



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:24 am BST

PDB ID : 3SLK  
Title : Structure of ketoreductase and enoylreductase didomain from modular polyketide synthase  
Authors : Zheng, J.; Gay, D.C.; Keatinge-Clay, A.T.  
Deposited on : 2011-06-24  
Resolution : 3.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

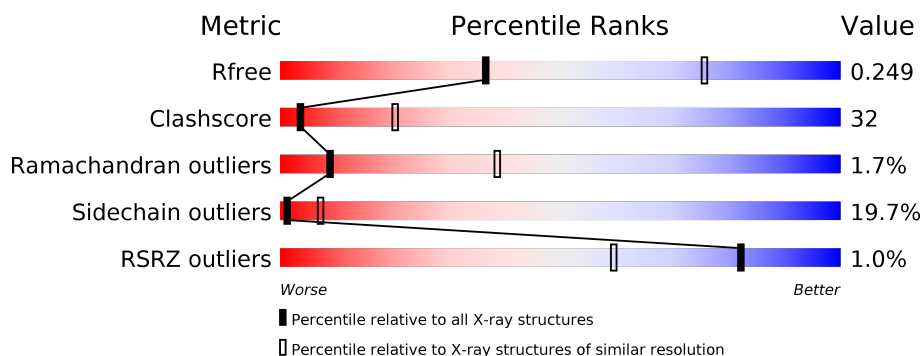
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	795	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>%</span> <span>51%</span> <span>34%</span> <span>8%</span> <span>• 6%</span> </div> </div>
1	B	795	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>%</span> <span>56%</span> <span>30%</span> <span>7%</span> <span>• 6%</span> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11217 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 Polyketide synthase extender module 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	747	Total	C	N	O	S	0	0	0
			5505	3457	990	1043	15			
1	B	747	Total	C	N	O	S	0	0	0
			5505	3457	990	1043	15			

There are 42 discrepancies between the modelled and reference sequences:

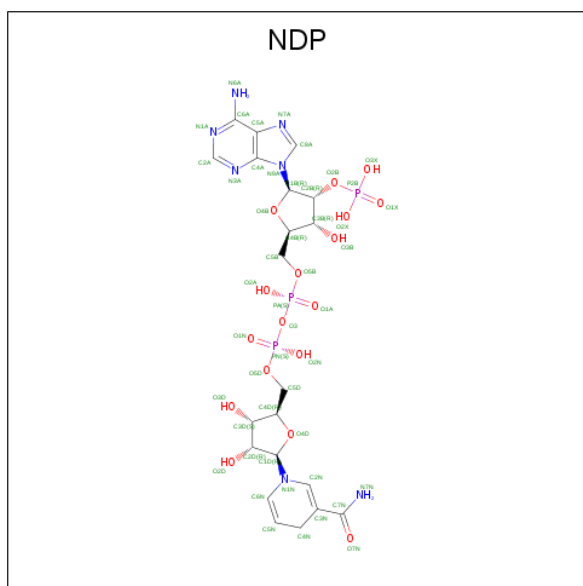
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP Q9ALM5
A	-19	GLY	-	EXPRESSION TAG	UNP Q9ALM5
A	-18	SER	-	EXPRESSION TAG	UNP Q9ALM5
A	-17	SER	-	EXPRESSION TAG	UNP Q9ALM5
A	-16	HIS	-	EXPRESSION TAG	UNP Q9ALM5
A	-15	HIS	-	EXPRESSION TAG	UNP Q9ALM5
A	-14	HIS	-	EXPRESSION TAG	UNP Q9ALM5
A	-13	HIS	-	EXPRESSION TAG	UNP Q9ALM5
A	-12	HIS	-	EXPRESSION TAG	UNP Q9ALM5
A	-11	HIS	-	EXPRESSION TAG	UNP Q9ALM5
A	-10	SER	-	EXPRESSION TAG	UNP Q9ALM5
A	-9	SER	-	EXPRESSION TAG	UNP Q9ALM5
A	-8	GLY	-	EXPRESSION TAG	UNP Q9ALM5
A	-7	LEU	-	EXPRESSION TAG	UNP Q9ALM5
A	-6	VAL	-	EXPRESSION TAG	UNP Q9ALM5
A	-5	PRO	-	EXPRESSION TAG	UNP Q9ALM5
A	-4	ARG	-	EXPRESSION TAG	UNP Q9ALM5
A	-3	GLY	-	EXPRESSION TAG	UNP Q9ALM5
A	-2	SER	-	EXPRESSION TAG	UNP Q9ALM5
A	-1	HIS	-	EXPRESSION TAG	UNP Q9ALM5
A	0	MET	-	EXPRESSION TAG	UNP Q9ALM5
B	-20	MET	-	EXPRESSION TAG	UNP Q9ALM5
B	-19	GLY	-	EXPRESSION TAG	UNP Q9ALM5
B	-18	SER	-	EXPRESSION TAG	UNP Q9ALM5
B	-17	SER	-	EXPRESSION TAG	UNP Q9ALM5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	EXPRESSION TAG	UNP Q9ALM5
B	-15	HIS	-	EXPRESSION TAG	UNP Q9ALM5
B	-14	HIS	-	EXPRESSION TAG	UNP Q9ALM5
B	-13	HIS	-	EXPRESSION TAG	UNP Q9ALM5
B	-12	HIS	-	EXPRESSION TAG	UNP Q9ALM5
B	-11	HIS	-	EXPRESSION TAG	UNP Q9ALM5
B	-10	SER	-	EXPRESSION TAG	UNP Q9ALM5
B	-9	SER	-	EXPRESSION TAG	UNP Q9ALM5
B	-8	GLY	-	EXPRESSION TAG	UNP Q9ALM5
B	-7	LEU	-	EXPRESSION TAG	UNP Q9ALM5
B	-6	VAL	-	EXPRESSION TAG	UNP Q9ALM5
B	-5	PRO	-	EXPRESSION TAG	UNP Q9ALM5
B	-4	ARG	-	EXPRESSION TAG	UNP Q9ALM5
B	-3	GLY	-	EXPRESSION TAG	UNP Q9ALM5
B	-2	SER	-	EXPRESSION TAG	UNP Q9ALM5
B	-1	HIS	-	EXPRESSION TAG	UNP Q9ALM5
B	0	MET	-	EXPRESSION TAG	UNP Q9ALM5

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



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

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

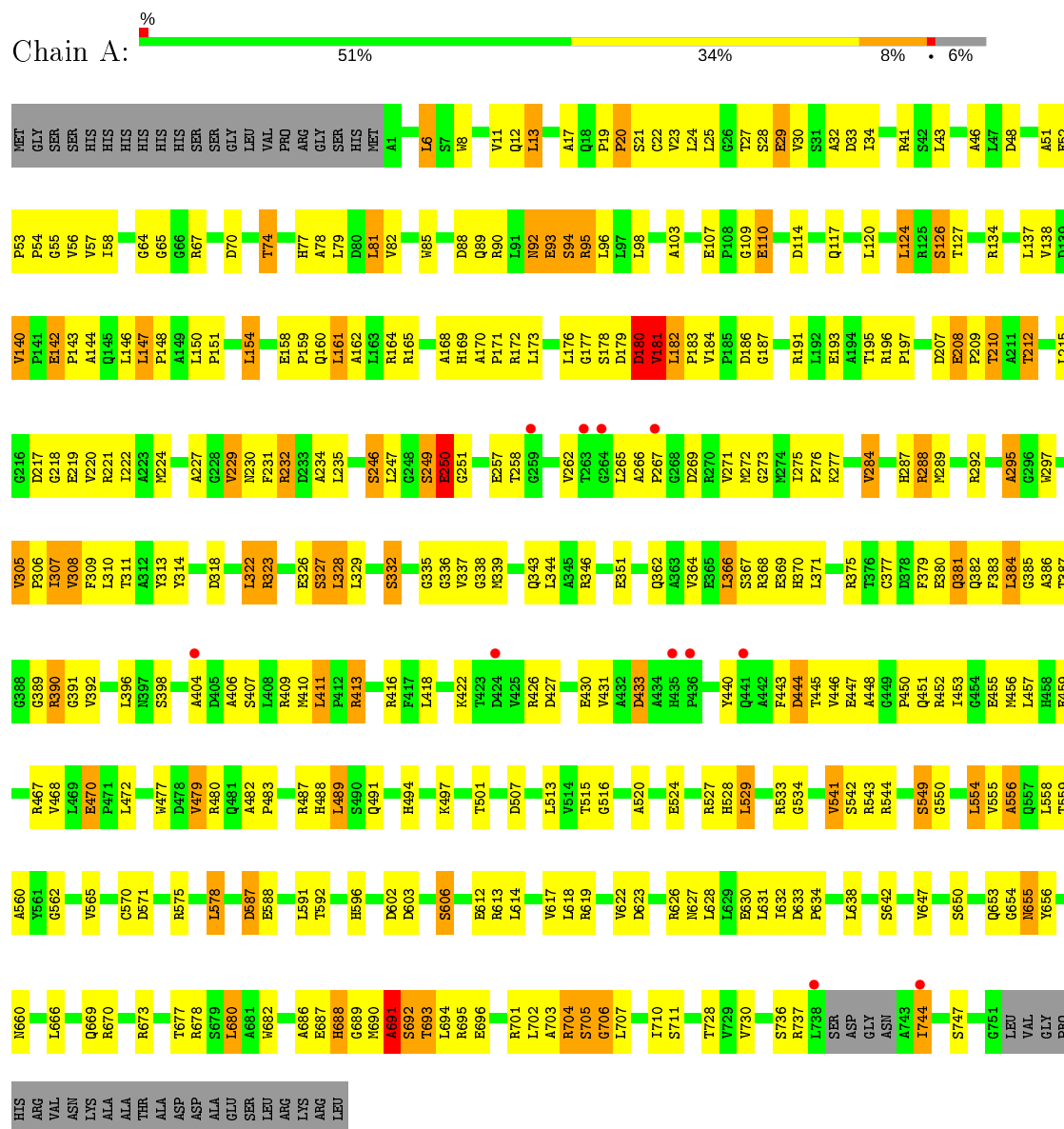


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

### 3 Residue-property plots

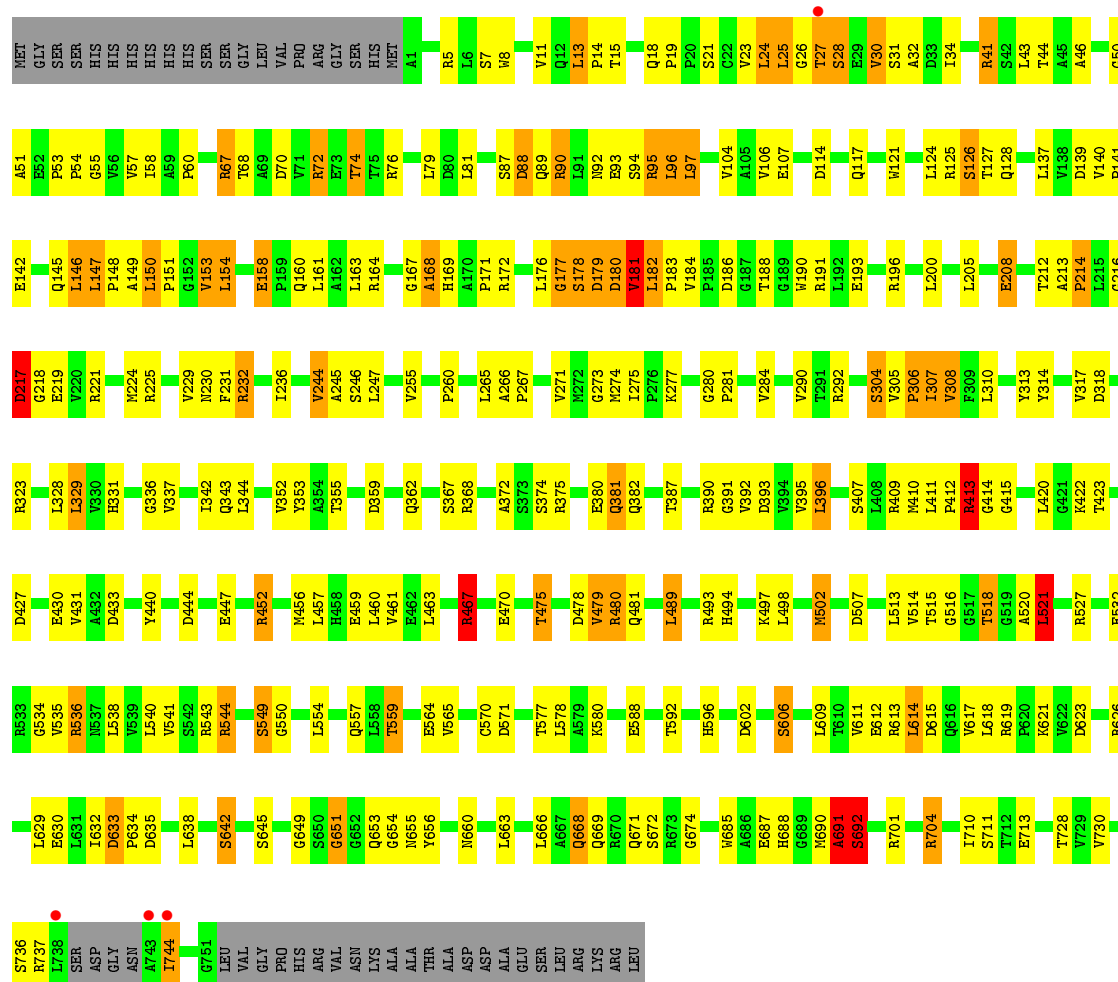
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Polyketide synthase extender module 2



- Molecule 1: Polyketide synthase extender module 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.10Å 110.19Å 202.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 45.26 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-3.00) 99.5 (45.26-3.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.21 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.210 , 0.256 0.207 , 0.249	Depositor DCC
$R_{free}$ test set	1698 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.0	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 56.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11217	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	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 40.36 % 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 2.7676e-04. 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	0.47	0/5614	0.50	0/7665
1	B	0.46	0/5614	0.50	1/7665 (0.0%)
All	All	0.46	0/11228	0.50	1/15330 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	6
All	All	0	11

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	521	LEU	CA-CB-CG	5.79	128.62	115.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	534	GLY	Peptide
1	A	549	SER	Peptide
1	A	686	ALA	Peptide
1	A	691	ALA	Peptide
1	A	89	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	B	413	ARG	Sidechain
1	B	50	GLY	Peptide
1	B	549	SER	Peptide
1	B	635	ASP	Peptide
1	B	651	GLY	Peptide
1	B	691	ALA	Peptide

## 5.2 Too-close contacts [i](#)

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	5505	0	5524	357	0
1	B	5505	0	5524	347	1
2	A	96	0	52	12	0
2	B	96	0	52	10	0
3	A	10	0	0	1	1
3	B	5	0	0	1	0
All	All	11217	0	11152	706	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 32.

