



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:38 PM UTC

PDB ID : 3CSF / pdb\_00003csf  
Title : Crystal structure of PI3K p110gamma catalytical domain in complex with organoruthenium inhibitor DW2  
Authors : Xie, P.; Marmorstein, R.  
Deposited on : 2008-04-09  
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

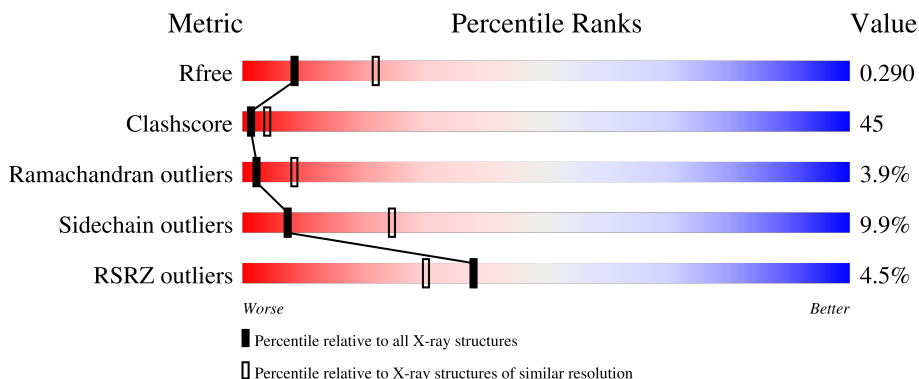
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of 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	966	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6938 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.

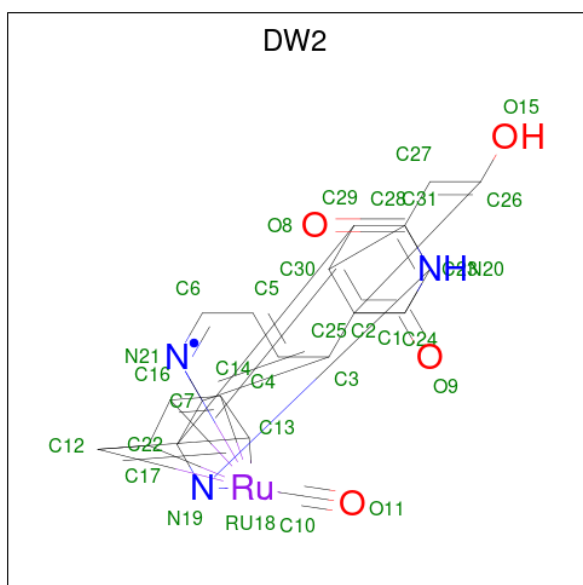
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	839	6801	4369	1159	1238	35	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	expression tag	UNP P48736
A	1103	HIS	-	expression tag	UNP P48736
A	1104	HIS	-	expression tag	UNP P48736
A	1105	HIS	-	expression tag	UNP P48736
A	1106	HIS	-	expression tag	UNP P48736
A	1107	HIS	-	expression tag	UNP P48736
A	1108	HIS	-	expression tag	UNP P48736

- Molecule 2 is RU-PYRIDOCARBAZOLE-2 (CCD ID: DW2) (formula:  $C_{23}H_{13}N_3O_4Ru$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	Ru		
2	A	1	31	23	3	4	1	0	0

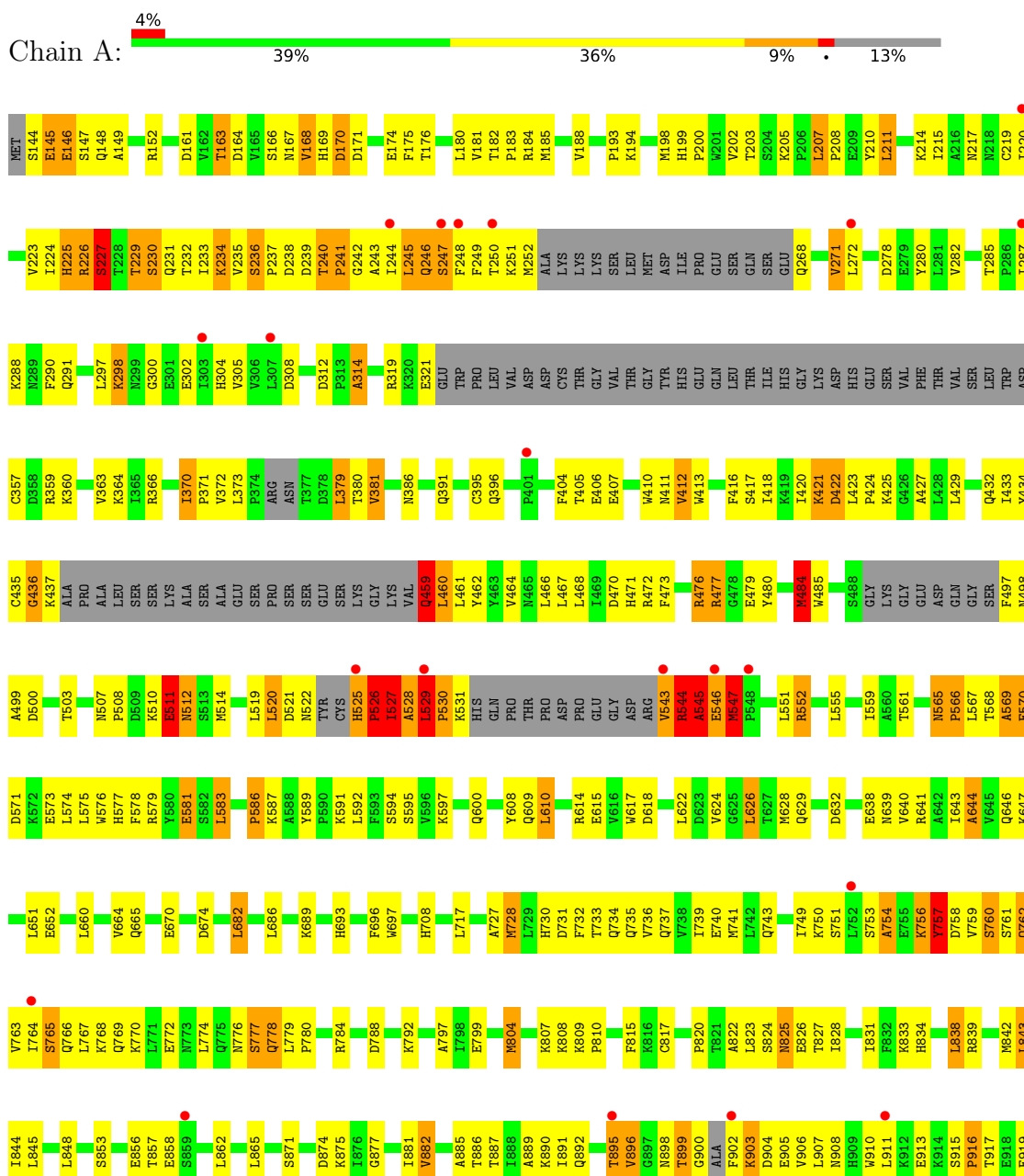
- Molecule 3 is water.

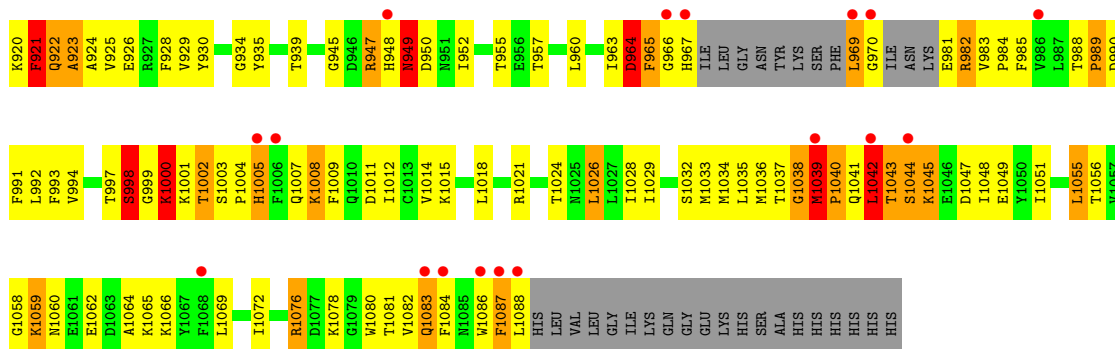
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	106	Total	O	0	0
			106	106		

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.63Å 68.08Å 106.27Å 90.00° 95.26° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.2 (50.00-2.80) 93.2 (50.00-2.80)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 2.81Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.252 , 0.287 0.257 , 0.290	Depositor DCC
$R_{free}$ test set	2457 reflections (9.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.9	Xtrriage
Anisotropy	0.407	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 71.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6938	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.90% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: DW2

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	0.73	13/6944 (0.2%)	1.24	75/9387 (0.8%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	756	LYS	CA-CB	-10.72	1.35	1.53
1	A	756	LYS	CB-CG	-9.67	1.23	1.52
1	A	1005	HIS	C-N	-7.75	1.23	1.33
1	A	526	PRO	C-N	7.74	1.44	1.33
1	A	527	ILE	CA-C	-6.87	1.44	1.52
1	A	547	MET	SD-CE	-6.72	1.62	1.79
1	A	530	PRO	N-CD	-6.55	1.38	1.47
1	A	921	PHE	C-N	-6.51	1.23	1.33
1	A	1004	PRO	C-N	6.18	1.41	1.33
1	A	895	THR	CA-C	6.11	1.57	1.52
1	A	528	ALA	CA-C	-6.05	1.44	1.53
1	A	804	MET	SD-CE	-5.74	1.65	1.79
1	A	528	ALA	CA-CB	-5.62	1.46	1.53

