:210:ALA:O	1:H:214:VAL:HG23	1.46	1.14
1:I:163:GLN:HE21	1:I:164:LYS:NZ	1.45	1.12
1:O:163:GLN:HE21	1:O:164:LYS:HD3	1.04	1.11
1:O:293:ASP:HB3	1:O:296:LEU:HD12	1.23	1.10
1:O:163:GLN:HE21	1:O:164:LYS:CD	1.65	1.10
1:M:21:LYS:H	1:M:21:LYS:HD3	1.14	1.08
1:C:183:ARG:HD2	1:C:187:ALA:HB3	1.14	1.08
1:C:159:LYS:O	1:C:163:GLN:HG3	1.50	1.08
1:A:202:ASN:HD21	1:C:281:ILE:HB	1.11	1.07
1:B:210:ALA:O	1:B:211:ALA:O	1.71	1.07
1:I:281:ILE:HB	1:M:202:ASN:HD21	1.20	1.06
1:O:281:ILE:HB	1:P:202:ASN:HD21	1.14	1.06
1:H:281:ILE:HB	1:L:202:ASN:HD21	1.21	1.05
1:O:281:ILE:HB	1:P:202:ASN:ND2	1.71	1.04
1:P:27:VAL:HG12	1:P:71:ILE:HD11	1.07	1.04
3:A:376:NDP:C4D	3:A:376:NDP:C1D	2.36	1.04
1:R:58:LYS:HB3	1:R:58:LYS:NZ	1.66	1.03
1:I:163:GLN:NE2	1:I:164:LYS:NZ	2.01	1.03
1:P:135:GLU:OE1	1:P:135:GLU:N	1.90	1.03
1:B:165:PHE:CA	1:B:248:LYS:HD3	1.87	1.03
1:C:80:VAL:HB	1:C:110:GLN:OE1	1.59	1.02
1:H:202:ASN:HD21	1:L:281:ILE:HB	1.23	1.02
1:H:169:LYS:HD2	1:L:301:GLY:HA3	1.40	1.02
1:I:202:ASN:HD21	1:M:281:ILE:HB	1.25	1.02
1:M:0:LYS:HD3	1:M:26:ASP:HB2	1.36	1.00
1:O:228:ILE:HD12	1:P:296:LEU:HD22	1.42	0.99
1:R:165:PHE:CA	1:R:248:LYS:HD2	1.92	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:165:PHE:HA	1:R:248:LYS:HD2	1.04	0.99
1:R:281:ILE:HB	1:Q:202:ASN:HD21	1.24	0.98
3:A:376:NDP:N1N	3:A:376:NDP:C2D	2.25	0.98
1:O:165:PHE:CD1	1:O:248:LYS:HD3	1.97	0.98
3:Q:375:NDP:C2D	3:Q:375:NDP:N1N	2.26	0.98
1:B:281:ILE:HB	1:D:202:ASN:HD21	1.30	0.97
1:P:134:GLU:HG2	1:P:135:GLU:OE1	1.63	0.97
1:P:208:THR:HG22	1:P:228:ILE:HA	1.43	0.97
1:A:188:SER:HB2	1:B:39:GLN:OE1	1.64	0.97
1:B:202:ASN:HD21	1:D:281:ILE:HB	1.26	0.96
1:O:281:ILE:CB	1:P:202:ASN:HD21	1.79	0.96
1:O:228:ILE:HG12	1:O:229:ALA:H	1.29	0.96
1:P:203:ILE:HG12	1:P:232:VAL:HG12	1.47	0.96
3:O:372:NDP:N1N	3:O:372:NDP:C2D	2.29	0.95
3:P:373:NDP:N1N	3:P:373:NDP:C2D	2.28	0.95
1:H:301:GLY:HA3	1:L:169:LYS:HD2	1.47	0.95
1:B:241:ASP:OD1	1:B:306:LYS:HE2	1.66	0.95
3:L:369:NDP:C2D	3:L:369:NDP:N1N	2.30	0.95
1:R:165:PHE:HA	1:R:248:LYS:CG	1.97	0.95
1:B:202:ASN:ND2	1:D:281:ILE:H	1.65	0.95
3:B:378:NDP:N1N	3:B:378:NDP:C2D	2.29	0.95
1:P:27:VAL:CG1	1:P:71:ILE:HD11	1.96	0.94
1:P:271:LEU:HD13	1:P:272:SER:N	1.82	0.94
1:R:165:PHE:CA	1:R:248:LYS:CD	2.44	0.94
1:L:158:VAL:CG1	1:L:221:LEU:HD11	1.97	0.94
1:P:222:LYS:HD3	1:P:223:GLY:N	1.83	0.94
1:P:27:VAL:HG12	1:P:71:ILE:CD1	1.98	0.94
3:C:365:NDP:C2D	3:C:365:NDP:N1N	2.30	0.93
1:M:0:LYS:CD	1:M:26:ASP:HB2	1.97	0.93
1:A:202:ASN:HD21	1:C:281:ILE:CB	1.81	0.93
1:O:293:ASP:CB	1:O:296:LEU:HD12	1.98	0.93
1:R:202:ASN:HD21	1:Q:281:ILE:HB	1.32	0.93
1:O:165:PHE:HD1	1:O:248:LYS:CD	1.82	0.92
1:A:169:LYS:HD2	1:C:301:GLY:HA3	1.48	0.92
1:O:301:GLY:HA3	1:P:169:LYS:HD2	1.48	0.92
1:M:0:LYS:NZ	1:M:0:LYS:CB	2.32	0.92
1:O:163:GLN:NE2	1:O:164:LYS:CD	2.31	0.92
1:B:165:PHE:HA	1:B:248:LYS:HD3	0.94	0.92
1:R:281:ILE:H	1:Q:202:ASN:HD22	1.15	0.92
1:A:202:ASN:ND2	1:C:281:ILE:HB	1.85	0.92
1:O:183:ARG:NH1	1:O:187:ALA:HB1	1.84	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:165:PHE:HA	1:O:248:LYS:HD2	1.50	0.91
1:I:281:ILE:H	1:M:202:ASN:ND2	1.68	0.91
1:O:165:PHE:HA	1:O:248:LYS:HG2	1.50	0.91
1:O:202:ASN:HD21	1:P:281:ILE:HB	1.34	0.91
1:B:139:HIS:CD2	1:B:333:GLN:HB2	2.05	0.91
1:C:77:ARG:NH1	3:C:365:NDP:C5A	2.34	0.91
1:C:110:GLN:NE2	1:I:106:GLY:HA3	1.85	0.91
1:Q:139:HIS:HE1	1:Q:332:TRP:CD2	1.89	0.91
1:O:163:GLN:NE2	1:O:164:LYS:CE	2.34	0.90
1:B:202:ASN:HD22	1:D:281:ILE:H	1.14	0.90
3:M:381:NDP:N1N	3:M:381:NDP:C2D	2.33	0.90
1:R:58:LYS:HB3	1:R:58:LYS:HZ3	1.35	0.90
3:A:376:NDP:N1N	3:A:376:NDP:O2D	2.04	0.90
1:I:202:ASN:ND2	1:M:281:ILE:H	1.69	0.90
1:R:139:HIS:O	1:R:139:HIS:HD2	1.54	0.90
3:I:380:NDP:N1N	3:I:380:NDP:C2D	2.33	0.89
1:R:139:HIS:HB3	1:R:333:GLN:OE1	1.73	0.89
1:B:172:MET:HE1	1:B:211:ALA:N	1.86	0.89
1:O:183:ARG:NH1	1:O:187:ALA:CB	2.35	0.89
1:B:38:LYS:HD3	1:B:59:THR:HG21	1.55	0.89
1:O:163:GLN:NE2	1:O:164:LYS:HD3	1.85	0.89
1:Q:191:ARG:H	1:Q:191:ARG:HD3	1.32	0.89
1:D:61:ASP:HB2	1:H:61:ASP:OD1	1.73	0.88
1:P:208:THR:HG22	1:P:228:ILE:CA	2.03	0.88
1:R:281:ILE:H	1:Q:202:ASN:ND2	1.72	0.88
1:B:169:LYS:HD2	1:D:301:GLY:HA3	1.55	0.88
1:H:281:ILE:HB	1:L:202:ASN:ND2	1.89	0.88
1:I:281:ILE:CB	1:M:202:ASN:HD21	1.87	0.88
1:B:281:ILE:HB	1:D:202:ASN:ND2	1.87	0.88
1:C:77:ARG:HH11	3:C:365:NDP:C5A	1.85	0.88
1:O:165:PHE:HA	1:O:248:LYS:CG	2.02	0.88
1:P:139:HIS:CD2	1:P:333:GLN:HG3	2.09	0.88
1:Q:191:ARG:CD	1:Q:191:ARG:N	1.92	0.87
1:A:202:ASN:HD22	1:C:281:ILE:H	1.20	0.87
1:O:228:ILE:HG12	1:O:229:ALA:N	1.87	0.87
1:R:164:LYS:O	1:R:248:LYS:CD	2.23	0.87
1:B:202:ASN:HD21	1:D:281:ILE:CB	1.88	0.87
1:O:281:ILE:H	1:P:202:ASN:ND2	1.73	0.87
1:C:183:ARG:HD2	1:C:187:ALA:CB	2.03	0.87
1:B:183:ARG:HE	1:B:187:ALA:HB3	1.37	0.86
1:A:202:ASN:ND2	1:C:281:ILE:H	1.73	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:202:ASN:HD22	1:M:281:ILE:H	1.18	0.86
1:I:281:ILE:HB	1:M:202:ASN:ND2	1.90	0.86
1:R:281:ILE:HB	1:Q:202:ASN:ND2	1.91	0.86
1:I:202:ASN:HD21	1:M:281:ILE:CB	1.88	0.86
1:R:281:ILE:CB	1:Q:202:ASN:HD21	1.88	0.86
1:Q:38:LYS:HD3	1:Q:59:THR:HG21	1.58	0.86
1:R:165:PHE:O	1:R:248:LYS:HG2	1.75	0.86
1:O:298:MET:HE1	1:P:226:ASN:OD1	1.76	0.85
1:P:209:GLY:HA3	2:P:364:SO4:O1	1.76	0.85
1:H:281:ILE:CB	1:L:202:ASN:HD21	1.89	0.85
1:H:77:ARG:NH1	3:H:379:NDP:C5A	2.40	0.85
1:O:165:PHE:HA	1:O:248:LYS:CD	2.07	0.85
1:I:281:ILE:H	1:M:202:ASN:HD22	1.20	0.84
1:Q:154:LEU:HD23	1:Q:214:VAL:HG21	1.59	0.84
1:Q:139:HIS:CE1	1:Q:332:TRP:HA	2.12	0.84
3:Q:375:NDP:O2D	3:Q:375:NDP:N1N	2.10	0.84
1:P:134:GLU:CG	1:P:135:GLU:OE1	2.25	0.84
1:D:61:ASP:HB2	1:H:61:ASP:CG	1.98	0.84
1:A:2:LYS:HB2	1:A:2:LYS:NZ	1.91	0.84
1:R:301:GLY:HA3	1:Q:169:LYS:HD2	1.58	0.84
1:A:39:GLN:OE1	1:B:188:SER:HB2	1.78	0.83
1:C:110:GLN:HE22	1:I:106:GLY:HA3	1.41	0.83
1:I:78:ASN:OD1	1:I:80:VAL:HG22	1.77	0.83
1:D:33:THR:HA	1:D:75:SER:OG	1.78	0.83
1:H:202:ASN:ND2	1:L:281:ILE:HB	1.94	0.83
1:O:202:ASN:ND2	1:P:281:ILE:HB	1.93	0.83
3:P:373:NDP:O2D	3:P:373:NDP:N1N	2.10	0.83
1:B:202:ASN:ND2	1:D:281:ILE:HB	1.94	0.83
1:H:148:SER:HB2	2:H:364:SO4:O1	1.77	0.83
1:C:77:ARG:HH12	3:C:365:NDP:C8A	1.91	0.82
1:I:202:ASN:ND2	1:M:281:ILE:HB	1.94	0.82
1:B:210:ALA:C	1:B:211:ALA:O	2.17	0.82
1:Q:164:LYS:O	1:Q:248:LYS:HD2	1.80	0.81
1:O:251:PHE:CB	2:O:371:SO4:O2	2.27	0.81
1:R:202:ASN:ND2	1:Q:281:ILE:HB	1.94	0.81
1:H:202:ASN:HD21	1:L:281:ILE:CB	1.93	0.81
1:B:164:LYS:O	1:B:248:LYS:HD3	1.80	0.81
1:A:281:ILE:HB	1:C:202:ASN:HD21	1.44	0.81
1:D:173:THR:HG23	1:D:228:ILE:CD1	2.10	0.81
1:M:0:LYS:CB	1:M:0:LYS:HZ3	1.91	0.80
1:C:38:LYS:HD3	1:C:59:THR:HG21	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:115:LYS:HE3	1:R:332:TRP:CZ3	2.16	0.80
1:O:164:LYS:O	1:O:248:LYS:HD2	1.82	0.80
1:O:165:PHE:CD1	1:O:248:LYS:CD	2.61	0.80
1:L:38:LYS:HD3	1:L:59:THR:HG21	1.64	0.80
1:A:163:GLN:NE2	1:A:164:LYS:HZ2	1.80	0.79
1:O:293:ASP:HB3	1:O:296:LEU:CD1	2.10	0.79
3:B:378:NDP:O2D	3:B:378:NDP:N1N	2.16	0.79
1:A:163:GLN:HE22	1:A:164:LYS:NZ	1.80	0.79
1:O:165:PHE:CA	1:O:248:LYS:HG2	2.13	0.79
1:R:139:HIS:O	1:R:139:HIS:CD2	2.34	0.79
1:H:135:GLU:HA	1:H:135:GLU:OE1	1.82	0.79
1:R:115:LYS:NZ	1:R:332:TRP:CZ3	2.50	0.79
1:P:187:ALA:O	1:Q:43:LEU:HD11	1.82	0.79
1:O:78:ASN:OD1	1:O:80:VAL:HG22	1.83	0.78
1:H:276:GLU:OE1	1:M:46:TYR:CE2	2.37	0.78
1:M:0:LYS:NZ	1:M:0:LYS:HB2	1.99	0.78
1:B:183:ARG:HE	1:B:187:ALA:CB	1.97	0.78
1:R:251:PHE:HB2	2:R:376:SO4:O2	1.83	0.78
1:Q:120:ALA:HB2	3:Q:375:NDP:H2D	1.66	0.78
1:R:1:LEU:CD1	1:R:90:ASP:HB2	2.14	0.78
1:A:2:LYS:HG2	1:A:89:ILE:HA	1.64	0.78
3:L:369:NDP:O2D	3:L:369:NDP:N1N	2.16	0.78
1:B:165:PHE:O	1:B:248:LYS:HG3	1.82	0.78
1:P:139:HIS:CG	1:P:333:GLN:HG3	2.19	0.77
1:C:77:ARG:NH1	3:C:365:NDP:N7A	2.32	0.77
1:O:232:VAL:HG21	1:P:203:ILE:HD11	1.65	0.77
1:P:139:HIS:HD2	1:P:333:GLN:OE1	1.67	0.77
1:Q:139:HIS:CE1	1:Q:332:TRP:CD2	2.73	0.77
1:B:165:PHE:CA	1:B:248:LYS:CD	2.52	0.77
1:Q:190:HIS:CE1	1:Q:191:ARG:HH11	2.02	0.77
1:Q:165:PHE:HA	1:Q:248:LYS:HD2	1.64	0.77
1:A:2:LYS:HD2	1:A:88:GLY:O	1.85	0.77
1:B:120:ALA:HB2	3:B:378:NDP:H2D	1.67	0.77
1:A:2:LYS:HD3	1:A:89:ILE:HD13	1.68	0.76
1:H:202:ASN:HD22	1:L:281:ILE:H	1.33	0.76
1:R:58:LYS:CB	1:R:58:LYS:NZ	2.48	0.76
1:H:281:ILE:H	1:L:202:ASN:HD22	1.30	0.76
1:R:251:PHE:CB	2:R:376:SO4:O2	2.33	0.76
1:I:301:GLY:HA3	1:M:169:LYS:HD2	1.67	0.76
1:R:58:LYS:HB3	1:R:58:LYS:HZ2	1.50	0.76
1:P:150:THR:HB	2:P:364:SO4:O3	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:202:ASN:HD21	1:Q:281:ILE:CB	1.99	0.76
1:R:164:LYS:O	1:R:248:LYS:HD2	1.83	0.76
1:B:165:PHE:HA	1:B:248:LYS:CG	2.16	0.75
1:B:281:ILE:CB	1:D:202:ASN:HD21	1.99	0.75
1:H:202:ASN:ND2	1:L:281:ILE:H	1.84	0.75
1:I:163:GLN:HE21	1:I:164:LYS:HZ2	0.77	0.75
1:Q:172:MET:HB2	1:Q:242:LEU:HD22	1.67	0.75
1:M:78:ASN:OD1	1:M:80:VAL:HG22	1.86	0.75
1:R:18(A):TRP:HH2	1:R:69:LYS:NZ	1.83	0.75
1:A:2:LYS:HB2	1:A:2:LYS:HZ3	1.50	0.75
1:A:281:ILE:HB	1:C:202:ASN:ND2	2.00	0.75
3:I:380:NDP:N1N	3:I:380:NDP:O2D	2.18	0.75
1:R:210:ALA:O	1:R:214:VAL:HG23	1.87	0.75
1:A:77:ARG:NH2	3:A:376:NDP:O1X	2.20	0.75
1:P:20:ARG:HH21	1:P:319:GLN:CD	1.91	0.74
1:Q:210:ALA:O	1:Q:214:VAL:HG23	1.87	0.74
1:R:18(A):TRP:CH2	1:R:69:LYS:NZ	2.56	0.74
1:L:158:VAL:HG11	1:L:221:LEU:CD1	2.17	0.74
1:R:60:ALA:O	1:R:60(A):GLY:C	2.22	0.74
1:C:183:ARG:CD	1:C:187:ALA:HB3	2.08	0.74
3:O:372:NDP:O2D	3:O:372:NDP:N1N	2.19	0.74
1:D:38:LYS:HD3	1:D:59:THR:HG21	1.69	0.73
1:P:82:LEU:HD13	1:P:84:TRP:CZ2	2.22	0.73
1:R:38:LYS:HD3	1:R:59:THR:HG21	1.70	0.73
1:Q:191:ARG:H	1:Q:191:ARG:HD2	0.57	0.73
1:O:120:ALA:HB2	3:O:372:NDP:H2D	1.70	0.73
1:R:173:THR:OG1	1:Q:306:LYS:NZ	2.21	0.73
3:M:381:NDP:O2D	3:M:381:NDP:N1N	2.20	0.73
1:O:169:LYS:HD2	1:P:301:GLY:HA3	1.71	0.73
1:R:115:LYS:CE	1:R:332:TRP:CZ3	2.71	0.73
1:O:281:ILE:H	1:P:202:ASN:HD22	1.34	0.73
1:Q:165:PHE:HD1	1:Q:248:LYS:CD	2.01	0.73
1:Q:328:VAL:CG1	1:Q:332:TRP:HZ3	2.01	0.73
1:P:20:ARG:NH2	1:P:319:GLN:OE1	2.20	0.72
3:C:365:NDP:N1N	3:C:365:NDP:O2D	2.20	0.72
1:C:77:ARG:NH1	3:C:365:NDP:C8A	2.52	0.72
1:H:172:MET:HE1	1:H:211:ALA:N	2.03	0.72
1:O:281:ILE:N	1:P:202:ASN:ND2	2.37	0.72
1:A:77:ARG:NH1	3:A:376:NDP:C5A	2.52	0.72
1:A:188:SER:CB	1:B:39:GLN:OE1	2.38	0.72
1:O:281:ILE:N	1:P:202:ASN:HD22	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ALA:C	1:B:211:ALA:C	2.47	0.72
1:H:281:ILE:H	1:L:202:ASN:ND2	1.88	0.72
1:R:165:PHE:CA	1:R:248:LYS:CG	2.67	0.71
1:I:210:ALA:N	2:I:366:SO4:O2	2.22	0.71
1:R:222:LYS:CD	1:R:223:GLY:N	2.53	0.71
1:L:158:VAL:CG1	1:L:221:LEU:CD1	2.69	0.71
1:O:286:THR:HG22	1:O:288:VAL:HG22	1.71	0.71
1:Q:183:ARG:HE	1:Q:187:ALA:HB3	1.54	0.71
1:D:78:ASN:OD1	1:D:80:VAL:HG22	1.90	0.71
1:P:134:GLU:CD	1:P:135:GLU:OE1	2.28	0.71
1:B:332:TRP:CD1	1:B:334:GLY:C	2.64	0.71
1:C:159:LYS:HE2	1:C:163:GLN:HE22	1.55	0.71
1:O:281:ILE:HG21	1:Q:48:SER:HA	1.70	0.71
1:O:165:PHE:CA	1:O:248:LYS:CG	2.69	0.71
1:O:232:VAL:CG2	1:P:203:ILE:HD11	2.20	0.71
1:L:210:ALA:O	1:L:214:VAL:HG23	1.91	0.70
1:L:77:ARG:NH2	3:L:369:NDP:O1X	2.24	0.70
1:B:210:ALA:C	1:B:211:ALA:CA	2.60	0.70
1:B:210:ALA:O	1:B:211:ALA:C	2.29	0.70
1:R:154:LEU:CD2	1:R:214:VAL:HG21	2.22	0.70
1:A:77:ARG:HH12	3:A:376:NDP:C5A	2.03	0.70
1:B:301:GLY:HA3	1:D:169:LYS:HD2	1.74	0.70
1:O:202:ASN:HD21	1:P:281:ILE:CB	2.04	0.70
1:Q:171:THR:O	1:Q:242:LEU:HD13	1.90	0.70
1:R:154:LEU:HD23	1:R:214:VAL:HG21	1.73	0.70
1:A:281:ILE:H	1:C:202:ASN:HD22	1.38	0.70
1:R:222:LYS:HD2	1:R:223:GLY:N	2.05	0.70
1:R:78:ASN:OD1	1:R:80:VAL:HG22	1.92	0.70
1:I:48:SER:HA	1:L:281:ILE:HG21	1.74	0.70
1:Q:139:HIS:HE1	1:Q:332:TRP:CE3	2.09	0.70
1:R:0:LYS:HB2	1:R:24:PRO:O	1.92	0.70
1:C:110:GLN:NE2	1:I:106:GLY:CA	2.55	0.69
1:Q:154:LEU:HD13	1:Q:240:VAL:HG11	1.73	0.69
1:A:301:GLY:HA3	1:C:169:LYS:HD2	1.74	0.69
1:C:57:VAL:C	1:C:58:LYS:HG2	2.11	0.69
1:O:293:ASP:CB	1:O:296:LEU:CD1	2.69	0.69
1:M:21:LYS:N	1:M:21:LYS:HD3	1.96	0.69
1:B:165:PHE:O	1:B:248:LYS:CG	2.41	0.69
1:B:29:VAL:HG23	1:B:72:LYS:O	1.93	0.69
1:Q:194:ARG:CD	1:Q:205:PRO:HD2	2.23	0.69
1:P:184:LEU:O	1:P:184:LEU:HD12	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:241:ASP:OD1	1:Q:306:LYS:HE3	1.94	0.68
1:R:169:LYS:HD2	1:Q:301:GLY:HA3	1.75	0.68
1:Q:194:ARG:HD2	1:Q:205:PRO:HD2	1.76	0.68
1:A:281:ILE:CB	1:C:202:ASN:HD21	2.06	0.68
1:O:172:MET:HG2	1:O:173:THR:N	2.09	0.68
1:O:202:ASN:HD22	1:P:281:ILE:H	1.38	0.68
1:D:139:HIS:CE1	1:D:333:GLN:H	2.11	0.68
1:I:154:LEU:HD13	1:I:240:VAL:HG21	1.75	0.68
1:O:226:ASN:ND2	1:P:300:MET:SD	2.67	0.68
1:B:212:LYS:NZ	1:B:226:ASN:CG	2.47	0.68
1:M:0:LYS:HZ3	1:M:0:LYS:HB3	1.58	0.68
1:R:139:HIS:CE1	1:R:333:GLN:H	2.12	0.68
1:P:208:THR:CG2	1:P:228:ILE:CA	2.70	0.68
1:Q:194:ARG:HD2	1:Q:205:PRO:O	1.94	0.68
1:H:34:GLY:HA3	1:H:39:GLN:OE1	1.94	0.68
1:B:46:TYR:HE2	1:C:276:GLU:OE1	1.77	0.67
1:P:39:GLN:OE1	1:Q:188:SER:HB2	1.94	0.67
1:P:222:LYS:CD	1:P:223:GLY:N	2.57	0.67
1:H:77:ARG:HH11	3:H:379:NDP:C5A	2.04	0.67
1:B:48:SER:HA	1:C:281:ILE:HG21	1.77	0.67
1:O:293:ASP:CG	1:O:296:LEU:HD11	2.15	0.67
1:C:78:ASN:OD1	1:C:80:VAL:HG22	1.96	0.66
1:C:77:ARG:NH2	3:C:365:NDP:O1X	2.27	0.66
1:L:129:VAL:H	1:L:133:ASN:HD21	1.43	0.66
1:L:77:ARG:NH1	3:L:369:NDP:C5A	2.58	0.66
1:C:159:LYS:HG2	1:C:163:GLN:NE2	2.10	0.66
1:H:24:PRO:HG2	1:H:25:LEU:HD23	1.76	0.66
1:O:165:PHE:CA	1:O:248:LYS:HD2	2.25	0.66
1:Q:328:VAL:CG1	1:Q:332:TRP:CZ3	2.78	0.66
1:R:1:LEU:HD23	1:R:329:ALA:HB2	1.77	0.66
1:A:78:ASN:OD1	1:A:80:VAL:HG22	1.95	0.66
1:B:210:ALA:CA	1:B:211:ALA:N	2.59	0.66
1:C:210:ALA:O	1:C:214:VAL:HG23	1.95	0.66
1:P:188:SER:HB2	1:Q:39:GLN:OE1	1.96	0.66
1:C:77:ARG:HH22	3:C:365:NDP:P2B	2.18	0.65
1:O:310:TRP:HZ2	1:P:205:PRO:HG2	1.60	0.65
1:M:0:LYS:HZ3	1:M:0:LYS:HB2	1.58	0.65
1:M:155:ALA:HB3	1:M:156:PRO:HD3	1.77	0.65
1:H:77:ARG:NH2	3:H:379:NDP:O1X	2.30	0.65
1:B:164:LYS:O	1:B:248:LYS:CD	2.44	0.65
1:I:281:ILE:HG21	1:L:48:SER:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:276:GLU:OE1	1:M:46:TYR:HE2	1.78	0.65
1:O:183:ARG:HH12	1:O:187:ALA:HB1	1.58	0.65
1:O:183:ARG:HH11	1:O:187:ALA:CB	2.09	0.65
1:D:173:THR:HG23	1:D:228:ILE:HD11	1.78	0.65
1:R:165:PHE:CD1	1:R:248:LYS:HD3	2.31	0.65
1:O:298:MET:CE	1:P:226:ASN:OD1	2.43	0.64
1:I:183:ARG:NH1	1:I:187:ALA:HB3	2.12	0.64
1:R:227:GLY:HA2	1:Q:298:MET:HE1	1.77	0.64
1:M:210:ALA:O	1:M:214:VAL:HG23	1.97	0.64
1:H:129:VAL:H	1:H:133:ASN:ND2	1.95	0.64
1:L:129:VAL:H	1:L:133:ASN:ND2	1.96	0.64
1:M:21:LYS:CD	1:M:21:LYS:H	2.00	0.64
1:H:78:ASN:OD1	1:H:80:VAL:HG22	1.97	0.64
1:C:106:GLY:HA3	1:I:110:GLN:HE22	1.63	0.64
1:O:183:ARG:NH1	1:O:187:ALA:HB3	2.11	0.64
1:Q:165:PHE:CD1	1:Q:248:LYS:CD	2.80	0.64
1:A:11:ILE:HG13	3:A:376:NDP:H1D	1.80	0.64
1:Q:165:PHE:HB3	1:Q:248:LYS:HG2	1.79	0.64
1:B:306:LYS:NZ	1:D:173:THR:OG1	2.20	0.64
1:R:139:HIS:CB	1:R:333:GLN:OE1	2.45	0.64
1:H:25:LEU:HD21	1:H:326:ASP:OD1	1.98	0.64
1:P:49:ILE:HD11	1:Q:185:LEU:HD22	1.80	0.64
1:R:48:SER:HA	1:P:281:ILE:HG21	1.80	0.64
1:D:173:THR:HG23	1:D:228:ILE:HD12	1.79	0.63
1:I:208:THR:CB	2:I:366:SO4:O3	2.46	0.63
1:P:150:THR:CB	2:P:364:SO4:O3	2.45	0.63
1:C:209:GLY:O	1:C:212:LYS:HG2	1.98	0.63
1:M:150:THR:OG1	2:M:370:SO4:O1	2.13	0.63
1:O:228:ILE:HD12	1:P:296:LEU:CD2	2.24	0.63
1:R:164:LYS:O	1:R:248:LYS:HD3	1.98	0.63
1:R:1:LEU:CD2	1:R:329:ALA:HB2	2.29	0.63
1:H:129:VAL:H	1:H:133:ASN:HD21	1.45	0.63
1:O:165:PHE:HB3	1:O:248:LYS:HG3	1.81	0.63
1:O:293:ASP:CG	1:O:296:LEU:CD1	2.67	0.63
1:P:261:GLU:OE1	1:P:261:GLU:C	2.36	0.63
1:L:84:TRP:CE3	1:L:84:TRP:HA	2.34	0.63
1:O:226:ASN:C	1:O:226:ASN:OD1	2.37	0.63
1:A:281:ILE:CG2	1:C:202:ASN:HD21	2.12	0.63
1:P:222:LYS:CD	1:P:222:LYS:C	2.68	0.63
1:Q:172:MET:SD	1:Q:227:GLY:HA3	2.39	0.63
1:I:203:ILE:HB	1:M:280:SER:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:64:ILE:HG13	1:P:71:ILE:HG22	1.81	0.62
1:B:77:ARG:NH2	3:B:378:NDP:O1X	2.32	0.62
1:I:183:ARG:NH1	1:I:187:ALA:CB	2.61	0.62
1:I:172:MET:CG	1:I:240:VAL:HG23	2.29	0.62
1:O:42:HIS:CD2	1:R:193:LEU:HD23	2.34	0.62
1:R:1:LEU:HD12	1:R:90:ASP:HB2	1.81	0.62
1:Q:128:TYR:HA	1:Q:133:ASN:HD21	1.64	0.62
1:Q:190:HIS:C	1:Q:191:ARG:HD2	2.14	0.62
1:O:281:ILE:CG2	1:Q:48:SER:HA	2.29	0.62
1:D:58:LYS:HB3	1:D:58:LYS:NZ	2.15	0.62
1:C:159:LYS:O	1:C:163:GLN:CG	2.38	0.62
1:H:276:GLU:CD	1:M:46:TYR:OH	2.38	0.62
1:I:280:SER:HB3	1:M:203:ILE:HB	1.82	0.62
1:H:48:SER:HA	1:M:281:ILE:HG21	1.82	0.62
1:R:195:ARG:NH1	2:R:363:SO4:O4	2.30	0.62
1:B:212:LYS:NZ	1:B:226:ASN:OD1	2.31	0.62
1:I:155:ALA:HB3	1:I:156:PRO:HD3	1.82	0.61
1:I:169:LYS:HD2	1:M:301:GLY:HA3	1.82	0.61
1:I:183:ARG:NH2	1:I:188:SER:O	2.34	0.61
1:O:310:TRP:HZ2	1:P:205:PRO:CG	2.12	0.61
1:R:300:MET:HE1	1:Q:226:ASN:HB2	1.82	0.61
1:O:37:VAL:HG21	1:O:61:ASP:O	2.01	0.61
1:P:187:ALA:O	1:P:196:ALA:HB1	2.00	0.61
1:Q:165:PHE:CD1	1:Q:248:LYS:HD2	2.36	0.61
1:O:48:SER:HA	1:Q:281:ILE:HG21	1.83	0.61
1:H:276:GLU:CD	1:M:46:TYR:HH	2.03	0.61
1:R:227:GLY:C	1:R:228:ILE:HG13	2.21	0.61
1:B:205:PRO:HG2	1:D:310:TRP:HZ2	1.66	0.61
1:D:139:HIS:CD2	1:D:332:TRP:HA	2.35	0.61
1:Q:172:MET:HE1	1:Q:211:ALA:N	2.15	0.61
1:R:222:LYS:HD3	1:R:223:GLY:N	2.16	0.61
1:R:18(A):TRP:HH2	1:R:69:LYS:HZ2	1.47	0.61
1:B:78:ASN:OD1	1:B:80:VAL:HG22	2.01	0.61
1:L:84:TRP:HE3	1:L:84:TRP:HA	1.65	0.61
1:P:236:ASN:O	1:P:237:VAL:HB	2.01	0.61
1:Q:77:ARG:NH2	3:Q:375:NDP:O1X	2.34	0.61
1:P:187:ALA:O	1:Q:43:LEU:CD1	2.49	0.60
1:L:158:VAL:HG12	1:L:221:LEU:HD11	1.81	0.60
1:O:183:ARG:HH11	1:O:187:ALA:HB3	1.66	0.60
1:O:42:HIS:CG	1:R:193:LEU:CD2	2.84	0.60
1:A:139:HIS:O	1:A:139:HIS:CD2	2.54	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:221:LEU:HD22	1:H:225:LEU:HD11	1.84	0.60
1:R:202:ASN:HD22	1:Q:281:ILE:H	1.48	0.60
1:Q:78:ASN:OD1	1:Q:80:VAL:HG22	2.01	0.60
1:A:2:LYS:CG	1:A:89:ILE:HA	2.30	0.60
1:L:85:GLY:C	1:L:87:MET:N	2.54	0.59
1:O:187:ALA:O	1:O:196:ALA:HB1	2.02	0.59
1:O:210:ALA:O	1:O:214:VAL:HG23	2.01	0.59
1:P:120:ALA:HB2	3:P:373:NDP:H2D	1.84	0.59
1:Q:209:GLY:O	1:Q:212:LYS:HG2	2.02	0.59
1:R:115:LYS:NZ	1:R:332:TRP:CE3	2.68	0.59
