



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:32 AM UTC

PDB ID : 2X6K / pdb_00002x6k
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

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>.

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)
Xtriage (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

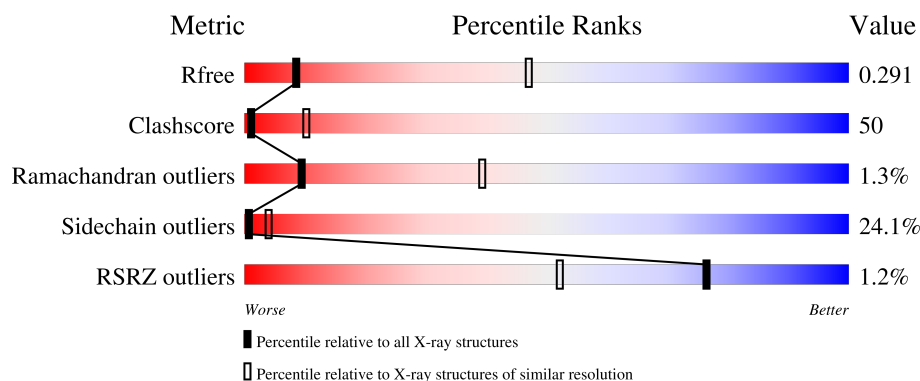
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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 ≥ 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	26% 34% 18% • 21%
1	B	696	30% 36% 12% • 21%

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
1	A	550	Total	C	N	O	S	0	0	0
			4497	2906	765	799	27			
1	B	550	Total	C	N	O	S	0	0	0
			4498	2907	766	798	27			

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 (CCD ID: SO4) (formula: O₄S).



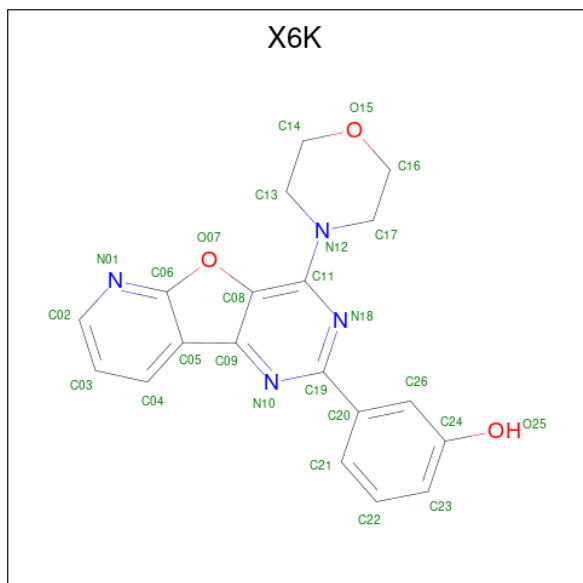
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