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	528	ALA	N-CA-C	22.08	137.26	108.34
1	A	756	LYS	CA-CB-CG	18.29	150.68	114.10
1	A	459	GLN	CA-C-N	15.16	143.07	121.24
1	A	459	GLN	C-N-CA	15.16	143.07	121.24
1	A	922	GLN	N-CA-C	-11.22	99.59	113.28
1	A	947	ARG	N-CA-C	11.19	125.06	109.29
1	A	525	HIS	CA-C-N	11.03	133.63	119.84
1	A	525	HIS	C-N-CA	11.03	133.63	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	459	GLN	O-C-N	-10.74	105.82	123.00
1	A	245	LEU	N-CA-C	-9.91	100.45	112.54
1	A	756	LYS	N-CA-CB	9.76	126.98	110.49
1	A	529	LEU	C-N-CD	-9.57	85.74	125.00
1	A	527	ILE	CA-C-N	-8.80	107.95	122.39
1	A	527	ILE	C-N-CA	-8.80	107.95	122.39
1	A	526	PRO	O-C-N	8.35	133.91	122.64
1	A	998	SER	O-C-N	8.26	133.57	122.59
1	A	527	ILE	N-CA-C	8.15	126.30	109.34
1	A	171	ASP	N-CA-C	7.71	121.14	112.97
1	A	923	ALA	N-CA-C	-7.64	102.52	112.68
1	A	761	SER	N-CA-C	-7.63	102.61	112.23
1	A	412	VAL	N-CA-C	7.58	118.79	108.17
1	A	756	LYS	N-CA-C	-7.58	94.66	110.80
1	A	1008	LYS	N-CA-C	-7.58	103.10	111.36
1	A	1043	THR	N-CA-C	-7.58	96.91	108.96
1	A	526	PRO	CB-CA-C	-7.24	99.62	111.56
1	A	145	GLU	N-CA-C	-7.19	103.48	111.82
1	A	547	MET	N-CA-C	-7.17	95.72	108.55
1	A	1042	LEU	N-CA-C	7.15	120.43	108.20
1	A	546	GLU	N-CA-C	7.12	120.89	109.86
1	A	762	GLN	N-CA-C	-7.12	103.22	110.97
1	A	1004	PRO	O-C-N	6.90	131.96	122.64
1	A	594	SER	N-CA-C	-6.89	104.84	113.18
1	A	756	LYS	CB-CG-CD	6.86	127.07	111.30
1	A	964	ASP	N-CA-C	6.72	125.11	110.80
1	A	565	ASN	CA-C-N	6.66	128.16	119.84
1	A	565	ASN	C-N-CA	6.66	128.16	119.84
1	A	146	GLU	N-CA-C	-6.65	103.28	111.33
1	A	247	SER	N-CA-C	-6.60	105.54	112.93
1	A	882	VAL	O-C-N	-6.56	115.52	122.67
1	A	460	LEU	N-CA-C	6.34	118.91	109.59
1	A	808	LYS	N-CA-C	-6.15	102.25	110.55
1	A	503	THR	N-CA-C	5.98	119.13	110.28
1	A	278	ASP	N-CA-C	-5.77	103.38	110.65
1	A	381	VAL	N-CA-C	5.77	118.47	108.90
1	A	670	GLU	CA-C-N	-5.75	113.83	119.64
1	A	670	GLU	C-N-CA	-5.75	113.83	119.64
1	A	896	VAL	CB-CA-C	-5.75	98.71	111.77
1	A	511	GLU	N-CA-C	5.68	118.68	111.69
1	A	1033	MET	N-CA-C	-5.68	104.71	111.69
1	A	547	MET	CA-C-N	5.64	126.89	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	547	MET	C-N-CA	5.64	126.89	119.84
1	A	499	ALA	N-CA-C	5.63	117.41	111.28
1	A	581	GLU	N-CA-C	-5.61	104.79	111.69
1	A	754	ALA	N-CA-C	-5.60	98.88	110.80
1	A	765	SER	N-CA-C	-5.58	105.28	111.36
1	A	644	ALA	N-CA-C	-5.55	104.92	110.97
1	A	530	PRO	N-CA-CB	5.53	109.06	103.25
1	A	527	ILE	CB-CA-C	-5.51	102.25	111.29
1	A	757	TYR	N-CA-C	5.46	122.42	110.80
1	A	484	MET	N-CA-C	5.42	118.44	110.59
1	A	236	SER	CA-C-N	5.33	126.50	119.84
1	A	236	SER	C-N-CA	5.33	126.50	119.84
1	A	545	ALA	O-C-N	5.33	129.67	122.59
1	A	949	ASN	N-CA-C	5.32	122.13	110.80
1	A	797	ALA	N-CA-C	-5.25	101.74	109.62
1	A	314	ALA	N-CA-C	-5.22	106.18	112.54
1	A	163	THR	N-CA-C	-5.19	106.35	113.30
1	A	788	ASP	CA-C-N	5.18	126.31	119.84
1	A	788	ASP	C-N-CA	5.18	126.31	119.84
1	A	423	LEU	N-CA-C	-5.17	103.07	109.64
1	A	825	ASN	N-CA-C	-5.16	105.66	112.94
1	A	638	GLU	N-CA-C	5.15	117.56	111.33
1	A	526	PRO	CA-C-N	-5.08	112.82	121.97
1	A	526	PRO	C-N-CA	-5.08	112.82	121.97
1	A	569	ALA	N-CA-C	-5.04	105.23	111.33

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6801	0	6850	616	0
2	A	31	0	12	3	0
3	A	106	0	0	15	0
All	All	6938	0	6862	616	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 45.

