



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 10:38 AM EDT

PDB ID : 2X6K  
Title : THE CRYSTAL STRUCTURE OF THE DROSOPHILA CLASS III PI3-KINASE VPS34 IN COMPLEX WITH PI-103  
Authors : Miller, S.; Tavshanjian, B.; Oleksy, A.; Perisic, O.; Houseman, B.T.; Shokat, K.M.; Williams, R.L.  
Deposited on : 2010-02-17  
Resolution : 3.50 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 : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 2.36.2  
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) : 2.36.2

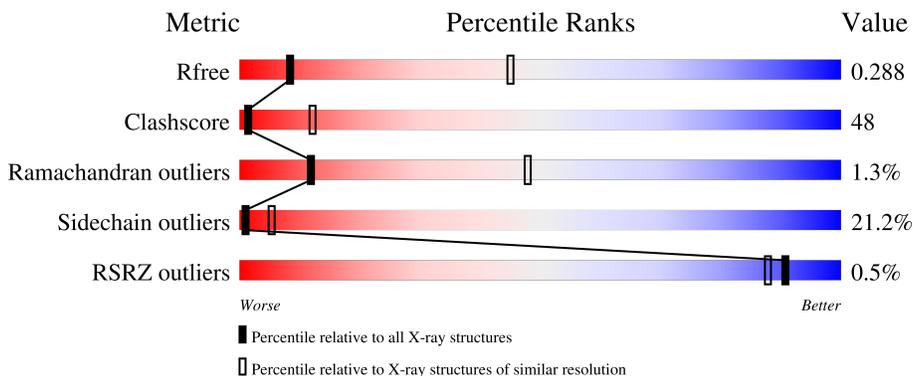
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	696	
1	B	696	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	X6K	B	1950	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9062 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.

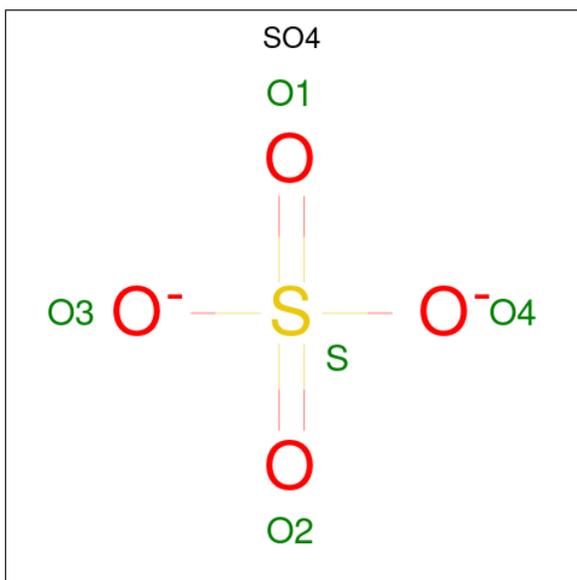
- Molecule 1 is a protein called PHOSPHOTIDYLINOSITOL 3 KINASE 59F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	550	4497	2906	765	799	27	0	0	0
1	B	550	4498	2907	766	798	27	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	455	ALA	GLY	engineered mutation	UNP Q9W1M7
B	455	ALA	GLY	engineered mutation	UNP Q9W1M7

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



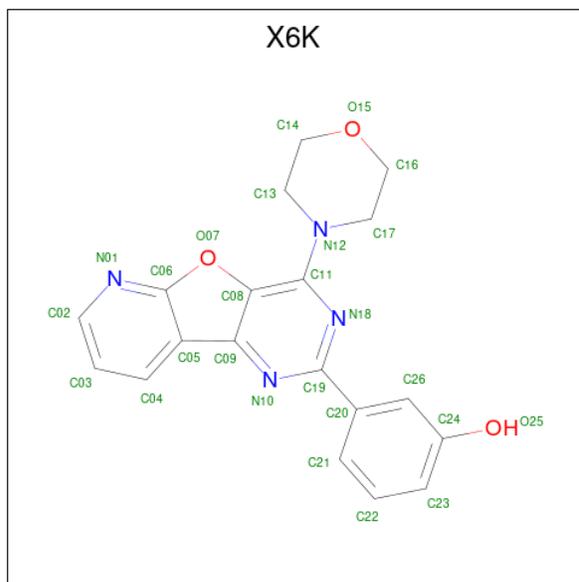
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

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

- Molecule 3 is 3-(4-MORPHOLIN-4-YLPYRIDO[3',2':4,5]FURO[3,2-D]PYRIMIDIN-2-YL)PHENOL (three-letter code: X6K) (formula: C<sub>19</sub>H<sub>16</sub>N<sub>4</sub>O<sub>3</sub>).

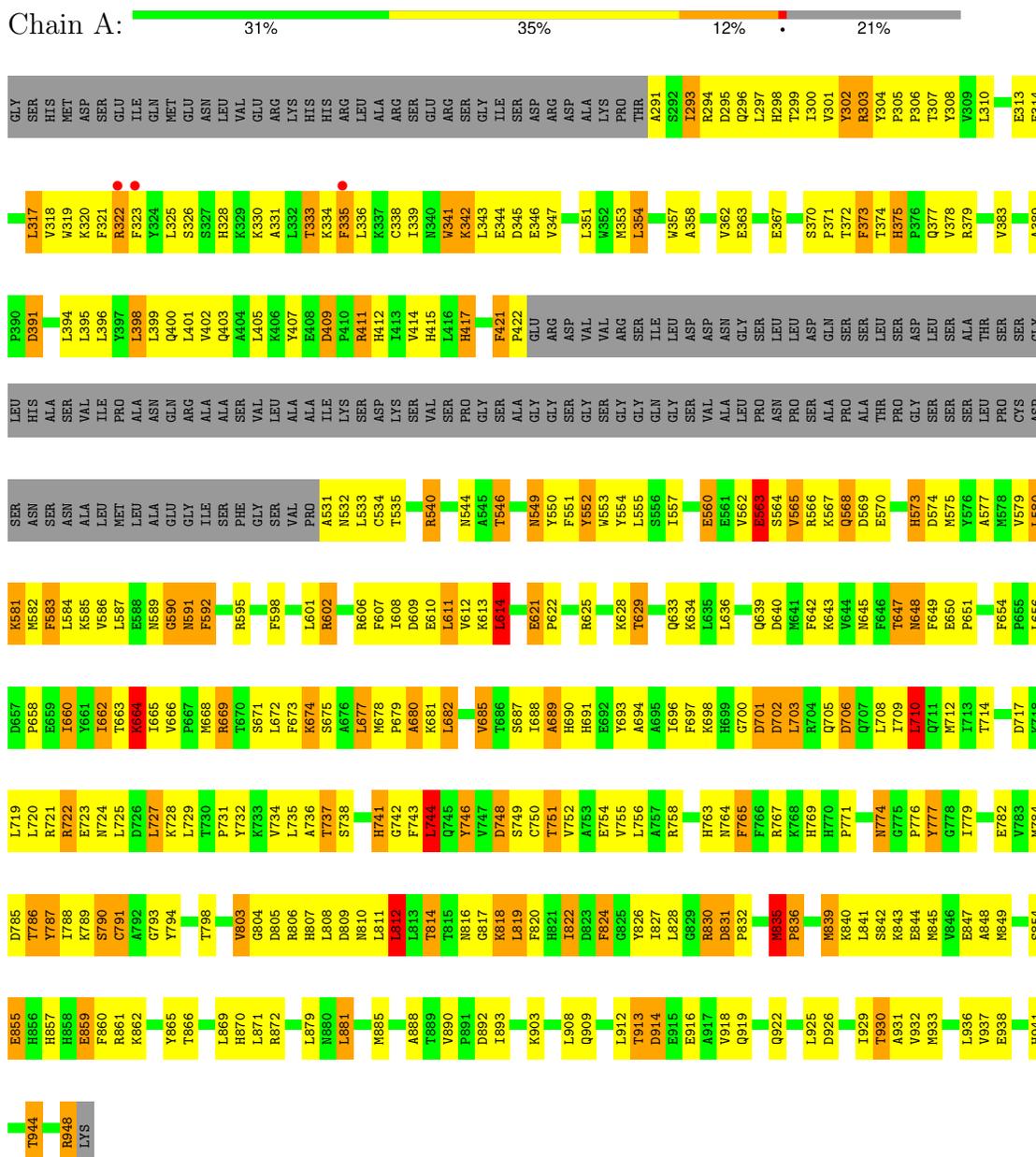


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			26	19	4	3		
3	B	1	Total	C	N	O	0	0
			26	19	4	3		

### 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: PHOSPHOTIDYLINOSITOL 3 KINASE 59F



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GLY	L317	L386	GLY	ASP	M575	P651	L729	G802	H874
SER	V316	D391	LEU	SER	Y576	I652	L730	V803	A675
HIS	K319	D392	HIS	ASN	M578	F653	P731	G804	H876
MET	K320	D393	ALA	SER	M581	P655	F732	D805	L880
ASP	F321	L394	VAL	ALA	K581	P658	K733	R806	L881
SER	R322	L395	ILE	LEU	M582		V734	D809	F882
GLU	F323	L396	PRO	MET	L587		L735	M810	S883
ILE		L398	ALA	LEU	L591		A736	L811	L884
GLN		L399	ASN	ALA	G590		T737	L812	V885
MET		L399	GLN	GLY	M591		S738	L813	V886
GLU		L400	ARG	GLY	F592		W739	T814	D887
MET		L401	ALA	ILE	R595		K740	T815	A888
GLU		V402	ALA	SER	R603		H741	M816	F888
ASN		Q403	ALA	PHE	S670		G742	F820	V890
LEU		A404	VAL	GLY	S671		F743	F820	P891
VAL		L405	VAL	SER	L672		L744	H821	D892
VAL		L406	LEU	SER	F599		Q745	I822	D892
GLY		L406	ALA	VAL	M600		Y746	D823	L895
HIS		L407	ALA	PRO	A531		V747	F824	L895
HIS		E408	ILE	A531	M532		D748	G825	K902
ARG		L339	LYS	M532	Q604		S749	Y826	E906
ARG		L339	SER	L533	R605		C750	I827	E906
LEU		N340	ASP	C534	Q605		T751	L828	N907
ALA		K341	LYS	T535	F607		G751	G829	L908
ARG		K342	SER	F536	L608		E754	R830	Q909
SER		L343	VAL	L537	D609		V755	K833	L912
GLU		E344	VAL	I538	E610		L756	P834	T913
ARG		D345	SER	Q539	L611		A757	F834	T913
ASP		E346	PRO	R540	V612		R758	R758	D914
GLY		A350	GLY	A541	K613		E759	M839	E915
ILE		L351	ALA	M544	L614		H690	L840	E916
SER		L354	GLY	A945			Y693	L841	A917
ASP		L354	GLY	T546			Y693	S842	V918
ASP		L354	SER	L547			H693	N764	S842
ASP		L354	GLY	A548			H693	F765	K843
LYS		L357	SER	M549			F697	F766	E844
PRO		A358	GLY	Y550			K698	R767	M845
THR		P359	GLY	F551			H699	V846	V846
THR		R360	ILE	Y552			G700	E847	E847
A291		E363	GLY	W553			D701	H770	A848
R294		L366	ASP	V554			D702	C772	L852
H298		L366	ASP	L555			L703	P771	L852
T299		L369	ASN	S556			R704	G775	H857
L300		S370	LEU	I557			Q705	P776	H858
Y301		F371	ASN	E560			D706	Y777	E859
Y302		T372	PRO	E561			Q707	F778	F860
R303		F373	PRO	V562			L708	L779	R861
Y304		T374	ALA	F563			I709	K862	K862
P305		H375	PRO	SER			L710	E863	C864
P306		F376	ALA	VAL			Q711	V783	C864
T307		Q377	THR	VAL			R712	V783	Y865
Y308		R378	PRO	K643			L713	T786	Y865
V309		R379	PRO	V644			T714	V787	T866
L310		K380	GLY	M645			L715	A867	T866
S311		Y381	LEU	Q568			L719	V868	Y868
S312		A382	SER	D569				L869	L869
S313		S383	ALA	E570				H870	H870
E314		V384	THR	H573				L871	L871
Q315		S384	LEU	F649				Y799	L871
D316		R385	PRO	E650				L801	L801
			CYS	D574				E723	H873

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.44Å 155.68Å 244.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.74 – 3.50 61.74 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (61.74-3.50) 99.5 (61.74-3.50)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 3.49Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.235 , 0.296 0.230 , 0.288	Depositor DCC
$R_{free}$ test set	1340 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	110.3	Xtrriage
Anisotropy	0.093	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 73.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9062	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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: X6K, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.58	1/4607 (0.0%)	0.86	6/6240 (0.1%)
1	B	0.51	1/4607 (0.0%)	0.68	2/6237 (0.0%)
All	All	0.55	2/9214 (0.0%)	0.77	8/12477 (0.1%)

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	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	311	SER	CB-OG	10.06	1.55	1.42
1	A	590	GLY	C-O	7.84	1.36	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	710	LEU	CA-CB-CG	-7.23	98.68	115.30
1	A	818	LYS	N-CA-C	-6.73	92.82	111.00
1	B	310	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	611	LEU	CA-CB-CG	5.14	127.13	115.30
1	A	744	LEU	CA-CB-CG	5.05	126.91	115.30
1	A	614	LEU	CA-CB-CG	5.03	126.88	115.30
1	A	710	LEU	CA-CB-CG	-5.03	103.74	115.30
1	A	812	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	589	ASN	Peptide
1	A	590	GLY	Mainchain
1	A	591	ASN	Mainchain
1	A	664	LYS	Peptide
1	A	680	ALA	Peptide
1	A	835	MET	Peptide
1	A	836	PRO	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	4497	0	4533	413	1
1	B	4498	0	4533	453	1
2	A	10	0	0	2	0
2	B	5	0	0	1	0
3	A	26	0	16	3	0
3	B	26	0	16	9	0
All	All	9062	0	9098	863	2

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 48.