All (706) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:LEU:HD21	1:A:410:MET:SD	1.59	1.42
1:B:691:ALA:CB	1:B:692:SER:HB2	1.51	1.37
1:B:691:ALA:HB3	1:B:692:SER:CB	1.61	1.28
1:A:691:ALA:HB3	1:A:692:SER:CB	1.64	1.25
1:B:178:SER:N	1:B:179:ASP:HA	1.37	1.23
1:A:692:SER:O	1:A:696:GLU:HG3	1.36	1.20
1:A:550:GLY:N	1:A:690:MET:HE3	1.54	1.19
1:B:160:GLN:O	1:B:161:LEU:HD23	1.42	1.18
1:A:487:ARG:O	1:A:491:GLN:HG3	1.44	1.17
1:A:208:GLU:OE1	1:A:210:THR:HG23	1.44	1.16
1:B:387:THR:HG21	1:B:391:GLY:H	1.05	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:LEU:C	1:B:148:PRO:HD2	1.66	1.15
1:A:181:VAL:HG13	1:A:182:LEU:N	1.60	1.15
1:A:691:ALA:CB	1:A:692:SER:HB2	1.76	1.14
1:A:507:ASP:HB3	1:A:592:THR:HG21	1.20	1.14
1:B:150:LEU:HD23	1:B:151:PRO:N	1.62	1.14
1:A:384:LEU:HD23	1:A:384:LEU:H	1.10	1.13
1:B:150:LEU:C	1:B:150:LEU:HD23	1.65	1.12
1:B:13:LEU:HD22	1:B:13:LEU:H	1.11	1.12
1:B:387:THR:HG21	1:B:391:GLY:N	1.63	1.11
1:A:691:ALA:CB	1:A:692:SER:CB	2.29	1.10
1:B:181:VAL:HG23	1:B:182:LEU:N	1.57	1.09
1:B:95:ARG:HH11	1:B:95:ARG:HG2	0.95	1.09
1:B:395:VAL:CG2	1:B:411:LEU:HD11	1.82	1.09
1:B:27:THR:OG1	1:B:28:SER:HA	1.53	1.08
1:A:217:ASP:HB2	1:A:218:GLY:HA3	1.35	1.08
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.00	1.08
1:A:95:ARG:HH11	1:A:95:ARG:HG2	1.13	1.08
1:B:181:VAL:CG2	1:B:182:LEU:H	1.67	1.07
1:A:691:ALA:HB3	1:A:692:SER:HB3	1.25	1.06
1:A:184:VAL:HG12	1:A:186:ASP:H	1.20	1.05
1:A:390:ARG:HB2	1:A:413:ARG:HB2	1.34	1.04
1:A:30:VAL:HG13	1:A:32:ALA:O	1.57	1.03
1:B:216:GLY:O	1:B:217:ASP:HB2	1.53	1.03
1:B:544:ARG:HG3	1:B:544:ARG:HH11	0.88	1.02
1:B:314:TYR:CA	1:B:456:MET:HE3	1.89	1.02
1:B:314:TYR:HA	1:B:456:MET:HE3	1.41	1.02
1:A:411:LEU:HG	1:A:411:LEU:O	1.58	1.01
1:B:507:ASP:HB3	1:B:592:THR:HG21	1.41	1.01
1:A:384:LEU:HD23	1:A:384:LEU:N	1.74	1.01
1:A:181:VAL:HG13	1:A:182:LEU:H	0.87	1.00
1:A:208:GLU:CD	1:A:210:THR:HG23	1.81	1.00
1:B:213:ALA:HA	1:B:221:ARG:NH2	1.77	1.00
1:A:550:GLY:N	1:A:690:MET:CE	2.26	0.99
1:A:380:GLU:O	1:A:384:LEU:HD23	1.62	0.98
1:A:181:VAL:CG1	1:A:182:LEU:H	1.73	0.98
1:B:25:LEU:CD2	1:B:25:LEU:N	2.28	0.97
1:A:375:ARG:HH11	1:A:375:ARG:HG3	1.22	0.97
1:A:410:MET:O	1:A:411:LEU:HD23	1.63	0.97
1:A:384:LEU:CD2	1:A:410:MET:SD	2.52	0.97
1:A:691:ALA:HB1	1:A:692:SER:HB2	1.45	0.97
1:A:392:VAL:O	1:A:411:LEU:HB2	1.64	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:GLY:H	1:A:690:MET:HE3	1.22	0.96
1:B:178:SER:N	1:B:179:ASP:CA	2.28	0.96
1:A:313:TYR:HD1	1:A:456:MET:CE	1.78	0.96
1:B:70:ASP:O	1:B:74:THR:HG23	1.65	0.95
1:B:158:GLU:HB3	1:B:161:LEU:HD21	1.47	0.95
1:B:395:VAL:HG23	1:B:411:LEU:HD11	1.46	0.95
1:A:384:LEU:N	1:A:384:LEU:CD2	2.27	0.95
1:B:181:VAL:HG23	1:B:182:LEU:H	0.80	0.94
1:A:314:TYR:CE1	1:A:448:ALA:HB2	2.03	0.94
1:A:308:VAL:HG11	1:A:336:GLY:C	1.86	0.94
1:A:314:TYR:HA	1:A:456:MET:HE1	1.49	0.93
1:B:691:ALA:CB	1:B:692:SER:CB	2.32	0.93
1:A:217:ASP:CB	1:A:218:GLY:HA3	1.99	0.93
1:A:95:ARG:HG2	1:A:95:ARG:NH1	1.74	0.92
1:B:544:ARG:CG	1:B:544:ARG:HH11	1.80	0.92
1:A:390:ARG:HB2	1:A:413:ARG:CB	1.98	0.92
1:B:146:LEU:C	1:B:148:PRO:CD	2.38	0.92
1:A:70:ASP:O	1:A:74:THR:HG23	1.71	0.91
1:A:232:ARG:CG	1:A:232:ARG:HH11	1.84	0.91
1:A:232:ARG:HG3	1:A:232:ARG:NH1	1.76	0.91
1:B:25:LEU:HD23	1:B:25:LEU:N	1.82	0.91
1:A:313:TYR:HD1	1:A:456:MET:HE3	1.33	0.91
1:B:314:TYR:CA	1:B:456:MET:CE	2.49	0.90
1:B:544:ARG:NH1	1:B:544:ARG:HG3	1.69	0.90
1:B:150:LEU:HD23	1:B:151:PRO:CA	2.01	0.90
1:B:95:ARG:CG	1:B:95:ARG:HH11	1.85	0.90
1:B:395:VAL:HG21	1:B:411:LEU:HD11	1.52	0.89
1:B:216:GLY:HA2	1:B:260:PRO:HD2	1.52	0.89
1:A:332:SER:OG	2:A:801:NDP:H4B	1.72	0.89
1:B:147:LEU:N	1:B:148:PRO:CD	2.36	0.89
1:B:95:ARG:HG2	1:B:95:ARG:NH1	1.67	0.89
1:B:179:ASP:OD2	1:B:180:ASP:HB3	1.72	0.88
1:B:13:LEU:CD2	1:B:13:LEU:H	1.86	0.88
1:B:13:LEU:N	1:B:13:LEU:HD22	1.88	0.88
1:B:216:GLY:C	1:B:218:GLY:HA2	1.93	0.87
1:A:308:VAL:CG1	1:A:336:GLY:C	2.43	0.87
1:B:121:TRP:O	1:B:125:ARG:HG3	1.75	0.87
1:B:150:LEU:CD2	1:B:151:PRO:N	2.37	0.87
1:B:178:SER:H	1:B:179:ASP:HA	1.40	0.86
1:A:292:ARG:HB3	1:B:737:ARG:HH12	1.39	0.85
1:A:543:ARG:HB2	2:A:802:NDP:O3X	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:ALA:CB	1:A:688:HIS:O	2.24	0.85
1:B:467:ARG:HH11	1:B:467:ARG:HB2	1.40	0.85
1:A:507:ASP:CB	1:A:592:THR:HG21	2.04	0.85
1:B:146:LEU:O	1:B:148:PRO:HD2	1.75	0.85
1:B:177:GLY:C	1:B:179:ASP:HA	1.96	0.85
1:B:182:LEU:HD12	1:B:183:PRO:CD	2.07	0.84
1:B:25:LEU:HD21	1:B:57:VAL:CG1	2.07	0.84
1:B:314:TYR:N	1:B:456:MET:CE	2.40	0.84
1:B:479:VAL:HG21	1:B:502:MET:HE3	1.58	0.84
1:B:217:ASP:N	1:B:218:GLY:HA2	1.92	0.84
1:A:313:TYR:CD1	1:A:456:MET:HE3	2.13	0.84
1:B:150:LEU:C	1:B:150:LEU:CD2	2.42	0.84
1:B:160:GLN:C	1:B:161:LEU:HD23	1.96	0.84
1:A:208:GLU:OE1	1:A:209:PRO:HD2	1.78	0.83
1:B:375:ARG:HG3	1:B:375:ARG:HH11	1.43	0.83
1:A:289:MET:CE	1:A:453:ILE:HD13	2.09	0.83
1:B:182:LEU:HD12	1:B:183:PRO:HD2	1.62	0.82
1:A:336:GLY:HA2	1:A:472:LEU:CD1	2.10	0.82
1:A:692:SER:H	1:A:695:ARG:HG3	1.43	0.82
1:B:30:VAL:HG13	1:B:32:ALA:H	1.45	0.81
1:A:217:ASP:H	1:A:219:GLU:H	1.26	0.81
1:A:250:GLU:HB3	1:A:307:ILE:HD13	1.61	0.81
1:A:390:ARG:HB2	1:A:413:ARG:CG	2.09	0.81
1:B:314:TYR:N	1:B:456:MET:HE1	1.96	0.81
1:A:332:SER:HG	2:A:801:NDP:C4B	1.94	0.80
1:A:308:VAL:HG12	1:A:337:VAL:HA	1.61	0.80
1:A:181:VAL:CG1	1:A:182:LEU:N	2.35	0.80
1:A:182:LEU:HB2	1:A:480:ARG:O	1.82	0.80
1:A:390:ARG:CB	1:A:413:ARG:CG	2.60	0.80
1:B:614:LEU:HD23	1:B:655:ASN:HB2	1.63	0.80
1:A:380:GLU:O	1:A:384:LEU:CD2	2.29	0.80
1:B:507:ASP:CB	1:B:592:THR:HG21	2.11	0.80
1:A:209:PRO:O	1:A:212:THR:HG23	1.82	0.79
1:B:181:VAL:CG2	1:B:182:LEU:N	2.31	0.79
1:B:314:TYR:CB	1:B:456:MET:HE3	2.13	0.79
1:B:150:LEU:HD22	1:B:151:PRO:HD3	1.63	0.78
1:B:381:GLN:HG3	1:B:382:GLN:N	1.95	0.78
2:A:801:NDP:H1B	2:A:801:NDP:O1X	1.83	0.78
1:B:343:GLN:HE22	1:B:470:GLU:H	1.32	0.77
1:A:332:SER:O	1:A:338:GLY:HA3	1.83	0.77
1:A:143:PRO:O	1:A:144:ALA:HB3	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:SER:O	1:A:690:MET:HE2	1.85	0.77
1:A:515:THR:HA	1:A:541:VAL:HG12	1.67	0.76
1:A:177:GLY:HA2	1:A:180:ASP:HA	1.68	0.76
1:B:150:LEU:HD22	1:B:151:PRO:CD	2.17	0.75
1:A:520:ALA:HB2	1:A:688:HIS:O	1.87	0.75
1:B:687:GLU:HG3	1:B:687:GLU:O	1.85	0.75
1:A:332:SER:OG	2:A:801:NDP:C4B	2.33	0.75
1:B:25:LEU:HD23	1:B:58:ILE:O	1.87	0.75
1:A:88:ASP:OD2	1:A:90:ARG:HD3	1.87	0.75
1:A:633:ASP:OD2	1:A:634:PRO:HD2	1.87	0.74
1:B:177:GLY:HA2	1:B:179:ASP:HB2	1.67	0.74
1:B:232:ARG:NH2	1:B:245:ALA:HB1	2.01	0.74
1:A:389:GLY:HA2	1:A:390:ARG:C	2.06	0.74
1:A:507:ASP:HB3	1:A:592:THR:CG2	2.10	0.74
1:B:95:ARG:CG	1:B:95:ARG:NH1	2.49	0.74
1:A:158:GLU:HB3	1:A:161:LEU:HD21	1.68	0.74
1:A:289:MET:HE3	1:A:453:ILE:HD13	1.68	0.74
1:A:549:SER:C	1:A:690:MET:CE	2.55	0.74
1:B:191:ARG:HH12	1:B:246:SER:HB2	1.53	0.74
2:A:801:NDP:C1B	2:A:801:NDP:O1X	2.35	0.74
1:A:655:ASN:HD22	1:A:655:ASN:N	1.84	0.73
1:B:41:ARG:O	1:B:44:THR:HB	1.87	0.73
1:B:314:TYR:HB2	1:B:456:MET:CE	2.18	0.73
1:B:124:LEU:HB3	1:B:137:LEU:HD21	1.70	0.73
1:B:275:ILE:HD11	1:B:290:VAL:HG11	1.71	0.73
1:A:687:GLU:O	1:A:688:HIS:HB2	1.86	0.73
1:B:27:THR:HG1	1:B:28:SER:HA	1.53	0.73
1:A:375:ARG:NH1	1:A:375:ARG:HG3	2.00	0.72
1:A:314:TYR:N	1:A:456:MET:HE2	2.03	0.72
1:A:392:VAL:O	1:A:411:LEU:CB	2.38	0.72
1:A:390:ARG:CB	1:A:413:ARG:HG2	2.19	0.72
1:A:195:THR:O	1:A:197:PRO:HD3	1.89	0.72
1:B:396:LEU:HD22	1:B:420:LEU:HD11	1.72	0.72
1:A:617:VAL:HG11	1:A:656:TYR:HA	1.71	0.72
1:A:710:ILE:HG22	1:A:711:SER:O	1.89	0.72
1:B:150:LEU:CD2	1:B:151:PRO:CD	2.66	0.72
1:B:457:LEU:O	1:B:461:VAL:HG23	1.89	0.72
1:A:549:SER:O	1:A:690:MET:CE	2.37	0.71
1:A:30:VAL:CG1	1:A:32:ALA:O	2.35	0.71
1:A:655:ASN:H	1:A:655:ASN:HD22	1.36	0.71
1:A:95:ARG:CG	1:A:95:ARG:HH11	1.95	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:PRO:HA	1:B:221:ARG:HH22	1.55	0.71