All (616) 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:988:THR:CG2	1:A:989:PRO:HD2	1.46	1.46
1:A:379:LEU:HG	1:A:435:CYS:SG	1.81	1.20
1:A:988:THR:CG2	1:A:989:PRO:CD	2.21	1.16
1:A:370:ILE:HG21	1:A:373:LEU:HG	1.26	1.14
1:A:988:THR:HG23	1:A:989:PRO:CD	1.79	1.11
1:A:511:GLU:HG2	1:A:512:ASN:HD22	0.96	1.10
1:A:988:THR:HG22	1:A:989:PRO:HD2	1.33	1.08
1:A:896:VAL:HG13	1:A:903:LYS:HE2	1.33	1.08
1:A:1034:MET:HG3	1:A:1039:MET:HE3	1.26	1.08
1:A:899:THR:HG22	1:A:900:GLY:H	1.13	1.08
1:A:1035:LEU:HD12	1:A:1048:ILE:HD13	1.30	1.08
1:A:181:VAL:HG13	1:A:185:MET:HE3	1.32	1.07
1:A:900:GLY:HA3	1:A:902:PHE:N	1.69	1.07
1:A:982:ARG:HH11	1:A:982:ARG:HG3	1.21	1.04
1:A:988:THR:HG23	1:A:989:PRO:HD2	1.07	1.02
1:A:511:GLU:HG2	1:A:512:ASN:ND2	1.75	1.01
1:A:181:VAL:HG13	1:A:185:MET:CE	1.89	1.00
1:A:433:ILE:HD12	1:A:484:MET:HE1	1.42	1.00
1:A:473:PHE:O	1:A:526:PRO:HB3	1.61	1.00
1:A:1000:LYS:HA	1:A:1076:ARG:NH2	1.79	0.98
1:A:1076:ARG:HG3	1:A:1076:ARG:HH11	1.22	0.98
1:A:1043:THR:CG2	1:A:1047:ASP:H	1.75	0.97
1:A:1000:LYS:HD3	1:A:1000:LYS:N	1.79	0.96
1:A:568:THR:HG22	1:A:570:GLU:H	1.30	0.96
1:A:1036:MET:HG2	1:A:1042:LEU:CD1	1.95	0.96
1:A:1014:VAL:HG11	1:A:1065:LYS:HE3	1.49	0.94
1:A:900:GLY:CA	1:A:902:PHE:N	2.30	0.94
1:A:997:THR:HG22	1:A:998:SER:H	1.31	0.94
1:A:370:ILE:HD13	1:A:371:PRO:HD2	1.49	0.94
1:A:1038:GLY:C	1:A:1040:PRO:HD3	1.92	0.93
1:A:988:THR:HG22	1:A:989:PRO:CD	1.93	0.93
1:A:231:GLN:HG3	1:A:232:THR:H	1.32	0.93
1:A:234:LYS:O	1:A:234:LYS:HD3	1.69	0.91
1:A:370:ILE:HG21	1:A:373:LEU:CG	1.98	0.91
1:A:466:LEU:HD11	1:A:476:ARG:HD3	1.51	0.91
1:A:916:PRO:HG2	1:A:917:THR:H	1.35	0.91
1:A:804:MET:HE3	1:A:810:PRO:HG2	1.49	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1039:MET:O	1:A:1041:GLN:N	2.04	0.90
1:A:900:GLY:C	1:A:902:PHE:N	2.30	0.90
1:A:198:MET:HE1	1:A:282:VAL:CG1	2.02	0.89
1:A:370:ILE:CG2	1:A:373:LEU:HG	2.02	0.89
1:A:246:GLN:O	1:A:250:THR:HG22	1.73	0.87
1:A:843:LEU:HD23	1:A:1039:MET:HE1	1.55	0.87
1:A:210:TYR:CD1	1:A:211:LEU:HD23	2.09	0.87
1:A:1043:THR:HG22	1:A:1047:ASP:CG	2.00	0.86
1:A:887:THR:HG22	1:A:889:ALA:H	1.39	0.86
1:A:1002:THR:CG2	1:A:1007:GLN:HE21	1.87	0.86
1:A:198:MET:HE1	1:A:282:VAL:HG11	1.56	0.86
1:A:760:SER:O	1:A:763:VAL:HG12	1.76	0.85
1:A:379:LEU:HD21	1:A:404:PHE:HD2	1.38	0.85
1:A:410:TRP:HB3	1:A:412:VAL:HG12	1.56	0.85
1:A:1036:MET:HG2	1:A:1042:LEU:HD12	1.58	0.85
1:A:899:THR:HG22	1:A:900:GLY:N	1.92	0.84
1:A:922:GLN:O	1:A:926:GLU:HG2	1.76	0.84
1:A:1011:ASP:OD2	1:A:1015:LYS:HE3	1.78	0.84
1:A:477:ARG:HD2	1:A:522:ASN:H	1.40	0.84
1:A:964:ASP:O	1:A:966:GLY:N	2.11	0.84
1:A:1060:ASN:HD21	1:A:1062:GLU:HB2	1.42	0.83
1:A:1002:THR:HG21	1:A:1007:GLN:HE21	1.41	0.83
1:A:895:THR:HB	1:A:903:LYS:HE3	1.60	0.83
1:A:462:TYR:HB3	1:A:484:MET:HE3	1.58	0.83
1:A:543:VAL:C	1:A:544:ARG:HD3	2.02	0.83
1:A:768:LYS:O	1:A:772:GLU:HG2	1.79	0.82
1:A:896:VAL:CG1	1:A:903:LYS:HE2	2.09	0.82
1:A:960:LEU:HD11	1:A:991:PHE:HE2	1.43	0.82
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.62	0.82
1:A:1078:LYS:HD3	3:A:1132:HOH:O	1.80	0.81
1:A:373:LEU:HD13	1:A:404:PHE:HZ	1.46	0.81
1:A:614:ARG:HG2	1:A:617:TRP:HB3	1.62	0.81
1:A:895:THR:C	1:A:903:LYS:HZ1	1.87	0.81
1:A:237:PRO:HA	1:A:287:ILE:HD11	1.61	0.81
1:A:185:MET:HE2	1:A:321:GLU:CD	2.06	0.81
1:A:207:LEU:HD23	1:A:208:PRO:HD2	1.63	0.81
1:A:1042:LEU:HD22	1:A:1042:LEU:C	2.06	0.81
1:A:433:ILE:CD1	1:A:484:MET:HE1	2.11	0.81
1:A:1042:LEU:C	1:A:1042:LEU:CD2	2.53	0.81
1:A:629:GLN:HG2	1:A:1029:ILE:HD13	1.63	0.81
1:A:997:THR:O	1:A:998:SER:HB3	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:917:THR:HB	1:A:919:GLU:OE1	1.80	0.80
1:A:1034:MET:CG	1:A:1039:MET:HE3	2.10	0.79
1:A:217:ASN:HD22	1:A:219:CYS:HB2	1.47	0.79
1:A:900:GLY:O	1:A:902:PHE:CG	2.35	0.79
1:A:484:MET:HE2	1:A:514:MET:HG2	1.65	0.79
1:A:148:GLN:O	1:A:152:ARG:HG3	1.81	0.79
1:A:1021:ARG:HE	1:A:1056:THR:CG2	1.97	0.78
1:A:380:THR:HG22	1:A:437:LYS:O	1.83	0.78
1:A:900:GLY:O	1:A:902:PHE:CD1	2.36	0.78
1:A:380:THR:HG22	1:A:437:LYS:C	2.09	0.78
1:A:757:TYR:H	1:A:757:TYR:HD2	1.29	0.77
1:A:224:ILE:HD13	1:A:233:ILE:HD13	1.65	0.77
1:A:462:TYR:CB	1:A:484:MET:HE3	2.14	0.77
1:A:760:SER:OG	1:A:762:GLN:HB3	1.83	0.77
1:A:227:SER:HB2	3:A:1144:HOH:O	1.83	0.77
1:A:484:MET:HE2	1:A:514:MET:CG	2.15	0.77
1:A:526:PRO:O	1:A:527:ILE:HG23	1.83	0.77
1:A:373:LEU:HD13	1:A:404:PHE:CZ	2.19	0.77
1:A:526:PRO:C	1:A:527:ILE:HG12	2.10	0.76
1:A:304:HIS:HB2	1:A:823:LEU:HD11	1.66	0.76
1:A:1043:THR:HG23	1:A:1043:THR:O	1.83	0.76
1:A:583:LEU:HD23	1:A:610:LEU:HD22	1.68	0.76
1:A:370:ILE:HD13	1:A:371:PRO:CD	2.16	0.76
1:A:379:LEU:HD21	1:A:404:PHE:CD2	2.21	0.75
1:A:804:MET:HE3	1:A:810:PRO:CG	2.15	0.75
1:A:547:MET:HB3	1:A:552:ARG:NH1	2.01	0.75
1:A:982:ARG:HH11	1:A:982:ARG:CG	1.99	0.74
1:A:1058:GLY:O	1:A:1059:LYS:O	2.05	0.74
1:A:217:ASN:ND2	1:A:219:CYS:HB2	2.02	0.73
1:A:1065:LYS:O	1:A:1069:LEU:HD23	1.88	0.73
1:A:1076:ARG:HG3	1:A:1076:ARG:NH1	1.99	0.73
1:A:997:THR:HG22	1:A:998:SER:N	2.04	0.72
1:A:1078:LYS:HG2	1:A:1082:VAL:HG23	1.71	0.72
1:A:226:ARG:HG2	1:A:226:ARG:HH11	1.53	0.72
1:A:529:LEU:HG	1:A:529:LEU:O	1.89	0.72
1:A:988:THR:HG22	1:A:989:PRO:N	2.04	0.72
1:A:223:VAL:HG12	1:A:225:HIS:CE1	2.25	0.71
1:A:1078:LYS:CE	1:A:1081:THR:HB	2.19	0.71
1:A:741:MET:HE1	1:A:778:GLN:O	1.91	0.71
1:A:792:LYS:HD2	3:A:1209:HOH:O	1.90	0.71
1:A:899:THR:CG2	1:A:900:GLY:H	1.98	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LEU:C	1:A:183:PRO:HD2	2.15	0.71
1:A:312:ASP:OD2	1:A:314:ALA:HB3	1.90	0.70
1:A:1078:LYS:HZ1	1:A:1081:THR:HG22	1.56	0.70
1:A:215:ILE:HD11	1:A:297:LEU:HD11	1.71	0.70
1:A:887:THR:HG21	1:A:950:ASP:HA	1.74	0.70
1:A:1021:ARG:HE	1:A:1056:THR:HG22	1.56	0.70
1:A:379:LEU:N	1:A:379:LEU:HD22	2.06	0.70
1:A:739:ILE:O	1:A:743:GLN:HG3	1.91	0.70
1:A:921:PHE:HA	1:A:924:ALA:HB3	1.72	0.69
1:A:210:TYR:CD1	1:A:211:LEU:CD2	2.76	0.69
1:A:576:TRP:CZ3	1:A:579:ARG:HD2	2.27	0.69
1:A:1038:GLY:C	1:A:1040:PRO:CD	2.65	0.69
1:A:547:MET:HB3	1:A:552:ARG:HH12	1.55	0.69
1:A:185:MET:HE2	1:A:321:GLU:OE1	1.93	0.69
1:A:181:VAL:CG1	1:A:185:MET:HE3	2.16	0.69
1:A:185:MET:CE	1:A:321:GLU:CD	2.65	0.69
1:A:1014:VAL:HG11	1:A:1065:LYS:CE	2.23	0.69
1:A:1009:PHE:HE2	1:A:1072:ILE:HD12	1.58	0.68
1:A:1078:LYS:HZ1	1:A:1081:THR:CG2	2.07	0.68
1:A:583:LEU:HD23	1:A:610:LEU:CD2	2.24	0.68
1:A:921:PHE:O	1:A:925:VAL:HG23	1.92	0.68
1:A:1036:MET:HG2	1:A:1042:LEU:HD11	1.73	0.68
1:A:180:LEU:O	1:A:183:PRO:HD2	1.93	0.68
1:A:640:VAL:O	1:A:643:ILE:HG12	1.94	0.68
1:A:964:ASP:O	1:A:965:PHE:C	2.36	0.68
1:A:420:ILE:HD13	1:A:522:ASN:HB3	1.74	0.67
1:A:1021:ARG:HG2	1:A:1055:LEU:CD2	2.24	0.67
1:A:1014:VAL:CG2	1:A:1069:LEU:HD21	2.24	0.67
1:A:1043:THR:C	1:A:1045:LYS:H	2.03	0.67
1:A:660:LEU:O	1:A:664:VAL:HG23	1.94	0.67
1:A:762:GLN:O	1:A:766:GLN:HG2	1.94	0.67
1:A:583:LEU:CD2	1:A:610:LEU:HD22	2.24	0.67
1:A:211:LEU:HD12	1:A:297:LEU:HD23	1.76	0.67