All (863) 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:B:664:LYS:CG	1:B:685:VAL:HG21	1.52	1.39
1:A:677:LEU:HD22	1:A:700:GLY:HA3	1.22	1.21
1:A:827:ILE:HG22	1:A:828:LEU:HG	1.25	1.11
1:A:591:ASN:O	1:A:595:ARG:HD3	1.48	1.11
1:B:672:LEU:HD21	1:B:678:MET:HB2	1.27	1.10
1:B:664:LYS:HG3	1:B:685:VAL:HG21	1.33	1.08
1:A:798:THR:HG22	1:A:803:VAL:HG23	1.33	1.07
1:A:806:ARG:HH21	1:A:810:ASN:HB3	1.21	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:785:ASP:OD2	1:A:789:LYS:HE3	1.58	1.04
1:B:664:LYS:HG2	1:B:685:VAL:HG21	1.12	1.04
1:B:664:LYS:HG2	1:B:685:VAL:CG2	1.87	1.03
1:B:318:VAL:HG12	1:B:322:ARG:HG3	1.41	1.03
1:B:319:TRP:O	1:B:323:PHE:HE2	1.41	1.02
1:B:398:LEU:HA	1:B:401:LEU:CD1	1.90	1.01
1:B:810:ASN:O	1:B:822:ILE:HG22	1.59	1.01
1:B:319:TRP:O	1:B:323:PHE:CE2	2.14	1.00
1:B:342:LYS:HB3	1:B:346:GLU:HG3	1.38	0.99
1:B:323:PHE:H	1:B:323:PHE:HD2	1.03	0.99
1:B:315:GLN:O	1:B:322:ARG:NH2	1.94	0.99
1:B:664:LYS:CG	1:B:685:VAL:CG2	2.40	0.98
1:B:806:ARG:NH1	1:B:823:ASP:O	1.96	0.98
1:B:712:MET:HA	1:B:712:MET:CE	1.94	0.97
1:A:664:LYS:HG3	1:A:685:VAL:CG2	1.92	0.97
1:A:319:TRP:HA	1:A:322:ARG:NE	1.79	0.97
1:B:311:SER:CB	1:B:314:GLU:HB3	1.94	0.97
1:B:664:LYS:H	1:B:685:VAL:HG23	1.28	0.96
1:B:606:ARG:HH12	1:B:643:LYS:HB3	1.28	0.95
1:B:302:TYR:CE2	1:B:303:ARG:HG2	2.01	0.95
1:A:664:LYS:HG3	1:A:685:VAL:HG21	1.46	0.95
1:A:342:LYS:H	1:A:342:LYS:HD2	1.30	0.95
1:B:310:LEU:HD23	1:B:311:SER:HB3	1.49	0.93
1:A:577:ALA:O	1:A:581:LYS:HD2	1.68	0.93
1:A:343:LEU:HB2	1:A:346:GLU:CG	1.99	0.93
1:B:305:PRO:HB3	1:B:308:TYR:CE2	2.05	0.92
1:B:417:HIS:ND1	1:B:578:MET:HB2	1.84	0.92
1:A:855:GLU:H	1:A:855:GLU:CD	1.73	0.92
1:A:318:VAL:O	1:A:322:ARG:HG2	1.69	0.91
1:B:311:SER:OG	1:B:314:GLU:HB3	1.70	0.91
1:A:669:ARG:NH2	2:A:1950:SO4:O1	2.03	0.91
1:B:308:TYR:CD1	1:B:310:LEU:HB3	2.06	0.91
1:A:798:THR:CG2	1:A:803:VAL:HG23	2.01	0.90
1:B:409:ASP:HB3	1:B:412:HIS:CD2	2.06	0.90
1:A:664:LYS:CG	1:A:685:VAL:HG21	2.02	0.90
1:B:398:LEU:HA	1:B:401:LEU:HD12	1.53	0.89
1:B:417:HIS:CE1	1:B:578:MET:HB2	2.07	0.89
1:B:319:TRP:CH2	1:B:346:GLU:OE1	2.26	0.89
1:B:842:SER:OG	1:B:845:MET:SD	2.31	0.89
1:B:633:GLN:NE2	1:B:668:MET:HA	1.88	0.89
1:B:705:GLN:NE2	1:B:824:PHE:O	2.06	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:LEU:HD11	1:A:844:GLU:HG2	1.55	0.89
1:A:806:ARG:NH2	1:A:810:ASN:HB3	1.87	0.89
1:A:591:ASN:O	1:A:595:ARG:CD	2.21	0.88
1:A:400:GLN:HG2	1:A:881:LEU:HD23	1.55	0.88
1:B:739:SER:O	1:B:740:LYS:HG2	1.74	0.88
1:B:782:GLU:O	1:B:786:THR:HG22	1.74	0.88
1:A:843:LYS:HE2	1:A:847:GLU:OE2	1.72	0.87
1:B:729:LEU:H	1:B:729:LEU:HD12	1.36	0.87
1:B:685:VAL:HG12	1:B:690:HIS:CE1	2.09	0.87
1:B:319:TRP:CA	1:B:322:ARG:HE	1.87	0.87
1:A:948:ARG:HH11	1:A:948:ARG:HB3	1.39	0.86
1:B:578:MET:O	1:B:582:MET:HG3	1.76	0.86
1:B:767:ARG:HD3	1:B:778:GLY:HA3	1.54	0.85
1:B:822:ILE:HD11	3:B:1950:X6K:N10	1.91	0.85
1:B:606:ARG:HH12	1:B:643:LYS:CB	1.88	0.85
1:B:677:LEU:HD11	1:B:700:GLY:HA3	1.57	0.85
1:A:602:ARG:NH1	1:A:606:ARG:HD2	1.92	0.85
1:B:335:PHE:HD2	1:B:335:PHE:C	1.79	0.85
3:B:1950:X6K:O07	3:B:1950:X6K:H132	1.77	0.85
1:B:363:GLU:HA	1:B:366:LEU:HD12	1.57	0.84
1:B:534:CYS:O	1:B:538:ILE:HD12	1.78	0.84
1:A:343:LEU:HB2	1:A:346:GLU:HG3	1.58	0.84
1:B:654:PHE:HD1	1:B:655:PRO:HD2	1.43	0.84
1:B:310:LEU:CD2	1:B:311:SER:HB3	2.07	0.84
1:B:681:LYS:NZ	2:B:1951:SO4:O3	2.11	0.83
1:A:728:LYS:HG3	1:A:786:THR:HB	1.61	0.83
1:B:322:ARG:NH2	1:B:338:CYS:SG	2.51	0.83
1:B:685:VAL:CG1	1:B:690:HIS:CE1	2.62	0.83
1:B:335:PHE:C	1:B:335:PHE:CD2	2.51	0.83
1:B:723:GLU:OE2	1:B:874:HIS:NE2	2.12	0.83
1:A:319:TRP:CD1	1:A:323:PHE:CE2	2.66	0.83
1:B:318:VAL:HG12	1:B:322:ARG:CG	2.08	0.82
1:B:305:PRO:CB	1:B:308:TYR:CD2	2.62	0.82
1:B:417:HIS:CE1	1:B:578:MET:CB	2.62	0.82
1:B:712:MET:HA	1:B:712:MET:HE3	1.60	0.82
1:B:766:PHE:HB3	1:B:779:ILE:HG21	1.59	0.82
1:A:830:ARG:HH11	1:A:830:ARG:HG2	1.44	0.82
1:B:766:PHE:HB3	1:B:779:ILE:CG2	2.09	0.82
1:A:798:THR:CG2	1:A:803:VAL:CG2	2.57	0.82
1:B:408:GLU:CB	1:B:409:ASP:HA	2.10	0.81
1:A:319:TRP:CD1	1:A:323:PHE:HE2	1.98	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:794:TYR:O	1:A:798:THR:OG1	1.96	0.81
1:B:305:PRO:HB3	1:B:308:TYR:HE2	1.40	0.81
1:B:876:ASN:N	1:B:876:ASN:HD22	1.78	0.81
1:A:930:THR:HA	1:A:936:LEU:CD1	2.10	0.81
1:B:319:TRP:HD1	1:B:323:PHE:CE2	1.98	0.81
1:A:553:TRP:O	1:A:557:ILE:HG13	1.81	0.80
1:B:308:TYR:HD1	1:B:310:LEU:HB3	1.46	0.80
1:B:398:LEU:HA	1:B:401:LEU:HD13	1.64	0.80
1:A:776:PRO:HD2	1:A:779:ILE:O	1.82	0.80
1:A:326:SER:HB2	1:A:357:TRP:CE2	2.17	0.79
1:A:609:ASP:O	1:A:613:LYS:HG3	1.83	0.79
1:A:741:HIS:ND1	1:A:741:HIS:N	2.31	0.79
1:B:606:ARG:NH1	1:B:643:LYS:HB3	1.96	0.79
1:A:798:THR:HG22	1:A:803:VAL:CG2	2.13	0.79
1:A:677:LEU:HD22	1:A:700:GLY:CA	2.09	0.79
1:A:855:GLU:CD	1:A:855:GLU:N	2.36	0.79
1:B:319:TRP:CD1	1:B:323:PHE:CZ	2.70	0.79
1:A:400:GLN:NE2	1:A:885:MET:SD	2.55	0.78
1:A:835:MET:HB3	1:A:836:PRO:O	1.83	0.78
1:A:735:LEU:HG	1:A:736:ALA:O	1.83	0.78
1:A:830:ARG:HG2	1:A:830:ARG:NH1	1.94	0.78
1:B:326:SER:O	1:B:357:TRP:CE2	2.37	0.78
1:A:565:VAL:HB	1:A:570:GLU:HG2	1.66	0.78
1:B:322:ARG:HH11	1:B:335:PHE:HA	1.48	0.78
1:B:776:PRO:C	1:B:777:TYR:HD2	1.87	0.78
1:A:351:LEU:HD11	1:A:377:GLN:HG2	1.66	0.78
1:B:392:GLU:HG2	1:B:393:ASP:N	1.98	0.78
1:B:667:PRO:O	1:B:670:THR:HG22	1.83	0.78
1:B:777:TYR:HD2	1:B:777:TYR:N	1.82	0.77
1:B:302:TYR:CE2	1:B:303:ARG:CG	2.67	0.77
1:A:723:GLU:OE1	1:A:723:GLU:HA	1.83	0.77
1:B:557:ILE:HD11	1:B:736:ALA:O	1.85	0.77
1:A:582:MET:O	1:A:586:VAL:HG23	1.85	0.77
1:B:305:PRO:CB	1:B:308:TYR:CE2	2.68	0.76
1:A:552:TYR:C	1:A:552:TYR:CD2	2.57	0.76
1:B:360:MET:CE	1:B:381:TYR:HB3	2.15	0.76
1:B:685:VAL:CG1	1:B:690:HIS:HE1	1.97	0.76
1:B:812:LEU:CD2	1:B:822:ILE:HB	2.15	0.76
3:A:1951:X6K:H132	3:A:1951:X6K:O07	1.85	0.75
1:A:341:TRP:HD1	1:A:342:LYS:HZ3	1.34	0.75
1:B:301:VAL:O	1:B:305:PRO:HD2	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:738:SER:HB3	1:B:741:HIS:CE1	2.21	0.75
1:A:948:ARG:HB3	1:A:948:ARG:NH1	2.01	0.75
1:B:685:VAL:HG11	1:B:690:HIS:HE1	1.51	0.75
1:B:777:TYR:O	1:B:779:ILE:N	2.18	0.75
1:A:814:THR:HG23	1:A:816:ASN:H	1.52	0.75
1:B:409:ASP:HB3	1:B:412:HIS:HD2	1.51	0.75
1:A:827:ILE:CG2	1:A:828:LEU:HG	2.12	0.75
1:B:822:ILE:HD11	3:B:1950:X6K:C09	2.17	0.75
1:A:746:TYR:CE2	1:A:748:ASP:HA	2.22	0.75
1:B:323:PHE:N	1:B:323:PHE:CD2	2.54	0.74
1:A:351:LEU:CD1	1:A:377:GLN:HG2	2.18	0.74
1:A:629:THR:O	1:A:633:GLN:HG3	1.87	0.74
1:A:552:TYR:C	1:A:552:TYR:HD2	1.91	0.74
1:B:704:ARG:NH1	1:B:889:THR:HG21	2.03	0.74
1:B:703:LEU:HB2	1:B:736:ALA:HB2	1.69	0.74
1:A:400:GLN:CG	1:A:881:LEU:HD23	2.18	0.74
1:B:305:PRO:HB2	1:B:308:TYR:HD2	1.52	0.74
1:A:861:ARG:HD3	1:A:865:TYR:OH	1.87	0.74
1:B:319:TRP:HA	1:B:322:ARG:HE	1.52	0.74
1:B:606:ARG:NH1	1:B:643:LYS:CB	2.49	0.73
1:B:664:LYS:HG3	1:B:685:VAL:CG2	2.13	0.73
1:B:734:VAL:HG22	1:B:744:LEU:HD22	1.69	0.73
1:B:876:ASN:HD22	1:B:876:ASN:H	1.34	0.73
1:A:342:LYS:HD2	1:A:342:LYS:N	2.02	0.73
1:B:763:HIS:CE1	1:B:777:TYR:CD1	2.77	0.73
1:B:322:ARG:NH1	1:B:335:PHE:HA	2.03	0.73
1:B:633:GLN:HE22	1:B:668:MET:HA	1.54	0.73
1:B:667:PRO:O	1:B:670:THR:CG2	2.35	0.73
1:A:930:THR:HA	1:A:936:LEU:HD13	1.70	0.73
1:B:765:PHE:C	1:B:765:PHE:CD2	2.62	0.73
1:A:866:THR:O	1:A:870:HIS:HD2	1.71	0.73
1:B:827:ILE:CG2	1:B:828:LEU:HG	2.19	0.73
1:A:357:TRP:HD1	1:A:358:ALA:O	1.72	0.72
1:B:398:LEU:CA	1:B:401:LEU:HD12	2.18	0.72
1:B:729:LEU:HD12	1:B:729:LEU:N	2.03	0.72
1:B:852:ILE:HA	1:B:857:HIS:CD2	2.23	0.72
1:B:803:VAL:CG1	1:B:806:ARG:HD3	2.19	0.72
1:B:322:ARG:CZ	1:B:338:CYS:SG	2.77	0.72
1:A:647:THR:O	1:A:664:LYS:HB3	1.89	0.72