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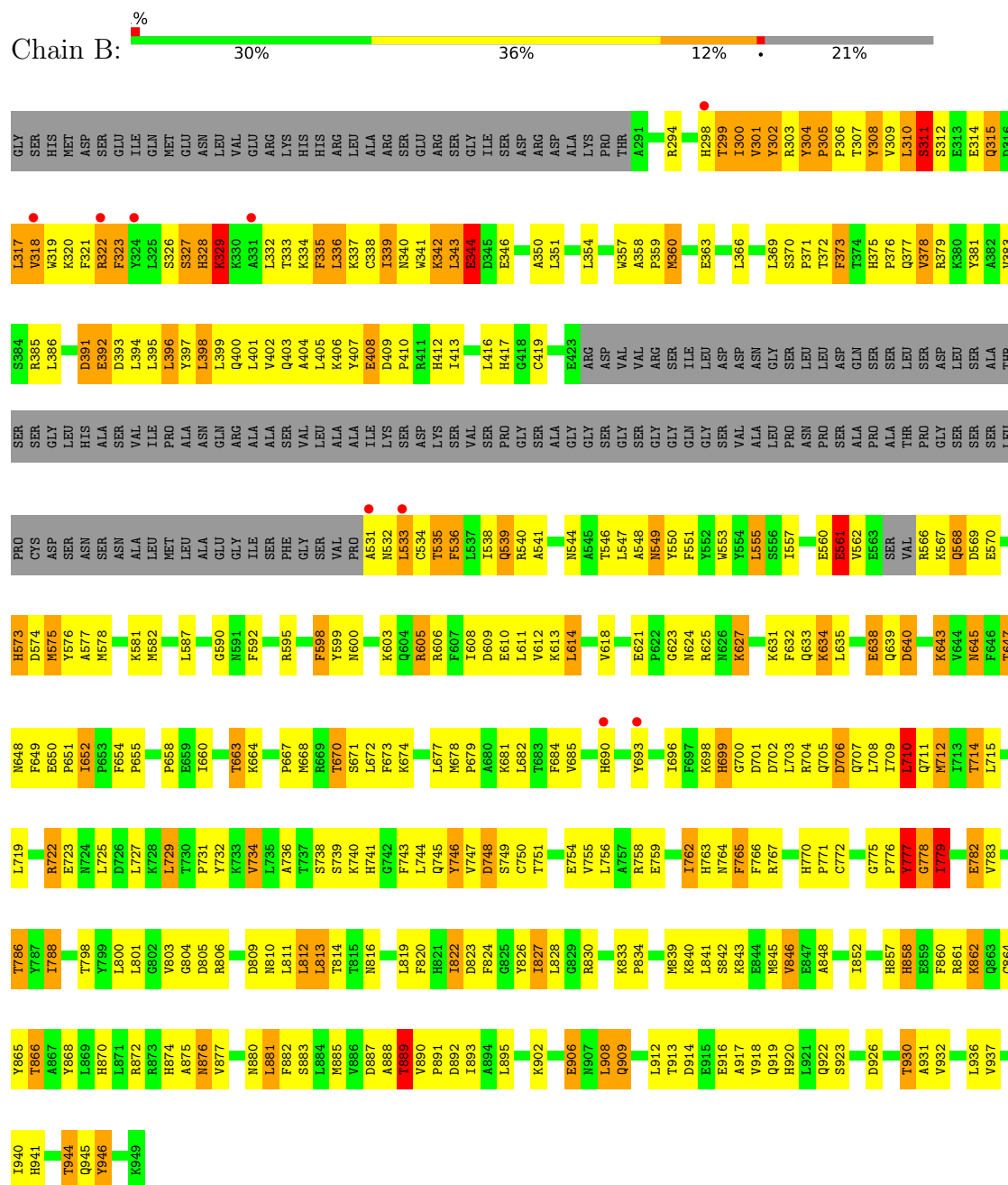
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 3-(4-MORPHOLIN-4-YLPYRIDO[3',2':4,5]FURO[3,2-D]PYRIMIDIN-2-YL)PHENOL (CCD ID: X6K) (formula: C₁₉H₁₆N₄O₃).



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		

● Molecule 1: PHOSPHOTIDYLINOSITOL 3 KINASE 59F



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.235 , 0.296 (Not available) , 0.291	Depositor DCC
R_{free} test set	1340 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	110.3	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 96.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9062	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.72	1/4607 (0.0%)	1.51	91/6240 (1.5%)
1	B	0.60	1/4607 (0.0%)	1.06	17/6237 (0.3%)
All	All	0.66	2/9214 (0.0%)	1.30	108/12477 (0.9%)

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	A	590	GLY	C-O	9.09	1.36	1.23
1	B	311	SER	CB-OG	6.59	1.55	1.42