1:B:25:LEU:HD23	1:B:25:LEU:H	1.55	0.71
1:B:314:TYR:HA	1:B:456:MET:CE	2.15	0.71
1:A:208:GLU:OE1	1:A:209:PRO:CD	2.38	0.71
1:B:273:GLY:HA3	1:B:290:VAL:HG12	1.71	0.71
1:A:144:ALA:HA	1:A:147:LEU:HD12	1.72	0.70
1:B:520:ALA:HB2	1:B:688:HIS:O	1.91	0.70
1:B:191:ARG:HE	1:B:208:GLU:HG2	1.56	0.70
1:A:208:GLU:OE2	1:A:210:THR:HG23	1.91	0.70
1:A:314:TYR:CD1	1:A:448:ALA:HB2	2.27	0.70
1:B:27:THR:N	1:B:28:SER:CB	2.55	0.70
1:A:702:LEU:O	1:A:707:LEU:HD12	1.91	0.70
1:B:164:ARG:HH11	1:B:164:ARG:HG2	1.57	0.70
1:A:314:TYR:CA	1:A:456:MET:HE1	2.21	0.70
1:A:602:ASP:OD2	1:A:613:ARG:HD2	1.92	0.70
1:B:127:THR:HG22	1:B:606:SER:OG	1.91	0.69
1:A:313:TYR:CD1	1:A:456:MET:CE	2.68	0.69
1:A:410:MET:O	1:A:411:LEU:CD2	2.37	0.69
1:B:213:ALA:HA	1:B:221:ARG:HH21	1.55	0.69
1:B:308:VAL:HG22	1:B:337:VAL:HA	1.74	0.69
1:B:147:LEU:N	1:B:148:PRO:HD3	2.07	0.69
1:B:72:ARG:HD3	1:B:615:ASP:OD2	1.93	0.69
1:A:250:GLU:HB3	1:A:307:ILE:CD1	2.23	0.69
1:A:208:GLU:CD	1:A:209:PRO:HD2	2.13	0.69
1:A:180:ASP:O	1:A:181:VAL:HG12	1.93	0.68
1:A:418:LEU:HB3	1:A:443:PHE:HE1	1.57	0.68
1:B:313:TYR:HD1	1:B:456:MET:HE2	1.58	0.68
1:B:633:ASP:OD2	1:B:634:PRO:HD2	1.93	0.68
1:A:544:ARG:HD3	2:A:802:NDP:O2X	1.91	0.68
1:B:274:MET:HG2	1:B:307:ILE:CD1	2.22	0.68
1:B:691:ALA:HB3	1:B:692:SER:HB2	0.72	0.68
1:B:444:ASP:O	1:B:447:GLU:HG3	1.93	0.68
1:A:444:ASP:O	1:A:447:GLU:HB2	1.94	0.68
1:B:27:THR:OG1	1:B:28:SER:CA	2.35	0.68
1:A:313:TYR:HD1	1:A:456:MET:HE2	1.59	0.68
1:B:191:ARG:NH1	1:B:246:SER:HB2	2.08	0.68
1:B:411:LEU:HD23	1:B:415:GLY:HA3	1.76	0.68
1:A:448:ALA:HB1	1:A:452:ARG:HG2	1.75	0.68
1:B:140:VAL:HG12	1:B:163:LEU:HB2	1.75	0.68
1:B:710:ILE:HG22	1:B:711:SER:O	1.94	0.68
1:B:184:VAL:HG12	1:B:186:ASP:H	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ASP:OD2	1:B:164:ARG:NH2	2.27	0.67
1:A:28:SER:OG	1:A:29:GLU:N	2.28	0.67
1:A:120:LEU:HD21	1:A:124:LEU:HD13	1.76	0.66
1:A:689:GLY:O	1:A:693:THR:HB	1.96	0.66
1:A:544:ARG:NH2	3:A:803:SO4:O3	2.21	0.66
1:B:27:THR:N	1:B:28:SER:HB3	2.11	0.66
1:A:430:GLU:O	1:A:433:ASP:HB2	1.95	0.66
1:B:72:ARG:NH1	1:B:611:VAL:CG1	2.59	0.66
1:A:142:GLU:HG2	1:A:142:GLU:O	1.94	0.66
1:A:308:VAL:CG1	1:A:337:VAL:N	2.59	0.66
1:B:150:LEU:HD23	1:B:151:PRO:HA	1.74	0.66
1:B:520:ALA:CB	1:B:688:HIS:O	2.44	0.66
1:A:179:ASP:O	1:A:180:ASP:HB3	1.96	0.65
1:A:691:ALA:HB3	1:A:692:SER:HB2	1.43	0.65
1:B:26:GLY:C	1:B:28:SER:OG	2.34	0.65
1:A:208:GLU:OE2	1:A:210:THR:CG2	2.44	0.65
1:A:411:LEU:O	1:A:411:LEU:CG	2.39	0.65
1:B:158:GLU:CB	1:B:161:LEU:HD21	2.24	0.65
1:A:23:VAL:HG22	1:A:57:VAL:HG22	1.79	0.65
1:B:150:LEU:HB3	1:B:151:PRO:HD3	1.79	0.65
1:A:406:ALA:HA	1:A:409:ARG:NH1	2.10	0.65
1:A:191:ARG:NH1	1:A:193:GLU:OE2	2.30	0.65
1:B:46:ALA:O	1:B:51:ALA:HB3	1.97	0.65
1:B:150:LEU:CD2	1:B:151:PRO:HD3	2.26	0.65
1:A:98:LEU:HD22	1:A:124:LEU:CD1	2.27	0.64
1:B:232:ARG:O	1:B:236:ILE:HG13	1.97	0.64
1:A:98:LEU:HD22	1:A:124:LEU:HD11	1.79	0.64
1:A:220:VAL:O	1:A:284:VAL:HG23	1.97	0.64
1:B:153:VAL:HG12	1:B:154:LEU:N	2.12	0.64
1:B:387:THR:CG2	1:B:391:GLY:H	1.97	0.64
1:B:412:PRO:HD2	1:B:413:ARG:HG2	1.78	0.64
1:B:617:VAL:HG11	1:B:656:TYR:HA	1.78	0.64
1:A:266:ALA:HB1	1:A:267:PRO:HD2	1.80	0.64
1:B:114:ASP:CG	1:B:117:GLN:HG3	2.18	0.64
1:B:390:ARG:O	1:B:413:ARG:HD3	1.97	0.64
1:B:314:TYR:H	1:B:456:MET:HE1	1.60	0.64
1:A:250:GLU:OE1	1:A:497:LYS:NZ	2.31	0.64
1:A:390:ARG:HB3	1:A:413:ARG:CG	2.27	0.64
1:B:395:VAL:HG21	1:B:411:LEU:CD1	2.25	0.64
1:A:179:ASP:O	1:A:180:ASP:CB	2.46	0.63
1:B:375:ARG:CG	1:B:375:ARG:HH11	2.10	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:VAL:HG11	1:A:336:GLY:O	1.98	0.63
1:A:704:ARG:NE	1:A:704:ARG:HA	2.13	0.63
1:B:559:THR:HG23	1:B:565:VAL:HB	1.80	0.63
1:A:575:ARG:NH1	1:A:630:GLU:HG2	2.14	0.63
1:B:390:ARG:O	1:B:413:ARG:NH1	2.26	0.63
1:A:177:GLY:HA2	1:A:180:ASP:CA	2.28	0.63
1:B:88:ASP:OD2	1:B:90:ARG:HD2	1.99	0.63
1:A:329:LEU:HB2	1:A:392:VAL:HG11	1.81	0.62
1:A:520:ALA:HB1	1:A:688:HIS:O	1.98	0.62
1:B:516:GLY:HA2	2:B:802:NDP:H1B	1.80	0.62
1:A:138:VAL:HG12	1:A:140:VAL:CG1	2.30	0.62
1:B:314:TYR:CB	1:B:456:MET:CE	2.74	0.62
1:A:275:ILE:CG2	1:A:276:PRO:HD2	2.29	0.62
1:A:558:LEU:HB2	1:A:565:VAL:HG21	1.82	0.62
1:B:25:LEU:HD21	1:B:57:VAL:HG13	1.79	0.62
1:A:375:ARG:CG	1:A:375:ARG:HH11	2.06	0.61
1:A:383:PHE:HA	1:A:386:ALA:HB3	1.82	0.61
1:A:92:ASN:C	1:A:94:SER:H	2.04	0.61
1:A:691:ALA:O	1:A:694:LEU:HB2	2.00	0.61
1:A:8:TRP:O	1:A:169:HIS:HD2	1.83	0.61
1:B:180:ASP:C	1:B:180:ASP:OD1	2.38	0.61
1:A:120:LEU:CD2	1:A:124:LEU:HD13	2.31	0.61
1:B:179:ASP:OD2	1:B:179:ASP:C	2.38	0.61
1:B:387:THR:CG2	1:B:390:ARG:HB3	2.31	0.61
1:A:92:ASN:HD22	1:A:93:GLU:H	1.49	0.60
1:B:72:ARG:HH12	1:B:611:VAL:CG1	2.12	0.60
1:A:266:ALA:HB1	1:A:267:PRO:CD	2.31	0.60
1:B:691:ALA:CA	1:B:692:SER:HB2	2.30	0.60
1:A:633:ASP:OD2	1:A:634:PRO:CD	2.50	0.60
1:A:98:LEU:HD13	1:A:124:LEU:HD22	1.82	0.60
1:B:124:LEU:O	1:B:128:GLN:HG3	2.01	0.60
1:B:375:ARG:NH1	2:B:801:NDP:O1X	2.34	0.60
1:A:275:ILE:HG22	1:A:276:PRO:HD2	1.84	0.60
1:A:452:ARG:O	1:A:456:MET:HG3	2.01	0.60
1:A:138:VAL:HG12	1:A:140:VAL:HG13	1.83	0.60
1:B:150:LEU:O	1:B:153:VAL:HB	2.01	0.60
1:B:8:TRP:CB	1:B:106:VAL:HG13	2.32	0.60
1:B:24:LEU:HD22	1:B:58:ILE:HB	1.83	0.60
1:B:444:ASP:HA	2:B:801:NDP:O7N	2.02	0.60
1:A:143:PRO:O	1:A:144:ALA:CB	2.48	0.59
1:B:164:ARG:O	1:B:167:GLY:CA	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:LEU:HD22	1:B:25:LEU:N	2.14	0.59
1:B:570:CYS:SG	1:B:577:THR:HG22	2.42	0.59
1:B:521:LEU:HD13	1:B:685:TRP:CE2	2.37	0.59
1:B:216:GLY:O	1:B:217:ASP:CB	2.38	0.59
1:A:177:GLY:HA2	1:A:180:ASP:N	2.17	0.59
1:A:147:LEU:HB2	1:A:148:PRO:CD	2.32	0.59
1:A:33:ASP:O	1:A:34:ILE:HG13	2.03	0.59
1:B:164:ARG:O	1:B:167:GLY:N	2.35	0.59
1:A:314:TYR:N	1:A:456:MET:CE	2.65	0.59
1:A:489:LEU:CD2	1:A:494:HIS:CE1	2.86	0.59
1:B:521:LEU:HD21	2:B:802:NDP:N7N	2.18	0.59
1:A:289:MET:HE1	1:A:453:ILE:HD13	1.85	0.59
1:A:124:LEU:HB3	1:A:137:LEU:HD21	1.84	0.58
1:A:655:ASN:H	1:A:655:ASN:ND2	2.00	0.58
1:B:381:GLN:HG3	1:B:382:GLN:H	1.68	0.58
1:B:507:ASP:HB3	1:B:592:THR:CG2	2.27	0.58
1:A:249:SER:HA	1:A:275:ILE:O	2.03	0.58
1:B:541:VAL:HG23	1:B:570:CYS:HB3	1.86	0.58
1:B:88:ASP:O	1:B:89:GLN:HB2	2.04	0.58
1:A:52:GLU:HG2	1:A:53:PRO:HD2	1.86	0.57
1:A:147:LEU:HB2	1:A:148:PRO:HD3	1.86	0.57
1:A:343:GLN:NE2	1:A:470:GLU:H	2.00	0.57
1:B:645:SER:O	1:B:649:GLY:HA2	2.04	0.57
1:A:336:GLY:HA2	1:A:472:LEU:HD12	1.85	0.57
1:A:617:VAL:CG1	1:A:656:TYR:HA	2.34	0.57
1:A:642:SER:HA	1:A:660:ASN:OD1	2.05	0.57
1:B:8:TRP:CH2	1:B:104:VAL:HG11	2.39	0.57
1:A:21:SER:HB2	1:A:55:GLY:H	1.70	0.57
1:A:308:VAL:CG1	1:A:336:GLY:O	2.52	0.57
1:A:308:VAL:HG12	1:A:337:VAL:CA	2.34	0.57
1:B:150:LEU:CD2	1:B:151:PRO:CA	2.78	0.57
1:B:27:THR:CB	1:B:28:SER:HA	2.35	0.57
1:B:407:SER:O	1:B:410:MET:HB2	2.05	0.57
1:A:418:LEU:HB3	1:A:443:PHE:CE1	2.38	0.57
1:B:24:LEU:C	1:B:25:LEU:HD22	2.24	0.57
1:B:21:SER:HB2	1:B:55:GLY:H	1.70	0.57
1:B:27:THR:H	1:B:28:SER:HB3	1.70	0.56
1:B:380:GLU:OE2	1:B:409:ARG:HD2	2.05	0.56
1:A:140:VAL:O	1:A:140:VAL:CG2	2.53	0.56
1:A:314:TYR:CA	1:A:456:MET:CE	2.83	0.56
1:B:182:LEU:HD12	1:B:183:PRO:N	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:VAL:O	1:A:497:LYS:HE2	2.05	0.56
1:A:305:VAL:O	1:A:309:PHE:HD2	1.88	0.56
1:B:150:LEU:HD21	1:B:154:LEU:HD11	1.87	0.56
1:A:231:PHE:HA	1:A:489:LEU:HD11	1.87	0.56
1:B:668:GLN:C	1:B:668:GLN:HE21	2.08	0.56
1:A:380:GLU:O	1:A:384:LEU:CG	2.53	0.56
1:B:387:THR:HG22	1:B:390:ARG:H	1.71	0.56
1:B:96:LEU:CD2	1:B:97:LEU:N	2.69	0.56
1:A:208:GLU:OE1	1:A:210:THR:N	2.34	0.55
1:A:515:THR:OG1	1:A:596:HIS:HD2	1.89	0.55
1:A:150:LEU:HD23	1:A:154:LEU:HD12	1.87	0.55
1:B:164:ARG:O	1:B:167:GLY:HA2	2.07	0.55
1:A:215:LEU:HD21	1:A:221:ARG:HB2	1.87	0.55