1:A:1028:ILE:HD12	1:A:1051:ILE:HG23	1.75	0.67
1:A:1043:THR:HG22	1:A:1047:ASP:OD2	1.95	0.67
1:A:960:LEU:CD1	1:A:991:PHE:HE2	2.08	0.66
1:A:235:VAL:HG11	1:A:244:ILE:HD13	1.77	0.66
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.76	0.66
1:A:741:MET:HE1	1:A:778:GLN:C	2.20	0.66
1:A:957:THR:HG22	1:A:957:THR:O	1.95	0.65
1:A:198:MET:HE3	1:A:280:TYR:CG	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:PRO:HD3	1:A:285:THR:O	1.95	0.65
1:A:1078:LYS:NZ	1:A:1081:THR:CG2	2.60	0.65
1:A:287:ILE:HD12	1:A:288:LYS:N	2.12	0.65
1:A:1021:ARG:HG2	1:A:1055:LEU:HD23	1.79	0.64
1:A:198:MET:HE1	1:A:282:VAL:HG13	1.79	0.64
1:A:198:MET:HE3	1:A:280:TYR:CB	2.27	0.64
1:A:357:CYS:O	1:A:421:LYS:HB2	1.98	0.64
1:A:526:PRO:O	1:A:527:ILE:HG12	1.97	0.64
1:A:215:ILE:HD11	1:A:297:LEU:CD1	2.27	0.64
1:A:926:GLU:OE1	1:A:1005:HIS:HE1	1.81	0.64
1:A:579:ARG:HG2	1:A:610:LEU:HD11	1.79	0.64
1:A:233:ILE:H	1:A:233:ILE:HD12	1.62	0.63
1:A:1043:THR:HG21	1:A:1047:ASP:H	1.60	0.63
1:A:169:HIS:HD2	1:A:170:ASP:HB3	1.61	0.63
1:A:998:SER:O	1:A:1001:LYS:HG3	1.97	0.63
1:A:235:VAL:HG12	1:A:236:SER:N	2.12	0.63
1:A:766:GLN:O	1:A:770:LYS:HG3	1.98	0.63
1:A:807:LYS:HG2	3:A:1177:HOH:O	1.97	0.63
1:A:928:PHE:CZ	1:A:991:PHE:HD2	2.17	0.63
1:A:1056:THR:HG23	1:A:1056:THR:O	1.98	0.63
1:A:464:VAL:HB	1:A:484:MET:HG2	1.81	0.63
1:A:547:MET:HE1	1:A:551:LEU:C	2.24	0.63
1:A:210:TYR:HD1	1:A:211:LEU:CD2	2.10	0.62
1:A:757:TYR:N	1:A:757:TYR:CD2	2.64	0.62
1:A:1000:LYS:N	1:A:1000:LYS:CD	2.58	0.62
1:A:1043:THR:O	1:A:1045:LYS:N	2.31	0.62
1:A:928:PHE:HZ	1:A:991:PHE:HD2	1.47	0.62
1:A:149:ALA:O	1:A:152:ARG:HB2	1.99	0.62
1:A:239:ASP:HB3	1:A:244:ILE:HD11	1.79	0.62
1:A:1009:PHE:CE2	1:A:1072:ILE:HD12	2.35	0.62
1:A:251:LYS:O	1:A:251:LYS:HD3	1.99	0.62
1:A:890:LYS:HZ2	2:A:1:DW2:H131	1.64	0.62
1:A:916:PRO:HG2	1:A:917:THR:N	2.13	0.62
1:A:239:ASP:CB	1:A:244:ILE:HD11	2.30	0.62
1:A:246:GLN:NE2	1:A:246:GLN:HA	2.14	0.62
1:A:1042:LEU:CD2	1:A:1043:THR:C	2.73	0.62
1:A:395:CYS:HB3	1:A:416:PHE:HD2	1.64	0.61
1:A:202:VAL:HG12	1:A:203:THR:N	2.15	0.61
1:A:302:GLU:HB2	1:A:304:HIS:CE1	2.35	0.61
1:A:569:ALA:O	1:A:573:GLU:HG3	2.00	0.61
1:A:997:THR:HG23	1:A:1002:THR:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:TRP:CH2	1:A:579:ARG:HD2	2.36	0.61
1:A:887:THR:CG2	1:A:950:ASP:HA	2.31	0.61
1:A:145:GLU:HA	1:A:148:GLN:CD	2.26	0.61
1:A:214:LYS:NZ	1:A:300:GLY:HA2	2.16	0.61
1:A:497:PHE:N	1:A:1044:SER:HG	1.99	0.61
1:A:989:PRO:HG2	1:A:1080:TRP:CD1	2.35	0.61
1:A:890:LYS:NZ	2:A:1:DW2:H131	2.15	0.61
1:A:168:VAL:HG13	1:A:170:ASP:H	1.64	0.60
1:A:1035:LEU:HA	1:A:1039:MET:HG2	1.82	0.60
1:A:202:VAL:HG11	1:A:285:THR:HG21	1.84	0.60
1:A:916:PRO:CG	1:A:917:THR:H	2.13	0.60
1:A:1078:LYS:HE3	1:A:1082:VAL:N	2.16	0.60
1:A:373:LEU:CD1	1:A:404:PHE:CZ	2.84	0.60
1:A:824:SER:OG	1:A:826:GLU:HG3	2.01	0.60
1:A:473:PHE:HB3	1:A:526:PRO:CB	2.32	0.59
1:A:379:LEU:HD23	1:A:379:LEU:C	2.28	0.59
1:A:462:TYR:CB	1:A:484:MET:CE	2.80	0.59
1:A:1078:LYS:HE3	1:A:1082:VAL:HG23	1.85	0.59
1:A:223:VAL:HG12	1:A:225:HIS:HE1	1.66	0.59
1:A:233:ILE:HD12	1:A:233:ILE:N	2.18	0.59
1:A:753:SER:HB3	1:A:809:LYS:HG3	1.84	0.59
1:A:240:THR:HG23	1:A:241:PRO:HD2	1.83	0.59
1:A:547:MET:CB	1:A:552:ARG:HH12	2.14	0.59
1:A:1018:LEU:HD23	1:A:1021:ARG:HD3	1.85	0.59
1:A:544:ARG:HD3	1:A:544:ARG:N	2.18	0.59
1:A:1043:THR:CG2	1:A:1043:THR:O	2.50	0.59
1:A:380:THR:CG2	1:A:437:LYS:O	2.51	0.58
1:A:960:LEU:HD11	1:A:991:PHE:CE2	2.31	0.58
1:A:1002:THR:HG22	1:A:1007:GLN:HE21	1.66	0.58
1:A:181:VAL:HG13	1:A:185:MET:HE1	1.79	0.58
1:A:472:ARG:O	1:A:473:PHE:HB2	2.02	0.58
1:A:891:ILE:HD12	1:A:910:TRP:CD1	2.37	0.58
1:A:484:MET:CE	1:A:514:MET:HG2	2.32	0.58
1:A:568:THR:HG22	1:A:570:GLU:N	2.11	0.58
1:A:886:THR:HG22	1:A:887:THR:N	2.19	0.58
1:A:1002:THR:HG22	1:A:1003:SER:H	1.68	0.58
1:A:363:VAL:HG23	1:A:520:LEU:CD1	2.33	0.58
1:A:903:LYS:HD2	1:A:906:VAL:HG22	1.84	0.58
1:A:930:TYR:HE1	1:A:1008:LYS:HE2	1.69	0.58
1:A:1003:SER:O	1:A:1007:GLN:HG3	2.03	0.58
1:A:1028:ILE:CD1	1:A:1051:ILE:HG23	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:HIS:HE1	3:A:1128:HOH:O	1.87	0.58
1:A:982:ARG:HG3	1:A:982:ARG:NH1	2.01	0.58
1:A:543:VAL:O	1:A:544:ARG:HB2	2.03	0.58
1:A:895:THR:HG22	1:A:903:LYS:NZ	2.18	0.58
1:A:1043:THR:HG23	1:A:1047:ASP:H	1.66	0.58
1:A:982:ARG:CG	1:A:982:ARG:NH1	2.63	0.57
1:A:215:ILE:HD11	1:A:297:LEU:HD21	1.84	0.57
1:A:843:LEU:HD23	1:A:1039:MET:CE	2.31	0.57
1:A:1078:LYS:CE	1:A:1082:VAL:HG23	2.35	0.57
1:A:733:THR:O	1:A:737:GLN:HG3	2.03	0.57
1:A:896:VAL:N	1:A:903:LYS:HZ1	2.02	0.57
1:A:207:LEU:CD2	1:A:208:PRO:HD2	2.32	0.57
1:A:231:GLN:HG3	1:A:232:THR:N	2.11	0.57
1:A:753:SER:OG	1:A:763:VAL:HG21	2.05	0.57
1:A:1018:LEU:HD21	1:A:1064:ALA:HB3	1.86	0.57
1:A:1000:LYS:HD3	1:A:1000:LYS:H	1.70	0.56
1:A:988:THR:HG21	1:A:1080:TRP:CE3	2.39	0.56
1:A:1026:LEU:O	1:A:1029:ILE:HG22	2.05	0.56
1:A:1078:LYS:CD	1:A:1081:THR:HB	2.35	0.56
1:A:234:LYS:HD3	1:A:234:LYS:C	2.31	0.56
1:A:930:TYR:CE1	1:A:1008:LYS:HE2	2.40	0.56
1:A:1024:THR:O	1:A:1028:ILE:HG12	2.05	0.56
1:A:237:PRO:HA	1:A:287:ILE:CD1	2.33	0.56
1:A:470:ASP:HB3	1:A:476:ARG:NH2	2.20	0.56
1:A:421:LYS:HZ2	1:A:527:ILE:HD11	1.71	0.56
1:A:831:ILE:HG13	1:A:881:ILE:HG12	1.87	0.56
1:A:181:VAL:CG1	1:A:185:MET:CE	2.75	0.56
1:A:202:VAL:CG1	1:A:285:THR:HG21	2.35	0.56
1:A:512:ASN:ND2	1:A:512:ASN:N	2.54	0.56
1:A:379:LEU:CG	1:A:435:CYS:SG	2.74	0.56
1:A:736:VAL:O	1:A:740:GLU:HB2	2.05	0.56
1:A:210:TYR:CE1	1:A:211:LEU:HD23	2.40	0.55
1:A:211:LEU:HD11	1:A:298:LYS:HB2	1.88	0.55
1:A:776:ASN:O	1:A:778:GLN:N	2.39	0.55
1:A:874:ASP:OD1	1:A:875:LYS:HG2	2.07	0.55
1:A:1045:LYS:O	1:A:1049:GLU:HG3	2.06	0.55
1:A:579:ARG:HG2	1:A:610:LEU:CD1	2.37	0.55
1:A:215:ILE:HD11	1:A:297:LEU:CD2	2.37	0.55
1:A:890:LYS:HG3	2:A:1:DW2:O11	2.06	0.55
1:A:963:ILE:O	1:A:965:PHE:N	2.38	0.55
1:A:1014:VAL:CG1	1:A:1065:LYS:HG3	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1036:MET:CG	1:A:1042:LEU:CD1	2.80	0.55
1:A:1038:GLY:O	1:A:1040:PRO:CD	2.55	0.55
1:A:435:CYS:HB3	1:A:461:LEU:CD1	2.37	0.55
1:A:1008:LYS:O	1:A:1012:ILE:HG12	2.07	0.55
1:A:765:SER:O	1:A:769:GLN:HG3	2.07	0.55
1:A:224:ILE:N	1:A:224:ILE:HD12	2.22	0.54
1:A:211:LEU:CD1	1:A:297:LEU:HD23	2.36	0.54
1:A:576:TRP:O	1:A:579:ARG:HD3	2.07	0.54
1:A:737:GLN:O	1:A:741:MET:HG3	2.06	0.54
1:A:896:VAL:N	1:A:903:LYS:CE	2.70	0.54
1:A:1060:ASN:ND2	1:A:1062:GLU:HB2	2.17	0.54
1:A:379:LEU:C	1:A:379:LEU:CD2	2.80	0.54
1:A:1043:THR:HG22	1:A:1047:ASP:CB	2.36	0.54
1:A:1078:LYS:CE	1:A:1082:VAL:CG2	2.85	0.54
1:A:223:VAL:CG1	1:A:225:HIS:HE1	2.20	0.54
1:A:544:ARG:O	1:A:545:ALA:CB	2.55	0.54
1:A:484:MET:HE2	1:A:514:MET:HG3	1.90	0.54
1:A:764:ILE:O	1:A:768:LYS:HG3	2.08	0.54
1:A:997:THR:HG23	1:A:1002:THR:H	1.70	0.54
1:A:892:GLN:O	1:A:896:VAL:HG22	2.08	0.54
1:A:1055:LEU:O	1:A:1056:THR:HG22	2.08	0.53
1:A:1084:PHE:O	1:A:1087:PHE:CE1	2.61	0.53
1:A:434:TYR:HD1	1:A:459:GLN:C	2.15	0.53