1:B:866:THR:O	1:B:870:HIS:HD2	1.71	0.72
1:A:664:LYS:HG3	1:A:685:VAL:HG22	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:MET:HG2	1:A:925:LEU:CD2	2.20	0.71
1:A:625:ARG:O	1:A:629:THR:HG23	1.90	0.71
1:A:608:ILE:O	1:A:612:VAL:HG23	1.91	0.71
1:B:319:TRP:CD1	1:B:323:PHE:CE2	2.78	0.71
1:B:648:ASN:HA	1:B:664:LYS:HB3	1.72	0.71
1:B:360:MET:HG2	1:B:385:ARG:HG3	1.72	0.71
1:A:648:ASN:HA	1:A:664:LYS:HB3	1.72	0.71
1:B:806:ARG:HH22	1:B:823:ASP:H	1.39	0.71
1:A:798:THR:HG23	1:A:803:VAL:HG21	1.70	0.71
1:B:335:PHE:CD1	1:B:357:TRP:HZ3	2.09	0.71
1:B:777:TYR:N	1:B:777:TYR:CD2	2.56	0.71
1:A:842:SER:OG	1:A:844:GLU:OE1	2.09	0.71
1:B:312:SER:O	1:B:315:GLN:HG2	1.92	0.70
1:B:560:GLU:OE1	1:B:739:SER:HB3	1.90	0.70
1:B:397:TYR:O	1:B:401:LEU:HD12	1.91	0.70
1:B:319:TRP:N	1:B:322:ARG:HE	1.89	0.70
1:B:299:THR:O	1:B:302:TYR:HD2	1.74	0.70
1:B:311:SER:HB2	1:B:314:GLU:HB3	1.74	0.70
1:B:743:PHE:O	1:B:744:LEU:HD23	1.92	0.69
1:B:763:HIS:NE2	1:B:848:ALA:HA	2.07	0.69
1:B:861:ARG:NH2	1:B:926:ASP:OD2	2.24	0.69
1:B:729:LEU:H	1:B:729:LEU:CD1	2.04	0.69
1:A:803:VAL:HG11	1:A:824:PHE:HD1	1.57	0.69
1:A:321:PHE:O	1:A:325:LEU:HD23	1.93	0.69
1:A:743:PHE:C	1:A:744:LEU:HD23	2.13	0.69
1:A:297:LEU:O	1:A:301:VAL:HG23	1.93	0.69
1:A:308:TYR:CD1	1:A:310:LEU:HB3	2.28	0.68
1:A:944:THR:HG23	1:B:931:ALA:O	1.93	0.68
1:B:561:GLU:OE1	1:B:561:GLU:HA	1.93	0.68
1:A:305:PRO:HB3	1:A:308:TYR:CZ	2.28	0.68
1:A:591:ASN:OD1	1:A:592:PHE:N	2.27	0.68
1:B:664:LYS:H	1:B:685:VAL:CG2	2.06	0.68
1:B:664:LYS:O	1:B:685:VAL:HG22	1.93	0.68
1:B:712:MET:HA	1:B:712:MET:HE2	1.74	0.68
1:A:412:HIS:HB3	1:A:531:ALA:N	2.09	0.68
1:A:728:LYS:O	1:A:818:LYS:HD3	1.93	0.68
1:B:930:THR:HG22	1:B:936:LEU:HB3	1.76	0.68
1:A:291:ALA:O	1:A:294:ARG:HG2	1.94	0.67
1:A:343:LEU:HB2	1:A:346:GLU:HG2	1.76	0.67
1:B:329:LYS:H	1:B:329:LYS:HD3	1.59	0.67
1:B:673:PHE:HB2	1:B:679:PRO:HD2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:842:SER:O	1:B:846:VAL:HG23	1.94	0.67
1:A:409:ASP:OD1	1:A:409:ASP:C	2.33	0.67
1:A:314:GLU:O	1:A:318:VAL:HG23	1.94	0.67
1:B:305:PRO:CB	1:B:308:TYR:HD2	2.07	0.67
1:A:819:LEU:HD23	1:A:820:PHE:HA	1.77	0.67
1:B:342:LYS:HB3	1:B:346:GLU:CG	2.22	0.67
1:B:806:ARG:NH2	1:B:810:ASN:HB3	2.09	0.66
1:B:315:GLN:CG	1:B:338:CYS:HB2	2.25	0.66
1:A:830:ARG:HH11	1:A:830:ARG:CG	2.08	0.66
1:A:854:SER:OG	1:A:857:HIS:N	2.28	0.66
1:B:396:LEU:H	1:B:396:LEU:HD12	1.61	0.66
1:A:672:LEU:HD23	1:A:680:ALA:HA	1.77	0.66
1:B:302:TYR:HE2	1:B:303:ARG:CG	2.08	0.66
1:A:737:THR:HG22	1:A:738:SER:O	1.96	0.66
1:B:708:LEU:HD12	1:B:885:MET:CE	2.26	0.66
1:A:375:HIS:HB3	1:A:378:VAL:HG13	1.78	0.66
1:B:573:HIS:C	1:B:573:HIS:CD2	2.69	0.65
1:B:599:TYR:HD2	1:B:599:TYR:O	1.79	0.65
1:B:319:TRP:HA	1:B:322:ARG:NE	2.12	0.65
1:A:319:TRP:NE1	1:A:323:PHE:CE2	2.64	0.65
1:B:308:TYR:CE1	1:B:310:LEU:HB3	2.31	0.65
1:B:398:LEU:CA	1:B:401:LEU:CD1	2.72	0.65
1:A:727:LEU:O	1:A:729:LEU:N	2.29	0.65
1:A:342:LYS:H	1:A:342:LYS:CD	2.01	0.65
1:A:689:ALA:HB3	1:A:691:HIS:CE1	2.32	0.65
1:B:798:THR:HG23	1:B:803:VAL:HB	1.79	0.65
1:A:752:VAL:HG11	1:A:808:LEU:HD12	1.78	0.65
1:B:375:HIS:CD2	1:B:377:GLN:H	2.15	0.65
1:A:930:THR:HA	1:A:936:LEU:HD12	1.78	0.65
1:B:624:ASN:H	1:B:627:LYS:HE2	1.62	0.65
1:A:314:GLU:O	1:A:317:LEU:HG	1.97	0.64
1:A:751:THR:HG23	1:A:754:GLU:HG3	1.79	0.64
1:B:654:PHE:CD1	1:B:655:PRO:HD2	2.29	0.64
1:A:806:ARG:NH2	1:A:822:ILE:O	2.29	0.64
1:A:421:PHE:HB2	1:A:422:PRO:HD3	1.79	0.64
1:A:737:THR:HG21	1:A:741:HIS:CD2	2.32	0.64
1:A:861:ARG:NH2	1:A:926:ASP:OD2	2.30	0.64
1:B:360:MET:HE1	1:B:381:TYR:HB3	1.79	0.64
1:B:722:ARG:HH11	1:B:722:ARG:HB3	1.62	0.64
1:A:737:THR:H	1:A:742:GLY:HA2	1.62	0.64
1:B:696:ILE:O	1:B:743:PHE:HA	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:784:MET:O	1:A:788:ILE:HG12	1.97	0.64
1:B:343:LEU:HB3	1:B:344:GLU:OE1	1.97	0.64
1:B:765:PHE:CD2	1:B:766:PHE:HD2	2.16	0.64
1:A:819:LEU:HD23	1:A:819:LEU:C	2.18	0.63
1:B:598:PHE:C	1:B:598:PHE:CD2	2.71	0.63
1:A:610:GLU:OE1	1:A:643:LYS:N	2.31	0.63
1:B:375:HIS:CD2	1:B:378:VAL:HG13	2.33	0.63
1:A:664:LYS:CG	1:A:685:VAL:CG2	2.66	0.63
1:B:319:TRP:HH2	1:B:346:GLU:CD	2.01	0.63
1:B:335:PHE:CD1	1:B:357:TRP:CZ3	2.86	0.63
1:B:413:ILE:HD13	1:B:575:MET:HG2	1.80	0.63
1:B:575:MET:SD	1:B:575:MET:C	2.77	0.63
1:A:307:THR:O	1:A:308:TYR:HD2	1.81	0.63
1:A:806:ARG:NH2	1:A:810:ASN:CB	2.61	0.63
1:A:672:LEU:CD2	1:A:680:ALA:HA	2.29	0.62
1:B:709:ILE:HG21	1:B:824:PHE:CD1	2.34	0.62
1:B:319:TRP:HH2	1:B:346:GLU:OE1	1.81	0.62
1:B:654:PHE:HD1	1:B:655:PRO:CD	2.11	0.62
1:A:749:SER:OG	1:A:812:LEU:HD12	1.98	0.62
1:A:347:VAL:O	1:A:351:LEU:HD23	2.00	0.62
1:A:709:ILE:CG1	1:A:827:ILE:HD11	2.30	0.62
1:B:379:ARG:O	1:B:383:VAL:HG23	2.00	0.62
1:B:397:TYR:C	1:B:401:LEU:HD12	2.20	0.62
1:A:373:PHE:H	1:A:373:PHE:HD2	1.48	0.62
1:B:763:HIS:CE1	1:B:777:TYR:HD1	2.16	0.61
1:A:746:TYR:HE2	1:A:748:ASP:CA	2.12	0.61
1:B:373:PHE:N	1:B:373:PHE:CD2	2.67	0.61
1:B:375:HIS:CD2	1:B:377:GLN:N	2.68	0.61
1:B:698:LYS:O	1:B:741:HIS:HA	2.01	0.61
1:A:362:VAL:HG21	1:A:389:ALA:HB2	1.82	0.61
1:A:305:PRO:O	1:A:334:LYS:NZ	2.20	0.61
1:A:294:ARG:HG3	1:A:295:ASP:N	2.16	0.61
1:A:640:ASP:N	1:A:645:ASN:OD1	2.33	0.61
1:B:633:GLN:NE2	1:B:668:MET:CA	2.62	0.61
1:A:765:PHE:HE1	1:A:769:HIS:CD2	2.19	0.61
1:A:798:THR:HG23	1:A:803:VAL:CG2	2.24	0.61
1:B:392:GLU:HG2	1:B:393:ASP:H	1.64	0.61
1:A:776:PRO:HB2	1:A:777:TYR:HD1	1.65	0.60
1:A:922:GLN:NE2	1:B:919:GLN:HB3	2.16	0.60
1:B:698:LYS:HZ2	3:B:1950:X6K:H25	1.49	0.60
1:B:708:LEU:C	1:B:708:LEU:HD23	2.21	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:PHE:HD1	1:A:583:PHE:O	1.83	0.60
1:A:746:TYR:HE2	1:A:748:ASP:CB	2.13	0.60
1:B:827:ILE:HG23	1:B:828:LEU:HG	1.84	0.60
1:A:319:TRP:HA	1:A:322:ARG:CZ	2.30	0.60
1:A:645:ASN:O	1:A:648:ASN:O	2.19	0.60
1:B:314:GLU:HA	1:B:317:LEU:HB3	1.81	0.60
1:B:338:CYS:SG	1:B:339:ILE:N	2.75	0.60
1:B:369:LEU:HD11	1:B:386:LEU:HD11	1.82	0.60
1:A:746:TYR:HE2	1:A:748:ASP:HA	1.66	0.60
1:B:416:LEU:C	1:B:582:MET:HE1	2.22	0.60
1:B:618:VAL:HG21	1:B:632:PHE:CD2	2.37	0.60
1:B:302:TYR:CD2	1:B:303:ARG:N	2.70	0.60
1:A:819:LEU:HD23	1:A:820:PHE:CA	2.32	0.60
1:B:406:LYS:NZ	1:B:887:ASP:O	2.33	0.60
1:B:417:HIS:HE1	1:B:578:MET:CB	2.12	0.60
1:B:876:ASN:N	1:B:876:ASN:ND2	2.49	0.60
1:B:373:PHE:N	1:B:373:PHE:HD2	2.00	0.60
1:B:618:VAL:HG11	1:B:632:PHE:HD2	1.67	0.60
1:A:319:TRP:HD1	1:A:323:PHE:CE2	2.19	0.59
1:B:318:VAL:O	1:B:322:ARG:N	2.35	0.59
1:A:776:PRO:CB	1:A:777:TYR:HD1	2.15	0.59
1:A:777:TYR:CD1	1:A:777:TYR:N	2.70	0.59
1:B:305:PRO:HG3	1:B:308:TYR:CE2	2.37	0.59
1:A:573:HIS:C	1:A:573:HIS:CD2	2.74	0.59
1:A:664:LYS:HG2	1:A:685:VAL:HG21	1.84	0.59
1:B:533:LEU:HG	1:B:534:CYS:N	2.16	0.59
1:A:371:PRO:HB3	1:A:407:TYR:CD1	2.37	0.59
1:B:311:SER:OG	1:B:311:SER:O	2.19	0.59
1:B:417:HIS:CE1	1:B:578:MET:HB3	2.37	0.59
1:B:663:THR:OG1	1:B:664:LYS:HG2	2.03	0.59
1:A:746:TYR:C	1:A:746:TYR:CD2	2.76	0.59
1:A:805:ASP:N	1:A:831:ASP:OD2	2.35	0.59
1:B:375:HIS:NE2	1:B:377:GLN:CB	2.65	0.59
1:A:723:GLU:O	1:A:724:ASN:CB	2.48	0.59
1:B:606:ARG:NH1	1:B:643:LYS:HB2	2.18	0.58
1:B:763:HIS:ND1	1:B:777:TYR:HD1	2.01	0.58
1:A:319:TRP:HA	1:A:322:ARG:CD	2.33	0.58
1:A:914:ASP:OD1	1:A:914:ASP:N	2.33	0.58
1:A:663:THR:HG22	1:A:664:LYS:H	1.68	0.58
1:B:578:MET:O	1:B:582:MET:CG	2.51	0.58
1:B:610:GLU:OE1	1:B:643:LYS:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:811:LEU:C	1:A:812:LEU:HD23	2.24	0.58
1:A:922:GLN:HE22	1:B:919:GLN:HB3	1.68	0.58
1:A:930:THR:HG22	1:A:936:LEU:HB3	1.85	0.58
1:B:315:GLN:HG3	1:B:338:CYS:HB2	1.83	0.58
1:B:783:VAL:HG13	1:B:816:ASN:O	2.02	0.58
1:B:743:PHE:C	1:B:744:LEU:HD23	2.23	0.58