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	818	LYS	N-CA-C	-13.13	92.82	110.55
1	B	532	ASN	N-CA-C	-9.14	101.20	111.71
1	A	857	HIS	N-CA-C	-8.60	101.12	111.69
1	A	835	MET	N-CA-C	8.44	122.46	110.40
1	A	592	PHE	N-CA-C	-8.39	103.56	113.88
1	A	318	VAL	N-CA-C	-8.37	102.08	110.62
1	A	595	ARG	N-CA-C	-8.36	102.25	111.36
1	A	641	MET	N-CA-C	-8.28	102.63	112.89
1	A	393	ASP	N-CA-C	-8.26	102.36	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	700	GLY	N-CA-C	7.96	121.74	112.50
1	A	836	PRO	N-CA-C	-7.81	101.17	110.70
1	B	623	GLY	N-CA-C	7.74	122.79	110.87
1	B	344	GLU	N-CA-C	7.71	122.70	112.13
1	A	784	MET	N-CA-C	-7.68	102.91	111.28
1	A	402	VAL	N-CA-C	-7.59	102.88	110.62
1	A	613	LYS	N-CA-C	-7.58	103.01	111.28
1	A	860	PHE	N-CA-C	-7.40	103.30	111.36
1	A	649	PHE	N-CA-C	7.36	118.90	108.74
1	A	551	PHE	N-CA-C	-7.35	103.35	111.36
1	A	766	PHE	N-CA-C	-7.12	103.56	111.82
1	A	594	LEU	N-CA-C	-7.01	103.40	112.23
1	B	701	ASP	N-CA-C	6.91	117.39	108.34
1	A	711	GLN	N-CA-C	-6.86	103.80	111.28
1	A	928	SER	N-CA-C	-6.79	103.96	111.36
1	A	297	LEU	N-CA-C	-6.67	103.83	112.23
1	A	409	ASP	CA-C-N	6.58	126.02	118.85
1	A	409	ASP	C-N-CA	6.58	126.02	118.85
1	A	858	HIS	N-CA-C	-6.54	104.15	111.28
1	A	308	TYR	N-CA-C	6.54	119.06	108.41
1	A	795	CYS	N-CA-C	-6.51	104.26	111.36
1	B	777	TYR	N-CA-C	-6.44	99.67	109.85
1	A	328	HIS	N-CA-C	6.32	118.78	109.24
1	A	790	SER	N-CA-C	-6.31	104.40	111.28
1	A	340	ASN	N-CA-C	6.25	117.78	110.97
1	A	854	SER	N-CA-C	-6.24	98.89	108.76
1	A	714	THR	N-CA-C	-6.18	104.62	111.36
1	A	800	LEU	N-CA-C	-6.18	104.66	111.82
1	A	721	ARG	N-CA-C	-6.13	104.71	111.82
1	A	788	ILE	N-CA-C	-6.11	104.39	110.62
1	A	681	LYS	N-CA-C	-6.09	100.36	110.17
1	A	798	THR	N-CA-C	-6.09	104.64	111.28
1	A	304	TYR	CA-C-N	-6.08	114.12	120.38
1	A	304	TYR	C-N-CA	-6.08	114.12	120.38
1	A	416	LEU	N-CA-C	-6.03	104.79	111.36
1	A	693	TYR	CA-C-N	-6.00	112.72	122.81
1	A	693	TYR	C-N-CA	-6.00	112.72	122.81
1	A	577	ALA	N-CA-C	-6.00	104.82	111.36
1	A	333	THR	N-CA-C	-5.98	104.84	111.36
1	A	866	THR	N-CA-C	-5.96	104.90	111.82
1	A	944	THR	N-CA-C	-5.89	104.99	111.82
1	A	820	PHE	N-CA-C	5.86	117.12	108.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	535	THR	N-CA-C	-5.85	104.99	111.71
1	A	775	GLY	CA-C-N	5.85	127.15	119.84