1:A:436:GLY:O	1:A:437:LYS:HG3	2.08	0.53
1:A:583:LEU:CD2	1:A:610:LEU:HD13	2.38	0.53
1:A:373:LEU:HD11	1:A:514:MET:HE2	1.90	0.53
1:A:220:ILE:HD11	1:A:237:PRO:HG3	1.89	0.53
1:A:249:PHE:CE1	1:A:268:GLN:HA	2.44	0.53
1:A:526:PRO:O	1:A:527:ILE:CG1	2.56	0.53
1:A:983:VAL:HG22	1:A:984:PRO:HD2	1.90	0.53
1:A:1032:SER:HB3	1:A:1048:ILE:HG23	1.90	0.53
1:A:1078:LYS:CG	1:A:1082:VAL:HG23	2.37	0.53
1:A:226:ARG:HH11	1:A:226:ARG:CG	2.20	0.53
1:A:467:LEU:O	1:A:476:ARG:HD2	2.09	0.53
1:A:215:ILE:HD12	1:A:215:ILE:N	2.22	0.53
1:A:592:LEU:O	1:A:595:SER:HB2	2.08	0.53
1:A:947:ARG:NH2	1:A:963:ILE:O	2.41	0.53
1:A:1036:MET:CG	1:A:1042:LEU:HD12	2.35	0.53
1:A:198:MET:HE3	1:A:280:TYR:HB3	1.90	0.53
1:A:381:VAL:HG13	1:A:404:PHE:HB2	1.91	0.53
1:A:144:SER:O	1:A:147:SER:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ARG:HH21	1:A:519:LEU:HD22	1.74	0.53
1:A:1062:GLU:O	1:A:1066:LYS:HG3	2.09	0.52
1:A:366:ARG:NH2	1:A:519:LEU:HD22	2.24	0.52
1:A:589:TYR:CD1	1:A:589:TYR:N	2.75	0.52
1:A:1034:MET:HG3	1:A:1039:MET:CE	2.19	0.52
1:A:547:MET:HE1	1:A:552:ARG:N	2.23	0.52
1:A:395:CYS:SG	1:A:418:ILE:HG13	2.50	0.52
1:A:886:THR:HG22	1:A:887:THR:H	1.73	0.52
1:A:1078:LYS:HE3	1:A:1082:VAL:CG2	2.40	0.52
1:A:168:VAL:CG1	1:A:169:HIS:N	2.73	0.52
1:A:555:LEU:O	1:A:559:ILE:HG12	2.09	0.52
1:A:229:THR:HB	3:A:1113:HOH:O	2.10	0.52
1:A:693:HIS:O	1:A:696:PHE:HB3	2.09	0.52
1:A:379:LEU:CD2	1:A:404:PHE:HD2	2.19	0.51
1:A:476:ARG:HG3	1:A:480:TYR:OH	2.10	0.51
1:A:561:THR:OG1	1:A:591:LYS:HE2	2.10	0.51
1:A:198:MET:CE	1:A:280:TYR:HB3	2.39	0.51
1:A:244:ILE:HA	1:A:247:SER:OG	2.10	0.51
1:A:905:GLU:HG3	1:A:993:PHE:CE2	2.44	0.51
1:A:568:THR:HB	1:A:571:ASP:OD2	2.10	0.51
1:A:828:ILE:N	1:A:828:ILE:HD12	2.26	0.51
1:A:915:SER:CB	1:A:921:PHE:HB2	2.40	0.51
1:A:949:ASN:HB2	1:A:1083:GLN:NE2	2.26	0.51
1:A:214:LYS:HD3	1:A:297:LEU:HD12	1.93	0.51
1:A:479:GLU:OE1	1:A:479:GLU:HA	2.11	0.51
1:A:566:PRO:O	1:A:567:LEU:HG	2.10	0.51
1:A:838:LEU:HD23	1:A:877:GLY:HA3	1.92	0.51
1:A:462:TYR:HB2	1:A:484:MET:CE	2.41	0.51
1:A:997:THR:CG2	1:A:1001:LYS:HB2	2.40	0.51
1:A:291:GLN:NE2	1:A:291:GLN:HA	2.25	0.51
1:A:928:PHE:HZ	1:A:991:PHE:CD2	2.26	0.51
1:A:161:ASP:O	1:A:164:ASP:HB3	2.11	0.51
1:A:1042:LEU:HD22	1:A:1043:THR:C	2.35	0.51
1:A:1078:LYS:HE2	1:A:1082:VAL:HG22	1.92	0.51
1:A:983:VAL:CG2	1:A:984:PRO:HD2	2.40	0.51
1:A:215:ILE:CD1	1:A:297:LEU:HD21	2.41	0.50
1:A:302:GLU:HB2	1:A:304:HIS:HE1	1.76	0.50
1:A:526:PRO:O	1:A:527:ILE:CG2	2.57	0.50
1:A:997:THR:HG23	1:A:1001:LYS:HB2	1.94	0.50
1:A:1014:VAL:HG11	1:A:1065:LYS:CD	2.42	0.50
1:A:1014:VAL:CG2	1:A:1065:LYS:HG3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:SER:O	1:A:510:LYS:HE3	2.11	0.50
1:A:839:ARG:HA	1:A:842:MET:HE3	1.93	0.50
1:A:997:THR:CG2	1:A:1002:THR:N	2.74	0.50
1:A:839:ARG:HA	1:A:842:MET:CE	2.41	0.50
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.92	0.50
1:A:586:PRO:HA	1:A:589:TYR:CE1	2.46	0.50
1:A:169:HIS:C	1:A:169:HIS:CD2	2.88	0.50
1:A:470:ASP:CB	1:A:476:ARG:NH2	2.75	0.50
1:A:750:LYS:NZ	1:A:834:HIS:HD2	2.10	0.50
1:A:777:SER:O	1:A:778:GLN:HG3	2.12	0.50
1:A:981:GLU:CD	1:A:1078:LYS:HZ3	2.19	0.50
1:A:1043:THR:C	1:A:1045:LYS:N	2.67	0.50
1:A:1014:VAL:HG21	1:A:1069:LEU:HD21	1.94	0.50
1:A:202:VAL:CG1	1:A:203:THR:N	2.74	0.50
1:A:233:ILE:H	1:A:233:ILE:CD1	2.25	0.49
1:A:939:THR:OG1	1:A:945:GLY:HA2	2.12	0.49
1:A:896:VAL:N	1:A:903:LYS:NZ	2.60	0.49
1:A:360:LYS:HE2	1:A:417:SER:HA	1.94	0.49
1:A:697:TRP:CH2	1:A:739:ILE:HD13	2.48	0.49
1:A:753:SER:O	1:A:754:ALA:HB3	2.12	0.49
1:A:774:LEU:C	1:A:776:ASN:H	2.20	0.49
1:A:1038:GLY:O	1:A:1040:PRO:HD3	2.11	0.49
1:A:185:MET:CE	1:A:321:GLU:OE2	2.60	0.49
1:A:287:ILE:HA	1:A:290:PHE:CD1	2.48	0.49
1:A:948:HIS:O	1:A:950:ASP:N	2.45	0.49
1:A:1021:ARG:NE	1:A:1056:THR:CG2	2.72	0.49
1:A:810:PRO:HB3	1:A:833:LYS:HB2	1.93	0.49
1:A:896:VAL:HA	1:A:903:LYS:NZ	2.27	0.49
1:A:935:TYR:O	1:A:939:THR:HG22	2.11	0.49
1:A:413:TRP:HD1	3:A:1187:HOH:O	1.96	0.49
1:A:760:SER:HG	1:A:763:VAL:H	1.57	0.49
1:A:1042:LEU:HD23	1:A:1043:THR:N	2.28	0.49
1:A:1078:LYS:HD2	1:A:1081:THR:HB	1.93	0.49
1:A:241:PRO:C	1:A:243:ALA:H	2.21	0.49
1:A:911:LEU:HD11	1:A:924:ALA:HB1	1.93	0.49
1:A:999:GLY:C	1:A:1000:LYS:HD3	2.36	0.49
1:A:370:ILE:HG21	1:A:373:LEU:CD1	2.40	0.48
1:A:425:LYS:HD2	1:A:473:PHE:CE2	2.48	0.48
1:A:547:MET:HE1	1:A:552:ARG:HA	1.94	0.48
1:A:379:LEU:HD22	1:A:379:LEU:H	1.74	0.48
1:A:459:GLN:NE2	1:A:460:LEU:H	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:ARG:HD2	1:A:618:ASP:OD1	2.14	0.48
1:A:920:LYS:O	1:A:921:PHE:CB	2.60	0.48
1:A:1035:LEU:HD23	1:A:1039:MET:HG3	1.96	0.48
1:A:473:PHE:HB3	1:A:526:PRO:HB3	1.95	0.48
1:A:895:THR:HG22	1:A:903:LYS:HZ2	1.79	0.48
1:A:689:LYS:HA	1:A:728:MET:HE1	1.95	0.48
1:A:1042:LEU:CD2	1:A:1043:THR:N	2.77	0.48
1:A:421:LYS:HZ1	1:A:527:ILE:HD13	1.79	0.48
1:A:1021:ARG:HE	1:A:1056:THR:HG23	1.77	0.48
1:A:462:TYR:HB2	1:A:484:MET:HE3	1.92	0.48
1:A:589:TYR:HD1	1:A:589:TYR:H	1.61	0.48
1:A:271:VAL:HG23	1:A:282:VAL:CG1	2.44	0.48
1:A:589:TYR:N	1:A:589:TYR:HD1	2.11	0.48
1:A:1038:GLY:O	1:A:1040:PRO:HD2	2.14	0.47
1:A:211:LEU:O	1:A:297:LEU:HD21	2.14	0.47
1:A:235:VAL:CG1	1:A:236:SER:N	2.77	0.47
1:A:241:PRO:O	1:A:243:ALA:N	2.48	0.47
1:A:381:VAL:HG12	1:A:435:CYS:HB2	1.96	0.47
1:A:885:ALA:HA	1:A:955:THR:HA	1.96	0.47
1:A:998:SER:O	1:A:1001:LYS:CG	2.62	0.47
1:A:1078:LYS:HE2	1:A:1082:VAL:CG2	2.44	0.47
1:A:246:GLN:C	1:A:248:PHE:H	2.20	0.47
1:A:319:ARG:HD3	3:A:1199:HOH:O	2.13	0.47
1:A:268:GLN:O	1:A:268:GLN:HG3	2.15	0.47
1:A:753:SER:CB	1:A:809:LYS:HG3	2.43	0.47
1:A:1000:LYS:CA	1:A:1076:ARG:NH2	2.64	0.47
1:A:614:ARG:HH11	1:A:646:GLN:HE22	1.62	0.47
1:A:856:GLU:C	1:A:858:GLU:H	2.21	0.47
1:A:948:HIS:CE1	1:A:1086:TRP:HB3	2.50	0.47
1:A:1032:SER:HB3	1:A:1048:ILE:CG2	2.45	0.47
1:A:521:ASP:C	1:A:521:ASP:OD1	2.57	0.47
1:A:597:LYS:HD2	1:A:600:GLN:OE1	2.14	0.47
1:A:831:ILE:HG13	1:A:881:ILE:CG1	2.45	0.47
1:A:1060:ASN:ND2	1:A:1062:GLU:H	2.12	0.47
1:A:198:MET:HE2	1:A:198:MET:HB3	1.50	0.47
1:A:689:LYS:HG2	1:A:728:MET:HE2	1.95	0.47
1:A:899:THR:CG2	1:A:900:GLY:N	2.65	0.47
1:A:948:HIS:ND1	1:A:1086:TRP:HB3	2.29	0.47
1:A:925:VAL:O	1:A:929:VAL:HG23	2.15	0.47
1:A:900:GLY:C	1:A:902:PHE:HB2	2.40	0.47
1:A:774:LEU:C	1:A:776:ASN:N	2.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:815:PHE:O	1:A:827:THR:HB	2.14	0.46
1:A:175:PHE:CG	1:A:471:HIS:CD2	3.03	0.46
1:A:235:VAL:HG11	1:A:244:ILE:CD1	2.44	0.46
1:A:241:PRO:C	1:A:243:ALA:N	2.71	0.46
1:A:167:ASN:O	1:A:167:ASN:CG	2.58	0.46
1:A:462:TYR:HB3	1:A:484:MET:CE	2.37	0.46
1:A:907:LEU:HD23	1:A:994:VAL:HG21	1.98	0.46
1:A:198:MET:CE	1:A:280:TYR:CB	2.92	0.46
1:A:207:LEU:HD22	1:A:211:LEU:HB2	1.97	0.46
1:A:1051:ILE:O	1:A:1055:LEU:HB2	2.15	0.46
1:A:245:LEU:HD21	1:A:272:LEU:HG	1.98	0.46
1:A:370:ILE:HG13	1:A:373:LEU:HD21	1.97	0.46
1:A:199:HIS:O	1:A:200:PRO:C	2.59	0.46
1:A:363:VAL:O	1:A:363:VAL:HG13	2.14	0.46
1:A:420:ILE:CD1	1:A:522:ASN:HB3	2.43	0.46