1:R:37:VAL:HB	1:R:61:ASP:OD2	2.01	0.59
1:R:58:LYS:CB	1:R:58:LYS:HZ2	2.10	0.59
1:A:139:HIS:CE1	1:A:333:GLN:H	2.20	0.59
1:I:208:THR:HB	2:I:366:SO4:O3	2.02	0.59
1:R:194:ARG:HD2	1:R:205:PRO:O	2.03	0.59
1:B:46:TYR:CE2	1:C:276:GLU:OE1	2.55	0.59
1:A:2:LYS:CD	1:A:89:ILE:HA	2.33	0.59
1:H:221:LEU:CD2	1:H:225:LEU:HD11	2.32	0.59
1:H:100:VAL:HG23	1:H:122(A):LYS:HG2	1.85	0.59
1:A:203:ILE:HB	1:C:280:SER:HB3	1.83	0.59
1:C:106:GLY:O	1:I:110:GLN:NE2	2.36	0.59
1:C:129:VAL:H	1:C:133:ASN:ND2	2.01	0.59
1:L:78:ASN:OD1	1:L:80:VAL:HG22	2.02	0.59
1:C:176:HIS:HB3	1:C:231:ARG:HD3	1.85	0.59
1:Q:165:PHE:HA	1:Q:248:LYS:CD	2.30	0.59
1:I:208:THR:OG1	2:I:366:SO4:O3	2.21	0.58
1:B:77:ARG:HH11	1:B:77:ARG:HG2	1.67	0.58
1:R:165:PHE:HA	1:R:248:LYS:HD3	1.70	0.58
1:A:2:LYS:HD2	1:A:88:GLY:C	2.21	0.58
1:B:27:VAL:HG12	1:B:71:ILE:HD13	1.84	0.58
1:M:150:THR:CB	2:M:370:SO4:O1	2.50	0.58
1:R:281:ILE:CG2	1:Q:202:ASN:HD21	2.17	0.58
1:H:276:GLU:OE2	1:M:46:TYR:OH	2.22	0.58
1:H:84:TRP:HE3	1:H:84:TRP:HA	1.69	0.58
1:M:154:LEU:HD23	1:M:214:VAL:HG21	1.86	0.58
1:C:32:ASP:O	1:C:75:SER:OG	2.21	0.58
1:B:281:ILE:CG2	1:D:202:ASN:HD21	2.16	0.58
1:H:84:TRP:CE3	1:H:84:TRP:HA	2.39	0.58
1:C:128:TYR:HA	1:C:133:ASN:HD21	1.68	0.58
1:D:139:HIS:NE2	1:D:332:TRP:HA	2.19	0.58
1:I:172:MET:HG3	1:I:240:VAL:CG2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:32:ASP:O	1:O:75:SER:OG	2.22	0.58
1:Q:129:VAL:H	1:Q:133:ASN:ND2	2.01	0.58
1:C:56:ASP:CG	1:C:58:LYS:HZ1	2.06	0.57
1:I:172:MET:HG2	1:I:173:THR:N	2.19	0.57
1:L:85:GLY:O	1:L:86:ASP:C	2.39	0.57
1:M:129:VAL:H	1:M:133:ASN:ND2	2.00	0.57
1:O:128:TYR:HA	1:O:133:ASN:HD21	1.69	0.57
1:B:281:ILE:H	1:D:202:ASN:HD22	1.50	0.57
1:I:210:ALA:O	1:I:214:VAL:HG23	2.04	0.57
1:I:58:LYS:NZ	1:I:58:LYS:HB3	2.18	0.57
1:R:222:LYS:HD3	1:R:223:GLY:H	1.69	0.57
1:A:205:PRO:HG2	1:C:310:TRP:HZ2	1.69	0.57
1:A:49:ILE:HD11	1:B:185:LEU:HD22	1.86	0.57
1:B:172:MET:HE2	1:B:210:ALA:HB3	1.85	0.57
1:B:1:LEU:HD23	1:B:3:VAL:CG2	2.34	0.57
1:H:77:ARG:HH12	3:H:379:NDP:C5A	2.17	0.57
1:O:278:LEU:O	1:P:194:ARG:HD3	2.04	0.57
1:R:228:ILE:HD11	1:Q:306:LYS:HE2	1.85	0.57
1:R:222:LYS:C	1:R:222:LYS:HD2	2.25	0.57
1:H:33:THR:HG21	1:H:77:ARG:HG2	1.86	0.57
1:P:208:THR:HG21	1:P:228:ILE:C	2.25	0.57
1:M:129:VAL:H	1:M:133:ASN:HD21	1.52	0.57
1:R:202:ASN:HD21	1:Q:281:ILE:CG2	2.18	0.57
1:R:115:LYS:HZ2	1:R:328:VAL:HG13	1.70	0.57
1:L:77:ARG:HH12	3:L:369:NDP:C5A	2.17	0.57
1:O:126:PRO:HG2	1:O:144:ILE:HG22	1.86	0.57
1:P:190:HIS:HA	1:P:191:ARG:NH1	2.19	0.57
1:R:160:VAL:O	1:R:164:LYS:HG2	2.05	0.57
1:C:129:VAL:H	1:C:133:ASN:HD21	1.53	0.56
1:H:281:ILE:HG21	1:M:48:SER:HA	1.86	0.56
1:M:128:TYR:HA	1:M:133:ASN:HD21	1.69	0.56
1:P:64:ILE:CG1	1:P:71:ILE:HG22	2.35	0.56
1:L:172:MET:HE1	1:L:211:ALA:N	2.20	0.56
1:B:165:PHE:CA	1:B:248:LYS:HG3	2.35	0.56
1:C:1:LEU:HD22	1:C:329:ALA:HB2	1.86	0.56
1:H:281:ILE:CG2	1:L:202:ASN:HD21	2.18	0.56
1:O:165:PHE:O	1:O:248:LYS:HG2	2.06	0.56
1:A:42:HIS:CG	1:B:193:LEU:HD13	2.41	0.56
1:P:129:VAL:H	1:P:133:ASN:ND2	2.03	0.56
1:P:139:HIS:CD2	1:P:333:GLN:OE1	2.56	0.56
1:R:310:TRP:HZ2	1:Q:205:PRO:HG2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:208:THR:HG22	1:I:228:ILE:HA	1.86	0.56
1:O:282:ASP:OD1	1:Q:46:TYR:HB3	2.05	0.56
1:A:236:ASN:O	1:A:237:VAL:HB	2.06	0.56
1:B:128:TYR:HA	1:B:133:ASN:HD21	1.71	0.56
1:A:194:ARG:HD3	1:C:278:LEU:O	2.06	0.56
1:M:58:LYS:HB3	1:M:58:LYS:NZ	2.20	0.56
1:R:222:LYS:CD	1:R:222:LYS:C	2.74	0.56
1:A:2:LYS:CD	1:A:89:ILE:HD13	2.36	0.56
1:H:148:SER:CB	2:H:364:SO4:O1	2.53	0.56
1:P:184:LEU:HD11	1:Q:178:TYR:CE1	2.41	0.56
1:L:187:ALA:O	1:L:196:ALA:HB1	2.06	0.56
1:C:77:ARG:NH1	3:C:365:NDP:C4A	2.68	0.56
1:P:221:LEU:HD22	1:P:225:LEU:HD11	1.87	0.56
3:P:373:NDP:O2D	3:P:373:NDP:C1D	2.35	0.56
1:A:155:ALA:HB3	1:A:156:PRO:HD3	1.87	0.55
1:H:172:MET:HE1	1:H:211:ALA:H	1.70	0.55
1:M:97:GLY:HA3	3:M:381:NDP:O3D	2.06	0.55
1:P:188:SER:CB	1:Q:39:GLN:OE1	2.54	0.55
1:A:197:ARG:HH21	1:B:48:SER:N	2.04	0.55
1:P:98:VAL:HG23	1:P:99:PHE:CD2	2.41	0.55
1:R:115:LYS:NZ	1:R:328:VAL:HG13	2.21	0.55
1:Q:139:HIS:ND1	1:Q:332:TRP:HA	2.21	0.55
1:H:77:ARG:HH12	3:H:379:NDP:C4A	2.19	0.55
1:L:194:ARG:HD2	1:L:205:PRO:O	2.07	0.55
1:L:97:GLY:HA3	3:L:369:NDP:O3D	2.06	0.55
1:I:129:VAL:H	1:I:133:ASN:HD21	1.55	0.55
1:R:155:ALA:HB3	1:R:156:PRO:HD3	1.87	0.55
1:R:165:PHE:HB3	1:R:248:LYS:HG3	1.89	0.55
1:O:97:GLY:HA3	3:O:372:NDP:O3D	2.07	0.55
1:B:209:GLY:O	1:B:213:ALA:HB3	2.07	0.55
1:P:185:LEU:HD22	1:Q:49:ILE:HD11	1.89	0.55
1:R:228:ILE:CD1	1:Q:306:LYS:NZ	2.70	0.55
1:B:251:PHE:CZ	1:B:254:GLU:HB2	2.42	0.55
1:I:183:ARG:CZ	1:I:188:SER:O	2.55	0.55
1:O:165:PHE:CD1	1:O:248:LYS:HD2	2.41	0.54
1:O:208:THR:HG22	1:O:228:ILE:HA	1.88	0.54
1:R:115:LYS:HE3	1:R:332:TRP:CH2	2.42	0.54
1:B:202:ASN:ND2	1:D:281:ILE:N	2.47	0.54
1:H:276:GLU:OE1	1:M:46:TYR:OH	2.25	0.54
1:R:100:VAL:HG23	1:R:122(A):LYS:HG2	1.89	0.54
1:L:33:THR:HA	1:L:75:SER:OG	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:117:LEU:HD23	1:O:117:LEU:C	2.28	0.54
1:O:97:GLY:CA	3:O:372:NDP:O3D	2.56	0.54
1:O:42:HIS:CG	1:R:193:LEU:HD22	2.43	0.54
1:A:2:LYS:HB2	1:A:2:LYS:HZ2	1.71	0.54
1:B:148:SER:HB2	2:B:364:SO4:O4	2.07	0.54
1:C:155:ALA:HB3	1:C:156:PRO:HD3	1.88	0.54
1:B:281:ILE:HG21	1:C:48:SER:HA	1.90	0.54
1:I:209:GLY:O	1:I:212:LYS:HG2	2.08	0.54
1:O:202:ASN:ND2	1:P:281:ILE:H	2.04	0.54
1:B:332:TRP:HD1	1:B:334:GLY:C	2.11	0.54
1:M:0:LYS:NZ	1:M:0:LYS:HB3	2.15	0.54
1:Q:251:PHE:CZ	1:Q:254:GLU:HB2	2.42	0.54
1:R:0:LYS:HD2	1:R:23:SER:O	2.07	0.54
1:D:82:LEU:HD13	1:D:84:TRP:CZ2	2.42	0.54
1:P:129:VAL:H	1:P:133:ASN:HD21	1.54	0.54
1:B:46:TYR:OH	1:C:276:GLU:OE2	2.25	0.54
1:I:163:GLN:HE21	1:I:164:LYS:CE	2.19	0.54
1:I:202:ASN:HD21	1:M:281:ILE:CG2	2.20	0.54
1:Q:242:LEU:HD12	1:Q:243:VAL:N	2.23	0.54
1:A:117:LEU:HD23	1:A:117:LEU:C	2.28	0.54
1:A:281:ILE:H	1:C:202:ASN:ND2	2.05	0.54
1:C:9:GLY:O	1:C:13:ARG:HG3	2.08	0.54
1:C:110:GLN:HE21	1:I:106:GLY:C	2.11	0.54
1:L:155:ALA:HB3	1:L:156:PRO:HD3	1.88	0.54
1:R:281:ILE:HG21	1:P:48:SER:HA	1.89	0.54
1:B:151:THR:OG1	1:B:209:GLY:O	2.26	0.54
1:B:31:ASN:ND2	3:B:378:NDP:H2A	2.23	0.54
1:L:1:LEU:HD22	1:L:329:ALA:HB2	1.90	0.54
1:O:82:LEU:HD13	1:O:84:TRP:CZ2	2.43	0.54
1:O:310:TRP:CZ2	1:P:205:PRO:CG	2.91	0.53
1:B:202:ASN:HD21	1:D:281:ILE:CG2	2.21	0.53
1:L:228:ILE:C	1:L:228:ILE:HD12	2.29	0.53
1:R:303:ASP:OD1	1:Q:169:LYS:HE3	2.07	0.53
1:B:129:VAL:H	1:B:133:ASN:ND2	2.06	0.53
1:A:129:VAL:H	1:A:133:ASN:ND2	2.06	0.53
1:A:208:THR:O	1:A:210:ALA:N	2.41	0.53
1:A:98:VAL:HG23	1:A:99:PHE:CD2	2.43	0.53
1:C:80:VAL:CB	1:C:110:GLN:OE1	2.47	0.53
1:H:24:PRO:HG2	1:H:25:LEU:CD2	2.38	0.53
1:I:236:ASN:O	1:I:237:VAL:HB	2.09	0.53
1:R:202:ASN:ND2	1:Q:281:ILE:H	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:GLY:HA3	1:C:212:LYS:HE2	1.90	0.53
1:C:272:SER:OG	1:C:288:VAL:HG11	2.09	0.53
1:I:172:MET:HG3	1:I:240:VAL:HG23	1.89	0.53
1:A:48:SER:HA	1:D:281:ILE:HG21	1.88	0.53
1:I:129:VAL:H	1:I:133:ASN:ND2	2.06	0.53
1:I:97:GLY:HA3	3:I:380:NDP:O3D	2.09	0.53
1:L:58:LYS:NZ	1:L:58:LYS:HB3	2.24	0.53
1:I:169:LYS:NZ	1:M:303:ASP:OD1	2.37	0.53
1:R:228:ILE:HD12	1:Q:306:LYS:NZ	2.24	0.53
1:D:103:ASP:OD1	1:D:103:ASP:N	2.42	0.53
1:D:129:VAL:H	1:D:133:ASN:HD21	1.56	0.53
1:D:228:ILE:HD12	1:D:228:ILE:C	2.30	0.53
1:P:139:HIS:CD2	1:P:333:GLN:CG	2.88	0.53
1:A:281:ILE:HG21	1:D:48:SER:HA	1.91	0.53
1:B:97:GLY:HA3	3:B:378:NDP:O3D	2.09	0.53
1:D:272:SER:OG	1:D:288:VAL:HG11	2.09	0.53
1:D:148:SER:HB2	2:D:364:SO4:O3	2.08	0.53
1:H:176:HIS:HB3	1:H:231:ARG:HD3	1.89	0.53
1:P:0:LYS:HB3	1:P:24:PRO:O	2.09	0.53
1:R:279:VAL:HG12	1:Q:205:PRO:HD3	1.91	0.53
1:A:0:LYS:HD3	1:A:1:LEU:N	2.22	0.52
1:I:202:ASN:ND2	1:M:281:ILE:N	2.50	0.52
1:O:277:PRO:O	1:P:194:ARG:HG2	2.09	0.52
1:Q:154:LEU:CD1	1:Q:242:LEU:CD2	2.41	0.52
1:B:28:VAL:C	1:B:71:ILE:HG23	2.30	0.52
1:B:77:ARG:HG2	1:B:77:ARG:NH1	2.24	0.52
1:H:272:SER:OG	1:H:288:VAL:HG11	2.09	0.52
1:H:58:LYS:HB3	1:H:58:LYS:NZ	2.24	0.52
1:P:9:GLY:O	1:P:13:ARG:HG3	2.10	0.52
1:R:227:GLY:HA2	1:Q:298:MET:CE	2.38	0.52
1:A:129:VAL:H	1:A:133:ASN:HD21	1.56	0.52
1:C:204:VAL:HB	1:C:231:ARG:HB2	1.92	0.52
1:D:148:SER:CB	2:D:364:SO4:O3	2.57	0.52
1:M:150:THR:HB	2:M:370:SO4:O1	2.09	0.52
1:D:210:ALA:O	1:D:214:VAL:HG23	2.09	0.52
1:B:203:ILE:HB	1:D:280:SER:HB3	1.91	0.52
1:H:128:TYR:HA	1:H:133:ASN:HD21	1.75	0.52
1:H:135:GLU:OE1	1:H:135:GLU:CA	2.56	0.52
1:M:97:GLY:CA	3:M:381:NDP:O3D	2.58	0.52
1:P:222:LYS:HD3	1:P:223:GLY:H	1.70	0.52
1:Q:248:LYS:O	1:Q:248:LYS:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:THR:OG1	1:C:98:VAL:HG22	2.09	0.52
1:I:281:ILE:N	1:M:202:ASN:HD22	2.00	0.52
1:O:125:ILE:HG23	1:O:126:PRO:HD2	1.91	0.52
1:Q:176:HIS:HB3	1:Q:231:ARG:HD3	1.91	0.52
1:D:11:ILE:HD11	3:D:365:NDP:H42N	1.92	0.52
1:C:106:GLY:C	1:I:110:GLN:NE2	2.62	0.52
1:I:11:ILE:HD11	3:I:380:NDP:H42N	1.91	0.52
1:L:95:GLY:O	3:L:369:NDP:H51A	2.09	0.52
1:I:281:ILE:N	1:M:202:ASN:ND2	2.49	0.52
1:O:281:ILE:CG2	1:P:202:ASN:HD21	2.22	0.52
1:D:172:MET:HE3	1:D:211:ALA:HB2	1.91	0.52
1:O:148:SER:HB2	2:O:364:SO4:O1	2.10	0.52
1:A:202:ASN:ND2	1:C:281:ILE:N	2.53	0.52
1:I:205:PRO:HG2	1:M:310:TRP:HZ2	1.74	0.52
1:M:241:ASP:OD1	1:M:306:LYS:HE2	2.10	0.52
1:H:276:GLU:OE1	1:M:46:TYR:CZ	2.62	0.52
1:O:282:ASP:CG	1:P:197:ARG:HH12	2.12	0.52
1:R:172:MET:HE1	1:R:211:ALA:N	2.25	0.52
1:R:97:GLY:HA3	3:R:377:NDP:O3D	2.10	0.52
1:O:129:VAL:H	1:O:133:ASN:ND2	2.08	0.52
1:O:155:ALA:HB3	1:O:156:PRO:HD3	1.91	0.52
1:O:165:PHE:CA	1:O:248:LYS:CD	2.85	0.52
1:Q:149:CYS:HB3	3:Q:375:NDP:H41N	1.91	0.52
1:A:2:LYS:NZ	1:A:2:LYS:CB	2.67	0.51
1:B:210:ALA:N	1:B:211:ALA:N	2.58	0.51
1:B:245:GLN:HE22	1:D:245:GLN:HE22	1.58	0.51
1:A:210:ALA:C	1:A:212:LYS:N	2.63	0.51
1:D:155:ALA:HB3	1:D:156:PRO:HD3	1.90	0.51
1:D:97:GLY:HA3	3:D:365:NDP:O3D	2.10	0.51
1:Q:95:GLY:O	3:Q:375:NDP:H51A	2.10	0.51
1:R:310:TRP:HZ2	1:Q:205:PRO:CG	2.22	0.51
1:B:159:LYS:O	1:B:163:GLN:HG3	2.08	0.51
1:H:58:LYS:HB3	1:H:58:LYS:HZ2	1.75	0.51
1:A:2:LYS:CG	1:A:89:ILE:HD13	2.40	0.51
1:C:97:GLY:HA3	3:C:365:NDP:O3D	2.11	0.51
1:M:0:LYS:HB2	1:M:0:LYS:HZ2	1.72	0.51
1:O:281:ILE:CB	1:P:202:ASN:ND2	2.50	0.51
1:P:195:ARG:NH1	2:P:363:SO4:O4	2.40	0.51
1:L:133:ASN:HD22	1:L:133:ASN:H	1.59	0.51
1:C:159:LYS:CG	1:C:163:GLN:NE2	2.73	0.51
1:C:57:VAL:N	1:C:58:LYS:HZ2	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:208:THR:CG2	1:P:228:ILE:C	2.79	0.51
1:B:280:SER:HB3	1:D:203:ILE:HB	1.93	0.51
1:D:129:VAL:H	1:D:133:ASN:ND2	2.09	0.51
1:H:33:THR:HA	1:H:75:SER:OG	2.10	0.51
1:M:0:LYS:CB	1:M:0:LYS:HZ2	2.18	0.51
1:R:300:MET:SD	1:Q:226:ASN:HB3	2.51	0.51
1:C:117:LEU:HD23	1:C:117:LEU:C	2.30	0.51
1:O:42:HIS:CB	1:R:193:LEU:CD2	2.88	0.51
1:A:194:ARG:HD2	1:A:205:PRO:O	2.11	0.51
1:C:228:ILE:HD12	1:C:228:ILE:C	2.31	0.51
1:H:172:MET:HE1	1:H:210:ALA:HB3	1.93	0.51
1:C:110:GLN:HE21	1:I:106:GLY:CA	2.24	0.51
1:Q:228:ILE:HD12	1:Q:228:ILE:C	2.32	0.51
1:P:188:SER:OG	3:Q:375:NDP:O3X	2.28	0.51
1:A:185:LEU:HD22	1:B:49:ILE:HD11	1.92	0.51
1:A:77:ARG:NH1	3:A:376:NDP:N7A	2.59	0.51
1:B:205:PRO:CG	1:D:310:TRP:HZ2	2.23	0.51
1:I:281:ILE:CG2	1:M:202:ASN:HD21	2.23	0.51
1:P:96:THR:OG1	1:P:98:VAL:HG22	2.11	0.51
1:C:159:LYS:HE2	1:C:163:GLN:NE2	2.25	0.50
1:D:128:TYR:HA	1:D:133:ASN:HD21	1.76	0.50
1:I:103:ASP:N	1:I:103:ASP:OD1	2.43	0.50
1:R:278:LEU:O	1:Q:194:ARG:HD3	2.10	0.50
1:Q:253:GLU:HA	1:Q:253:GLU:OE1	2.06	0.50
1:R:129:VAL:H	1:R:133:ASN:HD21	1.58	0.50
1:H:149:CYS:HB3	3:H:379:NDP:H41N	1.93	0.50
1:P:271:LEU:C	1:P:271:LEU:HD13	2.31	0.50
1:R:0:LYS:HG3	1:R:24:PRO:C	2.31	0.50
1:B:98:VAL:HG23	1:B:99:PHE:CD2	2.46	0.50
1:H:77:ARG:HH12	3:H:379:NDP:C8A	2.23	0.50
1:O:202:ASN:HD21	1:P:281:ILE:CG2	2.24	0.50
1:B:29:VAL:HA	1:B:72:LYS:O	2.11	0.50
1:A:184:LEU:HD21	1:B:199:ALA:HB3	1.93	0.50
1:L:100:VAL:HG23	1:L:122(A):LYS:HG2	1.93	0.50
1:P:117:LEU:C	1:P:117:LEU:HD23	2.31	0.50
1:D:154:LEU:HD23	1:D:214:VAL:HG21	1.93	0.50
1:P:157:PHE:HB2	1:P:259:PHE:CE1	2.47	0.50
1:R:233:PRO:HB2	1:Q:233:PRO:HB2	1.92	0.50
1:C:236:ASN:O	1:C:237:VAL:HB	2.12	0.50
1:M:103:ASP:OD1	1:M:104:GLY:N	2.45	0.50
1:R:128:TYR:HA	1:R:133:ASN:HD21	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:129:VAL:H	1:R:133:ASN:ND2	2.10	0.50
1:Q:139:HIS:CE1	1:Q:332:TRP:CG	3.00	0.50
1:Q:187:ALA:O	1:Q:196:ALA:HB1	2.11	0.50
1:R:203:ILE:HB	1:Q:280:SER:HB3	1.94	0.50
1:R:280:SER:HB3	1:Q:203:ILE:HB	1.93	0.50
1:C:80:VAL:HG13	1:C:107:LYS:HZ2	1.77	0.50
1:H:236:ASN:O	1:H:237:VAL:HB	2.12	0.50
1:H:77:ARG:NH1	3:H:379:NDP:N7A	2.59	0.50
1:L:33:THR:HG21	1:L:77:ARG:HG2	1.92	0.50
1:M:236:ASN:O	1:M:237:VAL:HB	2.12	0.50
1:P:155:ALA:HB3	1:P:156:PRO:HD3	1.93	0.50
1:Q:11:ILE:HD11	3:Q:375:NDP:H42N	1.93	0.50
1:A:202:ASN:HD21	1:C:281:ILE:CG2	2.23	0.49
1:O:1:LEU:HD22	1:O:329:ALA:HB2	1.93	0.49
1:A:133:ASN:HD22	1:A:133:ASN:N	2.09	0.49
1:D:58:LYS:HZ3	1:D:58:LYS:HB3	1.77	0.49
1:I:168:ILE:HD12	1:I:245:GLN:HG2	1.93	0.49
1:O:281:ILE:HD11	1:O:284:ARG:HD2	1.94	0.49
1:P:218:LEU:HB3	1:P:221:LEU:HD12	1.95	0.49
1:Q:129:VAL:H	1:Q:133:ASN:HD21	1.59	0.49
1:A:128:TYR:HA	1:A:133:ASN:HD21	1.77	0.49
1:C:209:GLY:CA	1:C:212:LYS:HE2	2.42	0.49
1:L:58:LYS:HZ2	1:L:58:LYS:HB3	1.77	0.49
1:O:129:VAL:H	1:O:133:ASN:HD21	1.60	0.49
1:Q:298:MET:HE2	1:Q:306:LYS:HD3	1.93	0.49
1:P:190:HIS:O	1:Q:39:GLN:NE2	2.44	0.49
1:R:226:ASN:HB3	1:Q:300:MET:SD	2.52	0.49
1:H:157:PHE:HB2	1:H:259:PHE:CE1	2.47	0.49
1:O:272:SER:OG	1:O:288:VAL:HG11	2.12	0.49
1:P:58:LYS:HB3	1:P:58:LYS:NZ	2.27	0.49
1:C:172:MET:C	1:C:172:MET:HE2	2.33	0.49
1:H:228:ILE:C	1:H:228:ILE:HD12	2.33	0.49
1:H:310:TRP:HZ2	1:L:205:PRO:HG2	1.77	0.49
1:L:240:VAL:HG13	1:L:311:TYR:CE1	2.47	0.49
1:Q:194:ARG:HD3	1:Q:205:PRO:HD2	1.91	0.49
1:A:9:GLY:HA3	3:A:376:NDP:O5B	2.12	0.49
1:I:241:ASP:OD1	1:I:306:LYS:HE2	2.12	0.49
1:O:176:HIS:HB3	1:O:231:ARG:HD3	1.93	0.49
1:A:154:LEU:HD21	1:A:172:MET:HE2	1.95	0.49
1:A:188:SER:CA	1:B:39:GLN:OE1	2.60	0.49
1:B:1:LEU:HD23	1:B:3:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:159:LYS:O	1:Q:163:GLN:HG3	2.13	0.49
1:A:193:LEU:HB3	1:B:42:HIS:CD2	2.48	0.49
1:A:82:LEU:HD13	1:A:84:TRP:CZ2	2.48	0.49
1:L:272:SER:OG	1:L:288:VAL:HG11	2.13	0.49
1:O:154:LEU:HD12	1:O:157:PHE:CZ	2.48	0.49
1:Q:165:PHE:CB	1:Q:248:LYS:HG2	2.42	0.49
1:B:172:MET:SD	1:B:227:GLY:HA3	2.52	0.49
1:Q:181:ASP:OD2	1:Q:195:ARG:NH1	2.43	0.49
1:A:97:GLY:CA	3:A:376:NDP:O3D	2.61	0.48
1:O:165:PHE:HB3	1:O:248:LYS:CG	2.42	0.48
1:O:165:PHE:C	1:O:248:LYS:HG2	2.33	0.48
1:P:184:LEU:C	1:P:184:LEU:HD12	2.33	0.48
1:P:98:VAL:HG23	1:P:99:PHE:CE2	2.47	0.48
1:R:236:ASN:O	1:R:237:VAL:HB	2.12	0.48
1:A:133:ASN:HD22	1:A:133:ASN:H	1.62	0.48
1:B:129:VAL:H	1:B:133:ASN:HD21	1.60	0.48
1:L:176:HIS:HB3	1:L:231:ARG:HD3	1.94	0.48
1:P:176:HIS:HB3	1:P:231:ARG:HD3	1.95	0.48
1:A:272:SER:OG	1:A:288:VAL:HG11	2.13	0.48
1:I:172:MET:HE2	1:I:172:MET:HB3	1.66	0.48
1:I:208:THR:OG1	2:I:366:SO4:O2	2.23	0.48
1:H:278:LEU:O	1:L:194:ARG:HD3	2.13	0.48
1:I:278:LEU:O	1:M:194:ARG:HD3	2.14	0.48
1:Q:212:LYS:O	1:Q:215:ALA:HB3	2.12	0.48
1:R:149:CYS:HB3	3:R:377:NDP:H41N	1.96	0.48
1:C:187:ALA:O	1:C:196:ALA:HB1	2.14	0.48
1:C:39:GLN:HG3	1:D:193:LEU:CD2	2.44	0.48
1:H:154:LEU:HD23	1:H:214:VAL:HG21	1.95	0.48
1:I:128:TYR:HA	1:I:133:ASN:HD21	1.79	0.48
1:Q:248:LYS:CG	1:Q:248:LYS:O	2.61	0.48
1:R:228:ILE:HD11	1:Q:306:LYS:CE	2.44	0.48
1:Q:328:VAL:HG12	1:Q:332:TRP:CZ3	2.47	0.48
1:H:172:MET:CE	1:H:210:ALA:HB3	2.44	0.48
1:H:77:ARG:HH22	3:H:379:NDP:P2B	2.36	0.48
1:A:205:PRO:HG2	1:C:310:TRP:CZ2	2.48	0.48
1:L:149:CYS:HB3	3:L:369:NDP:H41N	1.96	0.48
1:A:276:GLU:OE1	1:D:46:TYR:OH	2.20	0.48
1:B:187:ALA:O	1:B:196:ALA:HB1	2.13	0.48
1:M:29:VAL:HG22	1:M:30:ILE:N	2.29	0.48
1:B:165:PHE:C	1:B:248:LYS:HG3	2.34	0.48
1:C:56:ASP:CG	1:C:58:LYS:NZ	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:236:ASN:O	1:P:237:VAL:CB	2.62	0.48
1:R:248:LYS:HE2	1:R:248:LYS:HB3	1.67	0.48
1:L:77:ARG:HH12	3:L:369:NDP:C4A	2.26	0.48
1:M:272:SER:OG	1:M:288:VAL:HG11	2.14	0.48
1:P:128:TYR:HA	1:P:133:ASN:HD21	1.78	0.48
1:R:228:ILE:CD1	1:Q:306:LYS:HZ3	2.27	0.48
1:I:97:GLY:CA	3:I:380:NDP:O3D	2.62	0.48
1:I:310:TRP:HZ2	1:M:205:PRO:HG2	1.78	0.48
1:B:0:LYS:HE3	1:B:23:SER:O	2.14	0.47
1:L:188:SER:HB2	1:M:39:GLN:OE1	2.14	0.47
1:L:82:LEU:HD13	1:L:84:TRP:CZ2	2.49	0.47
1:P:228:ILE:C	1:P:228:ILE:HD12	2.35	0.47
1:Q:157:PHE:HB2	1:Q:259:PHE:CE1	2.49	0.47
1:Q:82:LEU:HD13	1:Q:84:TRP:CZ2	2.49	0.47
1:R:2:LYS:N	1:R:90:ASP:OD2	2.47	0.47
1:R:84:TRP:CE3	1:R:84:TRP:HA	2.49	0.47
1:D:157:PHE:HB2	1:D:259:PHE:CE1	2.48	0.47
1:H:281:ILE:CB	1:L:202:ASN:ND2	2.64	0.47
1:I:253:GLU:HA	2:I:379:SO4:O2	2.15	0.47
1:P:210:ALA:O	1:P:213:ALA:HB3	2.14	0.47
1:Q:164:LYS:O	1:Q:248:LYS:CD	2.59	0.47
1:A:210:ALA:HA	1:A:213:ALA:HB3	1.96	0.47
1:D:209:GLY:O	1:D:212:LYS:HG2	2.15	0.47
1:H:209:GLY:O	1:H:213:ALA:CB	2.62	0.47
1:I:95:GLY:O	3:I:380:NDP:H51A	2.15	0.47
1:Q:154:LEU:HD21	1:Q:242:LEU:HD21	1.95	0.47
1:H:97:GLY:HA3	3:H:379:NDP:O3D	2.14	0.47
1:Q:165:PHE:HD1	1:Q:248:LYS:CG	2.27	0.47
1:Q:261:GLU:OE1	1:Q:261:GLU:CA	2.62	0.47
1:C:82:LEU:HD13	1:C:84:TRP:CZ2	2.49	0.47
1:H:201:LEU:HD21	1:I:235:PRO:HG3	1.94	0.47
1:M:176:HIS:HB3	1:M:231:ARG:HD3	1.96	0.47
1:O:236:ASN:O	1:O:237:VAL:HB	2.13	0.47
1:O:42:HIS:HB3	1:R:193:LEU:CD2	2.45	0.47
1:Q:170:GLY:HA3	1:Q:244:VAL:HG12	1.96	0.47
1:A:184:LEU:O	1:A:184:LEU:HD12	2.15	0.47
1:A:97:GLY:HA3	3:A:376:NDP:O3D	2.15	0.47
1:B:228:ILE:C	1:B:228:ILE:HD12	2.35	0.47
1:C:33:THR:HG21	1:C:77:ARG:HG2	1.96	0.47
1:M:100:VAL:HG23	1:M:122(A):LYS:HG2	1.97	0.47
1:R:139:HIS:CG	1:R:333:GLN:OE1	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:84:TRP:HE3	1:R:84:TRP:HA	1.80	0.47
1:B:155:ALA:HB3	1:B:156:PRO:HD3	1.96	0.47
1:A:202:ASN:ND2	1:C:281:ILE:CB	2.60	0.47
1:D:238:SER:HB2	1:D:311:TYR:CZ	2.49	0.47
1:H:133:ASN:HD22	1:H:133:ASN:H	1.61	0.47
1:L:133:ASN:HD22	1:L:133:ASN:N	2.10	0.47
1:L:154:LEU:HD23	1:L:214:VAL:HG21	1.96	0.47