1	A	775	GLY	C-N-CA	5.85	127.15	119.84
1	A	678	MET	CA-C-N	5.83	125.59	119.76
1	A	678	MET	C-N-CA	5.83	125.59	119.76
1	A	664	LYS	N-CA-C	5.82	123.21	110.80
1	A	381	TYR	N-CA-C	-5.80	105.03	111.36
1	B	779	ILE	N-CA-C	5.78	117.49	109.80
1	A	369	LEU	N-CA-C	-5.78	104.95	112.23
1	A	764	ASN	N-CA-C	-5.78	105.06	111.71
1	A	367	GLU	N-CA-C	-5.77	105.07	111.71
1	A	816	ASN	CA-C-N	-5.76	113.47	122.51
1	A	816	ASN	C-N-CA	-5.76	113.47	122.51
1	A	627	LYS	N-CA-C	-5.71	105.03	112.23
1	A	717	ASP	N-CA-C	-5.71	105.06	111.28
1	A	299	THR	N-CA-C	-5.68	105.23	111.82
1	B	318	VAL	N-CA-C	-5.67	104.40	110.36
1	A	590	GLY	CA-C-N	-5.67	110.71	121.54
1	A	590	GLY	C-N-CA	-5.67	110.71	121.54
1	A	785	ASP	N-CA-C	-5.65	105.20	111.36
1	A	604	GLN	N-CA-C	-5.65	105.20	111.36
1	A	883	SER	N-CA-C	-5.64	105.22	111.71
1	A	722	ARG	N-CA-C	-5.62	105.15	111.28
1	A	691	HIS	N-CA-C	-5.60	102.35	110.64
1	B	561	GLU	N-CA-C	5.57	118.30	109.50
1	A	590	GLY	O-C-N	-5.50	115.55	122.70
1	A	786	THR	N-CA-C	-5.49	105.45	111.82
1	A	907	ASN	N-CA-C	-5.49	105.69	112.38
1	A	693	TYR	N-CA-C	-5.48	101.19	109.85
1	B	343	LEU	N-CA-C	5.41	116.86	111.07
1	A	905	GLU	N-CA-C	-5.35	105.61	111.82
1	A	931	ALA	N-CA-C	-5.32	106.29	112.89
1	A	676	ALA	N-CA-C	5.30	117.81	111.71
1	A	906	GLU	N-CA-C	-5.26	105.23	111.69
1	A	602	ARG	N-CA-C	-5.22	105.67	111.36
1	B	304	TYR	CA-C-N	-5.21	115.02	120.38
1	B	304	TYR	C-N-CA	-5.21	115.02	120.38
1	A	939	GLN	N-CA-C	-5.17	105.64	111.28
1	B	327	SER	N-CA-C	5.17	117.59	111.33
1	A	901	VAL	N-CA-C	-5.15	105.52	110.72
1	A	633	GLN	N-CA-C	-5.13	105.76	111.36
1	A	908	LEU	N-CA-C	-5.13	105.77	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	942	ARG	N-CA-C	-5.13	105.81	111.71
1	B	315	GLN	N-CA-C	-5.13	105.58	111.07
1	A	574	ASP	N-CA-C	-5.11	105.89	111.82
1	B	875	ALA	N-CA-C	-5.10	105.72	111.28
1	A	353	MET	N-CA-C	-5.10	105.80	111.36
1	B	329	LYS	N-CA-C	5.09	116.52	111.07
1	A	352	TRP	N-CA-C	-5.05	105.97	111.82
1	A	847	GLU	N-CA-C	-5.04	105.97	111.82
1	B	305	PRO	N-CA-C	5.04	116.85	110.70
1	A	871	LEU	N-CA-C	-5.04	105.87	111.36
1	B	710	LEU	CA-CB-CG	-5.04	98.68	116.30
1	A	739	SER	N-CA-C	5.03	116.78	110.24
1	A	548	ALA	N-CA-C	-5.03	105.80	111.28
1	A	859	GLU	N-CA-C	-5.03	105.99	111.82
1	A	782	GLU	N-CA-C	-5.02	105.88	111.36