1:A:295:ASP:OD1	1:A:296:GLN:N	2.37	0.58
1:B:605:ARG:O	1:B:609:ASP:OD1	2.22	0.58
1:B:746:TYR:C	1:B:746:TYR:CD2	2.77	0.58
1:B:803:VAL:HG12	1:B:806:ARG:HD3	1.84	0.58
1:B:865:TYR:CD1	1:B:918:VAL:HG13	2.38	0.58
1:B:920:HIS:O	1:B:923:SER:HB3	2.03	0.58
1:A:703:LEU:CD1	1:A:744:LEU:HD21	2.34	0.58
1:B:707:GLN:HB3	1:B:734:VAL:HG12	1.85	0.58
1:A:806:ARG:HH21	1:A:810:ASN:CB	2.06	0.57
1:A:827:ILE:N	1:A:892:ASP:OD2	2.37	0.57
1:B:704:ARG:CZ	1:B:889:THR:HG21	2.34	0.57
1:B:765:PHE:C	1:B:765:PHE:HD2	2.05	0.57
1:A:319:TRP:CH2	1:A:346:GLU:OE1	2.57	0.57
1:A:550:TYR:O	1:A:554:TYR:CD2	2.58	0.57
1:B:375:HIS:HD2	1:B:378:VAL:H	1.53	0.57
1:A:341:TRP:CD1	1:A:342:LYS:HA	2.39	0.57
1:B:706:ASP:OD2	3:B:1950:X6K:H22	2.04	0.57
1:B:888:ALA:O	1:B:889:THR:HB	2.04	0.57
1:A:587:LEU:HB3	1:A:598:PHE:HB2	1.86	0.57
1:A:872:ARG:NH2	1:A:912:LEU:O	2.38	0.57
1:B:767:ARG:CD	1:B:778:GLY:HA3	2.30	0.57
1:A:549:ASN:HD22	1:A:550:TYR:N	2.02	0.57
1:B:645:ASN:OD1	1:B:645:ASN:C	2.43	0.57
1:B:891:PRO:O	1:B:895:LEU:HD12	2.04	0.56
1:B:708:LEU:HD12	1:B:885:MET:HE3	1.88	0.56
1:B:763:HIS:HE1	1:B:777:TYR:CD1	2.22	0.56
1:A:552:TYR:CD2	1:A:552:TYR:O	2.57	0.56
1:B:412:HIS:ND1	1:B:531:ALA:HA	2.20	0.56
1:B:677:LEU:HD23	1:B:699:HIS:CE1	2.40	0.56
1:B:772:CYS:N	1:B:778:GLY:O	2.37	0.56
1:B:299:THR:O	1:B:302:TYR:CD2	2.56	0.56
1:B:335:PHE:HD1	1:B:357:TRP:HZ3	1.53	0.56
1:B:909:GLN:HG3	1:B:912:LEU:HG	1.88	0.56
1:A:417:HIS:ND1	1:A:417:HIS:C	2.59	0.56
1:B:319:TRP:HA	1:B:322:ARG:CD	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:PRO:O	1:B:334:LYS:NZ	2.25	0.56
1:A:566:ARG:O	1:A:567:LYS:HG2	2.06	0.56
1:B:889:THR:HG23	1:B:889:THR:O	2.05	0.56
1:A:298:HIS:HE1	1:A:318:VAL:HA	1.71	0.56
1:B:375:HIS:CD2	1:B:378:VAL:H	2.23	0.56
1:B:587:LEU:HB3	1:B:598:PHE:HB2	1.88	0.56
1:A:746:TYR:CE2	1:A:748:ASP:CA	2.89	0.56
1:B:765:PHE:HD2	1:B:766:PHE:N	2.03	0.56
1:A:306:PRO:HG3	1:A:879:LEU:HD13	1.88	0.56
1:B:398:LEU:HD23	1:B:399:LEU:N	2.22	0.55
1:B:712:MET:SD	1:B:882:PHE:HE2	2.28	0.55
1:B:739:SER:O	1:B:740:LYS:CG	2.52	0.55
1:A:373:PHE:N	1:A:373:PHE:CD2	2.73	0.55
1:A:677:LEU:HD12	1:A:677:LEU:H	1.70	0.55
1:A:776:PRO:C	1:A:777:TYR:CD1	2.80	0.55
1:B:405:LEU:HB3	1:B:575:MET:CE	2.36	0.55
1:B:710:LEU:O	1:B:714:THR:OG1	2.25	0.55
1:A:412:HIS:CB	1:A:531:ALA:N	2.69	0.55
1:B:372:THR:HG1	1:B:373:PHE:HD2	1.54	0.55
1:B:377:GLN:HG3	1:B:381:TYR:HE2	1.72	0.55
1:A:862:LYS:O	1:A:866:THR:HG23	2.07	0.55
1:A:703:LEU:N	1:A:703:LEU:HD23	2.22	0.55
1:B:319:TRP:N	1:B:322:ARG:NE	2.55	0.55
1:B:699:HIS:O	1:B:740:LYS:O	2.25	0.55
1:A:591:ASN:CG	1:A:592:PHE:H	2.06	0.55
1:A:804:GLY:O	1:A:805:ASP:HB3	2.06	0.55
1:A:565:VAL:HG12	1:A:569:ASP:HB2	1.89	0.55
1:B:868:TYR:O	1:B:872:ARG:HD3	2.06	0.55
1:A:400:GLN:O	1:A:403:GLN:HB2	2.07	0.55
1:A:948:ARG:HH11	1:A:948:ARG:CB	2.13	0.55
1:A:357:TRP:CD1	1:A:358:ALA:N	2.75	0.54
1:A:302:TYR:HA	1:A:334:LYS:HG3	1.89	0.54
1:A:709:ILE:HG13	1:A:827:ILE:HD11	1.89	0.54
1:A:787:TYR:HE1	1:A:791:CYS:SG	2.30	0.54
1:A:826:TYR:HD1	1:A:830:ARG:HB3	1.72	0.54
1:B:767:ARG:HD3	1:B:778:GLY:CA	2.32	0.54
1:A:562:VAL:C	1:A:564:SER:H	2.10	0.54
1:A:727:LEU:HB2	1:A:729:LEU:HD21	1.89	0.54
1:B:397:TYR:C	1:B:401:LEU:CD1	2.75	0.54
1:B:311:SER:HB2	1:B:314:GLU:CB	2.37	0.54
1:B:762:ILE:O	1:B:765:PHE:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:PRO:HB3	1:A:308:TYR:CE1	2.42	0.54
1:A:807:HIS:O	1:A:810:ASN:HB2	2.08	0.54
1:A:734:VAL:HG22	1:A:744:LEU:HD22	1.90	0.54
1:A:855:GLU:O	1:A:859:GLU:HB2	2.07	0.54
1:A:710:LEU:O	1:A:714:THR:OG1	2.24	0.54
1:B:614:LEU:O	1:B:618:VAL:HG23	2.08	0.54
1:B:329:LYS:HG2	1:B:359:PRO:O	2.07	0.53
1:A:621:GLU:O	1:A:628:LYS:HE2	2.09	0.53
1:A:673:PHE:HB2	1:A:679:PRO:HD2	1.90	0.53
1:B:338:CYS:O	1:B:341:TRP:HB3	2.08	0.53
1:B:788:ILE:HG13	1:B:860:PHE:HB2	1.90	0.53
1:B:876:ASN:H	1:B:876:ASN:ND2	2.05	0.53
1:A:719:LEU:O	1:A:722:ARG:HB2	2.07	0.53
1:A:765:PHE:CE1	1:A:769:HIS:CD2	2.96	0.53
1:B:335:PHE:HD2	1:B:336:LEU:N	2.06	0.53
1:A:583:PHE:CD1	1:A:583:PHE:C	2.81	0.53
1:A:633:GLN:OE1	1:A:668:MET:SD	2.66	0.53
1:A:808:LEU:H	1:A:808:LEU:HD22	1.73	0.53
1:B:906:GLU:O	1:B:909:GLN:OE1	2.25	0.53
1:A:790:SER:CB	1:A:819:LEU:H	2.22	0.53
1:A:717:ASP:OD1	1:A:721:ARG:NH1	2.30	0.53
1:B:672:LEU:HD21	1:B:678:MET:CB	2.20	0.53
1:A:302:TYR:CE1	1:A:303:ARG:HG3	2.44	0.53
1:A:313:GLU:OE1	1:A:313:GLU:HA	2.08	0.53
1:A:679:PRO:HG3	1:A:698:LYS:HG3	1.89	0.53
1:B:326:SER:HA	1:B:357:TRP:CH2	2.44	0.53
1:A:805:ASP:HB2	1:A:832:PRO:HD3	1.91	0.53
1:B:409:ASP:OD1	1:B:410:PRO:HD2	2.09	0.53
1:B:541:ALA:HB2	1:B:551:PHE:HD2	1.73	0.53
1:B:827:ILE:HG22	1:B:828:LEU:HG	1.90	0.53
1:A:357:TRP:CD1	1:A:358:ALA:O	2.59	0.53
1:A:777:TYR:HD1	1:A:777:TYR:N	2.06	0.53
1:B:334:LYS:O	1:B:337:LYS:HB2	2.09	0.52
1:A:549:ASN:C	1:A:549:ASN:ND2	2.62	0.52
1:B:842:SER:OG	1:B:845:MET:CG	2.57	0.52
1:A:787:TYR:O	1:A:787:TYR:CD1	2.62	0.52
1:B:705:GLN:HB2	1:B:890:VAL:HG13	1.92	0.52
1:B:860:PHE:CE1	1:B:864:CYS:SG	3.02	0.52
1:B:865:TYR:CD1	1:B:918:VAL:CG1	2.92	0.52
1:A:845:MET:O	1:A:848:ALA:HB3	2.10	0.52
1:B:328:HIS:CD2	1:B:329:LYS:HD3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:LEU:HD22	1:A:732:TYR:O	2.10	0.52
1:B:311:SER:OG	1:B:314:GLU:CB	2.50	0.52
1:B:319:TRP:CD1	1:B:323:PHE:HZ	2.23	0.52
1:B:621:GLU:HB2	1:B:631:LYS:NZ	2.25	0.52
1:B:810:ASN:HA	1:B:822:ILE:CG2	2.40	0.52
1:A:335:PHE:C	1:A:335:PHE:CD2	2.82	0.52
1:A:395:LEU:C	1:A:395:LEU:HD23	2.30	0.52
1:A:814:THR:HG23	1:A:816:ASN:N	2.23	0.52
1:B:319:TRP:CA	1:B:322:ARG:NE	2.66	0.52
1:B:323:PHE:HD2	1:B:323:PHE:N	1.85	0.52
1:A:610:GLU:OE1	1:A:642:PHE:HB3	2.09	0.52
1:A:776:PRO:C	1:A:777:TYR:HD1	2.13	0.52
1:B:673:PHE:HD2	1:B:679:PRO:HB2	1.75	0.52
1:A:320:LYS:HB2	1:A:321:PHE:CD2	2.45	0.52
1:A:649:PHE:HE1	1:A:662:ILE:HG13	1.75	0.52
1:A:614:LEU:C	1:A:614:LEU:HD12	2.30	0.52
1:A:866:THR:O	1:A:870:HIS:CD2	2.58	0.52
1:B:319:TRP:CH2	1:B:346:GLU:CD	2.82	0.52
1:B:326:SER:O	1:B:357:TRP:CZ2	2.62	0.52
1:B:417:HIS:N	1:B:582:MET:HE1	2.25	0.52
1:B:664:LYS:N	1:B:685:VAL:HG23	2.11	0.52
1:B:912:LEU:HD12	1:B:917:ALA:HA	1.92	0.52
1:A:702:ASP:OD2	1:A:702:ASP:C	2.48	0.51
1:A:786:THR:O	1:A:790:SER:OG	2.22	0.51
1:B:319:TRP:HH2	1:B:346:GLU:OE2	1.91	0.51
1:B:375:HIS:NE2	1:B:377:GLN:HB2	2.25	0.51
1:B:888:ALA:O	1:B:889:THR:CB	2.58	0.51
1:A:705:GLN:OE1	1:A:827:ILE:HD12	2.10	0.51
1:A:765:PHE:CE1	1:A:769:HIS:HD2	2.28	0.51
1:B:305:PRO:CG	1:B:308:TYR:CE2	2.93	0.51
1:B:326:SER:O	1:B:357:TRP:NE1	2.42	0.51
1:B:375:HIS:CD2	1:B:375:HIS:C	2.83	0.51
1:A:552:TYR:CD1	1:A:601:LEU:HD22	2.45	0.51
1:A:690:HIS:O	1:A:691:HIS:C	2.47	0.51
1:B:577:ALA:O	1:B:581:LYS:HD3	2.10	0.51
1:A:591:ASN:O	1:A:595:ARG:CG	2.59	0.51
1:B:391:ASP:OD2	1:B:540:ARG:NH2	2.44	0.51
1:B:412:HIS:CG	1:B:531:ALA:HA	2.46	0.51
1:B:746:TYR:HE2	1:B:748:ASP:HA	1.76	0.51
1:B:339:ILE:HD12	1:B:340:ASN:N	2.26	0.51
1:A:560:GLU:O	1:A:560:GLU:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:LEU:O	1:A:723:GLU:HG2	2.11	0.51
1:A:763:HIS:NE2	1:A:848:ALA:O	2.44	0.51
1:B:827:ILE:HB	1:B:892:ASP:OD2	2.11	0.51
1:A:396:LEU:C	1:A:396:LEU:HD23	2.31	0.51
1:A:723:GLU:O	1:A:724:ASN:HB3	2.10	0.51
1:A:339:ILE:O	1:A:342:LYS:HG2	2.11	0.51
1:A:649:PHE:O	1:A:663:THR:HG23	2.11	0.51
1:A:737:THR:HG23	1:A:738:SER:N	2.25	0.51
1:B:913:THR:HG22	1:B:916:GLU:CD	2.31	0.51
1:A:552:TYR:HD2	1:A:552:TYR:O	1.95	0.50
1:A:579:VAL:HA	1:A:582:MET:HE3	1.91	0.50
1:A:764:ASN:ND2	1:A:767:ARG:HH12	2.10	0.50
1:B:573:HIS:HD2	1:B:574:ASP:N	2.08	0.50
1:A:421:PHE:N	1:A:421:PHE:CD1	2.78	0.50
1:B:763:HIS:HD1	1:B:777:TYR:HD1	1.58	0.50
1:A:305:PRO:HB2	1:A:308:TYR:CD2	2.46	0.50
1:A:751:THR:HG23	1:A:754:GLU:CG	2.42	0.50