1:L:236:ASN:O	1:L:237:VAL:HB	2.15	0.47
1:P:133:ASN:H	1:P:133:ASN:HD22	1.63	0.47
1:A:187:ALA:O	1:A:196:ALA:HB1	2.15	0.47
1:A:11:ILE:HD11	3:A:376:NDP:H42N	1.95	0.47
1:B:176:HIS:HB3	1:B:231:ARG:HD3	1.96	0.47
1:B:33:THR:HA	1:B:75:SER:OG	2.15	0.47
1:H:77:ARG:NH1	3:H:379:NDP:C4A	2.77	0.47
1:O:84:TRP:CE3	1:O:84:TRP:HA	2.50	0.47
1:P:11:ILE:HG13	3:P:373:NDP:H1D	1.96	0.47
1:P:77:ARG:O	1:P:79:PRO:HD3	2.15	0.47
1:A:202:ASN:HD22	1:C:281:ILE:N	2.00	0.47
1:B:169:LYS:NZ	1:D:303:ASP:OD1	2.47	0.47
1:D:84:TRP:CE3	1:D:84:TRP:HA	2.50	0.47
1:L:126:PRO:HD2	1:L:143:ILE:O	2.15	0.47
1:L:128:TYR:HA	1:L:133:ASN:HD21	1.80	0.47
1:O:240:VAL:HG13	1:O:311:TYR:CE1	2.50	0.47
1:Q:96:THR:OG1	1:Q:98:VAL:HG22	2.15	0.47
1:B:149:CYS:HB3	3:B:378:NDP:H41N	1.96	0.46
1:H:207:SER:O	1:H:208:THR:HB	2.14	0.46
1:B:96:THR:OG1	1:B:98:VAL:HG22	2.15	0.46
1:C:97:GLY:CA	3:C:365:NDP:O3D	2.64	0.46
1:Q:190:HIS:CD2	1:Q:191:ARG:NH1	2.83	0.46
1:A:204:VAL:HB	1:A:231:ARG:HB2	1.98	0.46
1:C:154:LEU:HD12	1:C:157:PHE:CZ	2.50	0.46
1:O:42:HIS:CD2	1:R:193:LEU:CD2	2.97	0.46
1:P:271:LEU:HD13	1:P:272:SER:H	1.76	0.46
1:H:202:ASN:HD21	1:L:281:ILE:CG2	2.28	0.46
1:I:154:LEU:HD23	1:I:214:VAL:HG21	1.98	0.46
1:M:11:ILE:HD11	3:M:381:NDP:H42N	1.97	0.46
1:Q:155:ALA:HB3	1:Q:156:PRO:HD3	1.97	0.46
1:Q:190:HIS:HB3	1:Q:196:ALA:HB2	1.97	0.46
1:R:228:ILE:HG13	1:Q:298:MET:HE1	1.96	0.46
1:A:205:PRO:CG	1:C:310:TRP:HZ2	2.28	0.46
1:I:163:GLN:NE2	1:I:164:LYS:HZ3	2.07	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:16:LEU:HD23	1:I:16:LEU:O	2.15	0.46
1:P:194:ARG:HD2	1:P:205:PRO:O	2.15	0.46
1:Q:173:THR:HG23	1:Q:228:ILE:CD1	2.46	0.46
1:Q:183:ARG:HE	1:Q:187:ALA:CB	2.27	0.46
1:Q:98:VAL:HG23	1:Q:99:PHE:CD2	2.50	0.46
1:H:155:ALA:HB3	1:H:156:PRO:HD3	1.97	0.46
1:H:151:THR:OG1	1:H:210:ALA:HA	2.15	0.46
1:B:236:ASN:O	1:B:237:VAL:HB	2.15	0.46
1:L:97:GLY:CA	3:L:369:NDP:O3D	2.63	0.46
1:L:65:SER:HA	1:L:69:LYS:O	2.15	0.46
1:L:83:PRO:O	1:L:87:MET:HG3	2.15	0.46
1:O:209:GLY:O	1:O:212:LYS:HG2	2.16	0.46
1:P:97:GLY:HA3	3:P:373:NDP:O3D	2.16	0.46
1:R:272:SER:OG	1:R:288:VAL:HG11	2.16	0.46
1:A:320:ARG:NE	1:A:320:ARG:HA	2.31	0.46
1:D:149:CYS:HB3	3:D:365:NDP:H41N	1.98	0.46
1:R:165:PHE:C	1:R:248:LYS:HG2	2.36	0.46
1:B:191:ARG:HB3	1:B:191:ARG:NH1	2.31	0.46
1:H:250:THR:OG1	1:H:251:PHE:N	2.49	0.46
1:I:80:VAL:HB	1:I:110:GLN:OE1	2.15	0.46
1:P:133:ASN:N	1:P:133:ASN:HD22	2.13	0.46
1:Q:165:PHE:CA	1:Q:248:LYS:HD2	2.41	0.46
1:I:157:PHE:HB2	1:I:259:PHE:CE1	2.51	0.45
1:I:163:GLN:HG2	1:I:164:LYS:HD3	1.98	0.45
1:R:139:HIS:CD2	1:R:139:HIS:C	2.89	0.45
1:R:250:THR:OG1	1:R:251:PHE:N	2.50	0.45
1:R:137:TYR:CE2	1:R:331:LYS:HG3	2.51	0.45
1:A:208:THR:HG22	1:A:228:ILE:CA	2.46	0.45
1:H:183:ARG:HE	1:H:187:ALA:HB3	1.82	0.45
1:O:100:VAL:HG23	1:O:122(A):LYS:HG2	1.98	0.45
1:O:148:SER:CB	2:O:364:SO4:O1	2.63	0.45
1:O:96:THR:OG1	1:O:98:VAL:HG22	2.16	0.45
1:I:183:ARG:NH1	1:I:187:ALA:HB1	2.31	0.45
1:M:95:GLY:O	3:M:381:NDP:H51A	2.16	0.45
1:M:96:THR:OG1	1:M:98:VAL:HG22	2.15	0.45
1:O:190:HIS:HB3	1:O:196:ALA:HB2	1.98	0.45
1:O:84:TRP:HE3	1:O:84:TRP:HA	1.81	0.45
1:P:211:ALA:HB1	1:P:226:ASN:HA	1.98	0.45
1:R:126:PRO:HD2	1:R:143:ILE:O	2.16	0.45
1:A:84:TRP:CE3	1:A:84:TRP:HA	2.51	0.45
1:B:281:ILE:H	1:D:202:ASN:ND2	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:GLY:CA	3:B:378:NDP:O3D	2.65	0.45
1:A:96:THR:OG1	1:A:98:VAL:HG22	2.17	0.45
1:B:181:ASP:OD2	1:B:195:ARG:NH1	2.46	0.45
1:O:11:ILE:HG13	3:O:372:NDP:H1D	1.98	0.45
1:Q:172:MET:CB	1:Q:242:LEU:HD22	2.40	0.45
1:B:165:PHE:CA	1:B:248:LYS:CG	2.85	0.45
1:C:153:CYS:HA	1:C:290:SER:HB2	1.99	0.45
1:H:96:THR:OG1	1:H:98:VAL:HG22	2.16	0.45
1:Q:190:HIS:NE2	1:Q:191:ARG:NH1	2.65	0.45
1:R:29:VAL:HG22	1:R:30:ILE:N	2.32	0.45
1:P:184:LEU:CD1	1:Q:178:TYR:CE1	2.99	0.45
1:D:84:TRP:HE3	1:D:84:TRP:HA	1.80	0.45
1:I:272:SER:OG	1:I:288:VAL:HG11	2.17	0.45
1:M:58:LYS:HB3	1:M:58:LYS:HZ3	1.82	0.45
1:A:84:TRP:HE3	1:A:84:TRP:HA	1.81	0.45
1:I:100:VAL:HG23	1:I:122(A):LYS:HG2	1.99	0.45
1:I:163:GLN:HG2	1:I:164:LYS:N	2.32	0.45
1:L:170:GLY:HA3	1:L:244:VAL:HG12	1.99	0.45
1:O:204:VAL:HB	1:O:231:ARG:HB2	1.99	0.45
1:P:298:MET:CE	1:P:306:LYS:HD2	2.46	0.45
1:A:228:ILE:HD12	1:A:228:ILE:C	2.38	0.45
1:H:221:LEU:HD22	1:H:225:LEU:CD1	2.47	0.45
1:O:281:ILE:HD13	1:O:281:ILE:O	2.16	0.45
1:O:300:MET:SD	1:P:226:ASN:HB2	2.57	0.45
1:R:157:PHE:HB2	1:R:259:PHE:CE1	2.51	0.45
1:B:212:LYS:HZ3	1:B:226:ASN:CG	2.08	0.44
1:C:157:PHE:HB2	1:C:259:PHE:CE1	2.53	0.44
1:D:176:HIS:HB3	1:D:231:ARG:HD3	1.98	0.44
1:P:154:LEU:HD23	1:P:214:VAL:HG21	1.99	0.44
1:P:222:LYS:HD2	1:P:222:LYS:C	2.37	0.44
1:I:250:THR:OG1	1:I:251:PHE:N	2.49	0.44
1:O:126:PRO:HD2	1:O:143:ILE:O	2.17	0.44
1:Q:211:ALA:CB	1:Q:226:ASN:HA	2.46	0.44
1:Q:327:ILE:O	1:Q:331:LYS:HG2	2.17	0.44
1:A:194:ARG:HG2	1:C:277:PRO:O	2.18	0.44
1:O:11:ILE:HD11	3:O:372:NDP:H42N	1.98	0.44
1:P:34:GLY:HA3	1:P:39:GLN:OE1	2.17	0.44
1:Q:33:THR:HA	1:Q:75:SER:OG	2.18	0.44
1:A:266:GLU:HG2	1:A:267:LEU:HG	1.99	0.44
1:B:170:GLY:HA3	1:B:244:VAL:HG12	1.99	0.44
1:B:227:GLY:O	1:D:298:MET:HE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:TRP:CE3	1:C:84:TRP:HA	2.53	0.44
1:I:58:LYS:HZ3	1:I:58:LYS:HB3	1.82	0.44
1:A:103:ASP:OD1	1:A:103:ASP:O	2.35	0.44
1:B:172:MET:CE	1:B:211:ALA:N	2.72	0.44
1:I:84:TRP:CE3	1:I:84:TRP:HA	2.53	0.44
1:R:117:LEU:HD23	1:R:117:LEU:C	2.38	0.44
1:R:99:PHE:HZ	3:R:377:NDP:N6A	2.14	0.44
1:A:176:HIS:HB3	1:A:231:ARG:HD3	1.99	0.44
1:B:100:VAL:HG23	1:B:122(A):LYS:HG2	1.99	0.44
1:I:194:ARG:HD3	1:M:278:LEU:O	2.18	0.44
1:O:165:PHE:CB	1:O:248:LYS:CG	2.95	0.44
1:O:300:MET:HE2	1:P:224:LYS:O	2.18	0.44
1:Q:120:ALA:CB	3:Q:375:NDP:H2D	2.40	0.44
1:A:18:CYS:SG	1:A:319:GLN:HG2	2.58	0.44
1:H:77:ARG:HH11	3:H:379:NDP:C6A	2.30	0.44
1:P:204:VAL:HB	1:P:231:ARG:HB2	2.00	0.44
1:P:261:GLU:OE1	1:P:262:SER:N	2.50	0.44
1:A:0:LYS:HD3	1:A:0:LYS:C	2.37	0.44
1:B:9:GLY:HA3	3:B:378:NDP:O5B	2.18	0.44
1:B:281:ILE:CB	1:D:202:ASN:ND2	2.65	0.44
1:C:201:LEU:HD21	1:D:235:PRO:HG3	1.99	0.44
1:D:236:ASN:O	1:D:237:VAL:HB	2.18	0.44
1:O:191:ARG:HA	1:O:191:ARG:HD2	1.80	0.44
1:O:300:MET:HG3	1:P:170:GLY:O	2.18	0.44
1:P:84:TRP:HA	1:P:84:TRP:HE3	1.83	0.44
1:Q:320:ARG:NE	1:Q:320:ARG:HA	2.33	0.44
1:A:205:PRO:CG	1:C:310:TRP:CZ2	3.01	0.44
1:H:82:LEU:HD13	1:H:84:TRP:CZ2	2.53	0.44
1:B:204:VAL:HB	1:B:231:ARG:HB2	2.00	0.43
1:B:29:VAL:HG22	1:B:30:ILE:N	2.32	0.43
1:C:2:LYS:HD2	1:C:28:VAL:HG11	1.99	0.43
1:M:200:CYS:HB2	4:M:383:HOH:O	2.17	0.43
1:O:120:ALA:CB	3:O:372:NDP:H2D	2.44	0.43
1:Q:242:LEU:HD13	1:Q:242:LEU:HA	1.73	0.43
1:Q:31:ASN:ND2	3:Q:375:NDP:H2A	2.33	0.43
1:R:187:ALA:O	1:R:196:ALA:HB1	2.19	0.43
1:H:95:GLY:O	3:H:379:NDP:H51A	2.18	0.43
1:I:31:ASN:ND2	3:I:380:NDP:H2A	2.34	0.43
1:L:11:ILE:HD11	3:L:369:NDP:H42N	2.00	0.43
1:M:187:ALA:O	1:M:196:ALA:HB1	2.18	0.43
1:P:197:ARG:HH21	1:Q:48:SER:N	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:160:VAL:HG13	1:R:164:LYS:HZ2	1.83	0.43
1:A:153:CYS:SG	1:A:240:VAL:CG2	3.06	0.43
1:D:172:MET:CE	1:D:211:ALA:HB2	2.47	0.43
1:I:170:GLY:HA3	1:I:244:VAL:HG12	1.99	0.43
1:I:187:ALA:O	1:I:196:ALA:HB1	2.18	0.43
1:M:185:LEU:O	1:M:186:ASP:C	2.57	0.43
1:O:203:ILE:HB	1:P:280:SER:HB3	2.01	0.43
1:O:228:ILE:CG1	1:O:229:ALA:H	2.14	0.43
1:P:25:LEU:HD11	1:P:325:ALA:HB3	2.00	0.43
1:R:238:SER:HB2	1:R:311:TYR:CZ	2.53	0.43
1:A:98:VAL:HG23	1:A:99:PHE:CE2	2.52	0.43
1:B:154:LEU:HD23	1:B:214:VAL:HG21	1.99	0.43
1:D:172:MET:SD	1:D:227:GLY:HA3	2.58	0.43
1:L:179:THR:OG1	2:L:367:SO4:O4	2.22	0.43
1:M:251:PHE:CZ	1:M:254:GLU:HB2	2.53	0.43
1:P:135:GLU:N	1:P:135:GLU:CD	2.67	0.43
1:P:84:TRP:HA	1:P:84:TRP:CE3	2.53	0.43
1:Q:11:ILE:HG13	3:Q:375:NDP:H1D	2.01	0.43
1:R:178:TYR:HA	1:R:182:GLN:OE1	2.18	0.43
1:H:133:ASN:HD22	1:H:133:ASN:N	2.14	0.43
1:H:231:ARG:NH2	2:H:363:SO4:O2	2.36	0.43
1:M:170:GLY:HA3	1:M:244:VAL:HG12	2.00	0.43
1:Q:97:GLY:HA3	3:Q:375:NDP:O3D	2.18	0.43
1:R:165:PHE:CB	1:R:248:LYS:HG3	2.48	0.43
1:R:1:LEU:HD23	1:R:25:LEU:HD23	2.00	0.43
1:I:236:ASN:O	1:I:237:VAL:CB	2.66	0.43
1:M:120:ALA:HB2	3:M:381:NDP:C2D	2.49	0.43
1:B:117:LEU:C	1:B:117:LEU:HD23	2.39	0.43
1:B:241:ASP:OD1	1:B:306:LYS:CE	2.53	0.43
1:C:100:VAL:HG23	1:C:122(A):LYS:HG2	2.01	0.43
1:D:33:THR:HA	1:D:75:SER:HG	1.79	0.43
1:M:204:VAL:HB	1:M:231:ARG:HB2	2.00	0.43
1:O:248:LYS:HE2	1:O:248:LYS:HB2	1.64	0.43
1:P:149:CYS:HB3	3:P:373:NDP:H41N	2.01	0.43
1:P:33:THR:HA	1:P:75:SER:OG	2.18	0.43
1:A:289:SER:OG	1:A:320:ARG:HD2	2.18	0.43
1:L:9:GLY:O	1:L:13:ARG:HG3	2.19	0.43
1:M:31:ASN:ND2	3:M:381:NDP:H2A	2.33	0.43
1:O:281:ILE:CD1	1:O:284:ARG:HD2	2.49	0.43
1:R:169:LYS:NZ	1:Q:303:ASP:OD1	2.50	0.43
1:R:228:ILE:HD11	1:Q:306:LYS:NZ	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ASN:ND2	3:A:376:NDP:H2A	2.33	0.43
1:A:54:ASP:O	1:A:54:ASP:OD1	2.37	0.43
1:A:243:VAL:HG11	1:C:243:VAL:HG11	2.01	0.43
1:C:9:GLY:HA3	3:C:365:NDP:O5B	2.19	0.43
1:D:187:ALA:O	1:D:196:ALA:HB1	2.19	0.43
1:I:84:TRP:CD1	1:I:113:ALA:HB2	2.54	0.43
1:R:133:ASN:N	1:R:133:ASN:HD22	2.17	0.43
1:B:197:ARG:HH12	1:D:282:ASP:CG	2.22	0.43
1:I:172:MET:HG2	1:I:173:THR:H	1.83	0.43
1:I:9:GLY:HA3	3:I:380:NDP:O5B	2.19	0.43
1:L:157:PHE:HB2	1:L:259:PHE:CE1	2.54	0.43
1:P:186:ASP:OD1	1:Q:48:SER:HB2	2.19	0.43
1:Q:222:LYS:HD2	1:Q:222:LYS:HA	1.67	0.43
1:A:95:GLY:O	3:A:376:NDP:H51A	2.19	0.42
1:M:250:THR:OG1	1:M:251:PHE:N	2.51	0.42
1:P:97:GLY:CA	3:P:373:NDP:O3D	2.67	0.42
1:R:245:GLN:HE22	1:Q:245:GLN:HE22	1.65	0.42
1:R:202:ASN:ND2	1:Q:281:ILE:CB	2.70	0.42
1:B:98:VAL:HG23	1:B:99:PHE:CE2	2.54	0.42
1:C:106:GLY:HA3	1:I:110:GLN:NE2	2.33	0.42
1:C:235:PRO:HG3	1:D:201:LEU:HD21	2.01	0.42
1:A:224:LYS:O	1:C:300:MET:HE2	2.19	0.42
1:H:98:VAL:HG23	1:H:99:PHE:CD2	2.54	0.42
1:L:289:SER:OG	1:L:320:ARG:HD2	2.19	0.42
1:O:310:TRP:CZ2	1:P:205:PRO:HG2	2.49	0.42
1:A:163:GLN:HG2	1:A:164:LYS:N	2.35	0.42
1:A:188:SER:HA	1:B:39:GLN:OE1	2.19	0.42
1:C:106:GLY:CA	1:I:110:GLN:NE2	2.82	0.42
1:B:120:ALA:CB	3:B:378:NDP:H2D	2.43	0.42
1:D:0:LYS:HA	1:D:0:LYS:HD2	1.95	0.42
1:L:84:TRP:CA	1:L:84:TRP:CE3	3.02	0.42
1:O:95:GLY:O	3:O:372:NDP:H51A	2.19	0.42
1:R:300:MET:CE	1:Q:226:ASN:HB2	2.47	0.42
1:Q:45:LYS:HB3	2:Q:373:SO4:O1	2.19	0.42
1:R:106:GLY:O	1:R:109:LEU:N	2.48	0.42
1:R:137:TYR:HE2	1:R:331:LYS:HB2	1.84	0.42
1:A:157:PHE:HB2	1:A:259:PHE:CE1	2.55	0.42
1:A:194:ARG:CZ	1:C:277:PRO:HA	2.49	0.42
1:C:56:ASP:CA	1:C:58:LYS:HZ1	2.33	0.42
1:I:281:ILE:CB	1:M:202:ASN:ND2	2.65	0.42
1:I:202:ASN:ND2	1:M:281:ILE:CB	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:163:GLN:NE2	1:O:164:LYS:HZ3	2.02	0.42
1:O:281:ILE:HG21	1:Q:48:SER:CA	2.44	0.42
1:Q:236:ASN:O	1:Q:237:VAL:HB	2.18	0.42
1:R:327:ILE:O	1:R:331:LYS:HG2	2.20	0.42
1:A:163:GLN:CG	1:A:164:LYS:N	2.82	0.42
1:A:236:ASN:O	1:A:237:VAL:CB	2.67	0.42
1:B:320:ARG:NE	1:B:320:ARG:HA	2.35	0.42
1:I:226:ASN:ND2	1:M:298:MET:CE	2.82	0.42
1:I:48:SER:CA	1:L:281:ILE:HG21	2.48	0.42
1:P:208:THR:HG21	1:P:228:ILE:O	2.18	0.42
1:P:95:GLY:O	3:P:373:NDP:H51A	2.19	0.42
1:A:212:LYS:C	1:A:214:VAL:N	2.73	0.42
1:A:149:CYS:HB3	3:A:376:NDP:H41N	2.01	0.42
1:D:106:GLY:O	1:D:109:LEU:N	2.49	0.42
1:O:202:ASN:ND2	1:P:281:ILE:CB	2.71	0.42
1:O:282:ASP:OD2	1:P:197:ARG:NH1	2.52	0.42
1:P:29:VAL:HG22	1:P:30:ILE:N	2.35	0.42
3:O:372:NDP:O3X	1:R:188:SER:HB2	2.19	0.42
1:R:164:LYS:C	1:R:248:LYS:HD2	2.39	0.42
1:A:154:LEU:HD23	1:A:214:VAL:HG21	2.02	0.42
1:B:213:ALA:O	1:B:216:LEU:HB2	2.19	0.42
1:D:115:LYS:NZ	1:D:141:ASP:O	2.50	0.42
1:L:10:ARG:HH11	1:L:13:ARG:NH2	2.18	0.42
1:L:48:SER:N	1:M:197:ARG:HH21	2.17	0.42
1:O:9:GLY:HA3	3:O:372:NDP:O5B	2.20	0.42
1:Q:240:VAL:HG23	1:Q:311:TYR:CE1	2.55	0.42
1:A:154:LEU:HD12	1:A:157:PHE:CZ	2.55	0.42
1:H:194:ARG:HD3	1:L:278:LEU:O	2.20	0.42
1:I:191:ARG:HB3	1:I:191:ARG:NH1	2.34	0.42
1:I:1:LEU:HD22	1:I:329:ALA:HB2	2.02	0.42
1:M:190:HIS:HB3	1:M:196:ALA:HB2	2.02	0.42
1:O:303:ASP:OD1	1:P:169:LYS:NZ	2.51	0.42
1:P:42:HIS:CG	1:Q:193:LEU:HD13	2.54	0.42
1:Q:97:GLY:CA	3:Q:375:NDP:O3D	2.68	0.42
1:B:11:ILE:HG13	3:B:378:NDP:H1D	2.02	0.42
1:C:84:TRP:HE3	1:C:84:TRP:HA	1.84	0.42
1:D:133:ASN:HD22	1:D:133:ASN:N	2.18	0.42
1:D:240:VAL:HG13	1:D:311:TYR:CE1	2.55	0.42
1:M:236:ASN:O	1:M:237:VAL:CB	2.68	0.42
1:O:9:GLY:O	1:O:13:ARG:HG3	2.20	0.42
1:Q:248:LYS:HB2	1:Q:248:LYS:HE2	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:GLY:CA	1:I:110:GLN:HE22	2.30	0.41
1:L:158:VAL:HG11	1:L:221:LEU:HD13	1.99	0.41
1:Q:37:VAL:HG21	1:Q:62:SER:HA	2.02	0.41
1:A:33:THR:HA	1:A:75:SER:OG	2.20	0.41
1:D:117:LEU:HD23	1:D:117:LEU:C	2.40	0.41
1:H:79:PRO:HA	1:H:82:LEU:CD1	2.51	0.41
1:O:149:CYS:HB3	3:O:372:NDP:H41N	2.01	0.41
1:P:168:ILE:HG22	1:P:169:LYS:HD3	2.01	0.41
1:C:320:ARG:HA	1:C:320:ARG:NE	2.35	0.41
1:C:39:GLN:HG3	1:D:193:LEU:HD21	2.02	0.41
1:L:96:THR:OG1	1:L:98:VAL:HG22	2.19	0.41
1:Q:9:GLY:HA3	3:Q:375:NDP:O5B	2.20	0.41
1:B:30:ILE:HG13	1:B:71:ILE:HG21	2.02	0.41
1:C:80:VAL:HG13	1:C:107:LYS:NZ	2.34	0.41
1:H:289:SER:OG	1:H:320:ARG:HD2	2.20	0.41
1:I:168:ILE:HG22	1:I:169:LYS:HD3	2.01	0.41
1:M:191:ARG:NH1	1:M:191:ARG:HB3	2.35	0.41
1:O:228:ILE:CG1	1:O:229:ALA:N	2.68	0.41
1:O:320:ARG:NE	1:O:320:ARG:HA	2.36	0.41
1:O:97:GLY:HA2	3:O:372:NDP:O3D	2.20	0.41
1:O:300:MET:CG	1:P:171:THR:HG22	2.50	0.41
1:P:148:SER:OG	2:P:364:SO4:O3	2.38	0.41
1:D:133:ASN:ND2	1:D:133:ASN:C	2.73	0.41
1:D:133:ASN:HD22	1:D:133:ASN:H	1.67	0.41
1:H:280:SER:HB3	1:L:203:ILE:HB	2.01	0.41
1:H:252:ALA:N	2:H:378:SO4:O3	2.28	0.41
1:I:204:VAL:HB	1:I:231:ARG:HB2	2.02	0.41
1:I:9:GLY:O	1:I:13:ARG:HG3	2.20	0.41
1:M:157:PHE:HB2	1:M:259:PHE:CE1	2.55	0.41
1:O:220:ASN:N	1:O:220:ASN:OD1	2.54	0.41
1:O:63:ALA:HB1	1:O:71:ILE:O	2.20	0.41
1:Q:61:ASP:OD1	1:Q:61:ASP:C	2.58	0.41
1:B:185:LEU:O	1:B:186:ASP:C	2.57	0.41
1:I:183:ARG:HH12	1:I:187:ALA:HB1	1.85	0.41
1:P:208:THR:CG2	1:P:228:ILE:N	2.83	0.41
1:Q:120:ALA:HB1	1:Q:121:PRO:CD	2.51	0.41
1:R:253:GLU:OE1	1:R:253:GLU:HA	2.19	0.41
1:A:39:GLN:OE1	1:B:188:SER:CB	2.57	0.41
1:D:34:GLY:HA3	1:D:39:GLN:OE1	2.20	0.41
1:O:153:CYS:HA	1:O:290:SER:HB2	2.03	0.41
1:O:300:MET:HG3	1:P:171:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:256:ASN:OD1	2:P:372:SO4:O1	2.39	0.41
1:P:39:GLN:OE1	1:Q:188:SER:CB	2.67	0.41
1:R:281:ILE:N	1:Q:202:ASN:ND2	2.53	0.41
1:R:191:ARG:HB3	1:R:191:ARG:NH1	2.35	0.41
1:R:213:ALA:O	1:R:216:LEU:HB2	2.20	0.41
1:R:95:GLY:O	3:R:377:NDP:H51A	2.21	0.41
1:A:163:GLN:NE2	1:A:164:LYS:CE	2.71	0.41
1:A:197:ARG:HH12	1:C:282:ASP:CG	2.24	0.41
1:C:126:PRO:HD2	1:C:143:ILE:O	2.21	0.41
1:A:281:ILE:CB	1:C:202:ASN:ND2	2.72	0.41
1:D:159:LYS:O	1:D:163:GLN:HG3	2.19	0.41
1:D:208:THR:HG22	1:D:228:ILE:HA	2.02	0.41
1:H:209:GLY:O	1:H:213:ALA:HB2	2.20	0.41
1:I:228:ILE:HD12	1:I:228:ILE:C	2.41	0.41
1:I:232:VAL:HA	1:I:233:PRO:HD3	1.86	0.41
1:I:84:TRP:HA	1:I:84:TRP:HE3	1.85	0.41
1:P:184:LEU:HD21	1:Q:199:ALA:HB3	2.03	0.41
1:P:241:ASP:OD1	1:P:306:LYS:HE2	2.20	0.41
1:R:310:TRP:CZ2	1:Q:205:PRO:HG3	2.56	0.41
1:R:80:VAL:HG23	1:R:81:ASN:ND2	2.36	0.41
1:A:9:GLY:HA3	3:A:376:NDP:C5B	2.51	0.41
1:B:1:LEU:HD21	1:B:91:LEU:HB3	2.02	0.41
1:C:213:ALA:O	1:C:216:LEU:HB2	2.21	0.41
1:I:133:ASN:N	1:I:133:ASN:HD22	2.19	0.41
1:L:193:LEU:CD2	1:M:39:GLN:HG3	2.50	0.41
1:O:1:LEU:HA	1:O:1:LEU:HD12	1.70	0.41
1:O:298:MET:CE	1:P:226:ASN:CG	2.89	0.41
1:P:154:LEU:HD12	1:P:157:PHE:CZ	2.56	0.41
1:P:332:TRP:CD1	1:P:334:GLY:HA3	2.56	0.41
1:Q:261:GLU:HA	1:Q:261:GLU:OE1	2.20	0.41
1:R:205:PRO:HG2	1:Q:310:TRP:HZ2	1.85	0.41
1:D:95:GLY:O	3:D:365:NDP:H51A	2.21	0.41
1:I:226:ASN:HB2	1:M:300:MET:SD	2.61	0.41
1:P:27:VAL:CG1	1:P:71:ILE:CD1	2.79	0.41
1:R:172:MET:SD	1:R:227:GLY:HA3	2.61	0.41
1:A:56:ASP:OD1	1:A:58:LYS:HE2	2.21	0.41
1:A:80:VAL:HG23	1:A:81:ASN:ND2	2.36	0.41
1:B:194:ARG:HD3	1:D:278:LEU:O	2.21	0.41
1:C:186:ASP:HA	1:C:196:ALA:O	2.21	0.41
1:C:154:LEU:HD23	1:C:214:VAL:HG21	2.03	0.41
1:L:185:LEU:O	1:L:186:ASP:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:185:LEU:O	1:Q:186:ASP:C	2.59	0.41
1:B:150:THR:HB	2:B:364:SO4:O2	2.21	0.40
1:B:165:PHE:C	1:B:248:LYS:CG	2.90	0.40
1:C:77:ARG:HA	3:C:365:NDP:N1A	2.36	0.40
1:B:16:LEU:HD23	1:B:16:LEU:O	2.22	0.40
1:C:80:VAL:HG23	1:C:81:ASN:ND2	2.36	0.40
1:D:126:PRO:HD2	1:D:143:ILE:O	2.20	0.40
1:I:208:THR:CG2	1:I:228:ILE:HA	2.51	0.40
1:L:120:ALA:HB2	3:L:369:NDP:C2D	2.51	0.40
1:L:34:GLY:HA3	1:L:39:GLN:OE1	2.22	0.40
1:H:281:ILE:HG12	1:M:48:SER:HA	2.04	0.40
1:O:154:LEU:HD23	1:O:214:VAL:HG21	2.03	0.40
1:Q:117:LEU:HD23	1:Q:117:LEU:C	2.41	0.40
1:R:236:ASN:O	1:R:237:VAL:CB	2.69	0.40
1:B:190:HIS:HB3	1:B:196:ALA:HB2	2.03	0.40
1:H:159:LYS:O	1:H:163:GLN:HG3	2.22	0.40
1:M:84:TRP:HA	1:M:84:TRP:CE3	2.57	0.40
1:Q:261:GLU:O	1:Q:261:GLU:OE1	2.40	0.40
1:A:103:ASP:OD1	1:A:103:ASP:C	2.60	0.40
1:C:190:HIS:HB3	1:C:196:ALA:HB2	2.03	0.40
1:O:232:VAL:HA	1:O:233:PRO:HD3	1.82	0.40
1:A:193:LEU:HD13	1:B:42:HIS:CG	2.56	0.40
1:H:10:ARG:HH11	1:H:13:ARG:NH2	2.19	0.40
1:M:101:ASP:CG	1:M:103:ASP:OD1	2.59	0.40
1:M:9:GLY:O	1:M:13:ARG:HG3	2.22	0.40
1:P:37:VAL:HG21	1:P:62:SER:HA	2.03	0.40
1:P:82:LEU:HD13	1:P:84:TRP:CE2	2.54	0.40
1:R:282:ASP:CG	1:Q:197:ARG:HH12	2.23	0.40
1:Q:61:ASP:CG	1:Q:61:ASP:O	2.59	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:62:SER:OG	1:L:253:GLU:OE2[2_555]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/365 (92%)	308 (92%)	23 (7%)	4 (1%)	15	21
1	B	335/365 (92%)	313 (93%)	17 (5%)	5 (2%)	12	16
1	C	335/365 (92%)	315 (94%)	19 (6%)	1 (0%)	44	60
1	D	334/365 (92%)	318 (95%)	13 (4%)	3 (1%)	20	29
1	H	334/365 (92%)	314 (94%)	17 (5%)	3 (1%)	20	29
1	I	335/365 (92%)	316 (94%)	16 (5%)	3 (1%)	20	29
1	L	334/365 (92%)	315 (94%)	15 (4%)	4 (1%)	15	21
1	M	335/365 (92%)	312 (93%)	22 (7%)	1 (0%)	44	60
1	O	335/365 (92%)	317 (95%)	16 (5%)	2 (1%)	28	41
1	P	335/365 (92%)	312 (93%)	21 (6%)	2 (1%)	28	41
1	Q	335/365 (92%)	309 (92%)	25 (8%)	1 (0%)	44	60
1	R	335/365 (92%)	312 (93%)	19 (6%)	4 (1%)	15	21
All	All	4017/4380 (92%)	3761 (94%)	223 (6%)	33 (1%)	22	33