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	437	1
1	B	4498	0	4533	467	1
2	A	10	0	0	2	0
2	B	5	0	0	1	0
3	A	26	0	16	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	26	0	16	9	0
All	All	9062	0	9098	901	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 50.

All (901) 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
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:A:855:GLU:H	1:A:855:GLU:CD	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:335:PHE:HD2	1:B:335:PHE:C	1.79	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
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:335:PHE:C	1:B:335:PHE:CD2	2.51	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:B:712:MET:HA	1:B:712:MET:HE3	1.55	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:855:GLU:CD	1:A:855:GLU:N	2.36	0.83
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: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:776:PRO:C	1:B:777:TYR:HD2	1.87	0.82
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: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
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:552:TYR:C	1:A:552:TYR:CD2	2.57	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:552:TYR:C	1:A:552:TYR:HD2	1.91	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: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:B:417:HIS:ND1	1:B:578:MET:HE3	1.97	0.78
1:A:735:LEU:HG	1:A:736:ALA:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:765:PHE:C	1:B:765:PHE:CD2	2.62	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:341:TRP:HD1	1:A:342:LYS:HZ3	1.33	0.76
1:B:360:MET:CE	1:B:381:TYR:HB3	2.15	0.76
1:B:416:LEU:HB3	1:B:582:MET:HE1	1.67	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:B:301:VAL:O	1:B:305:PRO:HD2	1.87	0.75
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: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:A:743:PHE:C	1:A:744:LEU:HD23	2.13	0.73
1:B:606:ARG:NH1	1:B:643:LYS:CB	2.49	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:409:ASP:OD1	1:A:409:ASP:C	2.33	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
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:573:HIS:C	1:B:573:HIS:CD2	2.69	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:305:PRO:O	1:B:334:LYS:NZ	2.25	0.70
1:B:311:SER:HB2	1:B:314:GLU:HB3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:MET:HE1	1:B:381:TYR:HB3	1.72	0.69
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: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:B:598:PHE:C	1:B:598:PHE:CD2	2.71	0.68
1:A:819:LEU:HD23	1:A:819:LEU:C	2.18	0.68
1:B:319:TRP:HH2	1:B:346:GLU:CD	2.01	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: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
1:B:842:SER:O	1:B:846:VAL:HG23	1.94	0.67
1:B:575:MET:SD	1:B:575:MET:C	2.77	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:397:TYR:C	1:B:401:LEU:HD12	2.20	0.67
1:B:708:LEU:HD12	1:B:885:MET:HE2	1.77	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:B:708:LEU:C	1:B:708:LEU:HD23	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:405:LEU:HB3	1:B:575:MET:HE1	1.78	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:722:ARG:HH11	1:B:722:ARG:HB3	1.62	0.64
1:A:839:MET:HE2	1:A:925:LEU:HD21	1.79	0.64
1:A:573:HIS:C	1:A:573:HIS:CD2	2.74	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
1:B:765:PHE:C	1:B:765:PHE:HD2	2.05	0.64
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: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:A:746:TYR:C	1:A:746:TYR:CD2	2.76	0.63
1:B:335:PHE:CD1	1:B:357:TRP:CZ3	2.86	0.63
1:B:712:MET:HA	1:B:712:MET:HE2	1.79	0.63
1:B:413:ILE:HD13	1:B:575:MET:HG2	1.80	0.63
1:A:811:LEU:C	1:A:812:LEU:HD23	2.24	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:743:PHE:C	1:B:744:LEU:HD23	2.23	0.63
1:A:305:PRO:O	1:A:334:LYS:NZ	2.20	0.62