1:A:964:ASP:C	1:A:966:GLY:N	2.74	0.46
1:A:988:THR:HG21	1:A:1080:TRP:CZ3	2.51	0.46
1:A:511:GLU:HB3	3:A:1145:HOH:O	2.15	0.46
1:A:552:ARG:NH2	1:A:581:GLU:CD	2.74	0.46
1:A:565:ASN:O	1:A:566:PRO:O	2.33	0.46
1:A:1042:LEU:HD22	1:A:1042:LEU:O	2.16	0.46
1:A:784:ARG:HH11	1:A:784:ARG:HG2	1.81	0.46
1:A:947:ARG:HB3	1:A:948:HIS:H	1.48	0.46
1:A:211:LEU:HB3	1:A:297:LEU:HD23	1.97	0.45
1:A:366:ARG:NH2	1:A:519:LEU:HB2	2.31	0.45
1:A:528:ALA:HB1	1:A:529:LEU:H	1.49	0.45
1:A:817:CYS:HB2	1:A:828:ILE:HD11	1.98	0.45
1:A:220:ILE:CD1	1:A:237:PRO:HG3	2.46	0.45
1:A:163:THR:HB	3:A:1204:HOH:O	2.17	0.45
1:A:193:PRO:HA	3:A:1115:HOH:O	2.17	0.45
1:A:248:PHE:O	1:A:249:PHE:C	2.60	0.45
1:A:304:HIS:CB	1:A:823:LEU:HD11	2.42	0.45
1:A:214:LYS:HZ1	1:A:300:GLY:HA2	1.82	0.45
1:A:988:THR:HG23	1:A:989:PRO:HD3	1.88	0.45
1:A:371:PRO:HG2	1:A:511:GLU:O	2.16	0.45
1:A:1018:LEU:HD21	1:A:1064:ALA:CB	2.46	0.45
1:A:287:ILE:HA	1:A:290:PHE:HD1	1.80	0.45
1:A:184:ARG:O	1:A:188:VAL:HG23	2.17	0.45
1:A:435:CYS:SG	1:A:436:GLY:N	2.90	0.45
1:A:373:LEU:HD12	1:A:404:PHE:CE1	2.52	0.45
1:A:1042:LEU:C	1:A:1042:LEU:HD23	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1076:ARG:NH1	1:A:1076:ARG:CG	2.73	0.45
1:A:779:LEU:HD23	1:A:780:PRO:O	2.16	0.44
1:A:842:MET:HE2	1:A:871:SER:CB	2.47	0.44
1:A:862:LEU:CD2	1:A:862:LEU:N	2.80	0.44
1:A:967:HIS:NE2	1:A:970:GLY:HA2	2.32	0.44
1:A:1036:MET:CG	1:A:1042:LEU:HD11	2.43	0.44
1:A:215:ILE:CD1	1:A:297:LEU:HD11	2.43	0.44
1:A:731:ASP:O	1:A:735:GLN:HG3	2.16	0.44
1:A:739:ILE:HG13	1:A:740:GLU:N	2.31	0.44
1:A:992:LEU:HD11	1:A:1076:ARG:CD	2.48	0.44
1:A:641:ARG:O	1:A:644:ALA:HB3	2.17	0.44
1:A:732:PHE:O	1:A:736:VAL:HG23	2.18	0.44
1:A:903:LYS:HB2	1:A:906:VAL:HG23	1.99	0.44
1:A:960:LEU:CD1	1:A:991:PHE:CE2	2.96	0.44
1:A:552:ARG:HH11	1:A:552:ARG:HB2	1.82	0.44
1:A:421:LYS:NZ	1:A:527:ILE:CD1	2.80	0.44
1:A:614:ARG:O	1:A:615:GLU:C	2.61	0.44
1:A:1001:LYS:H	1:A:1076:ARG:HH22	1.64	0.44
1:A:182:THR:HB	1:A:183:PRO:HD3	1.98	0.44
1:A:235:VAL:HG12	1:A:236:SER:H	1.82	0.44
1:A:370:ILE:HD13	1:A:371:PRO:N	2.31	0.44
1:A:421:LYS:NZ	1:A:527:ILE:HD11	2.32	0.44
1:A:477:ARG:HD2	1:A:522:ASN:N	2.20	0.44
1:A:526:PRO:HG2	1:A:527:ILE:N	2.32	0.44
1:A:862:LEU:N	1:A:862:LEU:HD22	2.32	0.44
1:A:1086:TRP:O	1:A:1087:PHE:CD2	2.71	0.44
1:A:436:GLY:O	1:A:437:LYS:CB	2.66	0.44
1:A:632:ASP:C	1:A:632:ASP:OD1	2.60	0.44
1:A:853:SER:O	1:A:857:THR:HG23	2.17	0.44
1:A:957:THR:O	1:A:957:THR:CG2	2.65	0.44
1:A:820:PRO:C	1:A:822:ALA:H	2.25	0.44
1:A:175:PHE:CG	1:A:471:HIS:HD2	2.36	0.43
1:A:405:THR:C	1:A:407:GLU:N	2.75	0.43
1:A:916:PRO:CG	1:A:917:THR:N	2.75	0.43
1:A:226:ARG:O	1:A:227:SER:HB2	2.18	0.43
1:A:363:VAL:HG23	1:A:520:LEU:HD13	2.01	0.43
1:A:424:PRO:HG2	1:A:427:ALA:HB2	2.00	0.43
1:A:526:PRO:C	1:A:527:ILE:CG1	2.81	0.43
1:A:547:MET:HE1	1:A:552:ARG:CA	2.47	0.43
1:A:576:TRP:CE3	1:A:579:ARG:HD2	2.52	0.43
1:A:915:SER:HB3	1:A:921:PHE:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:GLU:HA	1:A:148:GLN:NE2	2.33	0.43
1:A:586:PRO:HA	1:A:589:TYR:CD1	2.54	0.43
1:A:882:VAL:HA	3:A:1120:HOH:O	2.18	0.43
1:A:1086:TRP:C	1:A:1087:PHE:CD2	2.96	0.43
1:A:410:TRP:HB3	1:A:412:VAL:CG1	2.39	0.43
1:A:531:LYS:HD3	1:A:609:GLN:HG2	2.01	0.43
1:A:194:LYS:HE3	3:A:1168:HOH:O	2.17	0.43
1:A:386:ASN:OD1	1:A:396:GLN:HG3	2.19	0.43
1:A:608:TYR:CZ	1:A:639:ASN:ND2	2.86	0.43
1:A:149:ALA:HA	1:A:152:ARG:HD2	2.01	0.43
1:A:250:THR:C	1:A:252:MET:H	2.27	0.43
1:A:168:VAL:HG13	1:A:169:HIS:N	2.34	0.43
1:A:622:LEU:HD21	1:A:651:LEU:CD2	2.49	0.43
1:A:682:LEU:HD22	1:A:686:LEU:CD1	2.49	0.43
1:A:981:GLU:C	1:A:982:ARG:HG2	2.43	0.43
1:A:1078:LYS:NZ	1:A:1081:THR:HB	2.34	0.43
1:A:577:HIS:CD2	3:A:1159:HOH:O	2.71	0.43
1:A:665:GLN:OE1	1:A:1037:THR:HB	2.18	0.43
1:A:727:ALA:O	1:A:730:HIS:HB3	2.19	0.43
1:A:842:MET:HE2	1:A:871:SER:HB3	2.00	0.43
1:A:948:HIS:O	1:A:949:ASN:C	2.62	0.43
1:A:1001:LYS:H	1:A:1076:ARG:NH2	2.16	0.43
1:A:308:ASP:N	1:A:308:ASP:OD1	2.52	0.43
1:A:432:GLN:HB3	1:A:460:LEU:CD1	2.49	0.43
1:A:435:CYS:HB3	1:A:461:LEU:HD11	1.99	0.43
1:A:904:ASP:O	1:A:990:ASP:HA	2.19	0.43
1:A:969:LEU:HD12	1:A:969:LEU:C	2.44	0.43
1:A:587:LYS:HA	1:A:626:LEU:HD11	2.01	0.42
1:A:862:LEU:HB3	1:A:934:GLY:HA3	2.00	0.42
1:A:184:ARG:NH2	1:A:321:GLU:OE1	2.52	0.42
1:A:824:SER:OG	1:A:825:ASN:N	2.52	0.42
1:A:844:ILE:HD13	1:A:1034:MET:SD	2.60	0.42
1:A:1014:VAL:HG11	1:A:1065:LYS:HG3	2.01	0.42
1:A:236:SER:HA	1:A:237:PRO:HD3	1.85	0.42
1:A:583:LEU:HD12	1:A:589:TYR:OH	2.18	0.42
1:A:885:ALA:HB2	1:A:955:THR:HG22	2.01	0.42
1:A:226:ARG:C	1:A:226:ARG:HD2	2.43	0.42
1:A:405:THR:O	1:A:407:GLU:N	2.53	0.42
1:A:751:SER:C	1:A:753:SER:H	2.26	0.42
1:A:379:LEU:HG	1:A:435:CYS:HG	1.72	0.42
1:A:983:VAL:HB	1:A:1082:VAL:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1078:LYS:HE3	1:A:1081:THR:HB	1.97	0.42
1:A:485:TRP:CH2	1:A:508:PRO:HD3	2.54	0.42
1:A:766:GLN:OE1	1:A:766:GLN:HA	2.19	0.42
1:A:908:ASN:HB2	1:A:993:PHE:HD2	1.84	0.42
1:A:185:MET:HE1	1:A:321:GLU:OE2	2.19	0.42
1:A:1078:LYS:HZ2	1:A:1081:THR:HG21	1.85	0.42
1:A:1000:LYS:HA	1:A:1076:ARG:CZ	2.46	0.42
1:A:359:ARG:HA	1:A:359:ARG:HD3	1.83	0.42
1:A:512:ASN:HD22	1:A:512:ASN:N	2.17	0.42
1:A:608:TYR:N	1:A:608:TYR:CD2	2.87	0.42
1:A:734:GLN:OE1	1:A:780:PRO:HB3	2.20	0.42
1:A:935:TYR:O	1:A:939:THR:CG2	2.67	0.42
1:A:1002:THR:HG21	1:A:1007:GLN:NE2	2.22	0.42
1:A:1069:LEU:HD13	1:A:1069:LEU:HA	1.84	0.42
1:A:205:LYS:NZ	1:A:652:GLU:OE1	2.53	0.42
1:A:1039:MET:O	1:A:1040:PRO:C	2.62	0.42
1:A:547:MET:HG2	1:A:578:PHE:CD2	2.55	0.41
1:A:507:ASN:HA	1:A:508:PRO:HD3	1.91	0.41
1:A:1039:MET:N	1:A:1040:PRO:CD	2.82	0.41
1:A:364:LYS:CE	1:A:411:ASN:OD1	2.68	0.41
1:A:436:GLY:O	1:A:437:LYS:CG	2.69	0.41
1:A:226:ARG:CG	1:A:226:ARG:NH1	2.80	0.41
1:A:370:ILE:HD12	1:A:372:VAL:O	2.21	0.41
1:A:875:LYS:HB3	1:A:875:LYS:HE3	1.74	0.41
1:A:896:VAL:HA	1:A:903:LYS:HZ3	1.85	0.41
1:A:900:GLY:O	1:A:902:PHE:CB	2.68	0.41
1:A:214:LYS:HD3	1:A:297:LEU:CD1	2.51	0.41
1:A:243:ALA:C	1:A:244:ILE:HG13	2.45	0.41
1:A:922:GLN:O	1:A:926:GLU:CG	2.59	0.41
1:A:985:PHE:CE1	1:A:1072:ILE:HD13	2.55	0.41
1:A:246:GLN:NE2	1:A:246:GLN:CA	2.81	0.41
1:A:500:ASP:HB3	1:A:708:HIS:CD2	2.56	0.41
1:A:624:VAL:O	1:A:628:MET:HG2	2.20	0.41
1:A:834:HIS:HA	1:A:875:LYS:O	2.21	0.41
1:A:921:PHE:C	1:A:923:ALA:N	2.73	0.41
1:A:224:ILE:O	1:A:230:SER:HA	2.21	0.40
1:A:887:THR:HB	1:A:890:LYS:HG3	2.03	0.40
1:A:1039:MET:N	1:A:1040:PRO:HD3	2.33	0.40
1:A:319:ARG:CD	3:A:1199:HOH:O	2.67	0.40
1:A:526:PRO:HB2	1:A:527:ILE:H	1.19	0.40
1:A:900:GLY:C	1:A:902:PHE:CB	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:CYS:HB3	1:A:461:LEU:HG	2.03	0.40
1:A:543:VAL:O	1:A:544:ARG:CB	2.70	0.40
1:A:856:GLU:C	1:A:858:GLU:N	2.79	0.40
1:A:498:ASN:OD1	1:A:498:ASN:C	2.64	0.40
1:A:512:ASN:ND2	1:A:512:ASN:H	2.18	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	817/966 (85%)	721 (88%)	64 (8%)	32 (4%)	<b>2</b> <b>8</b>