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	1	LEU
1	R	60(A)	GLY
1	P	209	GLY
1	A	209	GLY
1	A	211	ALA
1	B	207	SER
1	B	211	ALA
1	B	212	LYS
1	R	237	VAL
1	P	237	VAL
1	Q	237	VAL
1	A	237	VAL

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Mol	Chain	Res	Type
1	B	237	VAL
1	C	237	VAL
1	D	237	VAL
1	H	208	THR
1	H	237	VAL
1	I	237	VAL
1	L	237	VAL
1	M	237	VAL
1	O	237	VAL
1	I	62	SER
1	L	86	ASP
1	L	302	ASP
1	D	198	ALA
1	H	302	ASP
1	A	166	GLY
1	B	166	GLY
1	D	166	GLY
1	L	166	GLY
1	R	166	GLY
1	O	166	GLY
1	I	166	GLY

### 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	279/303 (92%)	262 (94%)	17 (6%)	22	34
1	B	279/303 (92%)	269 (96%)	10 (4%)	40	60
1	C	279/303 (92%)	267 (96%)	12 (4%)	33	52
1	D	279/303 (92%)	269 (96%)	10 (4%)	40	60
1	H	279/303 (92%)	264 (95%)	15 (5%)	26	41
1	I	279/303 (92%)	267 (96%)	12 (4%)	33	52
1	L	279/303 (92%)	269 (96%)	10 (4%)	40	60
1	M	279/303 (92%)	266 (95%)	13 (5%)	30	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	279/303 (92%)	262 (94%)	17 (6%)	22	34
1	P	279/303 (92%)	256 (92%)	23 (8%)	13	20
1	Q	279/303 (92%)	265 (95%)	14 (5%)	28	45
1	R	279/303 (92%)	262 (94%)	17 (6%)	22	34
All	All	3348/3636 (92%)	3178 (95%)	170 (5%)	28	44