1:A:672:LEU:CD2	1:A:680:ALA:HA	2.29	0.62
1:B:746:TYR:C	1:B:746:TYR:CD2	2.77	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:A:373:PHE:H	1:A:373:PHE:HD2	1.48	0.62
1:A:579:VAL:HA	1:A:582:MET:HE3	1.82	0.62
1:B:763:HIS:CE1	1:B:777:TYR:HD1	2.16	0.61
1:B:645:ASN:OD1	1:B:645:ASN:C	2.43	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: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:417:HIS:ND1	1:A:417:HIS:C	2.59	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: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:A:776:PRO:C	1:A:777:TYR:CD1	2.80	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:397:TYR:C	1:B:401:LEU:CD1	2.75	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: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:A:591:ASN:CG	1:A:592:PHE:H	2.06	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: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:562:VAL:C	1:A:564:SER:H	2.10	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
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:A:583:PHE:CD1	1:A:583:PHE:C	2.81	0.58
1:B:876:ASN:N	1:B:876:ASN:ND2	2.49	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:786:THR:O	1:A:790:SER:OG	2.22	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:A:549:ASN:C	1:A:549:ASN:ND2	2.62	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:A:335:PHE:C	1:A:335:PHE:CD2	2.82	0.56
1:A:395:LEU:C	1:A:395:LEU:HD23	2.30	0.56
1:B:891:PRO:O	1:B:895:LEU:HD12	2.04	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:A:614:LEU:C	1:A:614:LEU:HD12	2.30	0.56
1:A:776:PRO:C	1:A:777:TYR:HD1	2.13	0.56
1:B:319:TRP:CH2	1:B:346:GLU:CD	2.82	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:A:702:ASP:OD2	1:A:702:ASP:C	2.48	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:B:319:TRP:HA	1:B:322:ARG:CD	2.36	0.56
1:B:375:HIS:CD2	1:B:375:HIS:C	2.83	0.56
1:A:566:ARG:O	1:A:567:LYS:HG2	2.06	0.56
1:A:690:HIS:O	1:A:691:HIS:C	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:396:LEU:C	1:A:396:LEU:HD23	2.31	0.55
1:B:710:LEU:O	1:B:714:THR:OG1	2.25	0.55
1:B:913:THR:HG22	1:B:916:GLU:CD	2.31	0.55
1:A:412:HIS:CB	1:A:531:ALA:N	2.69	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:405:LEU:HB3	1:B:575:MET:CE	2.36	0.55
1:B:699:HIS:O	1:B:740:LYS:O	2.25	0.55
1:A:565:VAL:HG12	1:A:569:ASP:HB2	1.89	0.55
1:A:913:THR:CG2	1:A:916:GLU:CD	2.80	0.55
1:B:536:PHE:C	1:B:536:PHE:CD1	2.85	0.55
1:B:868:TYR:O	1:B:872:ARG:HD3	2.06	0.55
1:A:787:TYR:CD1	1:A:787:TYR:C	2.84	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:765:PHE:C	1:A:765:PHE:CD1	2.84	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:727:LEU:HB2	1:A:729:LEU:HD21	1.89	0.54
1:A:575:MET:SD	1:A:575:MET:C	2.91	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
1:A:804:GLY:O	1:A:805:ASP:HB3	2.06	0.54
1:B:315:GLN:C	1:B:322:ARG:NH2	2.65	0.54
1:A:305:PRO:HB3	1:A:308:TYR:CE1	2.42	0.54
1:A:871:LEU:HD22	1:A:878:MET:HE1	1.89	0.54
1:A:807:HIS:O	1:A:810:ASN:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:318:VAL:C	1:B:322:ARG:HG3	2.33	0.54
1:A:303:ARG:C	1:A:304:TYR:HD2	2.16	0.54
1:A:341:TRP:CD1	1:A:342:LYS:HZ3	2.22	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: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:B:746:TYR:C	1:B:746:TYR:HD2	2.15	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:398:LEU:C	1:A:398:LEU:HD12	2.34	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:B:614:LEU:HD12	1:B:614:LEU:C	2.34	0.52
1:A:544:ASN:C	1:A:544:ASN:OD1	2.52	0.52
1:B:842:SER:OG	1:B:845:MET:CG	2.57	0.52
1:B:315:GLN:HE22	1:B:341:TRP:CD1	2.27	0.52
1:B:810:ASN:C	1:B:822:ILE:HG22	2.33	0.52
1:A:787:TYR:CD1	1:A:787:TYR:O	2.62	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:710:LEU:HD22	1:A:732:TYR:O	2.10	0.52