1:A:528:HIS:O	1:A:533:ARG:HG2	2.07	0.55
1:A:126:SER:CB	1:A:654:GLY:HA2	2.36	0.55
1:B:24:LEU:C	1:B:25:LEU:CD2	2.75	0.55
1:A:140:VAL:O	1:A:140:VAL:HG23	2.06	0.55
1:A:390:ARG:HB3	1:A:413:ARG:HG3	1.89	0.55
1:A:575:ARG:NE	1:A:627:ASN:OD1	2.38	0.55
1:B:182:LEU:CD1	1:B:183:PRO:HD2	2.36	0.55
1:A:98:LEU:HD13	1:A:124:LEU:CD2	2.36	0.55
1:B:214:PRO:HA	1:B:221:ARG:NH2	2.21	0.55
1:B:25:LEU:HD21	1:B:57:VAL:HG12	1.88	0.55
1:B:96:LEU:HD22	1:B:97:LEU:N	2.22	0.54
1:A:384:LEU:CD2	1:A:410:MET:CE	2.85	0.54
1:B:177:GLY:CA	1:B:179:ASP:HB2	2.37	0.54
1:B:668:GLN:O	1:B:668:GLN:NE2	2.35	0.54
1:B:467:ARG:NH1	1:B:467:ARG:HB2	2.16	0.54
1:B:150:LEU:O	1:B:150:LEU:HD23	2.05	0.54
1:B:621:LYS:HD2	1:B:663:LEU:HD11	1.88	0.54
1:A:272:MET:HE1	1:A:305:VAL:HG11	1.89	0.54
1:A:127:THR:HG22	1:A:606:SER:OG	2.08	0.54
1:A:384:LEU:HD21	1:A:410:MET:CE	2.34	0.54
1:B:23:VAL:CG2	1:B:57:VAL:HG22	2.38	0.54
1:A:207:ASP:OD2	1:A:207:ASP:C	2.46	0.54
1:B:30:VAL:HG13	1:B:32:ALA:N	2.20	0.54
1:A:249:SER:O	1:A:250:GLU:HB3	2.08	0.53
1:B:230:ASN:OD1	1:B:307:ILE:HG21	2.08	0.53
1:B:744:ILE:HG13	1:B:744:ILE:O	2.07	0.53
1:B:153:VAL:HG12	1:B:154:LEU:HG	1.90	0.53
1:A:207:ASP:OD2	1:A:208:GLU:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:GLN:NE2	1:A:455:GLU:OE2	2.39	0.53
1:B:331:HIS:HD2	1:B:355:THR:OG1	1.91	0.53
1:B:521:LEU:HD21	2:B:802:NDP:H71N	1.74	0.53
1:B:58:ILE:HG22	1:B:60:PRO:HD3	1.91	0.53
1:A:308:VAL:HG11	1:A:336:GLY:CA	2.39	0.53
1:B:23:VAL:HG23	1:B:57:VAL:HG13	1.91	0.53
1:A:220:VAL:HG23	1:A:258:THR:HG22	1.90	0.53
1:A:313:TYR:CD1	1:A:456:MET:HE2	2.41	0.53
1:A:182:LEU:HD12	1:A:183:PRO:HD2	1.91	0.52
1:A:680:LEU:HD12	1:A:682:TRP:CZ2	2.44	0.52
1:B:191:ARG:CZ	1:B:277:LYS:HD3	2.39	0.52
1:B:232:ARG:NH2	1:B:245:ALA:CB	2.71	0.52
1:B:72:ARG:NH1	1:B:611:VAL:HG13	2.23	0.52
1:A:184:VAL:HG12	1:A:186:ASP:N	2.05	0.52
1:A:404:ALA:O	1:A:407:SER:HB2	2.09	0.52
1:A:618:LEU:HD22	1:A:622:VAL:HG21	1.92	0.52
1:B:515:THR:OG1	1:B:596:HIS:HD2	1.93	0.52
1:A:628:LEU:O	1:A:632:ILE:HB	2.10	0.52
1:B:88:ASP:OD2	1:B:88:ASP:C	2.48	0.52
1:A:120:LEU:HD21	1:A:124:LEU:CD1	2.39	0.52
1:A:222:ILE:HG21	1:A:224:MET:SD	2.50	0.52
1:A:295:ALA:HB3	1:A:297:TRP:CD1	2.45	0.52
1:A:336:GLY:HA2	1:A:472:LEU:HD11	1.88	0.52
1:B:190:TRP:O	1:B:281:PRO:HD2	2.10	0.52
1:B:691:ALA:HB1	1:B:692:SER:CB	2.35	0.52
1:B:704:ARG:HD2	1:B:704:ARG:N	2.25	0.52
1:B:150:LEU:CB	1:B:151:PRO:HD3	2.39	0.51
1:B:513:LEU:HD23	1:B:514:VAL:N	2.24	0.51
1:A:162:ALA:HB1	1:A:164:ARG:NH1	2.25	0.51
1:A:288:ARG:NH2	1:A:450:PRO:HB2	2.25	0.51
1:A:81:LEU:HD13	1:A:96:LEU:HD21	1.92	0.51
1:B:150:LEU:CD2	1:B:151:PRO:HA	2.39	0.51
1:A:541:VAL:HG22	1:A:570:CYS:HB3	1.93	0.51
1:B:633:ASP:OD2	1:B:634:PRO:CD	2.58	0.51
1:B:88:ASP:CG	1:B:90:ARG:HD2	2.31	0.51
1:A:48:ASP:HA	1:A:90:ARG:NH2	2.26	0.51
1:B:390:ARG:HG2	1:B:413:ARG:NH1	2.25	0.51
1:B:642:SER:HA	1:B:660:ASN:OD1	2.10	0.51
1:A:249:SER:O	1:A:250:GLU:CB	2.58	0.51
1:A:384:LEU:N	1:A:384:LEU:HD22	2.22	0.51
1:B:164:ARG:NH1	1:B:164:ARG:HG2	2.21	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:602:ASP:OD2	1:B:613:ARG:HD2	2.11	0.51
1:A:160:GLN:O	1:A:161:LEU:HD23	2.10	0.51
1:A:670:ARG:HD3	1:A:677:THR:OG1	2.10	0.51
1:A:632:ILE:HG23	1:A:633:ASP:O	2.11	0.51
1:A:382:GLN:O	1:A:386:ALA:N	2.44	0.50
1:B:88:ASP:OD2	1:B:90:ARG:CD	2.59	0.50
1:A:744:ILE:HG13	1:A:744:ILE:O	2.12	0.50
1:B:23:VAL:HG22	1:B:57:VAL:HG22	1.93	0.50
1:A:103:ALA:HB2	1:A:117:GLN:HB3	1.93	0.50
1:B:141:PRO:HD3	1:B:163:LEU:O	2.11	0.50
1:A:543:ARG:N	2:A:802:NDP:O3X	2.39	0.50
1:B:431:VAL:HG11	1:B:440:TYR:HB2	1.92	0.50
1:A:382:GLN:O	1:A:386:ALA:HB2	2.11	0.50
1:B:396:LEU:HD22	1:B:420:LEU:CD1	2.39	0.50
1:A:703:ALA:O	1:A:706:GLY:N	2.44	0.50
1:A:381:GLN:O	1:A:385:GLY:HA3	2.12	0.49
1:B:224:MET:HB2	1:B:280:GLY:O	2.12	0.49
1:B:520:ALA:HB3	2:B:802:NDP:O1N	2.11	0.49
1:A:177:GLY:HA2	1:A:180:ASP:H	1.76	0.49
1:A:13:LEU:HD21	1:A:168:ALA:CB	2.42	0.49
1:A:364:VAL:HG12	1:A:366:LEU:HB2	1.93	0.49
1:A:150:LEU:HB3	1:A:151:PRO:HD3	1.94	0.49
1:A:705:SER:O	1:A:707:LEU:HG	2.12	0.49
1:A:377:CYS:HA	1:A:379:PHE:CE1	2.47	0.49
1:B:387:THR:HG22	1:B:390:ARG:HB3	1.93	0.49
1:B:390:ARG:NH2	1:B:393:ASP:OD2	2.45	0.49
1:B:305:VAL:HB	1:B:306:PRO:HD3	1.93	0.49
1:B:467:ARG:CB	1:B:467:ARG:HH11	2.19	0.49
1:B:8:TRP:CZ2	1:B:104:VAL:HG13	2.47	0.49
1:A:587:ASP:OD1	1:A:587:ASP:N	2.46	0.49
1:B:179:ASP:O	1:B:180:ASP:OD1	2.30	0.49
1:B:687:GLU:CG	1:B:687:GLU:O	2.58	0.49
1:A:737:ARG:HG3	1:A:737:ARG:HH11	1.78	0.49
1:A:180:ASP:O	1:A:180:ASP:OD2	2.31	0.49
1:A:234:ALA:HB2	1:A:489:LEU:HD12	1.95	0.49
1:A:555:VAL:O	1:A:556:ALA:C	2.51	0.49
1:A:633:ASP:OD2	1:A:634:PRO:N	2.46	0.48
1:A:6:LEU:HD13	1:A:647:VAL:HG13	1.95	0.48
1:B:106:VAL:HG11	1:B:169:HIS:CD2	2.48	0.48
1:B:314:TYR:HB2	1:B:456:MET:HE3	1.79	0.48
1:A:120:LEU:CD2	1:A:124:LEU:CD1	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:GLU:O	1:A:688:HIS:CB	2.56	0.48
1:B:182:LEU:HG	1:B:205:LEU:HG	1.96	0.48
1:A:314:TYR:CE1	1:A:448:ALA:CB	2.88	0.48
1:A:633:ASP:OD2	1:A:633:ASP:C	2.51	0.48
1:B:180:ASP:O	1:B:181:VAL:HG22	2.13	0.48
1:B:216:GLY:O	1:B:218:GLY:HA2	2.11	0.48
1:B:308:VAL:HG22	1:B:337:VAL:CA	2.40	0.48
1:B:76:ARG:C	1:B:76:ARG:HD2	2.34	0.48
1:A:56:VAL:HG21	1:A:154:LEU:HD11	1.96	0.48
1:B:145:GLN:HA	1:B:148:PRO:HG3	1.96	0.48
1:A:230:ASN:OD1	1:A:307:ILE:HG21	2.14	0.48
1:B:390:ARG:HG2	1:B:413:ARG:CZ	2.43	0.48
1:B:8:TRP:CZ2	1:B:104:VAL:CG1	2.96	0.48
1:B:147:LEU:HG	1:B:147:LEU:H	1.37	0.48
1:B:68:THR:OG1	1:B:626:ARG:HG3	2.14	0.48
1:A:307:ILE:HG22	1:A:308:VAL:N	2.29	0.48
1:A:29:GLU:H	1:A:29:GLU:HG3	1.38	0.48
1:A:479:VAL:HG22	1:A:501:THR:O	2.14	0.48
1:B:126:SER:OG	1:B:651:GLY:HA2	2.14	0.48
1:A:208:GLU:OE2	1:A:277:LYS:NZ	2.46	0.47
1:A:150:LEU:HD23	1:A:150:LEU:O	2.14	0.47
1:A:489:LEU:HD22	1:A:494:HIS:CE1	2.48	0.47
1:B:513:LEU:HD21	1:B:541:VAL:HG12	1.96	0.47
1:B:518:THR:CG2	1:B:518:THR:O	2.62	0.47
1:A:179:ASP:O	1:A:180:ASP:OD1	2.32	0.47
1:A:571:ASP:C	1:A:571:ASP:OD1	2.52	0.47
1:A:737:ARG:HG3	1:A:737:ARG:NH1	2.29	0.47
1:B:737:ARG:HG3	1:B:737:ARG:NH1	2.29	0.47
1:A:366:LEU:HD22	1:A:370:HIS:HB2	1.96	0.47
1:B:390:ARG:NH2	1:B:393:ASP:OD1	2.48	0.47
1:A:246:SER:HB3	1:A:277:LYS:HG2	1.97	0.47
1:A:343:GLN:HE22	1:A:470:GLU:H	1.61	0.47
1:A:78:ALA:O	1:A:82:VAL:HG23	2.15	0.47
1:A:389:GLY:HA2	1:A:391:GLY:N	2.30	0.47
1:B:534:GLY:HA2	1:B:536:ARG:HH21	1.80	0.47
1:A:335:GLY:O	1:A:339:MET:HG3	2.15	0.47
1:B:633:ASP:OD2	1:B:633:ASP:C	2.52	0.47
1:A:162:ALA:HB1	1:A:164:ARG:HH12	1.80	0.47
1:A:617:VAL:HG11	1:A:656:TYR:CA	2.42	0.47
1:B:148:PRO:CD	1:B:149:ALA:H	2.27	0.47
1:B:67:ARG:HG3	3:B:803:SO4:O1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ARG:CZ	1:A:193:GLU:HB2	2.44	0.47
1:A:210:THR:HG21	1:A:277:LYS:NZ	2.30	0.47
1:B:212:THR:OG1	1:B:213:ALA:N	2.48	0.47
1:B:671:GLN:O	1:B:674:GLY:N	2.43	0.47
1:B:96:LEU:HD23	1:B:97:LEU:H	1.79	0.47
1:A:98:LEU:CD2	1:A:124:LEU:HD11	2.43	0.46
1:B:571:ASP:OD1	1:B:571:ASP:C	2.53	0.46
1:A:305:VAL:HG12	1:A:306:PRO:N	2.28	0.46
1:A:327:SER:HB3	1:A:351:GLU:HB3	1.96	0.46
1:B:179:ASP:O	1:B:180:ASP:CG	2.54	0.46
1:B:191:ARG:NH2	1:B:277:LYS:HD3	2.30	0.46
1:B:46:ALA:O	1:B:51:ALA:CB	2.63	0.46
1:A:107:GLU:HB2	1:A:110:GLU:OE2	2.16	0.46
1:A:8:TRP:HA	1:A:170:ALA:O	2.15	0.46
1:B:7:SER:O	1:B:171:PRO:HA	2.15	0.46
1:B:310:LEU:HD23	1:B:460:LEU:HD11	1.96	0.46
1:B:549:SER:HA	1:B:550:GLY:HA2	1.70	0.46
1:A:272:MET:CE	1:A:305:VAL:HG11	2.45	0.46
1:A:177:GLY:CA	1:A:180:ASP:H	2.29	0.46
1:A:578:LEU:HA	1:A:578:LEU:HD23	1.85	0.46
1:B:107:GLU:HB3	1:B:493:ARG:HH22	1.80	0.46
1:B:88:ASP:OD1	1:B:90:ARG:HD2	2.16	0.46
1:A:56:VAL:HG21	1:A:154:LEU:CD1	2.46	0.46
1:B:343:GLN:HE22	1:B:470:GLU:N	2.07	0.46
1:B:375:ARG:CG	1:B:375:ARG:NH1	2.74	0.46
1:A:13:LEU:HD21	1:A:168:ALA:HB2	1.98	0.46