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	0	LYS
1	O	53	PHE
1	O	61	ASP
1	O	75	SER
1	O	83	PRO
1	O	84	TRP
1	O	94	GLU
1	O	133	ASN
1	O	164	LYS
1	O	172	MET
1	O	191	ARG
1	O	208	THR
1	O	220	ASN
1	O	248	LYS
1	O	276	GLU
1	O	281	ILE
1	O	285	CYS
1	R	0	LYS
1	R	33	THR
1	R	58	LYS
1	R	62	SER
1	R	84	TRP
1	R	133	ASN
1	R	154	LEU
1	R	171	THR
1	R	172	MET
1	R	183	ARG
1	R	193	LEU
1	R	222	LYS
1	R	228	ILE
1	R	248	LYS
1	R	253	GLU

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Mol	Chain	Res	Type
1	R	261	GLU
1	R	285	CYS
1	P	0	LYS
1	P	58	LYS
1	P	84	TRP
1	P	94	GLU
1	P	133	ASN
1	P	135	GLU
1	P	138	THR
1	P	164	LYS
1	P	172	MET
1	P	184	LEU
1	P	190	HIS
1	P	191	ARG
1	P	193	LEU
1	P	208	THR
1	P	221	LEU
1	P	222	LYS
1	P	261	GLU
1	P	266	GLU
1	P	272	SER
1	P	276	GLU
1	P	281	ILE
1	P	285	CYS
1	P	333	GLN
1	Q	61	ASP
1	Q	84	TRP
1	Q	94	GLU
1	Q	133	ASN
1	Q	164	LYS
1	Q	169	LYS
1	Q	172	MET
1	Q	191	ARG
1	Q	242	LEU
1	Q	248	LYS
1	Q	253	GLU
1	Q	261	GLU
1	Q	285	CYS
1	Q	333	GLN
1	A	2	LYS
1	A	38	LYS
1	A	84	TRP

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Mol	Chain	Res	Type
1	A	94	GLU
1	A	133	ASN
1	A	163	GLN
1	A	164	LYS
1	A	172	MET
1	A	184	LEU
1	A	191	ARG
1	A	207	SER
1	A	208	THR
1	A	240	VAL
1	A	266	GLU
1	A	276	GLU
1	A	285	CYS
1	A	333	GLN
1	B	0	LYS
1	B	1	LEU
1	B	2	LYS
1	B	84	TRP
1	B	133	ASN
1	B	164	LYS
1	B	172	MET
1	B	188	SER
1	B	248	LYS
1	B	285	CYS
1	C	0	LYS
1	C	21	LYS
1	C	56	ASP
1	C	58	LYS
1	C	83	PRO
1	C	84	TRP
1	C	94	GLU
1	C	133	ASN
1	C	164	LYS
1	C	172	MET
1	C	253	GLU
1	C	285	CYS
1	D	58	LYS
1	D	75	SER
1	D	83	PRO
1	D	84	TRP
1	D	94	GLU
1	D	103	ASP

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Mol	Chain	Res	Type
1	D	133	ASN
1	D	164	LYS
1	D	172	MET
1	D	285	CYS
1	H	25	LEU
1	H	58	LYS
1	H	76	ASP
1	H	84	TRP
1	H	94	GLU
1	H	133	ASN
1	H	135	GLU
1	H	164	LYS
1	H	172	MET
1	H	206	THR
1	H	207	SER
1	H	212	LYS
1	H	221	LEU
1	H	247	SER
1	H	285	CYS
1	I	38	LYS
1	I	58	LYS
1	I	61	ASP
1	I	83	PRO
1	I	84	TRP
1	I	94	GLU
1	I	103	ASP
1	I	133	ASN
1	I	164	LYS
1	I	172	MET
1	I	208	THR
1	I	285	CYS
1	L	58	LYS
1	L	84	TRP
1	L	94	GLU
1	L	133	ASN
1	L	164	LYS
1	L	169	LYS
1	L	172	MET
1	L	188	SER
1	L	191	ARG
1	L	285	CYS
1	M	0	LYS

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Mol	Chain	Res	Type
1	M	21	LYS
1	M	58	LYS
1	M	61	ASP
1	M	84	TRP
1	M	94	GLU
1	M	133	ASN
1	M	163	GLN
1	M	164	LYS
1	M	172	MET
1	M	188	SER
1	M	228	ILE
1	M	285	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	42	HIS
1	O	81	ASN
1	O	133	ASN
1	O	152	ASN
1	O	163	GLN
1	O	202	ASN
1	O	256	ASN
1	O	330	ASN
1	R	81	ASN
1	R	133	ASN
1	R	139	HIS
1	R	152	ASN
1	R	202	ASN
1	R	245	GLN
1	R	256	ASN
1	R	330	ASN
1	P	42	HIS
1	P	133	ASN
1	P	139	HIS
1	P	152	ASN
1	P	202	ASN
1	P	256	ASN
1	P	330	ASN
1	Q	81	ASN
1	Q	133	ASN
1	Q	139	HIS

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Mol	Chain	Res	Type
1	Q	202	ASN
1	Q	256	ASN
1	Q	330	ASN
1	A	42	HIS
1	A	81	ASN
1	A	133	ASN
1	A	152	ASN
1	A	202	ASN
1	A	256	ASN
1	A	330	ASN
1	B	81	ASN
1	B	133	ASN
1	B	139	HIS
1	B	152	ASN
1	B	202	ASN
1	B	256	ASN
1	B	330	ASN
1	C	42	HIS
1	C	81	ASN
1	C	110	GLN
1	C	133	ASN
1	C	152	ASN
1	C	163	GLN
1	C	202	ASN
1	C	245	GLN
1	C	256	ASN
1	C	330	ASN
1	D	81	ASN
1	D	133	ASN
1	D	152	ASN
1	D	202	ASN
1	D	245	GLN
1	D	256	ASN
1	D	330	ASN
1	H	81	ASN
1	H	133	ASN
1	H	152	ASN
1	H	202	ASN
1	H	256	ASN
1	H	330	ASN
1	I	81	ASN
1	I	110	GLN

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Mol	Chain	Res	Type
1	I	133	ASN
1	I	152	ASN
1	I	163	GLN
1	I	202	ASN
1	I	256	ASN
1	I	330	ASN
1	L	81	ASN
1	L	133	ASN
1	L	152	ASN
1	L	202	ASN
1	L	256	ASN
1	L	330	ASN
1	M	81	ASN
1	M	110	GLN
1	M	133	ASN
1	M	152	ASN
1	M	202	ASN
1	M	256	ASN
1	M	330	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

46 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	363	-	4,4,4	0.31	0	6,6,6	0.09	0
2	SO4	A	364	-	4,4,4	0.40	0	6,6,6	0.09	0
2	SO4	A	375	-	4,4,4	0.32	0	6,6,6	0.09	0
3	NDP	A	376	-	43,52,52	4.89	26 (60%)	49,80,80	5.81	32 (65%)
2	SO4	B	363	-	4,4,4	0.28	0	6,6,6	0.08	0
2	SO4	B	364	-	4,4,4	0.38	0	6,6,6	0.09	0
2	SO4	B	377	-	4,4,4	0.27	0	6,6,6	0.08	0
3	NDP	B	378	-	43,52,52	4.15	24 (55%)	49,80,80	6.25	30 (61%)
2	SO4	C	363	-	4,4,4	0.31	0	6,6,6	0.09	0
2	SO4	C	364	-	4,4,4	0.40	0	6,6,6	0.09	0
3	NDP	C	365	-	43,52,52	4.13	23 (53%)	49,80,80	6.08	31 (63%)
2	SO4	D	363	-	4,4,4	0.32	0	6,6,6	0.09	0
2	SO4	D	364	-	4,4,4	0.41	0	6,6,6	0.09	0
3	NDP	D	365	-	43,52,52	4.23	24 (55%)	49,80,80	6.21	29 (59%)
2	SO4	H	363	-	4,4,4	0.31	0	6,6,6	0.09	0
2	SO4	H	364	-	4,4,4	0.41	0	6,6,6	0.09	0
2	SO4	H	378	-	4,4,4	0.31	0	6,6,6	0.10	0
3	NDP	H	379	-	43,52,52	4.17	23 (53%)	49,80,80	6.14	29 (59%)
2	SO4	I	365	-	4,4,4	0.30	0	6,6,6	0.08	0
2	SO4	I	366	-	4,4,4	0.39	0	6,6,6	0.09	0
2	SO4	I	379	-	4,4,4	0.40	0	6,6,6	0.09	0
3	NDP	I	380	-	43,52,52	4.11	24 (55%)	49,80,80	6.26	28 (57%)
2	SO4	L	367	-	4,4,4	0.31	0	6,6,6	0.09	0
2	SO4	L	368	-	4,4,4	0.39	0	6,6,6	0.10	0
3	NDP	L	369	-	43,52,52	4.31	22 (51%)	49,80,80	5.79	32 (65%)
2	SO4	M	369	-	4,4,4	0.31	0	6,6,6	0.09	0
2	SO4	M	370	-	4,4,4	0.37	0	6,6,6	0.08	0
2	SO4	M	380	-	4,4,4	0.31	0	6,6,6	0.09	0
3	NDP	M	381	-	43,52,52	4.11	23 (53%)	49,80,80	6.15	29 (59%)
2	SO4	O	363	-	4,4,4	0.30	0	6,6,6	0.09	0
2	SO4	O	364	-	4,4,4	0.39	0	6,6,6	0.09	0
2	SO4	O	371	-	4,4,4	0.39	0	6,6,6	0.09	0
3	NDP	O	372	-	43,52,52	4.55	23 (53%)	49,80,80	5.84	27 (55%)
2	SO4	P	363	-	4,4,4	0.31	0	6,6,6	0.09	0
2	SO4	P	364	-	4,4,4	0.38	0	6,6,6	0.09	0
2	SO4	P	372	-	4,4,4	0.38	0	6,6,6	0.09	0
3	NDP	P	373	-	43,52,52	4.23	26 (60%)	49,80,80	5.72	30 (61%)
2	SO4	Q	363	-	4,4,4	0.29	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	Q	364	-	4,4,4	0.40	0	6,6,6	0.09	0
2	SO4	Q	373	-	4,4,4	0.29	0	6,6,6	0.08	0
2	SO4	Q	374	-	4,4,4	0.40	0	6,6,6	0.09	0
3	NDP	Q	375	-	43,52,52	4.09	24 (55%)	49,80,80	6.10	32 (65%)
2	SO4	R	363	-	4,4,4	0.32	0	6,6,6	0.09	0
2	SO4	R	364	-	4,4,4	0.39	0	6,6,6	0.09	0
2	SO4	R	376	-	4,4,4	0.39	0	6,6,6	0.09	0
3	NDP	R	377	-	43,52,52	4.30	25 (58%)	49,80,80	6.07	29 (59%)