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	527	ILE
1	A	530	PRO
1	A	545	ALA
1	A	566	PRO
1	A	756	LYS
1	A	758	ASP
1	A	777	SER
1	A	916	PRO
1	A	949	ASN
1	A	964	ASP
1	A	965	PHE
1	A	998	SER
1	A	1040	PRO
1	A	1059	LYS
1	A	227	SER
1	A	230	SER

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Mol	Chain	Res	Type
1	A	921	PHE
1	A	526	PRO
1	A	899	THR
1	A	1044	SER
1	A	406	GLU
1	A	422	ASP
1	A	778	GLN
1	A	1000	LYS
1	A	1045	LYS
1	A	759	VAL
1	A	1038	GLY
1	A	544	ARG
1	A	241	PRO
1	A	242	GLY
1	A	436	GLY
1	A	1039	MET

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	755/864 (87%)	680 (90%)	75 (10%)	<b>7</b> <b>24</b>

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	GLU
1	A	168	VAL
1	A	170	ASP
1	A	174	GLU
1	A	207	LEU
1	A	211	LEU
1	A	225	HIS
1	A	226	ARG
1	A	227	SER
1	A	229	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	234	LYS
1	A	238	ASP
1	A	240	THR
1	A	246	GLN
1	A	271	VAL
1	A	298	LYS
1	A	370	ILE
1	A	379	LEU
1	A	391	GLN
1	A	421	LYS
1	A	422	ASP
1	A	459	GLN
1	A	476	ARG
1	A	477	ARG
1	A	484	MET
1	A	511	GLU
1	A	512	ASN
1	A	520	LEU
1	A	525	HIS
1	A	527	ILE
1	A	529	LEU
1	A	543	VAL
1	A	544	ARG
1	A	546	GLU
1	A	547	MET
1	A	552	ARG
1	A	570	GLU
1	A	574	LEU
1	A	575	LEU
1	A	583	LEU
1	A	586	PRO
1	A	610	LEU
1	A	626	LEU
1	A	647	LYS
1	A	682	LEU
1	A	717	LEU
1	A	728	MET
1	A	749	ILE
1	A	757	TYR
1	A	760	SER
1	A	767	LEU
1	A	799	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	838	LEU
1	A	843	LEU
1	A	845	LEU
1	A	848	LEU
1	A	865	LEU
1	A	898	ASN
1	A	903	LYS
1	A	913	GLU
1	A	952	ILE
1	A	969	LEU
1	A	982	ARG
1	A	989	PRO
1	A	998	SER
1	A	1000	LYS
1	A	1002	THR
1	A	1026	LEU
1	A	1039	MET
1	A	1042	LEU
1	A	1055	LEU
1	A	1076	ARG
1	A	1083	GLN
1	A	1087	PHE
1	A	1088	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	169	HIS
1	A	217	ASN
1	A	225	HIS
1	A	291	GLN
1	A	304	HIS
1	A	389	HIS
1	A	391	GLN
1	A	459	GLN
1	A	512	ASN
1	A	549	ASN
1	A	634	ASN
1	A	646	GLN
1	A	743	GLN
1	A	769	GLN
1	A	773	ASN

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Mol	Chain	Res	Type
1	A	834	HIS
1	A	898	ASN
1	A	908	ASN
1	A	951	ASN
1	A	1005	HIS
1	A	1007	GLN
1	A	1060	ASN
1	A	1085	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

1 ligand is 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	DW2	A	1	-	24,41,41	2.42	12 (50%)	30,90,90	1.44	3 (10%)

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	DW2	A	1	-	-	-	0/12/11/11

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	DW2	C6-N21	5.68	1.37	1.29
2	A	1	DW2	C5-C4	4.28	1.44	1.37
2	A	1	DW2	C27-C26	3.50	1.44	1.39
2	A	1	DW2	C3-C2	3.43	1.47	1.41
2	A	1	DW2	C24-C25	3.01	1.43	1.38
2	A	1	DW2	C30-C31	-2.91	1.40	1.49
2	A	1	DW2	C2-C1	-2.86	1.40	1.49
2	A	1	DW2	C28-C29	-2.45	1.41	1.46
2	A	1	DW2	C25-C26	2.25	1.43	1.39
2	A	1	DW2	C2-C30	2.16	1.45	1.40
2	A	1	DW2	C3-C7	2.12	1.44	1.40
2	A	1	DW2	C24-C23	2.01	1.42	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	DW2	C1-N20-C31	-4.24	108.90	112.59
2	A	1	DW2	C2-C3-C4	2.71	129.94	124.56
2	A	1	DW2	C29-C28-C23	2.07	108.58	106.49

There are no chirality outliers.