1:A:826:TYR:HB3	1:A:830:ARG:O	2.11	0.50
1:A:824:PHE:N	1:A:824:PHE:CD2	2.79	0.50
1:A:913:THR:CG2	1:A:916:GLU:CD	2.80	0.50
1:B:536:PHE:C	1:B:536:PHE:CD1	2.85	0.50
1:B:667:PRO:O	1:B:670:THR:HG23	2.12	0.50
1:A:787:TYR:CD1	1:A:787:TYR:C	2.84	0.50
1:A:872:ARG:NH1	1:A:909:GLN:O	2.39	0.50
1:B:749:SER:HB3	1:B:820:PHE:HZ	1.76	0.50
1:B:674:LYS:HG2	3:B:1950:X6K:H03	1.94	0.50
1:A:698:LYS:HZ1	3:A:1951:X6K:C24	2.24	0.50
1:A:765:PHE:C	1:A:765:PHE:CD1	2.84	0.50
1:B:906:GLU:HA	1:B:906:GLU:OE1	2.11	0.50
1:B:360:MET:HG2	1:B:385:ARG:CG	2.41	0.50
1:B:914:ASP:O	1:B:918:VAL:HG23	2.12	0.50
1:A:398:LEU:CD1	1:A:402:VAL:HG23	2.42	0.49
1:A:575:MET:SD	1:A:575:MET:C	2.91	0.49
1:A:665:ILE:HG22	1:A:666:VAL:N	2.25	0.49
1:B:302:TYR:HE2	1:B:303:ARG:HG3	1.76	0.49
1:B:677:LEU:HD23	1:B:699:HIS:HE1	1.77	0.49
1:A:647:THR:O	1:A:664:LYS:CB	2.58	0.49
1:B:712:MET:HE1	1:B:715:LEU:HD13	1.94	0.49
1:B:755:VAL:HG13	1:B:765:PHE:HD1	1.76	0.49
1:A:577:ALA:O	1:A:581:LYS:CD	2.51	0.49
1:B:876:ASN:O	1:B:880:ASN:ND2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:GLN:C	1:B:322:ARG:NH2	2.65	0.49
1:A:351:LEU:HD11	1:A:377:GLN:CG	2.40	0.49
1:A:885:MET:O	1:A:888:ALA:HB2	2.13	0.49
1:B:610:GLU:OE2	1:B:613:LYS:HD2	2.12	0.49
1:A:563:GLU:HA	1:A:563:GLU:OE1	2.11	0.49
1:A:814:THR:CG2	1:A:816:ASN:HB2	2.41	0.49
1:B:357:TRP:CD1	1:B:358:ALA:N	2.80	0.49
1:A:937:VAL:O	1:A:941:HIS:CD2	2.65	0.49
1:B:318:VAL:C	1:B:322:ARG:HG3	2.33	0.49
1:B:401:LEU:HA	1:B:404:ALA:HB3	1.94	0.49
1:A:303:ARG:C	1:A:304:TYR:HD2	2.16	0.49
1:A:844:GLU:OE1	1:A:844:GLU:N	2.43	0.49
1:A:861:ARG:NH2	1:A:929:ILE:HD12	2.27	0.49
1:A:308:TYR:HD1	1:A:310:LEU:HB3	1.78	0.49
1:B:751:THR:OG1	1:B:809:ASP:HA	2.12	0.49
1:A:803:VAL:HG11	1:A:824:PHE:CD1	2.42	0.49
1:B:377:GLN:O	1:B:381:TYR:HD2	1.96	0.49
1:A:398:LEU:C	1:A:398:LEU:HD12	2.34	0.48
1:A:412:HIS:HB3	1:A:531:ALA:CA	2.44	0.48
1:B:405:LEU:HB3	1:B:575:MET:HE1	1.94	0.48
1:B:541:ALA:O	1:B:548:ALA:HB2	2.14	0.48
1:B:573:HIS:CD2	1:B:574:ASP:N	2.81	0.48
1:B:631:LYS:O	1:B:635:LEU:HD23	2.12	0.48
1:B:756:LEU:HA	1:B:759:GLU:O	2.13	0.48
1:A:640:ASP:CA	1:A:645:ASN:OD1	2.61	0.48
1:A:654:PHE:CE2	1:A:693:TYR:CE1	3.00	0.48
1:A:737:THR:CG2	1:A:738:SER:N	2.76	0.48
1:B:360:MET:CG	1:B:385:ARG:HG3	2.43	0.48
1:B:375:HIS:CG	1:B:376:PRO:HD2	2.48	0.48
1:B:539:GLN:HG2	1:B:540:ARG:N	2.26	0.48
1:B:822:ILE:CD1	3:B:1950:X6K:C09	2.91	0.48
1:B:843:LYS:HA	1:B:932:VAL:CG1	2.43	0.48
1:A:294:ARG:HG3	1:A:295:ASP:H	1.79	0.48
1:A:814:THR:CG2	1:A:816:ASN:N	2.76	0.48
1:A:857:HIS:NE2	1:A:861:ARG:NH1	2.61	0.48
1:B:881:LEU:N	1:B:881:LEU:HD23	2.28	0.48
1:B:913:THR:CG2	1:B:916:GLU:HG3	2.43	0.48
1:A:709:ILE:HG12	1:A:827:ILE:HD11	1.95	0.48
1:B:746:TYR:C	1:B:746:TYR:HD2	2.15	0.48
1:A:295:ASP:O	1:A:299:THR:N	2.46	0.48
1:A:552:TYR:HD1	1:A:601:LEU:HD13	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:752:VAL:CG1	1:A:808:LEU:HD12	2.41	0.48
1:A:625:ARG:O	1:A:629:THR:CG2	2.59	0.48
1:A:709:ILE:O	1:A:712:MET:HB2	2.12	0.48
1:B:305:PRO:CG	1:B:308:TYR:CD2	2.96	0.48
1:B:336:LEU:HD11	1:B:354:LEU:HB2	1.94	0.48
1:B:614:LEU:HD12	1:B:614:LEU:C	2.34	0.48
1:B:634:LYS:HE3	1:B:638:GLU:OE2	2.13	0.48
1:A:575:MET:O	1:A:579:VAL:HG23	2.13	0.48
1:A:580:LEU:HD22	1:A:584:LEU:CD1	2.43	0.48
1:A:629:THR:HG22	1:A:672:LEU:HD12	1.94	0.48
1:A:703:LEU:CD1	1:A:744:LEU:CD2	2.92	0.48
1:A:811:LEU:N	1:A:811:LEU:HD23	2.28	0.48
1:A:296:GLN:O	1:A:299:THR:HG22	2.14	0.48
1:A:319:TRP:HH2	1:A:346:GLU:OE1	1.96	0.48
1:A:814:THR:HG21	1:A:816:ASN:HB2	1.95	0.48
1:A:819:LEU:HD23	1:A:820:PHE:N	2.27	0.48
1:A:826:TYR:CD1	1:A:830:ARG:HB3	2.49	0.48
1:B:709:ILE:HD12	1:B:801:LEU:HD13	1.95	0.48
1:A:544:ASN:C	1:A:544:ASN:OD1	2.52	0.48
1:A:787:TYR:CE1	1:A:791:CYS:SG	3.06	0.48
1:A:913:THR:HG22	1:A:916:GLU:OE1	2.14	0.48
1:B:332:LEU:HB2	1:B:357:TRP:CE2	2.49	0.48
1:B:843:LYS:CA	1:B:932:VAL:CG1	2.92	0.48
1:A:660:ILE:HG12	1:A:660:ILE:O	2.12	0.47
1:A:777:TYR:HB2	1:A:779:ILE:HD12	1.96	0.47
1:A:843:LYS:N	1:A:932:VAL:CG1	2.77	0.47
1:B:704:ARG:HA	1:B:707:GLN:HG2	1.96	0.47
1:B:810:ASN:C	1:B:822:ILE:HG22	2.33	0.47
1:A:294:ARG:O	1:A:298:HIS:HD2	1.97	0.47
1:A:353:MET:O	1:A:357:TRP:HB2	2.14	0.47
1:A:398:LEU:HD12	1:A:398:LEU:O	2.14	0.47
1:A:649:PHE:CE2	1:A:664:LYS:HA	2.48	0.47
1:B:399:LEU:HD12	1:B:399:LEU:O	2.13	0.47
1:B:776:PRO:C	1:B:777:TYR:CD2	2.78	0.47
1:B:902:LYS:O	1:B:906:GLU:HG2	2.13	0.47
1:A:673:PHE:HE2	1:A:696:ILE:HG12	1.79	0.47
1:A:806:ARG:HA	1:A:810:ASN:HD22	1.80	0.47
1:A:857:HIS:CD2	1:A:857:HIS:C	2.87	0.47
1:B:858:HIS:C	1:B:858:HIS:ND1	2.67	0.47
1:A:391:ASP:OD2	1:A:391:ASP:N	2.47	0.47
1:A:931:ALA:O	1:B:944:THR:OG1	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:712:MET:SD	1:B:882:PHE:CE2	3.07	0.47
1:A:335:PHE:CD2	1:A:335:PHE:O	2.68	0.47
1:A:814:THR:CG2	1:A:816:ASN:H	2.23	0.47
1:A:354:LEU:HD23	1:A:354:LEU:C	2.35	0.47
1:B:339:ILE:HD13	1:B:350:ALA:CB	2.45	0.47
1:B:710:LEU:HD22	1:B:732:TYR:O	2.15	0.47
1:A:293:ILE:O	1:A:296:GLN:N	2.45	0.47
1:A:551:PHE:CE1	1:A:555:LEU:HD11	2.49	0.47
1:B:332:LEU:HD13	1:B:357:TRP:CD2	2.49	0.47
1:B:708:LEU:HD12	1:B:885:MET:HE2	1.96	0.47
1:A:319:TRP:HD1	1:A:319:TRP:O	1.98	0.47
1:A:839:MET:HG2	1:A:925:LEU:HD23	1.95	0.47
1:B:400:GLN:OE1	1:B:711:GLN:OE1	2.33	0.47
1:A:379:ARG:O	1:A:383:VAL:HG23	2.15	0.46
1:B:417:HIS:HE1	1:B:578:MET:HB3	1.76	0.46
1:A:808:LEU:HD22	1:A:808:LEU:N	2.30	0.46
1:A:830:ARG:HH22	1:A:903:LYS:NZ	2.14	0.46
1:B:391:ASP:OD2	1:B:391:ASP:N	2.48	0.46
1:B:544:ASN:OD1	1:B:544:ASN:C	2.53	0.46
1:B:746:TYR:CE2	1:B:748:ASP:HA	2.49	0.46
1:A:614:LEU:HD21	1:A:636:LEU:HD23	1.98	0.46
1:A:744:LEU:HD23	1:A:744:LEU:N	2.31	0.46
1:A:865:TYR:CD1	1:A:918:VAL:HG13	2.50	0.46
1:B:302:TYR:CE2	1:B:303:ARG:HG3	2.48	0.46
1:A:872:ARG:HH12	1:A:909:GLN:C	2.18	0.46
1:A:913:THR:HG22	1:A:916:GLU:CD	2.36	0.46
1:A:300:ILE:O	1:A:304:TYR:HB2	2.15	0.46
1:A:567:LYS:HG3	1:A:568:GLN:H	1.80	0.46
1:B:363:GLU:HA	1:B:366:LEU:CD1	2.35	0.46
1:A:583:PHE:O	1:A:583:PHE:CD1	2.65	0.46
1:A:664:LYS:O	1:A:685:VAL:HG22	2.15	0.46
1:A:774:ASN:OD1	1:A:774:ASN:N	2.48	0.46
1:B:417:HIS:ND1	1:B:578:MET:CB	2.66	0.46
1:B:332:LEU:HB2	1:B:357:TRP:CD1	2.51	0.46
1:B:357:TRP:HD1	1:B:358:ALA:O	1.99	0.46
1:B:698:LYS:NZ	3:B:1950:X6K:O25	2.26	0.46
1:A:318:VAL:O	1:A:322:ARG:CG	2.52	0.46
1:B:800:LEU:HD13	1:B:908:LEU:HD21	1.97	0.46
1:B:813:LEU:HD12	1:B:813:LEU:HA	1.80	0.46
1:B:826:TYR:HB3	1:B:830:ARG:O	2.16	0.46
1:A:708:LEU:HD23	1:A:708:LEU:C	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:727:LEU:HD12	1:A:793:GLY:CA	2.46	0.46
1:A:763:HIS:O	1:A:767:ARG:HB2	2.16	0.46
1:A:330:LYS:O	1:A:333:THR:HG23	2.16	0.45
1:A:583:PHE:CE1	1:A:587:LEU:HD11	2.51	0.45
1:A:746:TYR:C	1:A:746:TYR:HD2	2.19	0.45
1:B:371:PRO:HB3	1:B:407:TYR:CD2	2.51	0.45
1:B:755:VAL:HG13	1:B:765:PHE:CD1	2.50	0.45
1:A:398:LEU:HD12	1:A:402:VAL:HG23	1.99	0.45
1:A:737:THR:CG2	1:A:741:HIS:CD2	2.98	0.45
1:A:755:VAL:CG1	1:A:765:PHE:CD2	2.99	0.45
1:B:541:ALA:CB	1:B:551:PHE:HD2	2.29	0.45
1:A:865:TYR:O	1:A:869:LEU:HG	2.17	0.45
1:B:405:LEU:HD23	1:B:533:LEU:HD11	1.96	0.45
1:B:674:LYS:HD3	3:B:1950:X6K:H03	1.98	0.45
1:B:779:ILE:H	1:B:779:ILE:HG12	1.32	0.45
1:A:331:ALA:HB3	1:A:357:TRP:HZ2	1.81	0.45
1:A:682:LEU:CD1	1:A:682:LEU:N	2.80	0.45
1:B:305:PRO:HG3	1:B:308:TYR:CD2	2.52	0.45
1:B:308:TYR:CE1	1:B:310:LEU:HD22	2.51	0.45
1:B:823:ASP:OD1	1:B:823:ASP:C	2.55	0.45
1:A:798:THR:HA	1:A:803:VAL:CG2	2.46	0.45
1:B:567:LYS:HG3	1:B:568:GLN:H	1.80	0.45
1:B:624:ASN:OD1	1:B:625:ARG:N	2.49	0.45
1:B:803:VAL:O	1:B:840:LYS:NZ	2.50	0.45
1:B:560:GLU:OE1	1:B:739:SER:CB	2.61	0.45