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	SO4	A	363	-	-	0/0/0/0	0/0/0/0
2	SO4	A	364	-	-	0/0/0/0	0/0/0/0
2	SO4	A	375	-	-	0/0/0/0	0/0/0/0
3	NDP	A	376	-	7/7/14/17	1/30/77/77	0/4/5/5
2	SO4	B	363	-	-	0/0/0/0	0/0/0/0
2	SO4	B	364	-	-	0/0/0/0	0/0/0/0
2	SO4	B	377	-	-	0/0/0/0	0/0/0/0
3	NDP	B	378	-	7/7/14/17	1/30/77/77	0/4/5/5
2	SO4	C	363	-	-	0/0/0/0	0/0/0/0
2	SO4	C	364	-	-	0/0/0/0	0/0/0/0
3	NDP	C	365	-	7/7/14/17	1/30/77/77	0/4/5/5
2	SO4	D	363	-	-	0/0/0/0	0/0/0/0
2	SO4	D	364	-	-	0/0/0/0	0/0/0/0
3	NDP	D	365	-	7/7/14/17	1/30/77/77	0/4/5/5
2	SO4	H	363	-	-	0/0/0/0	0/0/0/0
2	SO4	H	364	-	-	0/0/0/0	0/0/0/0
2	SO4	H	378	-	-	0/0/0/0	0/0/0/0
3	NDP	H	379	-	7/7/14/17	1/30/77/77	0/4/5/5
2	SO4	I	365	-	-	0/0/0/0	0/0/0/0
2	SO4	I	366	-	-	0/0/0/0	0/0/0/0
2	SO4	I	379	-	-	0/0/0/0	0/0/0/0
3	NDP	I	380	-	7/7/14/17	1/30/77/77	0/4/5/5
2	SO4	L	367	-	-	0/0/0/0	0/0/0/0
2	SO4	L	368	-	-	0/0/0/0	0/0/0/0
3	NDP	L	369	-	7/7/14/17	1/30/77/77	0/4/5/5
2	SO4	M	369	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	M	370	-	-	0/0/0/0	0/0/0/0
2	SO4	M	380	-	-	0/0/0/0	0/0/0/0
3	NDP	M	381	-	7/7/14/17	1/30/77/77	0/4/5/5
2	SO4	O	363	-	-	0/0/0/0	0/0/0/0
2	SO4	O	364	-	-	0/0/0/0	0/0/0/0
2	SO4	O	371	-	-	0/0/0/0	0/0/0/0
3	NDP	O	372	-	7/7/14/17	1/30/77/77	0/4/5/5
2	SO4	P	363	-	-	0/0/0/0	0/0/0/0
2	SO4	P	364	-	-	0/0/0/0	0/0/0/0
2	SO4	P	372	-	-	0/0/0/0	0/0/0/0
3	NDP	P	373	-	7/7/14/17	1/30/77/77	0/4/5/5
2	SO4	Q	363	-	-	0/0/0/0	0/0/0/0
2	SO4	Q	364	-	-	0/0/0/0	0/0/0/0
2	SO4	Q	373	-	-	0/0/0/0	0/0/0/0
2	SO4	Q	374	-	-	0/0/0/0	0/0/0/0
3	NDP	Q	375	-	7/7/14/17	1/30/77/77	0/4/5/5
2	SO4	R	363	-	-	0/0/0/0	0/0/0/0
2	SO4	R	364	-	-	0/0/0/0	0/0/0/0
2	SO4	R	376	-	-	0/0/0/0	0/0/0/0
3	NDP	R	377	-	7/7/14/17	1/30/77/77	0/4/5/5

All (287) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	377	NDP	O2D-C2D	-14.33	1.10	1.43
3	H	379	NDP	O2D-C2D	-13.78	1.11	1.43
3	D	365	NDP	O2D-C2D	-13.58	1.11	1.43
3	C	365	NDP	O2D-C2D	-13.57	1.11	1.43
3	B	378	NDP	O2D-C2D	-13.47	1.12	1.43
3	P	373	NDP	O2D-C2D	-13.42	1.12	1.43
3	I	380	NDP	O2D-C2D	-13.12	1.12	1.43
3	M	381	NDP	O2D-C2D	-13.01	1.13	1.43
3	L	369	NDP	O2D-C2D	-12.98	1.13	1.43
3	A	376	NDP	O2D-C2D	-12.87	1.13	1.43
3	Q	375	NDP	O2D-C2D	-12.60	1.13	1.43
3	O	372	NDP	O2D-C2D	-12.53	1.14	1.43
3	M	381	NDP	O4B-C1B	-6.77	1.31	1.41
3	R	377	NDP	O4B-C1B	-6.58	1.32	1.41
3	A	376	NDP	C8A-N7A	-5.94	1.23	1.34
3	O	372	NDP	C8A-N7A	-5.90	1.23	1.34
3	B	378	NDP	C8A-N7A	-5.88	1.23	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	376	NDP	C3D-C4D	-5.86	1.37	1.53
3	I	380	NDP	C8A-N7A	-5.86	1.23	1.34
3	C	365	NDP	C8A-N7A	-5.80	1.23	1.34
3	H	379	NDP	O4B-C1B	-5.76	1.33	1.41
3	Q	375	NDP	C8A-N7A	-5.71	1.24	1.34
3	M	381	NDP	C8A-N7A	-5.59	1.24	1.34
3	D	365	NDP	C8A-N7A	-5.55	1.24	1.34
3	I	380	NDP	C3D-C4D	-5.41	1.38	1.53
3	R	377	NDP	C8A-N7A	-5.37	1.24	1.34
3	D	365	NDP	O4B-C1B	-5.32	1.33	1.41
3	L	369	NDP	C3D-C4D	-5.28	1.39	1.53
3	I	380	NDP	O4B-C1B	-5.28	1.34	1.41
3	P	373	NDP	C8A-N7A	-5.24	1.24	1.34
3	H	379	NDP	C8A-N7A	-5.22	1.24	1.34
3	C	365	NDP	C3D-C4D	-5.17	1.39	1.53
3	I	380	NDP	C5D-C4D	-5.02	1.35	1.51
3	C	365	NDP	C5D-C4D	-5.01	1.35	1.51
3	M	381	NDP	C5D-C4D	-4.95	1.36	1.51
3	L	369	NDP	C8A-N7A	-4.95	1.25	1.34
3	P	373	NDP	C5D-C4D	-4.90	1.36	1.51
3	L	369	NDP	C5D-C4D	-4.80	1.36	1.51
3	O	372	NDP	C3D-C4D	-4.77	1.40	1.53
3	Q	375	NDP	C5D-C4D	-4.77	1.36	1.51
3	D	365	NDP	C3D-C4D	-4.75	1.40	1.53
3	H	379	NDP	C5D-C4D	-4.73	1.36	1.51
3	B	378	NDP	C5D-C4D	-4.66	1.36	1.51
3	H	379	NDP	C3D-C4D	-4.43	1.41	1.53
3	M	381	NDP	C3D-C4D	-4.39	1.41	1.53
3	O	372	NDP	O4B-C1B	-4.36	1.35	1.41
3	B	378	NDP	O4B-C1B	-4.35	1.35	1.41
3	R	377	NDP	C5D-C4D	-4.31	1.38	1.51
3	D	365	NDP	C5D-C4D	-4.19	1.38	1.51
3	A	376	NDP	C5D-C4D	-4.11	1.38	1.51
3	Q	375	NDP	C3D-C4D	-4.00	1.42	1.53
3	O	372	NDP	C5D-C4D	-3.97	1.39	1.51
3	R	377	NDP	C3D-C4D	-3.79	1.43	1.53
3	P	373	NDP	C3D-C4D	-3.72	1.43	1.53
3	L	369	NDP	O4B-C1B	-3.66	1.36	1.41
3	P	373	NDP	O4B-C1B	-3.66	1.36	1.41
3	A	376	NDP	O4B-C1B	-3.63	1.36	1.41
3	B	378	NDP	C3D-C4D	-3.61	1.43	1.53
3	C	365	NDP	C5B-C4B	-3.06	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	376	NDP	O4D-C4D	-3.06	1.38	1.45
3	P	373	NDP	C6N-N1N	-3.02	1.29	1.37
3	I	380	NDP	O4D-C4D	-2.97	1.38	1.45
3	O	372	NDP	C5B-C4B	-2.91	1.42	1.51
3	B	378	NDP	C5B-C4B	-2.90	1.42	1.51
3	H	379	NDP	C5B-C4B	-2.72	1.43	1.51
3	M	381	NDP	C5B-C4B	-2.71	1.43	1.51
3	L	369	NDP	C5B-C4B	-2.68	1.43	1.51
3	A	376	NDP	C5B-C4B	-2.68	1.43	1.51
3	R	377	NDP	C5B-C4B	-2.56	1.43	1.51
3	I	380	NDP	C5B-C4B	-2.53	1.43	1.51
3	C	365	NDP	O4B-C1B	-2.51	1.37	1.41
3	Q	375	NDP	O4B-C1B	-2.46	1.37	1.41
3	Q	375	NDP	C5B-C4B	-2.34	1.44	1.51
3	P	373	NDP	C5B-C4B	-2.31	1.44	1.51
3	P	373	NDP	C5A-N7A	2.02	1.46	1.39
3	R	377	NDP	C5A-N7A	2.05	1.46	1.39
3	A	376	NDP	C5A-N7A	2.06	1.46	1.39
3	C	365	NDP	O4D-C1D	2.13	1.47	1.42
3	D	365	NDP	C5A-C4A	2.14	1.45	1.40
3	D	365	NDP	C5A-N7A	2.15	1.46	1.39
3	Q	375	NDP	P2B-O2B	2.18	1.63	1.59
3	H	379	NDP	C4N-C5N	2.18	1.53	1.49
3	M	381	NDP	C5A-C4A	2.21	1.45	1.40
3	O	372	NDP	O5D-C5D	2.24	1.53	1.44
3	M	381	NDP	P2B-O3X	2.25	1.64	1.54
3	C	365	NDP	P2B-O3X	2.27	1.64	1.54
3	L	369	NDP	P2B-O3X	2.28	1.64	1.54
3	P	373	NDP	P2B-O3X	2.32	1.64	1.54
3	H	379	NDP	P2B-O3X	2.33	1.64	1.54
3	D	365	NDP	P2B-O2B	2.35	1.63	1.59
3	Q	375	NDP	C5A-C4A	2.36	1.45	1.40
3	O	372	NDP	C5A-C4A	2.40	1.45	1.40
3	M	381	NDP	C6A-N1A	2.40	1.48	1.37
3	I	380	NDP	P2B-O3X	2.41	1.64	1.54
3	I	380	NDP	C5A-C4A	2.42	1.45	1.40
3	C	365	NDP	P2B-O2B	2.42	1.63	1.59
3	P	373	NDP	C5A-C4A	2.42	1.46	1.40
3	C	365	NDP	O5D-C5D	2.42	1.54	1.44
3	Q	375	NDP	O4D-C1D	2.43	1.47	1.42
3	D	365	NDP	P2B-O3X	2.45	1.64	1.54
3	M	381	NDP	C4A-N3A	2.48	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	377	NDP	P2B-O3X	2.48	1.65	1.54
3	R	377	NDP	C5A-C4A	2.49	1.46	1.40
3	A	376	NDP	P2B-O3X	2.51	1.65	1.54
3	C	365	NDP	PN-O5D	2.54	1.70	1.59
3	B	378	NDP	C5A-C4A	2.55	1.46	1.40
3	O	372	NDP	P2B-O3X	2.57	1.65	1.54
3	M	381	NDP	C4N-C5N	2.57	1.54	1.49
3	I	380	NDP	C6A-N1A	2.60	1.48	1.37
3	B	378	NDP	P2B-O3X	2.64	1.65	1.54
3	H	379	NDP	C6A-N1A	2.65	1.49	1.37
3	A	376	NDP	C6A-N1A	2.65	1.49	1.37
3	C	365	NDP	C6A-N1A	2.65	1.49	1.37
3	B	378	NDP	P2B-O2B	2.65	1.64	1.59
3	L	369	NDP	C6A-N1A	2.65	1.49	1.37
3	Q	375	NDP	P2B-O3X	2.66	1.65	1.54
3	Q	375	NDP	C6A-N1A	2.67	1.49	1.37
3	B	378	NDP	O4D-C1D	2.68	1.48	1.42
3	P	373	NDP	C6A-N1A	2.71	1.49	1.37
3	B	378	NDP	C6A-N1A	2.74	1.49	1.37
3	R	377	NDP	P2B-O2B	2.81	1.64	1.59
3	I	380	NDP	C4N-C5N	2.86	1.55	1.49
3	D	365	NDP	C4N-C5N	2.87	1.55	1.49
3	O	372	NDP	O3D-C3D	2.88	1.49	1.43
3	O	372	NDP	PN-O5D	2.95	1.71	1.59
3	L	369	NDP	O5D-C5D	2.95	1.56	1.44
3	Q	375	NDP	C4N-C5N	2.99	1.55	1.49
3	Q	375	NDP	C3B-C2B	2.99	1.59	1.53
3	P	373	NDP	C4N-C5N	3.00	1.55	1.49
3	C	365	NDP	C4N-C5N	3.00	1.55	1.49
3	R	377	NDP	O5D-C5D	3.02	1.56	1.44
3	M	381	NDP	O5D-C5D	3.03	1.56	1.44
3	I	380	NDP	O5D-C5D	3.03	1.56	1.44
3	L	369	NDP	C5A-C4A	3.05	1.47	1.40
3	B	378	NDP	O5D-C5D	3.06	1.57	1.44
3	I	380	NDP	O4D-C1D	3.06	1.49	1.42
3	D	365	NDP	O5D-C5D	3.07	1.57	1.44
3	A	376	NDP	C4N-C5N	3.08	1.55	1.49
3	R	377	NDP	C6A-N1A	3.10	1.51	1.37
3	P	373	NDP	O5D-C5D	3.10	1.57	1.44
3	M	381	NDP	O4D-C1D	3.12	1.49	1.42
3	I	380	NDP	C4A-N3A	3.14	1.40	1.35
3	O	372	NDP	C6A-N1A	3.16	1.51	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	375	NDP	O5D-C5D	3.18	1.57	1.44
3	P	373	NDP	PN-O5D	3.20	1.72	1.59
3	A	376	NDP	C2N-C3N	3.22	1.44	1.34
3	D	365	NDP	C6A-N1A	3.23	1.51	1.37
3	A	376	NDP	O5D-C5D	3.24	1.57	1.44
3	I	380	NDP	C7N-N7N	3.26	1.42	1.33
3	B	378	NDP	C4N-C5N	3.26	1.56	1.49
3	D	365	NDP	C7N-N7N	3.27	1.42	1.33
3	I	380	NDP	PN-O5D	3.27	1.73	1.59
3	R	377	NDP	O4D-C1D	3.32	1.50	1.42
3	H	379	NDP	C5A-C4A	3.35	1.48	1.40
3	B	378	NDP	PN-O5D	3.36	1.73	1.59
3	O	372	NDP	C7N-N7N	3.36	1.42	1.33
3	O	372	NDP	O4D-C1D	3.36	1.50	1.42
3	D	365	NDP	O4D-C1D	3.37	1.50	1.42
3	B	378	NDP	C7N-N7N	3.38	1.42	1.33
3	P	373	NDP	C7N-N7N	3.40	1.42	1.33
3	R	377	NDP	PN-O5D	3.42	1.73	1.59
3	H	379	NDP	O5D-C5D	3.42	1.58	1.44
3	C	365	NDP	C7N-N7N	3.44	1.43	1.33
3	M	381	NDP	PN-O5D	3.45	1.73	1.59
3	L	369	NDP	C7N-N7N	3.47	1.43	1.33
3	H	379	NDP	C3B-C2B	3.47	1.60	1.53
3	M	381	NDP	C7N-N7N	3.48	1.43	1.33
3	O	372	NDP	C3B-C2B	3.50	1.60	1.53
3	D	365	NDP	PN-O5D	3.50	1.74	1.59
3	C	365	NDP	C3B-C2B	3.51	1.60	1.53
3	R	377	NDP	C7N-N7N	3.54	1.43	1.33
3	A	376	NDP	PN-O5D	3.55	1.74	1.59
3	H	379	NDP	C7N-N7N	3.57	1.43	1.33
3	R	377	NDP	C4N-C5N	3.57	1.56	1.49
3	A	376	NDP	P2B-O2B	3.57	1.65	1.59
3	Q	375	NDP	C7N-N7N	3.57	1.43	1.33
3	C	365	NDP	C4A-N3A	3.63	1.40	1.35
3	A	376	NDP	C3B-C2B	3.64	1.61	1.53
3	P	373	NDP	P2B-O2B	3.65	1.65	1.59
3	Q	375	NDP	PN-O5D	3.67	1.74	1.59
3	H	379	NDP	O4D-C1D	3.69	1.51	1.42
3	A	376	NDP	C4A-N3A	3.71	1.41	1.35
3	L	369	NDP	C3B-C2B	3.78	1.61	1.53
3	H	379	NDP	PN-O5D	3.85	1.75	1.59
3	A	376	NDP	C7N-N7N	3.85	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	369	NDP	PN-O5D	3.92	1.75	1.59
3	M	381	NDP	C3B-C2B	3.98	1.61	1.53
3	I	380	NDP	C3B-C2B	4.01	1.62	1.53
3	P	373	NDP	C3B-C2B	4.05	1.62	1.53
3	D	365	NDP	C4A-N3A	4.17	1.41	1.35
3	I	380	NDP	O3B-C3B	4.30	1.52	1.43
3	P	373	NDP	C4A-N3A	4.40	1.42	1.35
3	R	377	NDP	C4A-N3A	4.42	1.42	1.35
3	Q	375	NDP	C4A-N3A	4.43	1.42	1.35
3	B	378	NDP	C3B-C2B	4.48	1.63	1.53
3	D	365	NDP	C3B-C2B	4.51	1.63	1.53
3	D	365	NDP	PA-O5B	4.54	1.78	1.59
3	A	376	NDP	O3B-C3B	4.66	1.53	1.43
3	R	377	NDP	PA-O5B	4.67	1.79	1.59
3	P	373	NDP	O4D-C1D	4.70	1.53	1.42
3	L	369	NDP	O4D-C1D	4.81	1.53	1.42
3	I	380	NDP	PA-O5B	4.83	1.79	1.59
3	M	381	NDP	PA-O5B	4.86	1.79	1.59
3	B	378	NDP	C3B-C4B	4.86	1.65	1.53
3	A	376	NDP	C3B-C4B	4.88	1.65	1.53
3	R	377	NDP	C3B-C4B	4.89	1.65	1.53
3	Q	375	NDP	O3B-C3B	4.89	1.54	1.43
3	M	381	NDP	O3B-C3B	4.94	1.54	1.43
3	Q	375	NDP	PA-O5B	4.99	1.80	1.59
3	P	373	NDP	PA-O5B	5.03	1.80	1.59
3	O	372	NDP	O3B-C3B	5.03	1.54	1.43
3	I	380	NDP	C3B-C4B	5.03	1.66	1.53
3	M	381	NDP	C3B-C4B	5.09	1.66	1.53
3	H	379	NDP	PA-O5B	5.09	1.80	1.59
3	A	376	NDP	PA-O5B	5.11	1.80	1.59
3	D	365	NDP	C2D-C1D	5.13	1.69	1.53
3	R	377	NDP	C2D-C1D	5.17	1.69	1.53
3	L	369	NDP	C3B-C4B	5.17	1.66	1.53
3	O	372	NDP	C4A-N3A	5.18	1.43	1.35
3	B	378	NDP	C4A-N3A	5.19	1.43	1.35
3	C	365	NDP	O3B-C3B	5.25	1.55	1.43
3	B	378	NDP	PA-O5B	5.26	1.81	1.59
3	H	379	NDP	O3B-C3B	5.26	1.55	1.43
3	L	369	NDP	O3B-C3B	5.28	1.55	1.43
3	C	365	NDP	PA-O5B	5.34	1.81	1.59
3	O	372	NDP	C3B-C4B	5.46	1.67	1.53
3	H	379	NDP	C3B-C4B	5.46	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	375	NDP	C3B-C4B	5.52	1.67	1.53
3	D	365	NDP	C3B-C4B	5.53	1.67	1.53
3	P	373	NDP	C3B-C4B	5.63	1.67	1.53
3	B	378	NDP	O3B-C3B	5.70	1.56	1.43
3	R	377	NDP	C3B-C2B	5.71	1.65	1.53
3	P	373	NDP	O3B-C3B	5.73	1.56	1.43
3	L	369	NDP	PA-O5B	5.75	1.83	1.59
3	H	379	NDP	C2D-C1D	5.94	1.72	1.53
3	C	365	NDP	C3B-C4B	6.03	1.68	1.53
3	H	379	NDP	C4A-N3A	6.07	1.44	1.35
3	L	369	NDP	C4A-N3A	6.13	1.44	1.35
3	D	365	NDP	O3B-C3B	6.16	1.57	1.43
3	B	378	NDP	C2D-C3D	6.42	1.70	1.53
3	O	372	NDP	PA-O5B	6.50	1.86	1.59
3	R	377	NDP	O3B-C3B	6.69	1.58	1.43
3	P	373	NDP	C2D-C3D	6.77	1.71	1.53
3	R	377	NDP	C2D-C3D	6.94	1.71	1.53
3	H	379	NDP	C2D-C3D	7.02	1.72	1.53
3	A	376	NDP	C2D-C3D	7.02	1.72	1.53
3	I	380	NDP	C2A-N3A	7.07	1.43	1.32
3	B	378	NDP	C2A-N3A	7.21	1.44	1.32
3	C	365	NDP	C2A-N3A	7.23	1.44	1.32
3	M	381	NDP	C2D-C1D	7.24	1.76	1.53
3	L	369	NDP	C2A-N3A	7.25	1.44	1.32
3	P	373	NDP	C2A-N3A	7.28	1.44	1.32
3	A	376	NDP	C2A-N3A	7.32	1.44	1.32
3	Q	375	NDP	C2A-N3A	7.36	1.44	1.32
3	M	381	NDP	C2A-N3A	7.41	1.44	1.32
3	C	365	NDP	C2D-C3D	7.42	1.73	1.53
3	L	369	NDP	C2D-C3D	7.42	1.73	1.53
3	H	379	NDP	C2A-N3A	7.46	1.44	1.32
3	M	381	NDP	C2D-C3D	7.49	1.73	1.53
3	O	372	NDP	C2D-C3D	7.49	1.73	1.53
3	Q	375	NDP	C2D-C3D	7.58	1.73	1.53
3	I	380	NDP	C2D-C1D	7.74	1.77	1.53
3	I	380	NDP	C2D-C3D	7.81	1.74	1.53
3	B	378	NDP	C2D-C1D	7.99	1.78	1.53
3	D	365	NDP	C2A-N3A	7.99	1.45	1.32
3	R	377	NDP	C2A-N3A	8.08	1.45	1.32
3	A	376	NDP	O4B-C4B	8.36	1.63	1.45
3	C	365	NDP	C2D-C1D	8.38	1.79	1.53
3	C	365	NDP	O4B-C4B	8.59	1.64	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	369	NDP	O4B-C4B	8.60	1.64	1.45
3	P	373	NDP	O4B-C4B	8.63	1.64	1.45
3	I	380	NDP	O4B-C4B	8.64	1.64	1.45
3	P	373	NDP	C2D-C1D	8.70	1.80	1.53
3	D	365	NDP	C2D-C3D	8.72	1.76	1.53
3	Q	375	NDP	O4B-C4B	8.76	1.64	1.45
3	B	378	NDP	O4B-C4B	8.81	1.65	1.45
3	H	379	NDP	O4B-C4B	8.82	1.65	1.45
3	O	372	NDP	O4B-C4B	8.83	1.65	1.45
3	M	381	NDP	O4B-C4B	8.99	1.65	1.45
3	O	372	NDP	C2A-N3A	9.03	1.47	1.32
3	D	365	NDP	O4B-C4B	9.16	1.65	1.45
3	Q	375	NDP	C2D-C1D	9.18	1.82	1.53
3	R	377	NDP	O4B-C4B	9.20	1.65	1.45
3	L	369	NDP	C2D-C1D	10.31	1.85	1.53
3	A	376	NDP	O4D-C1D	10.41	1.67	1.42
3	O	372	NDP	C2D-C1D	13.73	1.96	1.53
3	A	376	NDP	C2D-C1D	16.12	2.04	1.53