1:A:311:THR:HA	1:A:445:THR:CG2	2.46	0.45
2:A:801:NDP:N3A	2:A:801:NDP:H2B	2.31	0.45
1:B:342:ILE:HG12	1:B:352:VAL:HG11	1.97	0.45
1:A:19:PRO:HA	1:A:20:PRO:HD3	1.71	0.45
1:A:655:ASN:ND2	1:A:656:TYR:H	2.13	0.45
1:B:411:LEU:HD23	1:B:415:GLY:CA	2.45	0.45
1:B:467:ARG:HG3	1:B:467:ARG:O	2.17	0.45
1:A:177:GLY:HA3	1:A:178:SER:C	2.35	0.45
1:B:53:PRO:HA	1:B:54:PRO:HD2	1.80	0.45
1:B:96:LEU:CD2	1:B:96:LEU:C	2.83	0.45
1:A:227:ALA:HA	1:A:251:GLY:HA2	1.98	0.45
1:A:231:PHE:HE2	1:A:235:LEU:HD21	1.81	0.45
1:A:383:PHE:HA	1:A:386:ALA:CB	2.45	0.45
1:A:687:GLU:OE1	1:A:687:GLU:O	2.34	0.45
1:B:182:LEU:CD1	1:B:183:PRO:CD	2.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:SER:O	1:A:706:GLY:C	2.54	0.45
1:B:273:GLY:CA	1:B:290:VAL:HG12	2.45	0.45
1:A:515:THR:OG1	1:A:596:HIS:HA	2.17	0.45
1:B:255:VAL:HG12	1:B:267:PRO:HA	1.98	0.45
1:B:554:LEU:HG	1:B:690:MET:CE	2.45	0.45
1:A:384:LEU:O	1:A:387:THR:O	2.34	0.45
1:B:88:ASP:OD2	1:B:90:ARG:N	2.35	0.45
1:B:13:LEU:HD21	1:B:168:ALA:HB2	1.99	0.45
1:B:387:THR:HG22	1:B:390:ARG:CB	2.46	0.45
1:B:331:HIS:CD2	1:B:355:THR:OG1	2.69	0.45
1:A:602:ASP:OD1	1:A:603:ASP:N	2.49	0.44
1:B:19:PRO:HB3	1:B:151:PRO:HG3	1.99	0.44
1:A:221:ARG:HG3	1:A:284:VAL:HB	1.99	0.44
1:A:543:ARG:CB	2:A:802:NDP:O3X	2.57	0.44
1:B:304:SER:OG	1:B:497:LYS:HB3	2.17	0.44
1:B:355:THR:HB	1:B:374:SER:HB3	1.98	0.44
1:B:313:TYR:CD1	1:B:456:MET:HG2	2.52	0.44
1:B:308:VAL:CG2	1:B:336:GLY:C	2.86	0.44
1:B:314:TYR:HB2	1:B:456:MET:HE1	1.95	0.44
1:A:326:GLU:CD	1:A:416:ARG:HH22	2.20	0.44
1:A:67:ARG:O	1:A:70:ASP:HB2	2.18	0.44
1:B:8:TRP:HB2	1:B:106:VAL:HG13	1.99	0.44
1:A:247:LEU:O	1:A:277:LYS:HA	2.18	0.44
1:A:482:ALA:N	1:A:483:PRO:CD	2.81	0.44
1:A:98:LEU:HD22	1:A:124:LEU:HD13	2.00	0.44
1:A:22:CYS:O	1:A:34:ILE:HG23	2.17	0.44
1:B:163:LEU:O	1:B:164:ARG:NH1	2.48	0.44
1:B:308:VAL:HG21	1:B:336:GLY:C	2.38	0.44
1:B:387:THR:HG22	1:B:390:ARG:N	2.33	0.44
1:B:479:VAL:C	1:B:481:GLN:H	2.21	0.44
1:B:158:GLU:CG	1:B:161:LEU:HD21	2.47	0.44
1:B:280:GLY:HA2	1:B:502:MET:CE	2.48	0.44
1:B:318:ASP:OD1	1:B:452:ARG:NH1	2.51	0.43
1:B:411:LEU:HD12	1:B:411:LEU:N	2.33	0.43
1:B:690:MET:O	1:B:691:ALA:O	2.35	0.43
1:A:322:LEU:HD11	1:A:328:LEU:HG	2.00	0.43
1:A:308:VAL:CG1	1:A:337:VAL:CA	2.96	0.43
1:A:631:LEU:HD23	1:A:631:LEU:HA	1.80	0.43
1:B:106:VAL:CG1	1:B:169:HIS:CD2	3.01	0.43
1:B:737:ARG:HH11	1:B:737:ARG:HG3	1.83	0.43
1:A:144:ALA:HA	1:A:147:LEU:CD1	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:LEU:HD23	1:B:97:LEU:N	2.33	0.43
1:A:250:GLU:HA	1:A:273:GLY:O	2.18	0.43
1:A:323:ARG:O	1:A:326:GLU:HB2	2.17	0.43
1:A:390:ARG:HB2	1:A:413:ARG:HG2	1.86	0.43
1:B:177:GLY:C	1:B:179:ASP:CA	2.79	0.43
1:B:232:ARG:HH21	1:B:245:ALA:HB1	1.80	0.43
1:B:475:THR:HB	1:B:498:LEU:HD22	2.00	0.43
1:A:406:ALA:HA	1:A:409:ARG:HH11	1.84	0.43
1:A:516:GLY:N	1:A:541:VAL:O	2.50	0.43
1:B:30:VAL:CG1	1:B:31:SER:N	2.81	0.43
1:A:335:GLY:O	1:A:339:MET:HB2	2.19	0.43
1:A:527:ARG:NH2	1:A:554:LEU:HD23	2.33	0.43
1:B:18:GLN:HA	1:B:19:PRO:HD2	1.85	0.43
1:B:216:GLY:O	1:B:219:GLU:N	2.51	0.43
1:A:375:ARG:CG	1:A:375:ARG:NH1	2.71	0.43
1:A:694:LEU:HA	1:A:694:LEU:HD23	1.87	0.43
1:A:262:VAL:HG13	1:A:287:HIS:CD2	2.54	0.43
1:A:560:ALA:C	1:A:562:GLY:H	2.22	0.43
1:A:231:PHE:HB3	2:A:801:NDP:H3D	2.00	0.43
1:B:30:VAL:HG13	1:B:31:SER:N	2.33	0.43
1:A:25:LEU:HG	1:A:57:VAL:CG1	2.49	0.42
1:B:182:LEU:HA	1:B:183:PRO:HD3	1.83	0.42
1:A:208:GLU:OE1	1:A:209:PRO:N	2.51	0.42
1:A:440:TYR:CD1	1:A:440:TYR:C	2.93	0.42
1:B:145:GLN:O	1:B:148:PRO:HG2	2.19	0.42
1:B:160:GLN:C	1:B:161:LEU:CD2	2.78	0.42
1:B:329:LEU:HA	1:B:353:TYR:O	2.20	0.42
1:B:57:VAL:O	1:B:96:LEU:HD23	2.19	0.42
1:A:20:PRO:O	1:A:21:SER:C	2.57	0.42
1:A:653:GLN:HB2	1:A:656:TYR:HB3	2.01	0.42
1:A:95:ARG:CG	1:A:95:ARG:NH1	2.56	0.42
1:B:704:ARG:HA	1:B:704:ARG:NE	2.34	0.42
1:A:687:GLU:O	1:A:687:GLU:CD	2.57	0.42
1:B:244:VAL:O	1:B:244:VAL:HG12	2.19	0.42
1:B:489:LEU:HD22	1:B:494:HIS:CE1	2.54	0.42
1:B:614:LEU:HD13	1:B:618:LEU:HD11	2.01	0.42
1:B:554:LEU:HB2	1:B:690:MET:CE	2.49	0.42
1:B:88:ASP:O	1:B:89:GLN:CB	2.68	0.42
1:A:46:ALA:O	1:A:51:ALA:HB3	2.20	0.42
1:A:669:GLN:O	1:A:673:ARG:HG2	2.19	0.42
1:B:231:PHE:HB3	2:B:801:NDP:H3D	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:ARG:HH21	1:B:554:LEU:HD23	1.83	0.42
1:B:690:MET:O	1:B:691:ALA:C	2.57	0.42
1:A:117:GLN:O	1:A:120:LEU:HB3	2.20	0.42
1:B:478:ASP:CG	1:B:480:ARG:HH21	2.23	0.42
1:A:28:SER:OG	1:A:29:GLU:HG3	2.19	0.42
1:A:305:VAL:N	1:A:306:PRO:CD	2.83	0.42
1:A:314:TYR:H	1:A:456:MET:HE2	1.84	0.42
1:B:177:GLY:CA	1:B:179:ASP:HA	2.50	0.42
1:B:304:SER:HA	1:B:497:LYS:HG2	2.02	0.42
1:A:176:LEU:HD23	1:A:176:LEU:HA	1.68	0.42
1:A:222:ILE:CG2	1:A:224:MET:SD	3.08	0.42
1:A:318:ASP:OD2	1:A:452:ARG:HD3	2.20	0.42
1:A:65:GLY:HA3	1:A:70:ASP:OD2	2.20	0.42
1:B:179:ASP:O	1:B:180:ASP:CB	2.67	0.42
1:B:308:VAL:HG22	1:B:337:VAL:N	2.35	0.42
1:B:72:ARG:HH11	1:B:611:VAL:HG13	1.84	0.42
1:A:58:ILE:HD11	1:A:150:LEU:HD11	2.02	0.42
1:B:145:GLN:C	1:B:148:PRO:CD	2.88	0.42
1:B:231:PHE:HA	1:B:489:LEU:HD11	2.02	0.42
1:B:645:SER:O	1:B:649:GLY:CA	2.68	0.42
1:B:304:SER:OG	1:B:497:LYS:HG2	2.20	0.42
1:B:126:SER:CB	1:B:654:GLY:HA2	2.50	0.42
1:A:215:LEU:HD22	1:A:284:VAL:HG21	2.02	0.41
1:A:380:GLU:O	1:A:384:LEU:HG	2.18	0.41
1:B:177:GLY:HA2	1:B:179:ASP:CB	2.45	0.41
1:B:355:THR:HA	1:B:372:ALA:O	2.20	0.41
1:A:150:LEU:CD2	1:A:154:LEU:HD12	2.50	0.41
1:A:427:ASP:HB3	1:A:430:GLU:HB2	2.02	0.41
1:A:54:PRO:O	1:A:94:SER:HB3	2.20	0.41
1:B:13:LEU:HA	1:B:14:PRO:HD2	1.89	0.41
1:B:427:ASP:OD2	1:B:430:GLU:HG3	2.20	0.41
1:B:606:SER:HA	1:B:609:LEU:HG	2.03	0.41
1:B:140:VAL:HA	1:B:141:PRO:HD3	1.84	0.41
1:B:479:VAL:C	1:B:481:GLN:N	2.72	0.41
1:A:109:GLY:HA3	1:A:488:HIS:NE2	2.35	0.41
1:A:390:ARG:HB3	1:A:413:ARG:HG2	1.94	0.41
1:A:427:ASP:O	1:A:431:VAL:HG23	2.20	0.41
1:A:542:SER:HA	2:A:802:NDP:N3A	2.35	0.41
1:A:633:ASP:CG	1:A:634:PRO:HD2	2.39	0.41
1:B:280:GLY:HA2	1:B:502:MET:HE1	2.02	0.41
1:B:392:VAL:O	1:B:411:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:GLU:HG3	1:A:159:PRO:HD2	2.02	0.41
1:A:310:LEU:HD21	1:A:457:LEU:HD23	2.01	0.41
1:B:266:ALA:HB1	1:B:267:PRO:HD2	2.00	0.41
1:B:307:ILE:HA	1:B:307:ILE:HD12	1.77	0.41
1:B:614:LEU:HD23	1:B:614:LEU:HA	1.92	0.41
1:A:692:SER:N	1:A:695:ARG:HG3	2.23	0.41
1:B:554:LEU:HB2	1:B:690:MET:HE2	2.02	0.41
1:B:25:LEU:CD2	1:B:58:ILE:O	2.64	0.41
1:B:96:LEU:HD22	1:B:96:LEU:C	2.40	0.41
1:A:17:ALA:O	1:A:19:PRO:HD3	2.20	0.41
1:A:266:ALA:O	1:A:269:ASP:HB2	2.21	0.41
1:A:489:LEU:HD22	1:A:494:HIS:HE1	1.85	0.41
1:A:85:TRP:CZ3	1:A:96:LEU:HD13	2.55	0.41
1:A:390:ARG:CB	1:A:413:ARG:HG3	2.47	0.41
1:A:689:GLY:O	1:A:690:MET:C	2.58	0.41
1:B:176:LEU:HA	1:B:176:LEU:HD23	1.85	0.41
1:B:479:VAL:HG11	1:B:502:MET:CE	2.50	0.41
1:A:383:PHE:C	1:A:386:ALA:H	2.24	0.41
1:B:164:ARG:H	1:B:167:GLY:HA2	1.86	0.41
1:A:95:ARG:HA	1:A:134:ARG:O	2.20	0.41
1:B:150:LEU:HD21	1:B:154:LEU:CD1	2.50	0.41
1:B:544:ARG:NH1	2:B:802:NDP:O2X	2.54	0.41
1:A:407:SER:O	1:A:410:MET:HB2	2.21	0.41
1:A:626:ARG:HE	1:A:626:ARG:HB3	1.68	0.41
1:A:6:LEU:HD21	1:A:171:PRO:HB2	2.03	0.41
1:B:8:TRP:HB3	1:B:106:VAL:HG13	2.03	0.40
1:B:179:ASP:OD2	1:B:179:ASP:O	2.39	0.40
1:B:126:SER:HB2	1:B:654:GLY:HA2	2.03	0.40
1:B:541:VAL:CG2	1:B:570:CYS:HB3	2.50	0.40
1:A:173:LEU:HA	1:A:173:LEU:HD23	1.79	0.40
1:A:529:LEU:HD12	1:A:529:LEU:HA	1.89	0.40
1:B:444:ASP:HA	2:B:801:NDP:H72N	1.86	0.40
1:A:232:ARG:CG	1:A:232:ARG:NH1	2.55	0.40
1:A:571:ASP:OD2	1:A:619:ARG:NH1	2.54	0.40
1:B:191:ARG:NH1	1:B:193:GLU:HB2	2.36	0.40
1:B:274:MET:HG2	1:B:307:ILE:HD12	2.01	0.40
1:B:543:ARG:NE	2:B:802:NDP:O3X	2.41	0.40
1:A:64:GLY:N	1:A:114:ASP:OD2	2.44	0.40
1:A:221:ARG:NH1	1:A:257:GLU:OE2	2.41	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:B:413:ARG:NH2	3:A:804:SO4:O1[2_564]	2.19	0.01