1:A:544:ASN:OD1	1:A:546:THR:N	2.50	0.45
1:A:727:LEU:HB2	1:A:729:LEU:CD2	2.47	0.45
1:B:639:GLN:O	1:B:640:ASP:CB	2.65	0.45
1:B:908:LEU:HD23	1:B:908:LEU:HA	1.74	0.45
1:B:300:ILE:O	1:B:304:TYR:HB2	2.17	0.45
1:B:342:LYS:CB	1:B:346:GLU:HG3	2.29	0.45
1:B:722:ARG:HB3	1:B:722:ARG:NH1	2.30	0.45
1:B:319:TRP:O	1:B:323:PHE:CD2	2.67	0.44
1:B:598:PHE:HD2	1:B:599:TYR:N	2.15	0.44
1:A:614:LEU:HD12	1:A:614:LEU:O	2.17	0.44
1:A:675:SER:HA	2:A:1949:SO4:O1	2.17	0.44
1:B:862:LYS:O	1:B:866:THR:HG22	2.18	0.44
1:A:326:SER:HB2	1:A:357:TRP:CD2	2.52	0.44
1:A:807:HIS:CD2	1:A:809:ASP:HB2	2.52	0.44
1:A:861:ARG:O	1:A:865:TYR:CD2	2.71	0.44
1:A:948:ARG:HD2	1:A:948:ARG:C	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:LYS:H	1:A:674:LYS:HG2	1.56	0.44
1:A:723:GLU:OE1	1:A:723:GLU:CA	2.58	0.44
1:A:830:ARG:HA	1:A:830:ARG:HD3	1.81	0.44
1:B:804:GLY:O	1:B:805:ASP:HB3	2.16	0.44
1:B:392:GLU:O	1:B:396:LEU:HD12	2.18	0.44
1:B:605:ARG:HA	1:B:605:ARG:HD3	1.82	0.44
1:B:751:THR:HG23	1:B:754:GLU:CB	2.47	0.44
1:A:398:LEU:O	1:A:401:LEU:N	2.51	0.44
1:B:319:TRP:HD1	1:B:323:PHE:HE2	1.58	0.44
1:B:765:PHE:HD2	1:B:766:PHE:HD2	1.64	0.44
1:B:843:LYS:N	1:B:932:VAL:HG11	2.33	0.44
1:B:305:PRO:HB3	1:B:308:TYR:CD2	2.36	0.44
1:B:395:LEU:O	1:B:398:LEU:HB3	2.18	0.44
1:B:392:GLU:CG	1:B:393:ASP:N	2.73	0.44
1:B:865:TYR:HB3	1:B:918:VAL:HG13	2.00	0.44
1:A:343:LEU:O	1:A:347:VAL:HG23	2.18	0.44
1:A:533:LEU:HD23	1:A:534:CYS:N	2.33	0.44
1:A:585:LYS:HD2	1:A:585:LYS:HA	1.70	0.44
1:B:318:VAL:CG1	1:B:322:ARG:HG3	2.29	0.44
1:B:335:PHE:HD1	1:B:357:TRP:CZ3	2.30	0.44
1:A:776:PRO:CB	1:A:777:TYR:CD1	2.99	0.43
1:A:922:GLN:OE1	1:B:922:GLN:OE1	2.35	0.43
1:B:549:ASN:ND2	1:B:550:TYR:N	2.65	0.43
1:B:603:LYS:HB3	1:B:652:ILE:HD11	2.00	0.43
1:B:702:ASP:OD2	1:B:704:ARG:HB2	2.18	0.43
1:B:712:MET:HE2	1:B:712:MET:CA	2.44	0.43
1:A:398:LEU:O	1:A:399:LEU:C	2.56	0.43
1:A:566:ARG:HB2	1:A:567:LYS:HE3	1.99	0.43
1:B:403:GLN:NE2	1:B:888:ALA:HA	2.34	0.43
1:B:608:ILE:O	1:B:612:VAL:HG23	2.19	0.43
1:B:684:PHE:HB2	1:B:693:TYR:O	2.18	0.43
1:B:866:THR:O	1:B:870:HIS:CD2	2.61	0.43
1:A:763:HIS:CE1	1:A:777:TYR:CD2	3.06	0.43
1:B:314:GLU:HG3	1:B:314:GLU:O	2.18	0.43
1:B:664:LYS:N	1:B:685:VAL:CG2	2.78	0.43
1:B:767:ARG:HG2	1:B:778:GLY:HA3	2.01	0.43
1:B:777:TYR:O	1:B:778:GLY:C	2.56	0.43
1:A:409:ASP:OD1	1:A:411:ARG:N	2.51	0.43
1:A:701:ASP:OD2	1:A:702:ASP:N	2.52	0.43
1:A:728:LYS:CG	1:A:786:THR:HB	2.40	0.43
1:A:822:ILE:HD11	3:A:1951:X6K:H162	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:LEU:O	1:B:336:LEU:HD22	2.17	0.43
1:A:351:LEU:HD12	1:A:377:GLN:HG2	1.96	0.43
1:A:743:PHE:O	1:A:744:LEU:HD23	2.19	0.43
1:A:820:PHE:N	1:A:820:PHE:CD2	2.86	0.43
1:A:341:TRP:CD1	1:A:342:LYS:N	2.86	0.43
1:A:591:ASN:CG	1:A:592:PHE:N	2.72	0.43
1:B:621:GLU:HB2	1:B:631:LYS:HZ3	1.83	0.43
1:B:732:TYR:HB2	1:B:745:GLN:HB3	2.00	0.43
1:A:363:GLU:H	1:A:363:GLU:CD	2.20	0.43
1:A:398:LEU:HA	1:A:401:LEU:HG	2.00	0.43
1:A:403:GLN:HG3	1:A:885:MET:SD	2.59	0.43
1:A:656:LEU:HA	1:A:656:LEU:HD23	1.66	0.43
1:A:842:SER:HB3	1:A:845:MET:SD	2.59	0.43
1:B:913:THR:HG23	1:B:916:GLU:HG3	2.00	0.43
1:A:861:ARG:O	1:A:865:TYR:CE2	2.71	0.43
1:B:310:LEU:HD23	1:B:311:SER:CB	2.34	0.43
1:B:751:THR:HG23	1:B:754:GLU:HB2	2.01	0.43
1:B:770:HIS:O	1:B:779:ILE:HA	2.19	0.43
1:B:858:HIS:HE1	1:B:862:LYS:NZ	2.16	0.43
1:A:294:ARG:HH11	1:A:321:PHE:HE1	1.66	0.43
1:B:751:THR:HA	1:B:812:LEU:CD1	2.49	0.43
1:B:912:LEU:HB3	1:B:916:GLU:HB2	2.00	0.43
1:A:395:LEU:HD23	1:A:395:LEU:O	2.19	0.42
1:B:329:LYS:O	1:B:332:LEU:HB3	2.18	0.42
1:B:360:MET:HE2	1:B:381:TYR:HB3	1.98	0.42
1:A:663:THR:O	1:A:664:LYS:O	2.37	0.42
1:A:720:LEU:HD23	1:A:720:LEU:N	2.34	0.42
1:B:553:TRP:O	1:B:557:ILE:HG13	2.20	0.42
1:B:599:TYR:HD2	1:B:599:TYR:C	2.22	0.42
1:B:648:ASN:OD1	1:B:649:PHE:N	2.52	0.42
1:A:682:LEU:O	1:A:694:ALA:HB1	2.19	0.42
1:B:310:LEU:CG	1:B:311:SER:HB3	2.49	0.42
1:B:381:TYR:O	1:B:385:ARG:HG2	2.18	0.42
1:A:621:GLU:HA	1:A:622:PRO:HD3	1.84	0.42
1:A:696:ILE:CG2	1:A:697:PHE:N	2.83	0.42
1:A:845:MET:O	1:A:849:MET:HG3	2.20	0.42
1:A:299:THR:O	1:A:303:ARG:HB2	2.19	0.42
1:A:326:SER:HB2	1:A:357:TRP:CZ2	2.53	0.42
1:B:416:LEU:HB3	1:B:582:MET:HE1	2.02	0.42
1:A:654:PHE:HE2	1:A:693:TYR:HE1	1.67	0.42
1:A:708:LEU:HD23	1:A:708:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:PRO:CG	1:A:879:LEU:HD13	2.49	0.42
1:A:666:VAL:HB	1:A:669:ARG:HB2	2.00	0.42
1:B:763:HIS:HE1	1:B:777:TYR:CE1	2.37	0.42
1:A:305:PRO:HB3	1:A:308:TYR:CE2	2.55	0.42
1:A:341:TRP:CD1	1:A:342:LYS:CA	3.03	0.42
1:A:807:HIS:H	1:A:810:ASN:HB2	1.84	0.42
1:B:294:ARG:O	1:B:298:HIS:HD2	2.02	0.42
1:B:332:LEU:HB2	1:B:357:TRP:NE1	2.35	0.42
1:B:764:ASN:HA	1:B:767:ARG:NH1	2.35	0.42
1:B:398:LEU:N	1:B:401:LEU:CD1	2.83	0.42
1:B:549:ASN:ND2	1:B:658:PRO:CG	2.83	0.42
1:B:551:PHE:CE1	1:B:555:LEU:HG	2.54	0.42
1:B:575:MET:SD	1:B:576:TYR:N	2.93	0.42
1:A:362:VAL:CG2	1:A:389:ALA:HB2	2.47	0.41
1:A:835:MET:C	1:A:836:PRO:O	2.58	0.41
1:A:835:MET:HA	1:A:836:PRO:HD3	1.94	0.41
1:B:645:ASN:OD1	1:B:647:THR:HG23	2.20	0.41
1:B:845:MET:O	1:B:848:ALA:HB3	2.20	0.41
1:A:567:LYS:CG	1:A:568:GLN:H	2.33	0.41
1:A:727:LEU:HD23	1:A:727:LEU:N	2.35	0.41
1:B:590:GLY:O	1:B:595:ARG:NE	2.53	0.41
1:A:580:LEU:HD22	1:A:584:LEU:HD11	2.02	0.41
1:B:549:ASN:CG	1:B:658:PRO:HG3	2.40	0.41
1:A:394:LEU:HD23	1:A:540:ARG:HH11	1.85	0.41
1:A:400:GLN:OE1	1:A:881:LEU:HD23	2.20	0.41
1:A:871:LEU:HD23	1:A:871:LEU:HA	1.97	0.41
1:B:311:SER:OG	1:B:314:GLU:HG2	2.20	0.41
1:B:777:TYR:C	1:B:779:ILE:N	2.74	0.41
1:B:811:LEU:HD12	1:B:845:MET:SD	2.60	0.41
1:A:671:SER:O	1:A:672:LEU:HD23	2.20	0.41
1:A:681:LYS:C	1:A:682:LEU:HD12	2.41	0.41
1:A:705:GLN:HB2	1:A:890:VAL:HG13	2.02	0.41
1:A:727:LEU:HD12	1:A:793:GLY:HA3	2.03	0.41
1:A:755:VAL:HG11	1:A:765:PHE:HD2	1.85	0.41
1:B:569:ASP:OD1	1:B:570:GLU:N	2.54	0.41
1:A:755:VAL:HG11	1:A:765:PHE:CD2	2.56	0.41
1:A:765:PHE:CD1	1:A:765:PHE:O	2.73	0.41
1:A:930:THR:CG2	1:A:936:LEU:HD13	2.51	0.41
1:B:375:HIS:NE2	1:B:377:GLN:HB3	2.35	0.41
1:B:833:LYS:HB3	1:B:834:PRO:CD	2.50	0.41
1:B:303:ARG:HB2	1:B:304:TYR:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:775:GLY:O	1:B:776:PRO:C	2.58	0.41
1:A:843:LYS:CE	1:A:847:GLU:OE2	2.56	0.41
1:A:937:VAL:O	1:A:941:HIS:HD2	2.02	0.41
1:A:375:HIS:O	1:A:378:VAL:HG22	2.21	0.41
1:A:933:MET:HB2	1:A:936:LEU:HD12	2.02	0.41
1:B:299:THR:O	1:B:303:ARG:HG3	2.21	0.41
1:B:315:GLN:HB2	1:B:338:CYS:CB	2.51	0.41
1:B:329:LYS:HE3	1:B:329:LYS:HB2	1.82	0.41
1:B:649:PHE:CG	1:B:650:GLU:N	2.89	0.41
1:B:708:LEU:CD1	1:B:885:MET:HG3	2.51	0.41
1:B:812:LEU:HD21	1:B:822:ILE:HB	1.98	0.41
1:B:833:LYS:HB3	1:B:834:PRO:HD2	2.03	0.41
1:B:314:GLU:O	1:B:317:LEU:HB3	2.21	0.41
1:B:336:LEU:HD11	1:B:354:LEU:HD12	2.03	0.41
1:B:551:PHE:C	1:B:551:PHE:CD1	2.95	0.41
1:B:555:LEU:HD22	1:B:555:LEU:HA	1.92	0.41
1:A:607:PHE:CD1	1:A:607:PHE:C	2.95	0.40
1:B:315:GLN:HB2	1:B:338:CYS:HB2	2.04	0.40
1:B:566:ARG:O	1:B:570:GLU:OE2	2.39	0.40
1:A:405:LEU:HD23	1:A:533:LEU:CD2	2.50	0.40
1:A:662:ILE:H	1:A:662:ILE:HG12	1.71	0.40
1:B:403:GLN:NE2	1:B:406:LYS:HE3	2.36	0.40
1:B:416:LEU:HD22	1:B:535:THR:HG22	2.03	0.40
1:A:533:LEU:HD23	1:A:533:LEU:C	2.41	0.40
1:A:706:ASP:O	1:A:710:LEU:HD12	2.21	0.40
1:A:724:ASN:O	1:A:724:ASN:ND2	2.54	0.40
1:A:776:PRO:HB2	1:A:777:TYR:CD1	2.50	0.40
1:A:861:ARG:HH22	1:A:929:ILE:HD12	1.86	0.40
1:B:567:LYS:HG3	1:B:568:GLN:N	2.37	0.40
1:A:549:ASN:CG	1:A:658:PRO:HG3	2.42	0.40
1:A:650:GLU:HA	1:A:651:PRO:HD3	1.94	0.40
1:A:814:THR:HG22	1:A:817:GLY:N	2.36	0.40
1:A:400:GLN:CD	1:A:881:LEU:HD23	2.42	0.40
1:B:332:LEU:HD13	1:B:357:TRP:CG	2.56	0.40
1:B:678:MET:HA	1:B:679:PRO:HD3	1.72	0.40