All (358) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	376	NDP	O4D-C1D-C2D	-17.75	67.36	106.64
3	O	372	NDP	O4D-C1D-C2D	-13.93	75.80	106.64
3	A	376	NDP	C2D-C1D-N1N	-13.76	77.91	113.32
3	L	369	NDP	O4D-C1D-C2D	-12.54	78.89	106.64
3	A	376	NDP	C1D-N1N-C2N	-12.30	100.23	121.09
3	O	372	NDP	C1D-N1N-C2N	-11.99	100.75	121.09
3	O	372	NDP	C2D-C1D-N1N	-11.92	82.65	113.32
3	Q	375	NDP	C1D-N1N-C6N	-11.30	96.23	120.77
3	M	381	NDP	C1D-N1N-C6N	-11.19	96.46	120.77
3	I	380	NDP	C1D-N1N-C6N	-10.89	97.11	120.77
3	Q	375	NDP	O4D-C1D-C2D	-10.71	82.94	106.64
3	P	373	NDP	O4D-C1D-C2D	-10.68	83.01	106.64
3	C	365	NDP	O4D-C1D-C2D	-10.65	83.08	106.64
3	L	369	NDP	C2D-C1D-N1N	-10.40	86.55	113.32
3	B	378	NDP	C1D-N1N-C6N	-10.36	98.27	120.77
3	Q	375	NDP	C2D-C1D-N1N	-10.17	87.14	113.32
3	P	373	NDP	C2D-C1D-N1N	-10.05	87.46	113.32
3	I	380	NDP	O4D-C1D-C2D	-9.99	84.54	106.64
3	B	378	NDP	O4D-C1D-C2D	-9.85	84.83	106.64
3	H	379	NDP	C1D-N1N-C6N	-9.45	100.25	120.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	373	NDP	C1D-N1N-C2N	-9.12	105.62	121.09
3	B	378	NDP	C2D-C1D-N1N	-9.07	89.97	113.32
3	C	365	NDP	C2D-C1D-N1N	-8.96	90.27	113.32
3	D	365	NDP	C1D-N1N-C6N	-8.92	101.39	120.77
3	M	381	NDP	O4D-C1D-C2D	-8.68	87.43	106.64
3	I	380	NDP	C2D-C1D-N1N	-8.60	91.18	113.32
3	A	376	NDP	C1D-N1N-C6N	-8.44	102.44	120.77
3	D	365	NDP	O4D-C1D-C2D	-8.18	88.53	106.64
3	R	377	NDP	O4D-C1D-C2D	-8.14	88.62	106.64
3	H	379	NDP	O4D-C1D-C2D	-8.09	88.73	106.64
3	M	381	NDP	C2D-C1D-N1N	-8.01	92.69	113.32
3	A	376	NDP	C2D-C3D-C4D	-7.66	87.69	102.62
3	D	365	NDP	C2D-C3D-C4D	-7.64	87.74	102.62
3	O	372	NDP	C1D-N1N-C6N	-7.63	104.20	120.77
3	R	377	NDP	C2D-C3D-C4D	-7.57	87.87	102.62
3	C	365	NDP	C1D-N1N-C6N	-7.51	104.47	120.77
3	L	369	NDP	C1D-N1N-C2N	-7.49	108.38	121.09
3	R	377	NDP	C1D-N1N-C6N	-7.48	104.53	120.77
3	L	369	NDP	C1D-N1N-C6N	-7.29	104.93	120.77
3	P	373	NDP	C2D-C3D-C4D	-7.24	88.52	102.62
3	L	369	NDP	C2D-C3D-C4D	-7.17	88.66	102.62
3	C	365	NDP	C2D-C3D-C4D	-7.02	88.94	102.62
3	Q	375	NDP	C2D-C3D-C4D	-6.97	89.04	102.62
3	H	379	NDP	C2D-C1D-N1N	-6.96	95.41	113.32
3	B	378	NDP	C2D-C3D-C4D	-6.95	89.09	102.62
3	M	381	NDP	C2D-C3D-C4D	-6.87	89.24	102.62
3	R	377	NDP	C2D-C1D-N1N	-6.87	95.65	113.32
3	P	373	NDP	C4D-O4D-C1D	-6.84	94.21	109.47
3	O	372	NDP	C2D-C3D-C4D	-6.83	89.32	102.62
3	H	379	NDP	C2D-C3D-C4D	-6.76	89.46	102.62
3	D	365	NDP	C2D-C1D-N1N	-6.72	96.02	113.32
3	I	380	NDP	C2D-C3D-C4D	-6.40	90.15	102.62
3	C	365	NDP	C1D-N1N-C2N	-6.17	110.62	121.09
3	R	377	NDP	C4D-O4D-C1D	-5.88	96.35	109.47
3	D	365	NDP	C4D-O4D-C1D	-5.53	97.13	109.47
3	L	369	NDP	C4D-O4D-C1D	-5.31	97.63	109.47
3	P	373	NDP	C1D-N1N-C6N	-5.09	109.72	120.77
3	R	377	NDP	O3X-P2B-O2B	-4.86	83.88	106.00
3	B	378	NDP	O3X-P2B-O2B	-4.70	84.62	106.00
3	C	365	NDP	O3X-P2B-O2B	-4.70	84.64	106.00
3	C	365	NDP	C4D-O4D-C1D	-4.62	99.16	109.47
3	D	365	NDP	O3X-P2B-O2B	-4.62	85.00	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	375	NDP	O3X-P2B-O2B	-4.57	85.21	106.00
3	I	380	NDP	O3X-P2B-O2B	-4.55	85.29	106.00
3	Q	375	NDP	C1D-N1N-C2N	-4.51	113.44	121.09
3	P	373	NDP	O3X-P2B-O2B	-4.39	86.05	106.00
3	M	381	NDP	O3X-P2B-O2B	-4.35	86.23	106.00
3	R	377	NDP	C2B-C3B-C4B	-4.27	92.23	101.95
3	O	372	NDP	O3X-P2B-O2B	-4.24	86.70	106.00
3	I	380	NDP	C1D-N1N-C2N	-4.18	113.99	121.09
3	A	376	NDP	O3X-P2B-O2B	-4.10	87.34	106.00
3	H	379	NDP	O3X-P2B-O2B	-3.98	87.92	106.00
3	I	380	NDP	O2B-C2B-C1B	-3.94	95.36	110.06
3	H	379	NDP	C4D-O4D-C1D	-3.90	100.76	109.47
3	L	369	NDP	O3X-P2B-O2B	-3.88	88.38	106.00
3	H	379	NDP	C2B-C3B-C4B	-3.86	93.17	101.95
3	A	376	NDP	O2B-C2B-C1B	-3.85	95.70	110.06
3	M	381	NDP	C2B-C3B-C4B	-3.85	93.20	101.95
3	D	365	NDP	C2B-C3B-C4B	-3.85	93.20	101.95
3	B	378	NDP	C2B-C3B-C4B	-3.78	93.36	101.95
3	A	376	NDP	C4D-O4D-C1D	-3.77	101.05	109.47
3	O	372	NDP	C4D-O4D-C1D	-3.77	101.07	109.47
3	P	373	NDP	C2B-C3B-C4B	-3.74	93.44	101.95
3	O	372	NDP	O2B-C2B-C1B	-3.73	96.17	110.06
3	A	376	NDP	O4D-C4D-C3D	-3.71	97.80	105.17
3	P	373	NDP	O2B-C2B-C1B	-3.59	96.67	110.06
3	M	381	NDP	O4B-C4B-C3B	-3.59	98.03	105.17
3	H	379	NDP	C4B-O4B-C1B	-3.58	105.96	109.77
3	O	372	NDP	C4B-O4B-C1B	-3.58	105.96	109.77
3	O	372	NDP	C2B-C3B-C4B	-3.53	93.92	101.95
3	L	369	NDP	C2B-C3B-C4B	-3.51	93.96	101.95
3	B	378	NDP	C1D-N1N-C2N	-3.51	115.14	121.09
3	I	380	NDP	C2B-C3B-C4B	-3.50	94.00	101.95
3	M	381	NDP	O2B-C2B-C1B	-3.48	97.09	110.06
3	D	365	NDP	O4B-C4B-C3B	-3.46	98.28	105.17
3	R	377	NDP	O4B-C4B-C3B	-3.46	98.30	105.17
3	I	380	NDP	O4B-C4B-C3B	-3.44	98.33	105.17
3	C	365	NDP	O2B-C2B-C1B	-3.43	97.26	110.06
3	Q	375	NDP	C4B-O4B-C1B	-3.43	106.12	109.77
3	C	365	NDP	C2B-C3B-C4B	-3.42	94.17	101.95
3	A	376	NDP	C2B-C3B-C4B	-3.38	94.25	101.95
3	O	372	NDP	C5A-C6A-N1A	-3.36	109.54	119.70
3	Q	375	NDP	O2B-C2B-C1B	-3.30	97.76	110.06
3	O	372	NDP	O4B-C4B-C3B	-3.28	98.64	105.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	377	NDP	C1D-N1N-C2N	-3.27	115.55	121.09
3	H	379	NDP	O2B-C2B-C1B	-3.22	98.06	110.06
3	H	379	NDP	O4B-C4B-C3B	-3.19	98.82	105.17
3	D	365	NDP	O2B-C2B-C1B	-3.17	98.24	110.06
3	L	369	NDP	O2B-C2B-C1B	-3.17	98.24	110.06
3	C	365	NDP	C4B-O4B-C1B	-3.13	106.44	109.77
3	Q	375	NDP	C2B-C3B-C4B	-3.12	94.85	101.95
3	M	381	NDP	C4B-O4B-C1B	-3.10	106.47	109.77
3	R	377	NDP	O2B-C2B-C1B	-3.08	98.57	110.06
3	L	369	NDP	C4B-O4B-C1B	-3.06	106.51	109.77
3	B	378	NDP	C4B-O4B-C1B	-3.05	106.53	109.77
3	I	380	NDP	C4B-O4B-C1B	-3.04	106.54	109.77
3	B	378	NDP	O2B-C2B-C1B	-2.97	98.99	110.06
3	M	381	NDP	C4D-O4D-C1D	-2.93	102.93	109.47
3	B	378	NDP	C4D-O4D-C1D	-2.93	102.94	109.47
3	B	378	NDP	O4B-C4B-C3B	-2.85	99.49	105.17
3	L	369	NDP	O4B-C4B-C3B	-2.72	99.77	105.17
3	C	365	NDP	O4B-C4B-C3B	-2.68	99.83	105.17
3	Q	375	NDP	O4B-C4B-C3B	-2.65	99.89	105.17
3	A	376	NDP	O4B-C4B-C3B	-2.59	100.01	105.17
3	C	365	NDP	O5D-PN-O1N	-2.53	99.05	109.25
3	R	377	NDP	C4B-O4B-C1B	-2.45	107.16	109.77
3	A	376	NDP	C4B-O4B-C1B	-2.39	107.23	109.77
3	R	377	NDP	C5A-C6A-N1A	-2.38	112.49	119.70
3	P	373	NDP	O4B-C4B-C3B	-2.37	100.45	105.17
3	D	365	NDP	C5A-C6A-N1A	-2.30	112.75	119.70
3	Q	375	NDP	C4D-O4D-C1D	-2.28	104.38	109.47
3	M	381	NDP	C5A-C6A-N1A	-2.27	112.83	119.70
3	D	365	NDP	C4B-O4B-C1B	-2.27	107.36	109.77
3	H	379	NDP	C5A-C6A-N1A	-2.24	112.94	119.70
3	I	380	NDP	C5A-C6A-N1A	-2.22	112.98	119.70
3	P	373	NDP	O2A-PA-O1A	-2.19	100.93	112.28
3	Q	375	NDP	C5A-C6A-N1A	-2.15	113.20	119.70
3	B	378	NDP	C5A-C6A-N1A	-2.14	113.24	119.70
3	L	369	NDP	C5A-C6A-N1A	-2.13	113.26	119.70
3	I	380	NDP	C4D-O4D-C1D	-2.12	104.74	109.47
3	H	379	NDP	O2A-PA-O1A	-2.06	101.61	112.28
3	Q	375	NDP	O2A-PA-O1A	-2.06	101.62	112.28
3	L	369	NDP	O2A-PA-O1A	-2.06	101.64	112.28
3	C	365	NDP	C5A-C6A-N1A	-2.05	113.49	119.70
3	A	376	NDP	C5A-C6A-N1A	-2.03	113.55	119.70
3	P	373	NDP	C5A-C6A-N1A	-2.03	113.55	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	376	NDP	O2A-PA-O1A	-2.01	101.89	112.28
3	M	381	NDP	C3N-C2N-N1N	2.03	126.02	123.08
3	C	365	NDP	N6A-C6A-N1A	2.03	122.79	118.77
3	D	365	NDP	O4D-C4D-C5D	2.05	116.33	109.40
3	C	365	NDP	C3D-C2D-C1D	2.05	105.37	101.43
3	P	373	NDP	C3N-C2N-N1N	2.08	126.09	123.08
3	M	381	NDP	O5B-PA-O1A	2.10	117.72	109.25
3	A	376	NDP	N6A-C6A-N1A	2.10	122.94	118.77
3	R	377	NDP	O3B-C3B-C4B	2.14	117.33	111.09
3	A	376	NDP	C3N-C2N-N1N	2.14	126.18	123.08
3	I	380	NDP	C3D-C2D-C1D	2.14	105.54	101.43
3	B	378	NDP	O3B-C3B-C4B	2.16	117.39	111.09
3	L	369	NDP	O3B-C3B-C4B	2.18	117.45	111.09
3	M	381	NDP	C5A-C6A-N6A	2.19	124.93	120.47
3	H	379	NDP	N6A-C6A-N1A	2.25	123.22	118.77
3	I	380	NDP	C3N-C2N-N1N	2.25	126.35	123.08
3	M	381	NDP	O3B-C3B-C4B	2.27	117.72	111.09
3	I	380	NDP	N6A-C6A-N1A	2.27	123.28	118.77
3	Q	375	NDP	O4D-C4D-C5D	2.28	117.11	109.40
3	D	365	NDP	O5B-PA-O1A	2.29	118.49	109.25
3	C	365	NDP	O3B-C3B-C4B	2.30	117.81	111.09
3	Q	375	NDP	O3B-C3B-C4B	2.32	117.86	111.09
3	D	365	NDP	O3B-C3B-C4B	2.33	117.89	111.09
3	Q	375	NDP	N6A-C6A-N1A	2.33	123.39	118.77
3	L	369	NDP	N6A-C6A-N1A	2.34	123.41	118.77
3	L	369	NDP	O5B-PA-O1A	2.36	118.78	109.25
3	P	373	NDP	O3B-C3B-C4B	2.36	117.99	111.09
3	L	369	NDP	C3D-C2D-C1D	2.38	106.00	101.43
3	C	365	NDP	O5B-PA-O1A	2.39	118.88	109.25
3	P	373	NDP	O5B-PA-O1A	2.40	118.92	109.25
3	P	373	NDP	O2N-PN-O1N	2.40	124.71	112.28
3	M	381	NDP	O2N-PN-O1N	2.40	124.72	112.28
3	A	376	NDP	O2N-PN-O1N	2.41	124.75	112.28
3	A	376	NDP	O5B-C5B-C4B	2.41	117.55	109.00
3	H	379	NDP	O3B-C3B-C4B	2.42	118.16	111.09
3	C	365	NDP	O7N-C7N-N7N	2.48	128.94	122.92
3	P	373	NDP	C3D-C2D-C1D	2.50	106.22	101.43
3	R	377	NDP	O7N-C7N-N7N	2.50	129.00	122.92
3	H	379	NDP	O5B-PA-O1A	2.50	119.35	109.25
3	Q	375	NDP	C3N-C2N-N1N	2.51	126.72	123.08
3	A	376	NDP	O5B-PA-O1A	2.51	119.38	109.25
3	P	373	NDP	O5B-C5B-C4B	2.52	117.92	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	365	NDP	C3D-C2D-C1D	2.52	106.27	101.43
3	B	378	NDP	N6A-C6A-N1A	2.53	123.77	118.77
3	I	380	NDP	O2N-PN-O1N	2.53	125.39	112.28
3	H	379	NDP	O5B-C5B-C4B	2.53	117.99	109.00
3	L	369	NDP	O2N-PN-O1N	2.56	125.55	112.28
3	O	372	NDP	O2N-PN-O1N	2.57	125.56	112.28
3	B	378	NDP	O5B-C5B-C4B	2.57	118.12	109.00
3	C	365	NDP	O5B-C5B-C4B	2.57	118.13	109.00
3	H	379	NDP	O2N-PN-O1N	2.58	125.62	112.28
3	C	365	NDP	O2N-PN-O1N	2.59	125.66	112.28
3	B	378	NDP	O7N-C7N-N7N	2.59	129.20	122.92
3	D	365	NDP	O2N-PN-O1N	2.59	125.70	112.28
3	R	377	NDP	O5B-PA-O1A	2.60	119.72	109.25
3	D	365	NDP	O7N-C7N-N7N	2.60	129.23	122.92
3	Q	375	NDP	O2N-PN-O1N	2.61	125.81	112.28
3	D	365	NDP	N6A-C6A-N1A	2.63	123.98	118.77
3	O	372	NDP	N3A-C2A-N1A	2.65	131.17	128.86
3	Q	375	NDP	O5B-C5B-C4B	2.66	118.44	109.00
3	R	377	NDP	N6A-C6A-N1A	2.69	124.09	118.77
3	I	380	NDP	O5B-C5B-C4B	2.69	118.54	109.00
3	R	377	NDP	O5B-C5B-C4B	2.70	118.57	109.00
3	O	372	NDP	N6A-C6A-N1A	2.70	124.12	118.77
3	Q	375	NDP	C3D-C2D-C1D	2.72	106.64	101.43
3	A	376	NDP	O7N-C7N-N7N	2.73	129.55	122.92
3	P	373	NDP	O4D-C4D-C5D	2.73	118.63	109.40
3	Q	375	NDP	O5B-PA-O1A	2.74	120.30	109.25
3	L	369	NDP	O2B-P2B-O1X	2.74	120.00	109.26
3	Q	375	NDP	O7N-C7N-N7N	2.74	129.58	122.92
3	L	369	NDP	O5B-C5B-C4B	2.75	118.74	109.00
3	P	373	NDP	O7N-C7N-N7N	2.76	129.62	122.92
3	M	381	NDP	C3D-C2D-C1D	2.76	106.73	101.43
3	R	377	NDP	O2N-PN-O1N	2.76	126.57	112.28
3	M	381	NDP	O7N-C7N-N7N	2.81	129.74	122.92
3	D	365	NDP	O5B-C5B-C4B	2.84	119.07	109.00
3	B	378	NDP	C3N-C2N-N1N	2.85	127.21	123.08
3	B	378	NDP	O5B-PA-O1A	2.85	120.76	109.25
3	H	379	NDP	O2B-P2B-O1X	2.87	120.52	109.26
3	M	381	NDP	O5B-C5B-C4B	2.87	119.19	109.00
3	O	372	NDP	C5A-C6A-N6A	2.87	126.33	120.47
3	L	369	NDP	O4D-C4D-C5D	2.93	119.30	109.40
3	B	378	NDP	O2N-PN-O1N	2.94	127.51	112.28
3	I	380	NDP	O7N-C7N-N7N	2.96	130.10	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	376	NDP	C3D-C2D-C1D	2.97	107.13	101.43
3	H	379	NDP	O7N-C7N-N7N	3.12	130.50	122.92
3	M	381	NDP	O2B-P2B-O1X	3.13	121.53	109.26
3	D	365	NDP	O2B-P2B-O1X	3.20	121.79	109.26
3	L	369	NDP	O7N-C7N-N7N	3.21	130.71	122.92
3	I	380	NDP	O2B-P2B-O1X	3.21	121.85	109.26
3	L	369	NDP	C3N-C2N-N1N	3.24	127.78	123.08
3	O	372	NDP	O2B-P2B-O1X	3.25	121.98	109.26
3	R	377	NDP	C3D-C2D-C1D	3.28	107.73	101.43
3	B	378	NDP	C3D-C2D-C1D	3.29	107.74	101.43
3	A	376	NDP	O2B-P2B-O1X	3.33	122.30	109.26
3	P	373	NDP	O2B-P2B-O1X	3.42	122.66	109.26
3	C	365	NDP	O2B-P2B-O1X	3.44	122.74	109.26
3	H	379	NDP	C3D-C2D-C1D	3.46	108.07	101.43
3	R	377	NDP	O2B-P2B-O1X	3.51	123.01	109.26
3	Q	375	NDP	O2B-P2B-O1X	3.51	123.03	109.26
3	B	378	NDP	C5B-C4B-C3B	3.62	129.06	115.29
3	A	376	NDP	C5B-C4B-C3B	3.62	129.10	115.29
3	Q	375	NDP	C5B-C4B-C3B	3.63	129.11	115.29
3	L	369	NDP	C5B-C4B-C3B	3.70	129.40	115.29
3	I	380	NDP	C5B-C4B-C3B	3.74	129.55	115.29
3	C	365	NDP	C5B-C4B-C3B	3.75	129.56	115.29
3	R	377	NDP	C5B-C4B-C3B	3.78	129.67	115.29
3	B	378	NDP	O2B-P2B-O1X	3.79	124.13	109.26
3	H	379	NDP	C5B-C4B-C3B	3.81	129.79	115.29
3	P	373	NDP	C5B-C4B-C3B	3.82	129.82	115.29
3	A	376	NDP	O4D-C4D-C5D	3.85	122.41	109.40
3	M	381	NDP	C5B-C4B-C3B	3.95	130.34	115.29
3	D	365	NDP	C5B-C4B-C3B	3.96	130.37	115.29
3	O	372	NDP	C5B-C4B-C3B	3.98	130.45	115.29
3	C	365	NDP	C3N-C2N-N1N	4.20	129.17	123.08
3	O	372	NDP	C3N-C2N-N1N	4.33	129.36	123.08
3	A	376	NDP	O3D-C3D-C2D	4.47	126.15	111.83
3	B	378	NDP	O3D-C3D-C2D	4.49	126.22	111.83
3	C	365	NDP	O3D-C3D-C2D	4.64	126.69	111.83
3	H	379	NDP	O3D-C3D-C2D	4.66	126.76	111.83
3	P	373	NDP	O3D-C3D-C2D	4.68	126.81	111.83
3	O	372	NDP	O3D-C3D-C2D	4.69	126.85	111.83
3	R	377	NDP	O3D-C3D-C2D	4.69	126.86	111.83
3	L	369	NDP	O3D-C3D-C2D	4.73	126.98	111.83
3	Q	375	NDP	O3D-C3D-C2D	4.74	127.02	111.83
3	I	380	NDP	O3D-C3D-C2D	4.89	127.50	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	381	NDP	O3D-C3D-C2D	4.99	127.83	111.83
3	D	365	NDP	O3D-C3D-C2D	5.15	128.31	111.83
3	D	365	NDP	C5D-C4D-C3D	5.16	134.95	115.29
3	H	379	NDP	C5D-C4D-C3D	5.20	135.09	115.29
3	Q	375	NDP	C5D-C4D-C3D	5.25	135.29	115.29
3	L	369	NDP	C5D-C4D-C3D	5.26	135.34	115.29
3	M	381	NDP	C5D-C4D-C3D	5.27	135.36	115.29
3	P	373	NDP	C5D-C4D-C3D	5.31	135.50	115.29
3	R	377	NDP	C5D-C4D-C3D	5.36	135.71	115.29
3	B	378	NDP	C5D-C4D-C3D	5.42	135.93	115.29
3	A	376	NDP	C5D-C4D-C3D	5.43	136.00	115.29
3	I	380	NDP	C5D-C4D-C3D	5.52	136.33	115.29
3	C	365	NDP	C5D-C4D-C3D	5.63	136.73	115.29
3	O	372	NDP	O3B-C3B-C2B	5.64	127.21	111.18
3	Q	375	NDP	O3B-C3B-C2B	5.66	127.28	111.18
3	H	379	NDP	O3B-C3B-C2B	5.70	127.40	111.18
3	L	369	NDP	O3B-C3B-C2B	5.70	127.41	111.18
3	C	365	NDP	O3B-C3B-C2B	5.77	127.58	111.18
3	B	378	NDP	O2D-C2D-C3D	5.81	130.43	111.83
3	C	365	NDP	O2D-C2D-C3D	5.82	130.47	111.83
3	I	380	NDP	O3B-C3B-C2B	5.87	127.88	111.18
3	O	372	NDP	C5D-C4D-C3D	5.93	137.88	115.29
3	D	365	NDP	O3B-C3B-C2B	5.96	128.13	111.18
3	O	372	NDP	O2D-C2D-C3D	5.99	131.01	111.83
3	M	381	NDP	O3B-C3B-C2B	6.02	128.31	111.18
3	R	377	NDP	O2D-C2D-C3D	6.14	131.51	111.83
3	Q	375	NDP	O2D-C2D-C3D	6.15	131.53	111.83
3	H	379	NDP	O2D-C2D-C3D	6.17	131.60	111.83
3	L	369	NDP	O2D-C2D-C3D	6.18	131.61	111.83
3	A	376	NDP	O3B-C3B-C2B	6.22	128.86	111.18
3	M	381	NDP	O2D-C2D-C3D	6.37	132.23	111.83
3	B	378	NDP	O3B-C3B-C2B	6.46	129.56	111.18
3	P	373	NDP	O3B-C3B-C2B	6.52	129.72	111.18
3	I	380	NDP	O2D-C2D-C3D	6.53	132.75	111.83
3	R	377	NDP	O3B-C3B-C2B	6.69	130.20	111.18
3	D	365	NDP	O2D-C2D-C3D	6.73	133.39	111.83
3	R	377	NDP	C3B-C2B-C1B	6.87	116.20	102.75
3	P	373	NDP	O2D-C2D-C3D	6.91	133.95	111.83
3	I	380	NDP	C3B-C2B-C1B	6.94	116.32	102.75
3	M	381	NDP	C3B-C2B-C1B	6.99	116.43	102.75
3	L	369	NDP	C3B-C2B-C1B	7.04	116.52	102.75
3	O	372	NDP	C3B-C2B-C1B	7.05	116.54	102.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	365	NDP	C3B-C2B-C1B	7.14	116.72	102.75
3	B	378	NDP	C3B-C2B-C1B	7.16	116.75	102.75
3	H	379	NDP	C3B-C2B-C1B	7.20	116.83	102.75
3	Q	375	NDP	C3B-C2B-C1B	7.23	116.90	102.75
3	A	376	NDP	C3B-C2B-C1B	7.28	116.99	102.75
3	C	365	NDP	C3B-C2B-C1B	7.30	117.03	102.75
3	P	373	NDP	C3B-C2B-C1B	7.72	117.86	102.75
3	H	379	NDP	C1B-N9A-C4A	8.11	140.64	126.64
3	O	372	NDP	C1B-N9A-C4A	8.21	140.82	126.64
3	A	376	NDP	O2D-C2D-C3D	8.35	138.57	111.83
3	P	373	NDP	C1B-N9A-C4A	8.39	141.13	126.64
3	L	369	NDP	C1B-N9A-C4A	8.45	141.24	126.64
3	B	378	NDP	C1B-N9A-C4A	8.45	141.24	126.64
3	A	376	NDP	C1B-N9A-C4A	8.46	141.25	126.64
3	Q	375	NDP	C1B-N9A-C4A	8.47	141.27	126.64
3	C	365	NDP	C1B-N9A-C4A	8.49	141.30	126.64
3	M	381	NDP	C1B-N9A-C4A	8.68	141.64	126.64
3	I	380	NDP	C1B-N9A-C4A	8.71	141.68	126.64
3	H	379	NDP	O2B-C2B-C3B	8.80	144.20	111.63
3	B	378	NDP	O2B-C2B-C3B	8.80	144.21	111.63
3	Q	375	NDP	O2B-C2B-C3B	8.88	144.52	111.63
3	D	365	NDP	O2B-C2B-C3B	8.89	144.56	111.63
3	D	365	NDP	C1B-N9A-C4A	8.91	142.03	126.64
3	C	365	NDP	O2B-C2B-C3B	8.95	144.79	111.63
3	L	369	NDP	O2B-C2B-C3B	8.96	144.82	111.63
3	R	377	NDP	C1B-N9A-C4A	9.00	142.18	126.64
3	P	373	NDP	O2B-C2B-C3B	9.00	144.97	111.63
3	R	377	NDP	O2B-C2B-C3B	9.02	145.05	111.63
3	M	381	NDP	O2B-C2B-C3B	9.07	145.22	111.63
3	O	372	NDP	O2B-C2B-C3B	9.15	145.53	111.63
3	I	380	NDP	O2B-C2B-C3B	9.27	145.95	111.63
3	A	376	NDP	O2B-C2B-C3B	9.39	146.39	111.63
3	A	376	NDP	O4D-C1D-N1N	17.39	143.09	108.07
3	O	372	NDP	O4D-C1D-N1N	23.57	155.54	108.07
3	P	373	NDP	O4D-C1D-N1N	25.82	160.08	108.07
3	L	369	NDP	O4D-C1D-N1N	26.39	161.22	108.07
3	Q	375	NDP	O4D-C1D-N1N	30.20	168.91	108.07
3	C	365	NDP	O4D-C1D-N1N	30.90	170.30	108.07
3	R	377	NDP	O4D-C1D-N1N	31.86	172.24	108.07
3	M	381	NDP	O4D-C1D-N1N	31.97	172.46	108.07
3	B	378	NDP	O4D-C1D-N1N	32.50	173.52	108.07
3	I	380	NDP	O4D-C1D-N1N	32.54	173.61	108.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	365	NDP	O4D-C1D-N1N	33.10	174.73	108.07
3	H	379	NDP	O4D-C1D-N1N	33.14	174.82	108.07