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	743/795 (94%)	657 (88%)	73 (10%)	13 (2%)	9	39
1	B	743/795 (94%)	684 (92%)	47 (6%)	12 (2%)	9	40
All	All	1486/1590 (94%)	1341 (90%)	120 (8%)	25 (2%)	9	39

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	ASP
1	A	691	ALA
1	B	217	ASP
1	B	691	ALA
1	A	295	ALA
1	B	467	ARG
1	A	20	PRO
1	A	93	GLU
1	A	187	GLY
1	A	688	HIS
1	B	414	GLY
1	B	480	ARG
1	A	181	VAL
1	A	250	GLU
1	A	369	GLU
1	A	692	SER
1	B	168	ALA
1	B	181	VAL
1	B	692	SER
1	A	556	ALA

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Mol	Chain	Res	Type
1	A	706	GLY
1	B	177	GLY
1	B	306	PRO
1	B	317	VAL
1	B	214	PRO

### 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	566/605 (94%)	460 (81%)	106 (19%)	1	8
1	B	566/605 (94%)	449 (79%)	117 (21%)	1	6
All	All	1132/1210 (94%)	909 (80%)	223 (20%)	1	7

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	11	VAL
1	A	12	GLN
1	A	13	LEU
1	A	24	LEU
1	A	27	THR
1	A	29	GLU
1	A	41	ARG
1	A	43	LEU
1	A	74	THR
1	A	77	HIS
1	A	79	LEU
1	A	81	LEU
1	A	92	ASN
1	A	94	SER
1	A	95	ARG
1	A	110	GLU
1	A	124	LEU

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Mol	Chain	Res	Type
1	A	126	SER
1	A	140	VAL
1	A	142	GLU
1	A	146	LEU
1	A	147	LEU
1	A	154	LEU
1	A	161	LEU
1	A	165	ARG
1	A	172	ARG
1	A	180	ASP
1	A	181	VAL
1	A	182	LEU
1	A	196	ARG
1	A	208	GLU
1	A	210	THR
1	A	212	THR
1	A	229	VAL
1	A	232	ARG
1	A	246	SER
1	A	249	SER
1	A	250	GLU
1	A	265	LEU
1	A	271	VAL
1	A	284	VAL
1	A	288	ARG
1	A	305	VAL
1	A	307	ILE
1	A	308	VAL
1	A	322	LEU
1	A	323	ARG
1	A	327	SER
1	A	328	LEU
1	A	332	SER
1	A	344	LEU
1	A	346	ARG
1	A	362	GLN
1	A	366	LEU
1	A	367	SER
1	A	368	ARG
1	A	371	LEU
1	A	381	GLN
1	A	384	LEU

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Mol	Chain	Res	Type
1	A	390	ARG
1	A	396	LEU
1	A	398	SER
1	A	411	LEU
1	A	413	ARG
1	A	422	LYS
1	A	426	ARG
1	A	433	ASP
1	A	444	ASP
1	A	446	VAL
1	A	459	GLU
1	A	467	ARG
1	A	468	VAL
1	A	470	GLU
1	A	477	TRP
1	A	479	VAL
1	A	489	LEU
1	A	513	LEU
1	A	524	GLU
1	A	529	LEU
1	A	541	VAL
1	A	554	LEU
1	A	559	THR
1	A	578	LEU
1	A	587	ASP
1	A	588	GLU
1	A	591	LEU
1	A	606	SER
1	A	612	GLU
1	A	614	LEU
1	A	623	ASP
1	A	638	LEU
1	A	650	SER
1	A	655	ASN
1	A	666	LEU
1	A	678	ARG
1	A	680	LEU
1	A	693	THR
1	A	701	ARG
1	A	704	ARG
1	A	705	SER
1	A	728	THR

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Mol	Chain	Res	Type
1	A	730	VAL
1	A	736	SER
1	A	744	ILE
1	A	747	SER
1	B	5	ARG
1	B	11	VAL
1	B	13	LEU
1	B	15	THR
1	B	24	LEU
1	B	25	LEU
1	B	27	THR
1	B	28	SER
1	B	30	VAL
1	B	34	ILE
1	B	41	ARG
1	B	43	LEU
1	B	67	ARG
1	B	72	ARG
1	B	74	THR
1	B	79	LEU
1	B	81	LEU
1	B	87	SER
1	B	88	ASP
1	B	90	ARG
1	B	92	ASN
1	B	93	GLU
1	B	94	SER
1	B	95	ARG
1	B	96	LEU
1	B	97	LEU
1	B	126	SER
1	B	142	GLU
1	B	146	LEU
1	B	147	LEU
1	B	150	LEU
1	B	153	VAL
1	B	154	LEU
1	B	158	GLU
1	B	172	ARG
1	B	178	SER
1	B	179	ASP
1	B	180	ASP

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Mol	Chain	Res	Type
1	B	181	VAL
1	B	182	LEU
1	B	188	THR
1	B	196	ARG
1	B	200	LEU
1	B	208	GLU
1	B	217	ASP
1	B	225	ARG
1	B	229	VAL
1	B	232	ARG
1	B	244	VAL
1	B	247	LEU
1	B	265	LEU
1	B	271	VAL
1	B	284	VAL
1	B	292	ARG
1	B	304	SER
1	B	307	ILE
1	B	308	VAL
1	B	323	ARG
1	B	328	LEU
1	B	329	LEU
1	B	344	LEU
1	B	359	ASP
1	B	362	GLN
1	B	367	SER
1	B	368	ARG
1	B	381	GLN
1	B	396	LEU
1	B	413	ARG
1	B	422	LYS
1	B	423	THR
1	B	433	ASP
1	B	452	ARG
1	B	459	GLU
1	B	463	LEU
1	B	467	ARG
1	B	475	THR
1	B	479	VAL
1	B	489	LEU
1	B	502	MET
1	B	518	THR

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Mol	Chain	Res	Type
1	B	521	LEU
1	B	532	GLU
1	B	535	VAL
1	B	536	ARG
1	B	538	LEU
1	B	540	LEU
1	B	544	ARG
1	B	557	GLN
1	B	559	THR
1	B	564	GLU
1	B	578	LEU
1	B	580	LYS
1	B	588	GLU
1	B	606	SER
1	B	612	GLU
1	B	614	LEU
1	B	619	ARG
1	B	623	ASP
1	B	629	LEU
1	B	630	GLU
1	B	632	ILE
1	B	633	ASP
1	B	638	LEU
1	B	642	SER
1	B	653	GLN
1	B	666	LEU
1	B	668	GLN
1	B	669	GLN
1	B	672	SER
1	B	692	SER
1	B	701	ARG
1	B	704	ARG
1	B	713	GLU
1	B	728	THR
1	B	730	VAL
1	B	736	SER
1	B	744	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN

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Mol	Chain	Res	Type
1	A	35	GLN
1	A	92	ASN
1	A	128	GLN
1	A	169	HIS
1	A	343	GLN
1	A	370	HIS
1	A	382	GLN
1	A	441	GLN
1	A	494	HIS
1	A	557	GLN
1	A	596	HIS
1	A	653	GLN
1	A	655	ASN
1	B	331	HIS
1	B	343	GLN
1	B	382	GLN
1	B	441	GLN
1	B	557	GLN
1	B	596	HIS

### 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 ⓘ

7 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	NDP	A	802	-	45,52,52	1.42	3 (6%)	53,80,80	1.47	10 (18%)
3	SO4	A	804	-	4,4,4	0.33	0	6,6,6	0.13	0
3	SO4	B	803	-	4,4,4	0.33	0	6,6,6	0.10	0
2	NDP	A	801	-	45,52,52	1.33	3 (6%)	53,80,80	1.31	2 (3%)
2	NDP	B	801	-	45,52,52	1.38	4 (8%)	53,80,80	1.50	4 (7%)
3	SO4	A	803	-	4,4,4	0.37	0	6,6,6	0.15	0
2	NDP	B	802	-	45,52,52	1.43	4 (8%)	53,80,80	1.46	7 (13%)

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	NDP	A	801	-	-	11/30/77/77	0/5/5/5
2	NDP	B	802	-	-	5/30/77/77	0/5/5/5
2	NDP	A	802	-	-	4/30/77/77	0/5/5/5
2	NDP	B	801	-	-	12/30/77/77	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	802	NDP	C4N-C3N	-5.91	1.38	1.49
2	A	802	NDP	C4N-C3N	-5.77	1.38	1.49
2	A	801	NDP	C4N-C3N	-5.64	1.38	1.49
2	B	801	NDP	C4N-C3N	-5.56	1.39	1.49
2	A	802	NDP	C4N-C5N	-4.01	1.38	1.48
2	B	802	NDP	C4N-C5N	-3.99	1.38	1.48
2	A	801	NDP	C4N-C5N	-3.76	1.39	1.48
2	B	801	NDP	C4N-C5N	-3.75	1.39	1.48
2	B	801	NDP	C6N-C5N	3.70	1.39	1.33
2	A	802	NDP	C6N-C5N	3.56	1.39	1.33
2	A	801	NDP	C6N-C5N	3.33	1.39	1.33
2	B	802	NDP	C6N-C5N	3.18	1.39	1.33
2	B	801	NDP	O4B-C1B	2.20	1.44	1.41
2	B	802	NDP	O4B-C1B	2.13	1.44	1.41

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	NDP	PN-O3-PA	-6.25	111.38	132.83
2	B	802	NDP	N3A-C2A-N1A	-4.98	120.90	128.68
2	A	801	NDP	N3A-C2A-N1A	-4.94	120.96	128.68
2	B	801	NDP	N3A-C2A-N1A	-4.84	121.11	128.68
2	A	802	NDP	N3A-C2A-N1A	-4.63	121.44	128.68
2	A	801	NDP	PN-O3-PA	-4.32	118.01	132.83
2	A	802	NDP	O3B-C3B-C2B	-3.35	101.64	111.17
2	B	801	NDP	O4D-C1D-N1N	3.25	114.41	108.06
2	B	802	NDP	PN-O3-PA	-3.16	121.99	132.83
2	A	802	NDP	O3B-C3B-C4B	-2.87	102.75	111.05
2	B	802	NDP	O3B-C3B-C2B	-2.78	103.28	111.17
2	A	802	NDP	PN-O3-PA	-2.75	123.40	132.83
2	B	802	NDP	O3B-C3B-C4B	-2.74	103.12	111.05
2	B	802	NDP	O4D-C1D-N1N	2.66	113.26	108.06
2	A	802	NDP	O2D-C2D-C3D	-2.45	103.89	111.82
2	B	802	NDP	C3N-C2N-N1N	-2.36	119.73	123.10
2	B	802	NDP	C2D-C1D-N1N	-2.31	107.52	113.30
2	A	802	NDP	O2N-PN-O1N	2.26	123.40	112.24
2	A	802	NDP	C3B-C2B-C1B	-2.24	98.67	102.89
2	B	801	NDP	O3X-P2B-O2X	2.15	115.85	107.64
2	A	802	NDP	C3N-C2N-N1N	-2.14	120.05	123.10
2	A	802	NDP	C2B-C3B-C4B	2.12	106.60	101.99
2	A	802	NDP	C4A-C5A-N7A	-2.05	107.27	109.40