All (2) 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:A:391:ASP:OD2	1:A:724:ASN:OD1[6_555]	1.87	0.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:600:ASN:ND2	1:B:782:GLU:OE2[8_565]	2.11	0.09

### 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	546/696 (78%)	507 (93%)	34 (6%)	5 (1%)	17 56
1	B	544/696 (78%)	519 (95%)	16 (3%)	9 (2%)	9 42
All	All	1090/1392 (78%)	1026 (94%)	50 (5%)	14 (1%)	12 48

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	664	LYS
1	A	731	PRO
1	B	408	GLU
1	B	778	GLY
1	A	563	GLU
1	B	889	THR
1	A	689	ALA
1	B	640	ASP
1	B	946	TYR
1	A	771	PRO
1	B	592	PHE
1	B	771	PRO
1	B	306	PRO
1	B	731	PRO

#### 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	495/612 (81%)	382 (77%)	113 (23%)	1	4
1	B	494/612 (81%)	397 (80%)	97 (20%)	1	7
All	All	989/1224 (81%)	779 (79%)	210 (21%)	1	5

All (210) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	293	ILE
1	A	302	TYR
1	A	303	ARG
1	A	317	LEU
1	A	322	ARG
1	A	328	HIS
1	A	333	THR
1	A	335	PHE
1	A	336	LEU
1	A	338	CYS
1	A	341	TRP
1	A	342	LYS
1	A	344	GLU
1	A	345	ASP
1	A	354	LEU
1	A	367	GLU
1	A	370	SER
1	A	372	THR
1	A	373	PHE
1	A	374	THR
1	A	375	HIS
1	A	391	ASP
1	A	398	LEU
1	A	409	ASP
1	A	411	ARG
1	A	414	VAL
1	A	415	HIS
1	A	417	HIS
1	A	421	PHE
1	A	532	ASN
1	A	535	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	540	ARG
1	A	546	THR
1	A	549	ASN
1	A	552	TYR
1	A	560	GLU
1	A	563	GLU
1	A	565	VAL
1	A	568	GLN
1	A	573	HIS
1	A	574	ASP
1	A	580	LEU
1	A	581	LYS
1	A	583	PHE
1	A	592	PHE
1	A	602	ARG
1	A	611	LEU
1	A	614	LEU
1	A	621	GLU
1	A	629	THR
1	A	634	LYS
1	A	639	GLN
1	A	647	THR
1	A	648	ASN
1	A	660	ILE
1	A	662	ILE
1	A	669	ARG
1	A	674	LYS
1	A	677	LEU
1	A	678	MET
1	A	682	LEU
1	A	685	VAL
1	A	687	SER
1	A	688	ILE
1	A	701	ASP
1	A	702	ASP
1	A	703	LEU
1	A	706	ASP
1	A	710	LEU
1	A	722	ARG
1	A	725	LEU
1	A	727	LEU
1	A	737	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	741	HIS
1	A	744	LEU
1	A	746	TYR
1	A	748	ASP
1	A	750	CYS
1	A	751	THR
1	A	758	ARG
1	A	765	PHE
1	A	774	ASN
1	A	777	TYR
1	A	782	GLU
1	A	786	THR
1	A	787	TYR
1	A	790	SER
1	A	791	CYS
1	A	803	VAL
1	A	812	LEU
1	A	814	THR
1	A	819	LEU
1	A	822	ILE
1	A	824	PHE
1	A	830	ARG
1	A	831	ASP
1	A	835	MET
1	A	839	MET
1	A	840	LYS
1	A	841	LEU
1	A	855	GLU
1	A	859	GLU
1	A	860	PHE
1	A	881	LEU
1	A	893	ILE
1	A	908	LEU
1	A	913	THR
1	A	914	ASP
1	A	919	GLN
1	A	930	THR
1	A	938	GLU
1	A	944	THR
1	A	948	ARG
1	B	299	THR
1	B	302	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	307	THR
1	B	308	TYR
1	B	310	LEU
1	B	311	SER
1	B	317	LEU
1	B	320	LYS
1	B	321	PHE
1	B	322	ARG
1	B	323	PHE
1	B	327	SER
1	B	328	HIS
1	B	329	LYS
1	B	333	THR
1	B	335	PHE
1	B	336	LEU
1	B	342	LYS
1	B	344	GLU
1	B	351	LEU
1	B	360	MET
1	B	366	LEU
1	B	370	SER
1	B	372	THR
1	B	373	PHE
1	B	378	VAL
1	B	391	ASP
1	B	394	LEU
1	B	396	LEU
1	B	398	LEU
1	B	419	CYS
1	B	533	LEU
1	B	536	PHE
1	B	539	GLN
1	B	546	THR
1	B	549	ASN
1	B	551	PHE
1	B	555	LEU
1	B	561	GLU
1	B	562	VAL
1	B	568	GLN
1	B	573	HIS
1	B	575	MET
1	B	598	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	599	TYR
1	B	605	ARG
1	B	609	ASP
1	B	611	LEU
1	B	614	LEU
1	B	627	LYS
1	B	634	LYS
1	B	638	GLU
1	B	645	ASN
1	B	647	THR
1	B	652	ILE
1	B	654	PHE
1	B	663	THR
1	B	670	THR
1	B	671	SER
1	B	682	LEU
1	B	699	HIS
1	B	706	ASP
1	B	710	LEU
1	B	712	MET
1	B	714	THR
1	B	719	LEU
1	B	722	ARG
1	B	729	LEU
1	B	746	TYR
1	B	747	VAL
1	B	748	ASP
1	B	750	CYS
1	B	758	ARG
1	B	765	PHE
1	B	777	TYR
1	B	779	ILE
1	B	782	GLU
1	B	786	THR
1	B	788	ILE
1	B	812	LEU
1	B	814	THR
1	B	822	ILE
1	B	827	ILE
1	B	839	MET
1	B	841	LEU
1	B	846	VAL

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Mol	Chain	Res	Type
1	B	862	LYS
1	B	866	THR
1	B	876	ASN
1	B	881	LEU
1	B	883	SER
1	B	889	THR
1	B	909	GLN
1	B	930	THR
1	B	937	VAL
1	B	941	HIS
1	B	944	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	HIS
1	A	340	ASN
1	A	403	GLN
1	A	412	HIS
1	A	549	ASN
1	A	573	HIS
1	A	639	GLN
1	A	691	HIS
1	A	764	ASN
1	A	769	HIS
1	A	810	ASN
1	A	863	GLN
1	A	870	HIS
1	A	919	GLN
1	A	941	HIS
1	B	298	HIS
1	B	328	HIS
1	B	356	ASN
1	B	403	GLN
1	B	415	HIS
1	B	549	ASN
1	B	573	HIS
1	B	633	GLN
1	B	690	HIS
1	B	711	GLN
1	B	810	ASN
1	B	858	HIS

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Mol	Chain	Res	Type
1	B	870	HIS
1	B	876	ASN
1	B	880	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 monosaccharides in this entry.

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

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	1950	-	4,4,4	0.35	0	6,6,6	0.29	0
2	SO4	A	1949	-	4,4,4	0.24	0	6,6,6	0.17	0
3	X6K	B	1950	-	27,30,30	2.42	10 (37%)	27,43,43	1.90	6 (22%)
2	SO4	B	1951	-	4,4,4	0.24	0	6,6,6	0.07	0
3	X6K	A	1951	-	27,30,30	2.43	10 (37%)	27,43,43	1.77	8 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	X6K	B	1950	-	-	2/4/16/16	0/5/5/5
3	X6K	A	1951	-	-	2/4/16/16	0/5/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1951	X6K	C06-N01	5.37	1.45	1.35
3	B	1950	X6K	C19-N10	5.35	1.44	1.35
3	A	1951	X6K	C19-N10	5.33	1.44	1.35
3	B	1950	X6K	C06-N01	5.25	1.44	1.35
3	B	1950	X6K	C11-N18	4.28	1.34	1.30
3	B	1950	X6K	C22-C23	4.19	1.46	1.38
3	A	1951	X6K	C11-N18	3.99	1.34	1.30
3	A	1951	X6K	C22-C23	3.97	1.45	1.38
3	A	1951	X6K	C05-C09	3.50	1.52	1.42
3	A	1951	X6K	C26-C20	3.46	1.49	1.42
3	B	1950	X6K	C26-C20	3.39	1.49	1.42
3	B	1950	X6K	C05-C09	3.29	1.51	1.42
3	A	1951	X6K	C05-C06	-2.66	1.35	1.42
3	B	1950	X6K	C05-C06	-2.45	1.36	1.42
3	B	1950	X6K	C22-C21	2.22	1.41	1.36
3	B	1950	X6K	C19-N18	-2.20	1.32	1.36
3	A	1951	X6K	C21-C20	-2.16	1.37	1.42
3	A	1951	X6K	C19-N18	-2.14	1.32	1.36
3	A	1951	X6K	C11-N12	2.13	1.46	1.39
3	B	1950	X6K	C21-C20	-2.10	1.37	1.42

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1950	X6K	C17-N12-C13	4.83	122.44	111.57
3	A	1951	X6K	C17-N12-C11	3.85	129.60	116.86
3	B	1950	X6K	C17-N12-C11	3.68	129.05	116.86
3	A	1951	X6K	C17-N12-C13	3.21	118.79	111.57
3	A	1951	X6K	C05-C06-N01	-3.07	119.84	124.94
3	B	1950	X6K	C05-C06-N01	-2.90	120.11	124.94
3	A	1951	X6K	C02-N01-C06	2.82	120.01	116.63
3	B	1950	X6K	C03-C02-N01	-2.67	120.05	123.97
3	B	1950	X6K	C13-N12-C11	-2.52	108.52	116.86
3	A	1951	X6K	C03-C02-N01	-2.47	120.34	123.97
3	A	1951	X6K	C11-N18-C19	2.29	120.53	117.11
3	B	1950	X6K	C02-N01-C06	2.22	119.29	116.63
3	A	1951	X6K	C26-C20-C21	2.13	120.81	118.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1951	X6K	C08-C11-N18	-2.11	119.38	122.93

There are no chirality outliers.

All (4) torsion outliers are listed below:

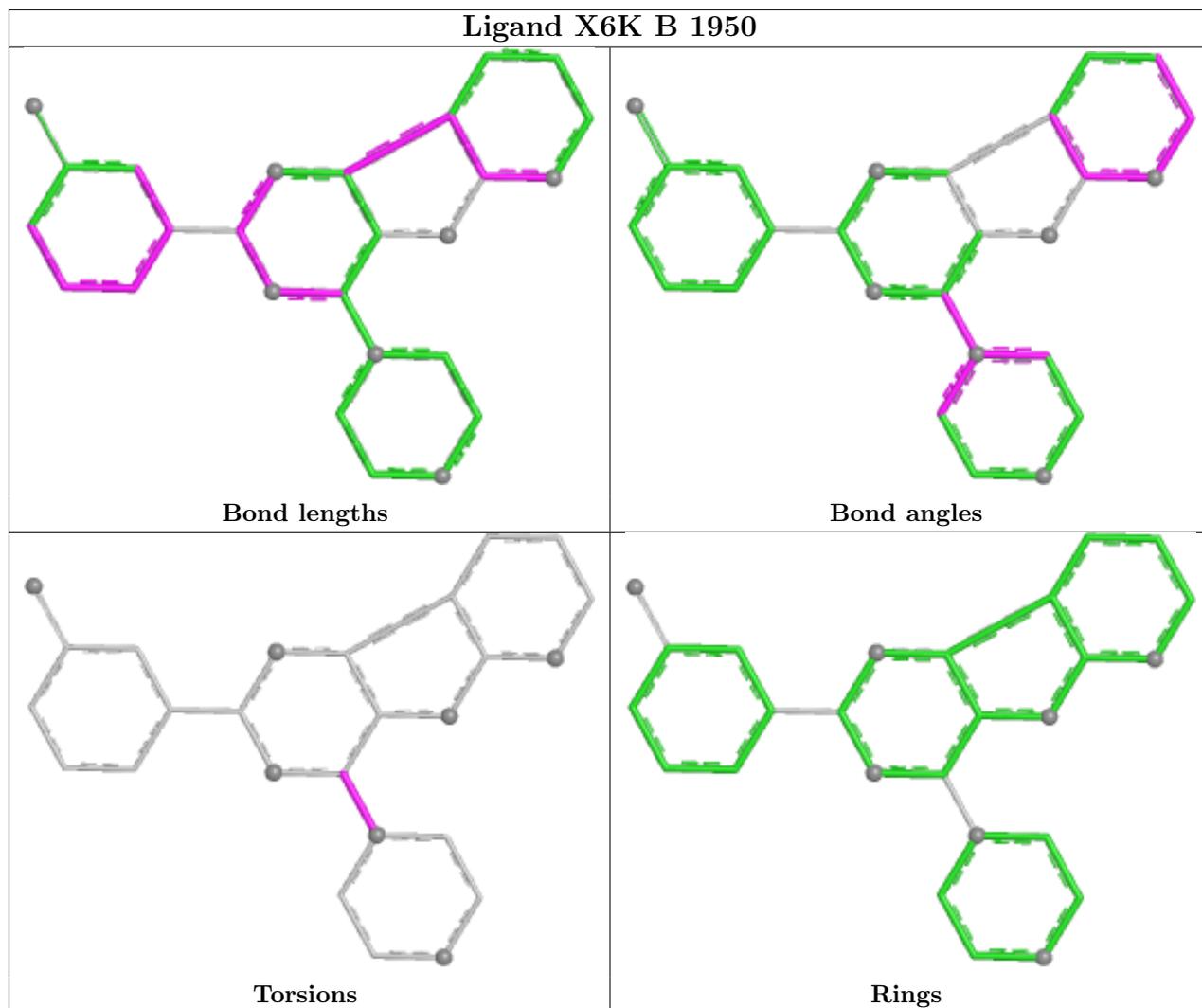
Mol	Chain	Res	Type	Atoms
3	A	1951	X6K	C08-C11-N12-C13
3	A	1951	X6K	N18-C11-N12-C13
3	B	1950	X6K	C08-C11-N12-C13
3	B	1950	X6K	N18-C11-N12-C13