All (84) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	378	NDP	C1B
3	B	378	NDP	C3D
3	B	378	NDP	C2B
3	B	378	NDP	C4D
3	B	378	NDP	C2D
3	B	378	NDP	C1D
3	B	378	NDP	C4B
3	O	372	NDP	C1B
3	O	372	NDP	C3D
3	O	372	NDP	C2B
3	O	372	NDP	C4D
3	O	372	NDP	C1D
3	O	372	NDP	C2D
3	O	372	NDP	C4B
3	M	381	NDP	C1B
3	M	381	NDP	C3D
3	M	381	NDP	C2B
3	M	381	NDP	C4D
3	M	381	NDP	C2D
3	M	381	NDP	C1D
3	M	381	NDP	C4B
3	I	380	NDP	C1B
3	I	380	NDP	C3D
3	I	380	NDP	C2B
3	I	380	NDP	C4D
3	I	380	NDP	C2D
3	I	380	NDP	C1D
3	I	380	NDP	C4B
3	R	377	NDP	C1B
3	R	377	NDP	C3D
3	R	377	NDP	C2B
3	R	377	NDP	C4D
3	R	377	NDP	C2D
3	R	377	NDP	C1D
3	R	377	NDP	C4B
3	A	376	NDP	C1B

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
3	A	376	NDP	C3D
3	A	376	NDP	C2B
3	A	376	NDP	C4D
3	A	376	NDP	C1D
3	A	376	NDP	C2D
3	A	376	NDP	C4B
3	L	369	NDP	C1B
3	L	369	NDP	C3D
3	L	369	NDP	C2B
3	L	369	NDP	C4D
3	L	369	NDP	C1D
3	L	369	NDP	C2D
3	L	369	NDP	C4B
3	D	365	NDP	C1B
3	D	365	NDP	C3D
3	D	365	NDP	C2B
3	D	365	NDP	C4D
3	D	365	NDP	C2D
3	D	365	NDP	C1D
3	D	365	NDP	C4B
3	H	379	NDP	C1B
3	H	379	NDP	C3D
3	H	379	NDP	C2B
3	H	379	NDP	C4D
3	H	379	NDP	C2D
3	H	379	NDP	C1D
3	H	379	NDP	C4B
3	Q	375	NDP	C1B
3	Q	375	NDP	C3D
3	Q	375	NDP	C2B
3	Q	375	NDP	C4D
3	Q	375	NDP	C2D
3	Q	375	NDP	C1D
3	Q	375	NDP	C4B
3	P	373	NDP	C1B
3	P	373	NDP	C3D
3	P	373	NDP	C2B
3	P	373	NDP	C4D
3	P	373	NDP	C1D
3	P	373	NDP	C2D
3	P	373	NDP	C4B
3	C	365	NDP	C1B

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Mol	Chain	Res	Type	Atom
3	C	365	NDP	C3D
3	C	365	NDP	C2B
3	C	365	NDP	C4D
3	C	365	NDP	C2D
3	C	365	NDP	C1D
3	C	365	NDP	C4B

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	R	377	NDP	PA-O5B-C5B-C4B
3	A	376	NDP	PA-O5B-C5B-C4B
3	O	372	NDP	PA-O5B-C5B-C4B
3	D	365	NDP	PA-O5B-C5B-C4B
3	I	380	NDP	PA-O5B-C5B-C4B
3	B	378	NDP	PA-O5B-C5B-C4B
3	M	381	NDP	PA-O5B-C5B-C4B
3	P	373	NDP	PA-O5B-C5B-C4B
3	Q	375	NDP	PA-O5B-C5B-C4B
3	C	365	NDP	PA-O5B-C5B-C4B
3	H	379	NDP	PA-O5B-C5B-C4B
3	L	369	NDP	PA-O5B-C5B-C4B

There are no ring outliers.

29 monomers are involved in 181 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	376	NDP	19	0
2	B	364	SO4	2	0
3	B	378	NDP	13	0
3	C	365	NDP	16	0
2	D	364	SO4	2	0
3	D	365	NDP	6	0
2	H	363	SO4	1	0
2	H	364	SO4	2	0
2	H	378	SO4	1	0
3	H	379	NDP	14	0
2	I	366	SO4	5	0
2	I	379	SO4	1	0
3	I	380	NDP	10	0
2	L	367	SO4	1	0
3	L	369	NDP	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	370	SO4	3	0
3	M	381	NDP	10	0
2	O	364	SO4	2	0
2	O	371	SO4	2	0
3	O	372	NDP	15	0
2	P	363	SO4	1	0
2	P	364	SO4	4	0
2	P	372	SO4	1	0
3	P	373	NDP	11	0
2	Q	373	SO4	1	0
3	Q	375	NDP	16	0
2	R	363	SO4	1	0
2	R	376	SO4	2	0
3	R	377	NDP	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	1
1	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	210:ALA	C	211:ALA	N	1.68
1	A	206:THR	C	207:SER	N	1.18
1	L	205:PRO	C	206:THR	N	1.16
1	B	333:GLN	C	334:GLY	N	1.12

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	337/365 (92%)	0.12	2 (0%) 89 87	7, 24, 42, 53	1 (0%)
1	B	337/365 (92%)	0.02	1 (0%) 93 93	7, 18, 35, 54	1 (0%)
1	C	337/365 (92%)	-0.06	1 (0%) 93 93	6, 16, 31, 43	1 (0%)
1	D	336/365 (92%)	0.25	12 (3%) 43 42	7, 27, 56, 65	1 (0%)
1	H	336/365 (92%)	0.28	9 (2%) 55 52	9, 28, 55, 67	1 (0%)
1	I	337/365 (92%)	-0.00	1 (0%) 93 93	7, 22, 37, 50	1 (0%)
1	L	336/365 (92%)	0.32	14 (4%) 37 35	11, 30, 57, 73	1 (0%)
1	M	337/365 (92%)	0.01	0 100 100	10, 21, 38, 44	1 (0%)
1	O	337/365 (92%)	-0.04	2 (0%) 89 87	6, 17, 32, 47	1 (0%)
1	P	337/365 (92%)	0.18	4 (1%) 79 77	9, 25, 42, 54	1 (0%)
1	Q	337/365 (92%)	-0.04	1 (0%) 93 93	7, 18, 34, 44	1 (0%)
1	R	337/365 (92%)	0.30	13 (3%) 40 39	6, 26, 55, 68	1 (0%)
All	All	4041/4380 (92%)	0.11	60 (1%) 74 72	6, 22, 50, 73	12 (0%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	332	TRP	5.1
1	H	332	TRP	4.0
1	L	61	ASP	3.6
1	D	80	VAL	3.5
1	L	60(A)	GLY	3.3
1	H	61	ASP	3.3
1	R	77	ARG	3.2
1	D	77	ARG	3.1
1	D	332	TRP	3.0
1	P	139	HIS	3.0
1	L	103	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	R	68	GLY	3.0
1	R	333	GLN	2.9
1	L	85	GLY	2.9
1	R	83	PRO	2.9
1	L	116	VAL	2.8
1	H	86	ASP	2.8
1	R	332	TRP	2.8
1	L	86	ASP	2.7
1	H	60(A)	GLY	2.6
1	H	78	ASN	2.6
1	D	98	VAL	2.5
1	L	110	GLN	2.5
1	R	1	LEU	2.5
1	H	143	ILE	2.5
1	L	0	LYS	2.4
1	L	333	GLN	2.4
1	L	72	LYS	2.4
1	L	89	ILE	2.4
1	R	86	ASP	2.3
1	B	56	ASP	2.3
1	R	72	LYS	2.3
1	A	61	ASP	2.3
1	D	78	ASN	2.2
1	R	88	GLY	2.2
1	O	62	SER	2.2
1	D	329	ALA	2.2
1	H	211	ALA	2.2
1	L	78	ASN	2.2
1	I	191	ARG	2.2
1	A	215	ALA	2.2
1	R	209	GLY	2.2
1	P	333	GLN	2.2
1	D	83	PRO	2.2
1	D	0	LYS	2.1
1	D	2	LYS	2.1
1	R	111	ALA	2.1
1	P	140	ALA	2.1
1	H	1	LEU	2.1
1	R	78	ASN	2.1
1	R	329	ALA	2.1
1	P	212	LYS	2.1
1	D	85	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	Q	61	ASP	2.1
1	D	91	LEU	2.1
1	H	209	GLY	2.0
1	L	211	ALA	2.0
1	C	62	SER	2.0
1	D	191	ARG	2.0
1	O	122(A)	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	O	371	5/5	0.49	0.88	27.18	148,148,148,148	5
2	SO4	M	370	5/5	0.78	0.48	8.58	70,71,71,71	5
2	SO4	M	380	5/5	0.92	0.41	7.90	65,65,66,66	5
2	SO4	I	366	5/5	0.76	0.38	6.14	69,69,70,70	5
2	SO4	Q	373	5/5	0.84	0.43	5.64	74,74,74,75	5
2	SO4	I	379	5/5	0.92	0.23	3.81	64,64,65,65	0
2	SO4	B	377	5/5	0.85	0.36	3.81	77,77,77,77	5
2	SO4	H	364	5/5	0.82	0.26	2.42	55,57,57,58	5
2	SO4	Q	374	5/5	0.95	0.24	2.30	51,52,52,52	5
2	SO4	O	364	5/5	0.93	0.21	2.00	56,56,56,57	5
2	SO4	D	364	5/5	0.89	0.22	1.60	54,54,55,55	5
2	SO4	Q	364	5/5	0.95	0.17	1.49	40,41,42,42	0
3	NDP	I	380	48/48	0.94	0.19	1.48	19,26,42,46	0
2	SO4	B	364	5/5	0.94	0.23	1.47	40,42,43,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	R	364	5/5	0.92	0.23	1.45	50,50,51,51	5
3	NDP	C	365	48/48	0.93	0.20	1.33	17,24,40,43	0
2	SO4	L	368	5/5	0.91	0.21	1.29	49,50,51,53	0
3	NDP	O	372	48/48	0.92	0.20	1.25	16,25,39,43	0
3	NDP	H	379	48/48	0.89	0.23	1.17	31,38,54,57	0
3	NDP	B	378	48/48	0.93	0.19	1.04	17,23,45,46	0
3	NDP	L	369	48/48	0.89	0.22	0.96	31,40,58,60	0
3	NDP	Q	375	48/48	0.93	0.19	0.88	25,30,49,51	0
3	NDP	M	381	48/48	0.93	0.18	0.85	21,26,41,43	0
2	SO4	C	364	5/5	0.87	0.17	0.80	57,57,59,59	0
3	NDP	R	377	48/48	0.90	0.23	0.73	30,43,53,54	0
2	SO4	A	364	5/5	0.95	0.21	0.60	48,49,51,51	0
3	NDP	D	365	48/48	0.92	0.22	0.49	30,40,55,57	0
3	NDP	P	373	48/48	0.94	0.17	0.29	11,26,45,47	0
3	NDP	A	376	48/48	0.93	0.17	0.26	19,25,47,48	0
2	SO4	P	364	5/5	0.96	0.18	0.16	44,44,45,45	0
2	SO4	R	376	5/5	0.93	0.17	0.10	62,63,63,63	0
2	SO4	A	375	5/5	0.97	0.16	-0.16	55,55,55,56	0
2	SO4	H	378	5/5	0.94	0.17	-0.31	55,56,56,56	0
2	SO4	P	372	5/5	0.97	0.13	-0.94	61,61,62,62	0
2	SO4	D	363	5/5	0.94	0.22	-	60,60,61,62	0
2	SO4	C	363	5/5	0.95	0.19	-	62,62,63,63	0
2	SO4	H	363	5/5	0.96	0.20	-	60,61,61,62	0
2	SO4	R	363	5/5	0.95	0.22	-	35,36,37,37	5
2	SO4	I	365	5/5	0.96	0.19	-	64,65,65,66	0
2	SO4	Q	363	5/5	0.94	0.19	-	51,51,52,53	0
2	SO4	P	363	5/5	0.95	0.20	-	60,60,61,62	0
2	SO4	B	363	5/5	0.94	0.23	-	52,53,54,54	0
2	SO4	A	363	5/5	0.87	0.28	-	56,56,57,58	5
2	SO4	L	367	5/5	0.95	0.22	-	63,63,64,65	0
2	SO4	O	363	5/5	0.94	0.25	-	50,51,51,52	5
2	SO4	M	369	5/5	0.93	0.23	-	60,60,61,62	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.