There are no torsion outliers.

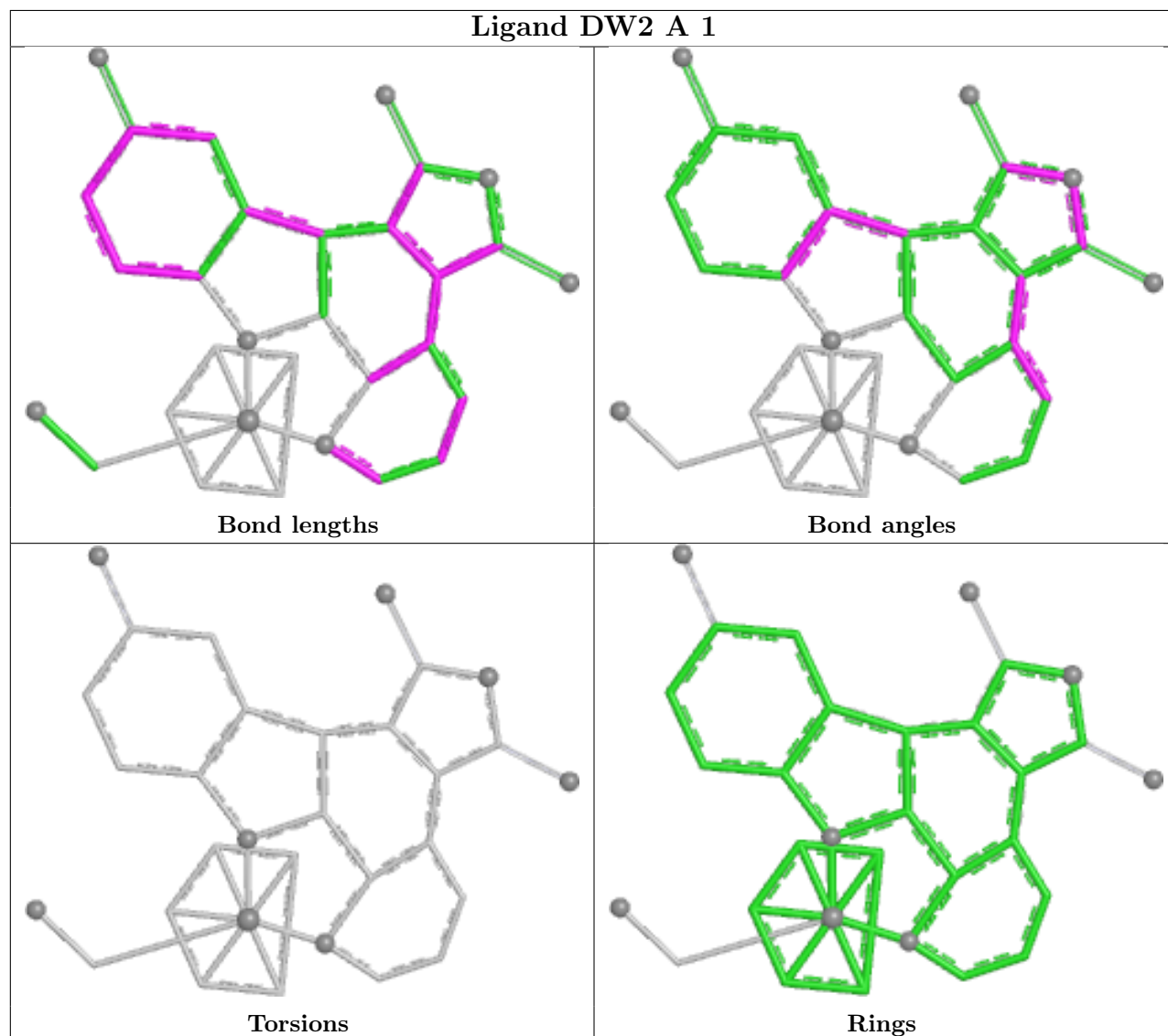
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	DW2	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	839/966 (86%)	0.42	38 (4%) <span style="border: 1px solid red; padding: 2px;">38</span> <span style="border: 1px solid red; padding: 2px;">30</span>	20, 90, 141, 163	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	967	HIS	4.6
1	A	948	HIS	3.8
1	A	1084	PHE	3.7
1	A	543	VAL	3.6
1	A	911	LEU	3.5
1	A	1088	LEU	3.2
1	A	970	GLY	3.1
1	A	966	GLY	3.1
1	A	1044	SER	3.0
1	A	220	ILE	2.9
1	A	969	LEU	2.8
1	A	764	ILE	2.7
1	A	307	LEU	2.7
1	A	525	HIS	2.6
1	A	244	ILE	2.6
1	A	1068	PHE	2.6
1	A	1039	MET	2.6
1	A	248	PHE	2.6
1	A	1086	TRP	2.5
1	A	303	ILE	2.5
1	A	902	PHE	2.5
1	A	859	SER	2.5
1	A	1042	LEU	2.4
1	A	1087	PHE	2.4
1	A	529	LEU	2.3
1	A	986	VAL	2.2
1	A	401	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	546	GLU	2.1
1	A	287	ILE	2.1
1	A	548	PRO	2.1
1	A	1005	HIS	2.1
1	A	1006	PHE	2.1
1	A	895	THR	2.1
1	A	752	LEU	2.0
1	A	247	SER	2.0
1	A	1083	GLN	2.0
1	A	272	LEU	2.0
1	A	250	THR	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](#)

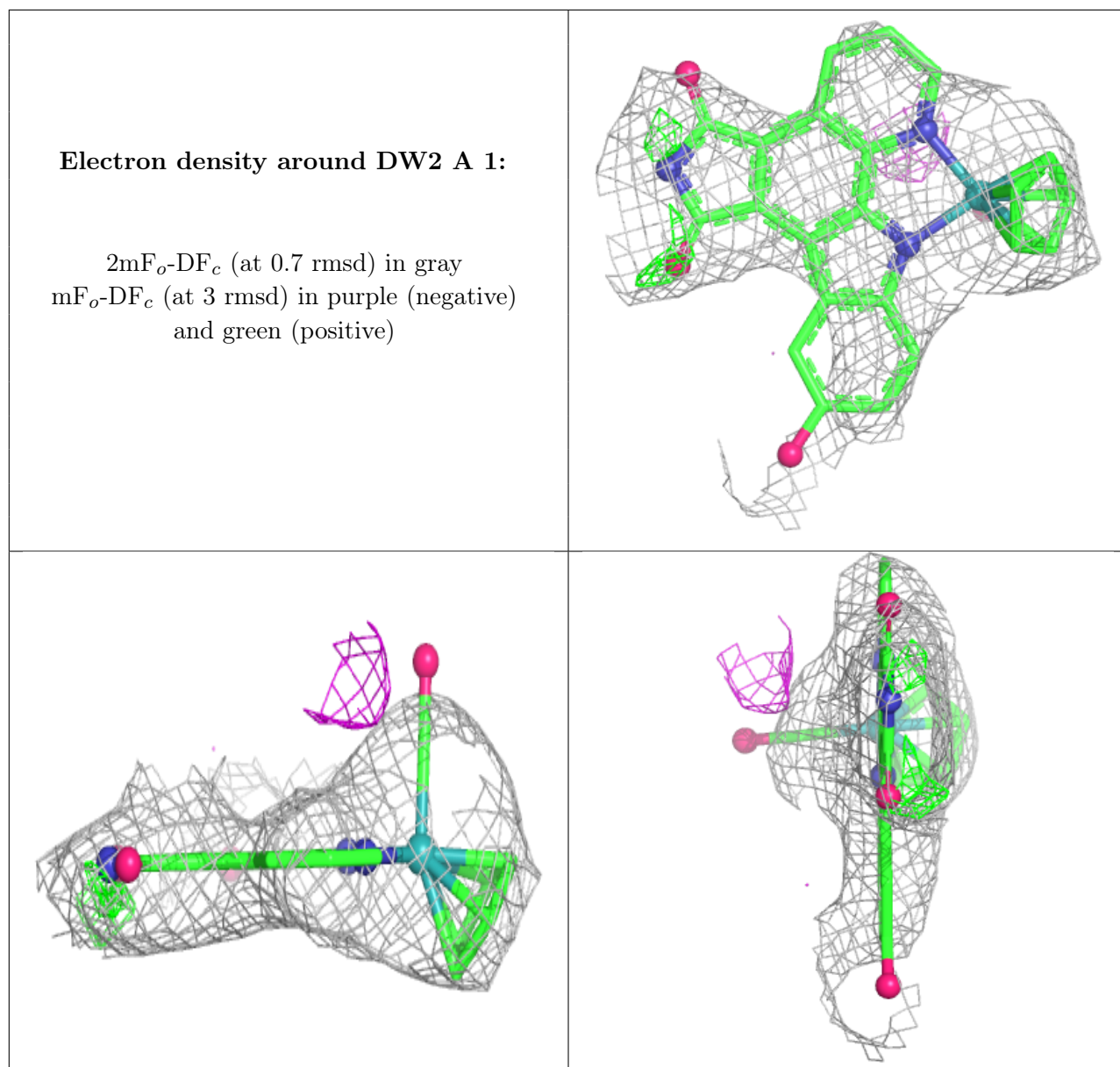
There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	DW2	A	1	31/31	0.90	0.18	158,161,191,191	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.