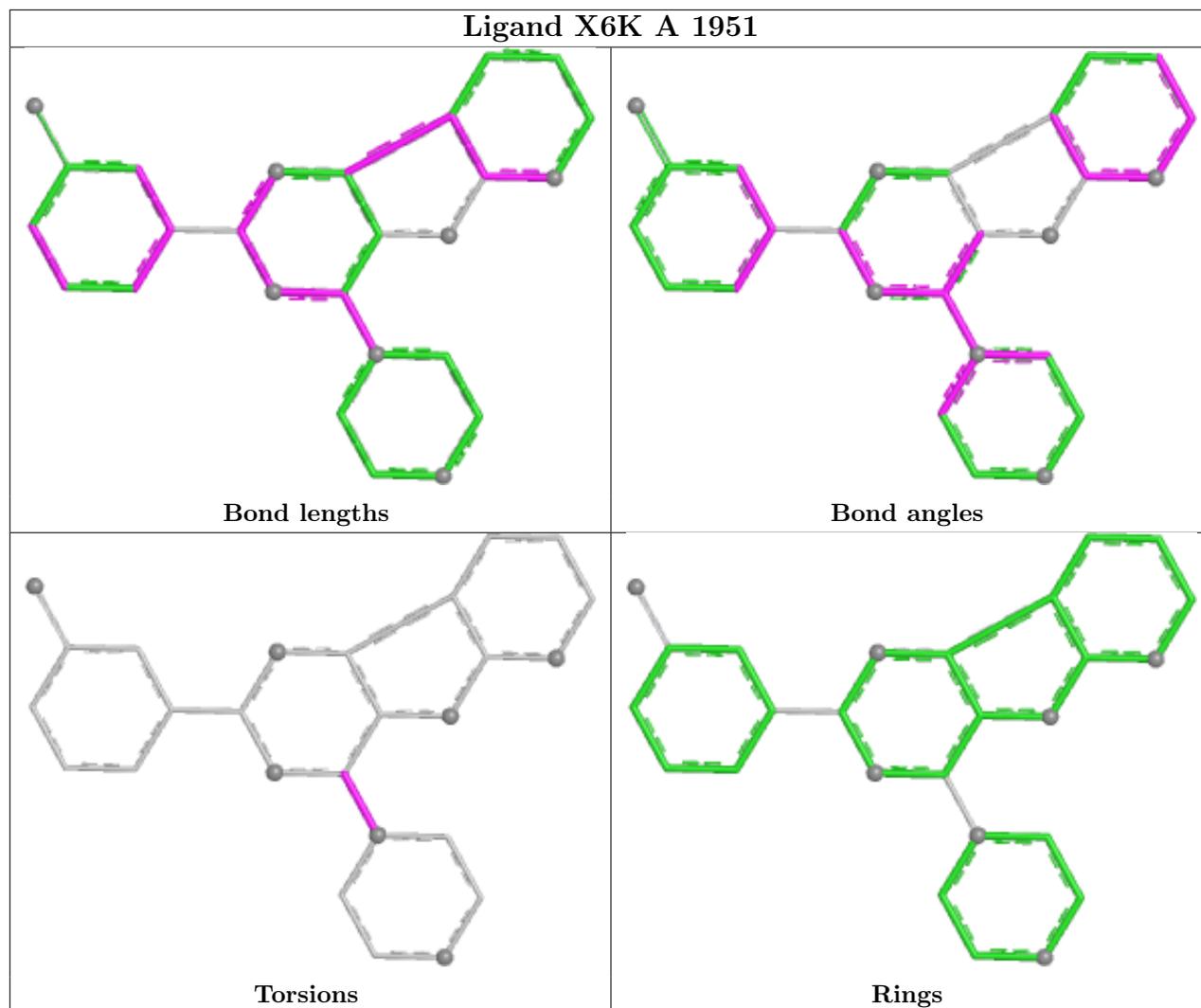
There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1950	SO4	1	0
2	A	1949	SO4	1	0
3	B	1950	X6K	9	0
2	B	1951	SO4	1	0
3	A	1951	X6K	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 [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	550/696 (79%)	-0.26	3 (0%) 91 88	18, 62, 117, 129	0
1	B	550/696 (79%)	-0.21	3 (0%) 91 88	48, 75, 126, 135	0
All	All	1100/1392 (79%)	-0.24	6 (0%) 91 88	18, 69, 121, 135	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	690	HIS	2.8
1	A	322	ARG	2.5
1	A	323	PHE	2.3
1	B	341	TRP	2.2
1	A	335	PHE	2.1
1	B	676	ALA	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](#)

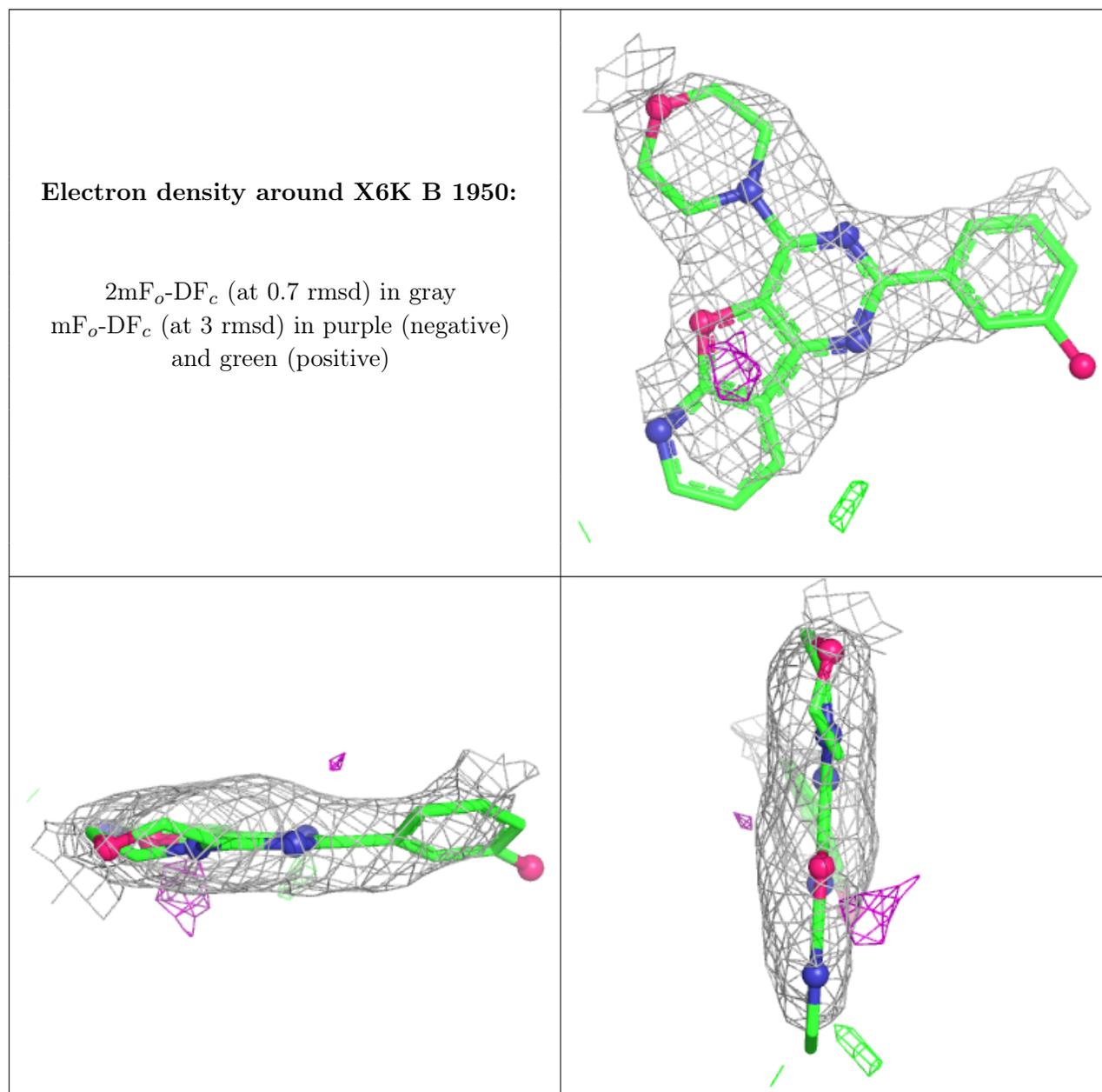
There are no monosaccharides in this entry.

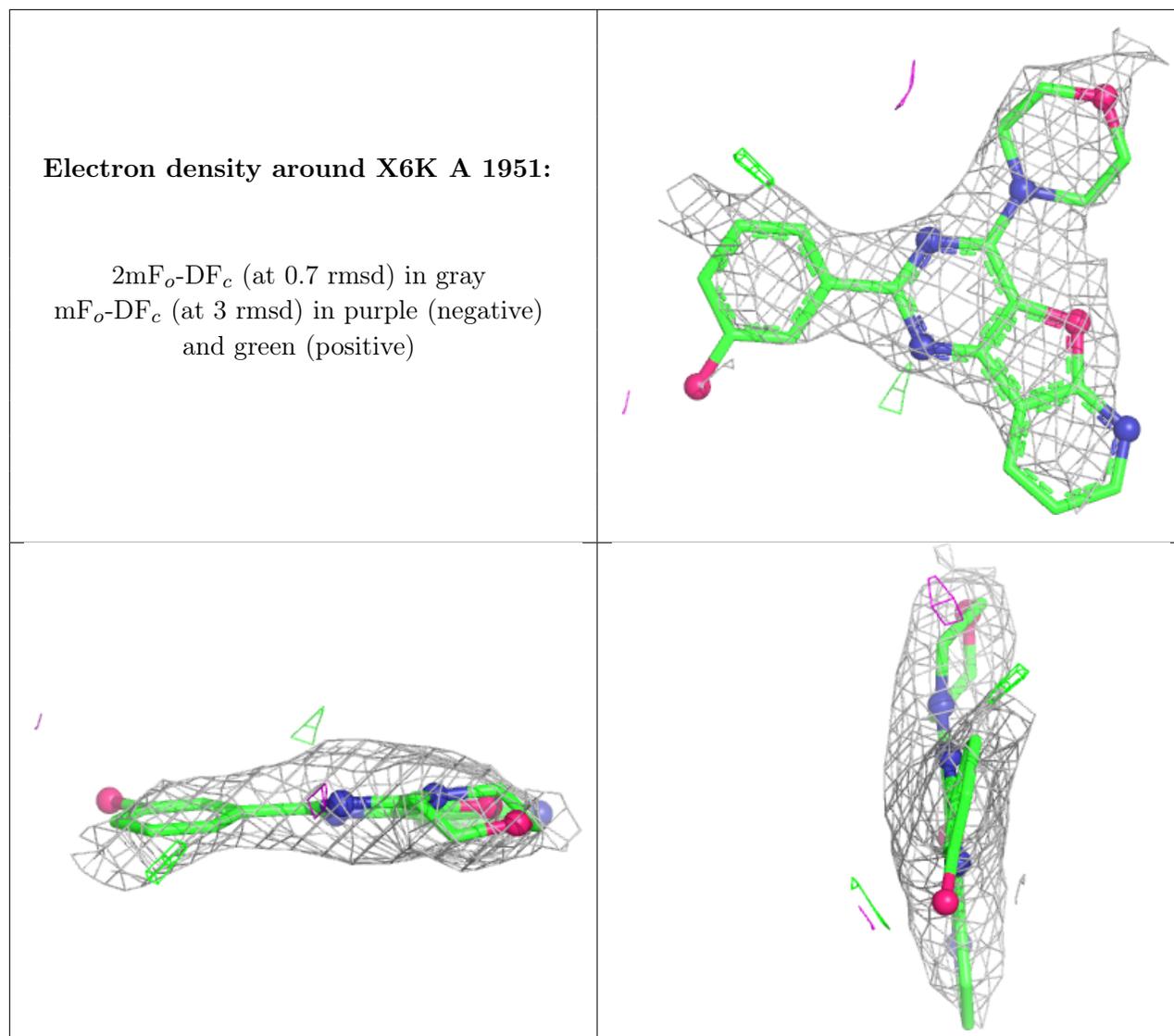
### 6.4 Ligands [i](#)

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( $\text{\AA}^2$ )	Q<0.9
2	SO4	B	1951	5/5	0.65	0.17	194,194,194,194	0
3	X6K	B	1950	26/26	0.85	0.52	113,121,125,125	0
2	SO4	A	1949	5/5	0.87	0.23	145,145,145,146	0
3	X6K	A	1951	26/26	0.89	0.35	114,119,123,123	0
2	SO4	A	1950	5/5	0.93	0.35	146,147,147,147	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.