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	NDP	C5B-O5B-PA-O1A
2	B	801	NDP	C5D-O5D-PN-O3
2	B	801	NDP	C5D-O5D-PN-O2N
2	B	801	NDP	O4D-C4D-C5D-O5D
2	A	802	NDP	O4D-C1D-N1N-C6N
2	B	802	NDP	O4D-C1D-N1N-C6N
2	B	801	NDP	C3D-C4D-C5D-O5D
2	A	801	NDP	C1B-C2B-O2B-P2B
2	B	801	NDP	O4D-C1D-N1N-C2N
2	A	801	NDP	O4D-C1D-N1N-C2N
2	B	801	NDP	PA-O3-PN-O1N
2	B	801	NDP	O4B-C4B-C5B-O5B
2	A	801	NDP	C4B-C5B-O5B-PA
2	B	801	NDP	C4B-C5B-O5B-PA
2	A	801	NDP	PA-O3-PN-O2N

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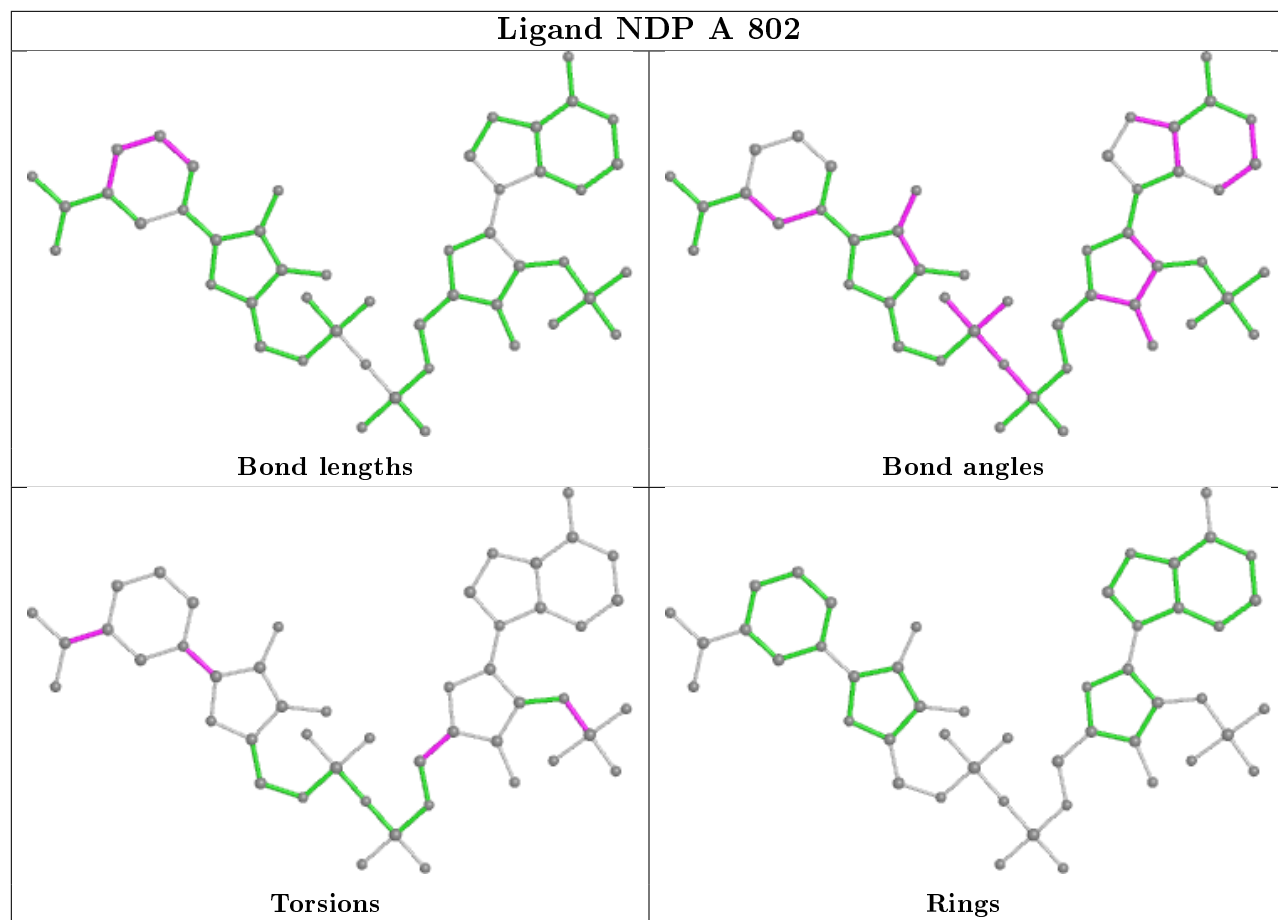
Mol	Chain	Res	Type	Atoms
2	B	801	NDP	C5D-O5D-PN-O1N
2	A	801	NDP	C3B-C2B-O2B-P2B
2	B	801	NDP	PA-O3-PN-O2N
2	B	802	NDP	O4B-C4B-C5B-O5B
2	A	801	NDP	PA-O3-PN-O1N
2	B	801	NDP	C3B-C4B-C5B-O5B
2	A	802	NDP	C2B-O2B-P2B-O1X
2	A	801	NDP	C2B-O2B-P2B-O1X
2	A	801	NDP	C5B-O5B-PA-O3
2	B	802	NDP	C5D-O5D-PN-O3
2	A	802	NDP	O4B-C4B-C5B-O5B
2	A	801	NDP	O4B-C4B-C5B-O5B
2	A	802	NDP	C2N-C3N-C7N-N7N
2	A	801	NDP	C2N-C3N-C7N-N7N
2	B	801	NDP	C2N-C3N-C7N-N7N
2	B	802	NDP	C5D-O5D-PN-O1N
2	B	802	NDP	C2N-C3N-C7N-N7N

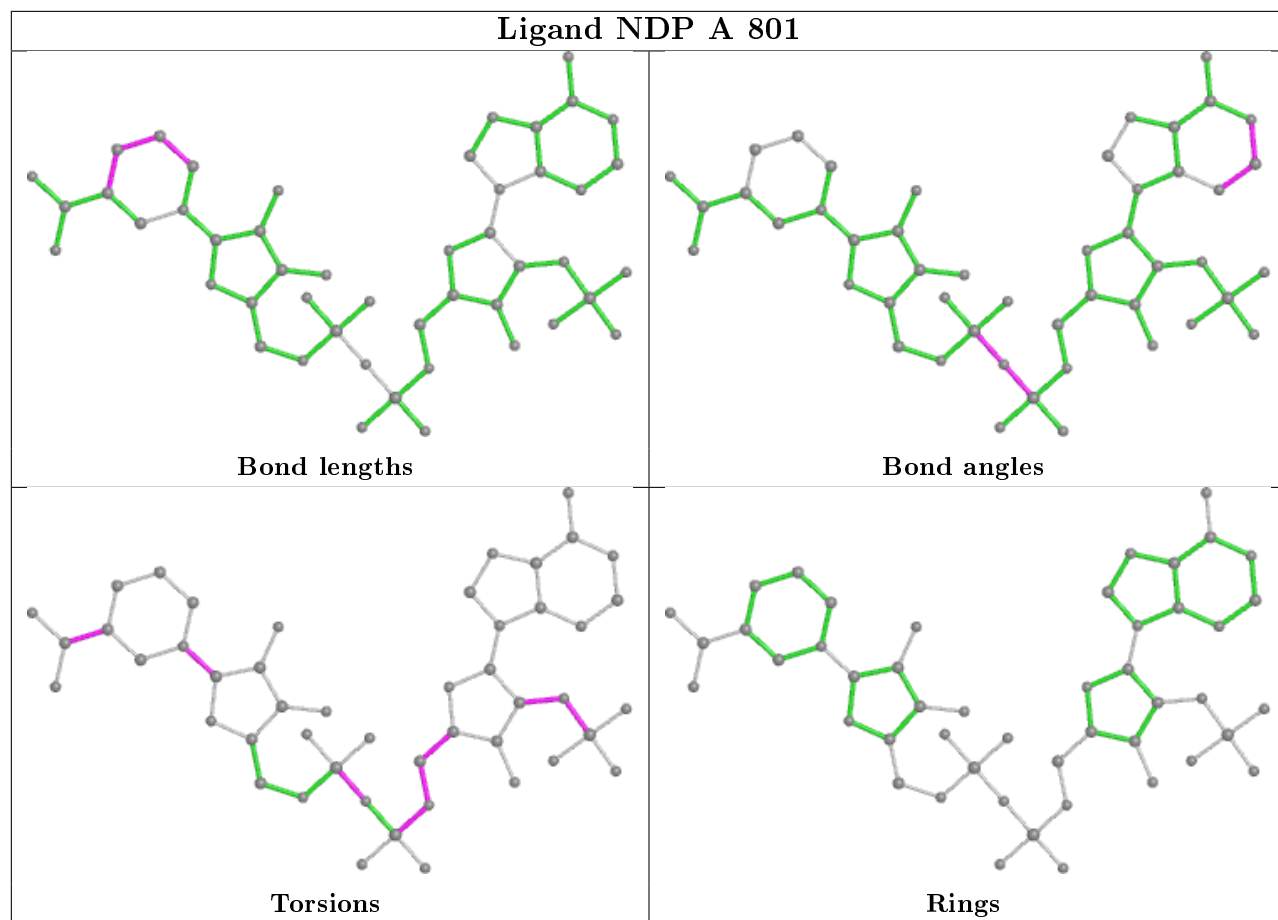
There are no ring outliers.

7 monomers are involved in 25 short contacts:

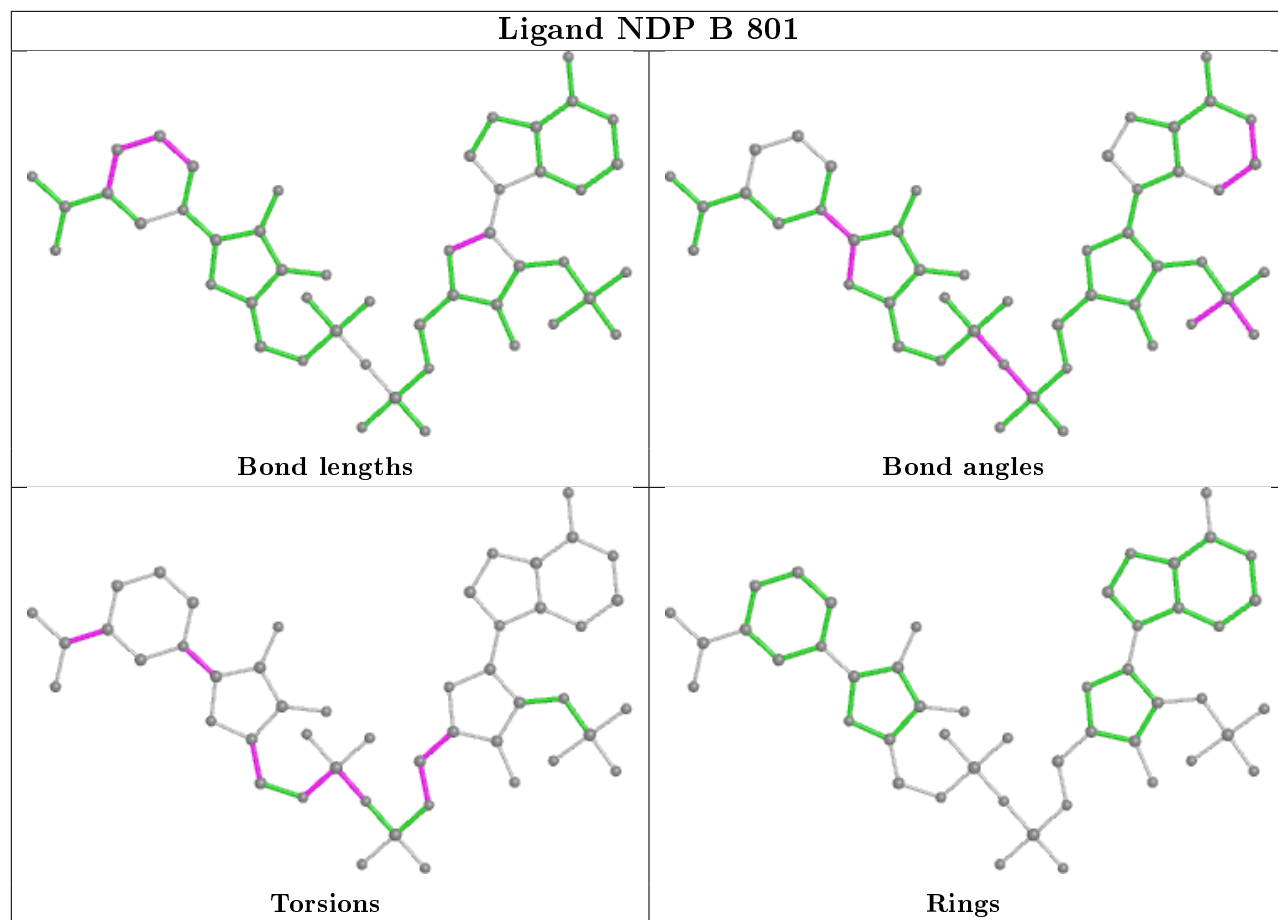
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	802	NDP	5	0
3	A	804	SO4	0	1
3	B	803	SO4	1	0
2	A	801	NDP	7	0
2	B	801	NDP	4	0
3	A	803	SO4	1	0
2	B	802	NDP	6	0

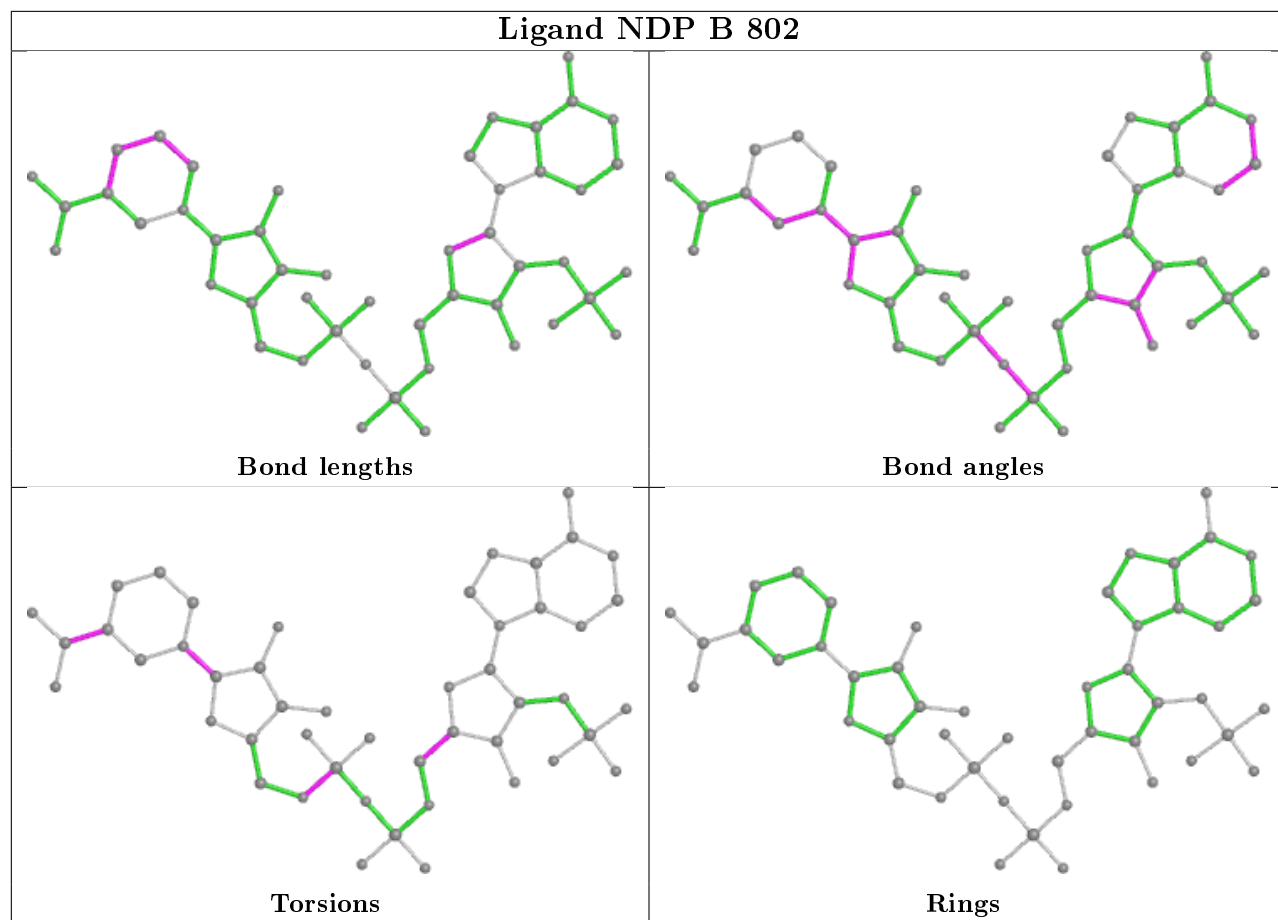
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	747/795 (93%)	-0.20	11 (1%) 73 46	33, 73, 145, 182	0
1	B	747/795 (93%)	-0.40	4 (0%) 91 75	36, 63, 112, 171	0
All	All	1494/1590 (93%)	-0.30	15 (1%) 82 59	33, 67, 136, 182	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	743	ALA	4.9
1	A	259	GLY	3.7
1	A	435	HIS	3.3
1	A	264	GLY	2.9
1	B	744	ILE	2.9
1	A	436	PRO	2.8
1	A	441	GLN	2.5
1	A	263	THR	2.5
1	A	738	LEU	2.5
1	A	267	PRO	2.5
1	A	744	ILE	2.4
1	B	738	LEU	2.2
1	B	27	THR	2.2
1	A	404	ALA	2.1
1	A	424	ASP	2.1

### 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](#)

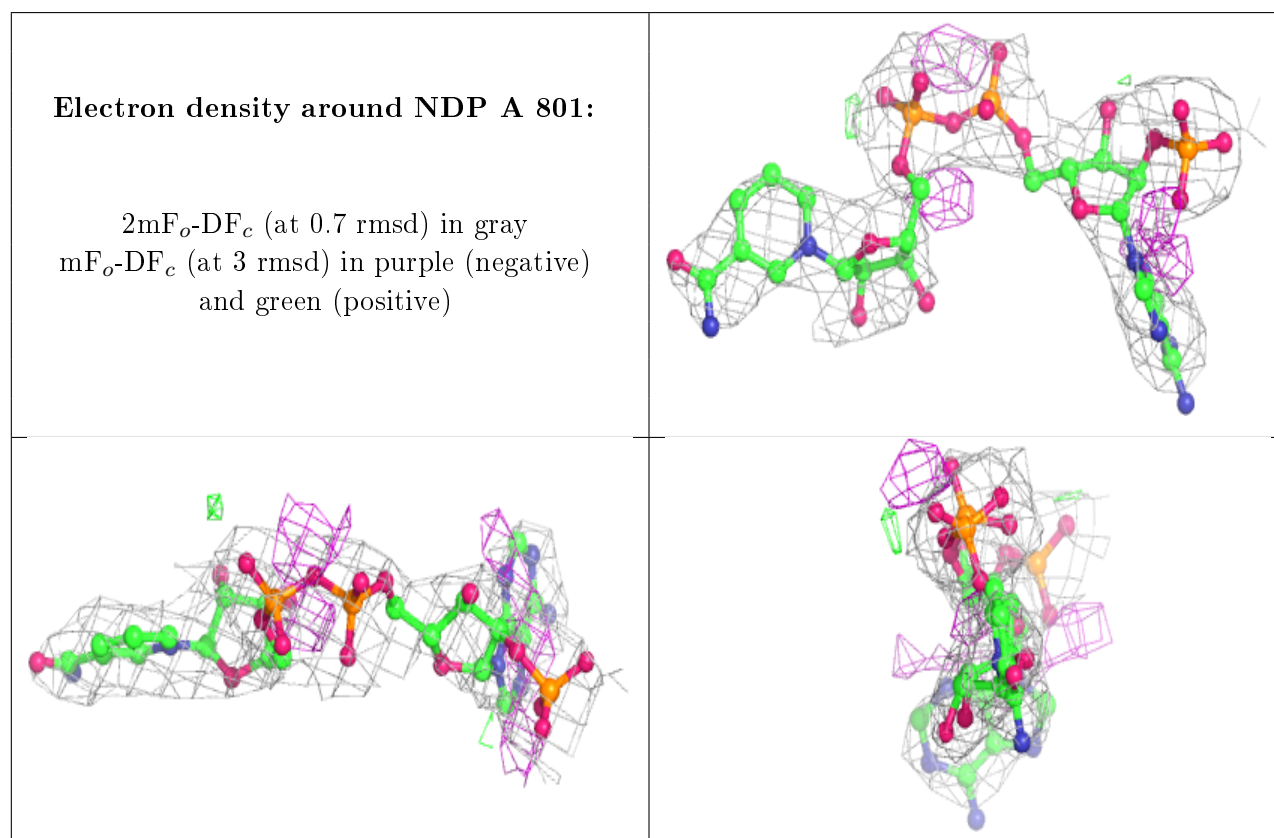
There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

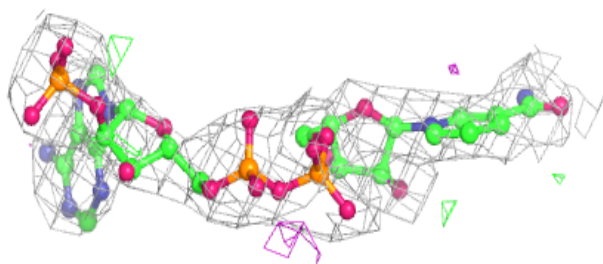
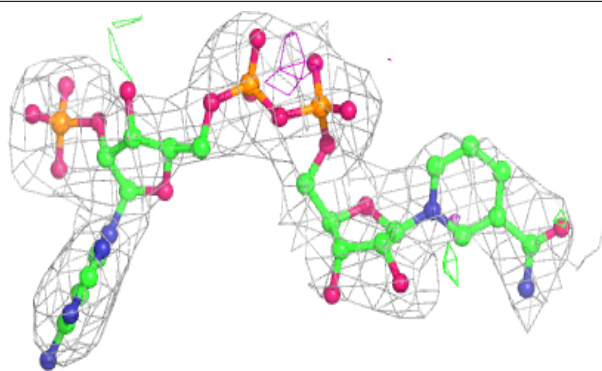
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NDP	A	801	48/48	0.91	0.25	83,100,111,119	0
3	SO4	B	803	5/5	0.92	0.17	69,69,94,111	0
2	NDP	B	801	48/48	0.94	0.21	64,83,95,98	0
3	SO4	A	804	5/5	0.98	0.09	42,45,47,48	0
2	NDP	A	802	48/48	0.98	0.13	25,31,37,40	0
2	NDP	B	802	48/48	0.98	0.11	24,29,34,40	0
3	SO4	A	803	5/5	0.99	0.17	25,27,33,36	0

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

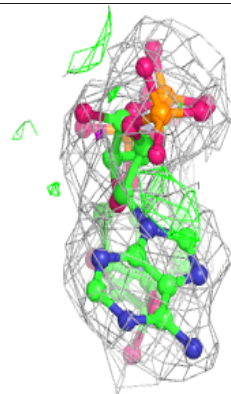
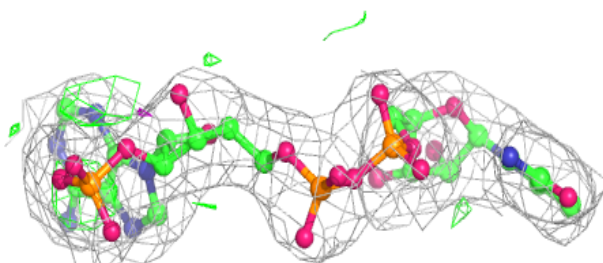
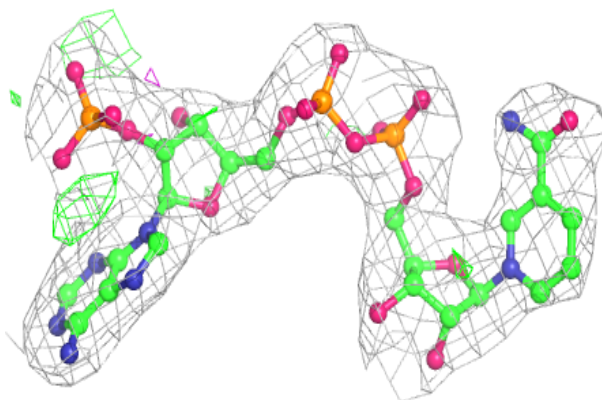


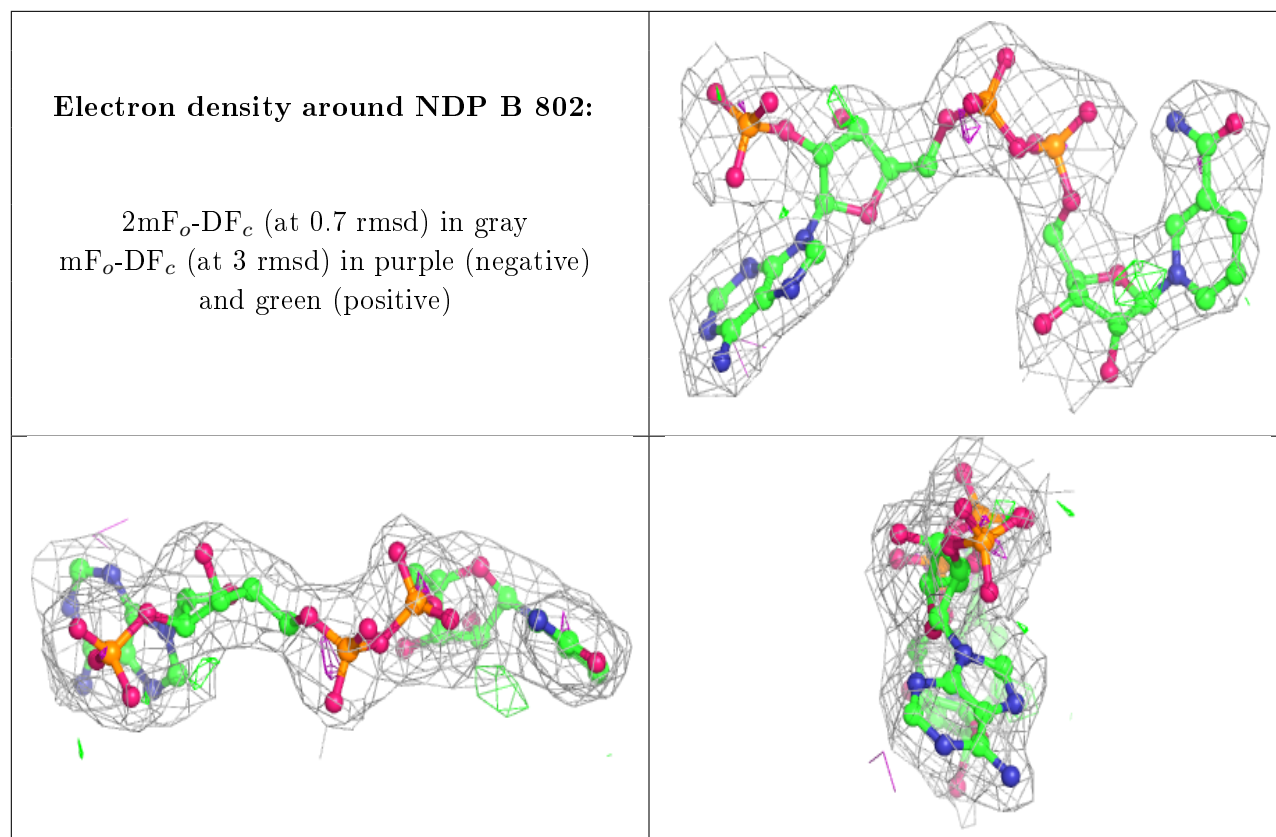
**Electron density around NDP B 801:**

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

**Electron density around NDP A 802:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.