1:A:857:HIS:C	1:A:857:HIS:CD2	2.87	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:B:858:HIS:C	1:B:858:HIS:ND1	2.67	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: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:866:THR:O	1:A:870:HIS:CD2	2.58	0.52
1:B:326:SER:O	1:B:357:TRP:CZ2	2.62	0.52
1:B:664:LYS:N	1:B:685:VAL:HG23	2.11	0.52
1:B:776:PRO:C	1:B:777:TYR:CD2	2.78	0.52
1:B:912:LEU:HD12	1:B:917:ALA:HA	1.92	0.52
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:416:LEU:C	1:B:582:MET:HE1	2.35	0.51
1:A:552:TYR:CD1	1:A:601:LEU:HD22	2.45	0.51
1:B:577:ALA:O	1:B:581:LYS:HD3	2.10	0.51
1:B:712:MET:HE1	1:B:715:LEU:HD13	1.92	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:A:872:ARG:HH12	1:A:909:GLN:C	2.18	0.51
1:A:913:THR:HG22	1:A:916:GLU:CD	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:354:LEU:HD23	1:A:354:LEU:C	2.35	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:A:552:TYR:HD2	1:A:552:TYR:O	1.95	0.50
1:A:764:ASN:ND2	1:A:767:ARG:HH12	2.10	0.50
1:B:544:ASN:OD1	1:B:544:ASN:C	2.53	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:A:708:LEU:HD23	1:A:708:LEU:C	2.36	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:746:TYR:C	1:A:746:TYR:HD2	2.19	0.50
1:B:667:PRO:O	1:B:670:THR:HG23	2.12	0.50
1:B:698:LYS:HZ2	3:B:1950:X6K:H25	1.49	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: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:416:LEU:CB	1:B:582:MET:HE1	2.38	0.50
1:B:823:ASP:OD1	1:B:823:ASP:C	2.55	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: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:417:HIS:HA	1:B:582:MET:HE3	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: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:A:948:ARG:HD2	1:A:948:ARG:C	2.38	0.49
1:B:401:LEU:HA	1:B:404:ALA:HB3	1.94	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:412:HIS:HB3	1:A:531:ALA:CA	2.44	0.48
1:A:931:ALA:O	1:B:944:THR:OG1	2.26	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:363:GLU:H	1:A:363:GLU:CD	2.20	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:398:LEU:O	1:A:399:LEU:C	2.56	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: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
1:A:752:VAL:CG1	1:A:808:LEU:HD12	2.41	0.48
1:B:777:TYR:O	1:B:778:GLY:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:698:LYS:NZ	3:A:1951:X6K:O25	2.37	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:591:ASN:CG	1:A:592:PHE:N	2.72	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: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: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:391:ASP:OD2	1:A:391:ASP:N	2.47	0.47
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:B:599:TYR:HD2	1:B:599:TYR:C	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:681:LYS:C	1:A:682:LEU:HD12	2.41	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:B:549:ASN:CG	1:B:658:PRO:HG3	2.40	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:777:TYR:C	1:B:779:ILE:N	2.74	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: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:B:775:GLY:O	1:B:776:PRO:C	2.58	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: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:B:405:LEU:CB	1:B:575:MET:HE1	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:LEU:HD12	1:A:402:VAL:HG23	1.99	0.45
1:A:607:PHE:CD1	1:A:607:PHE:C	2.95	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:583:PHE:HD1	1:A:583:PHE:C	2.23	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:A:533:LEU:C	1:A:533:LEU:HD23	2.41	0.45
1:A:549:ASN:CG	1:A:658:PRO:HG3	2.42	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:A:400:GLN:CD	1:A:881:LEU:HD23	2.42	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:A:409:ASP:CG	1:A:412:HIS:CD2	2.95	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:748:ASP:C	1:B:748:ASP:OD2	2.59	0.45
1:B:319:TRP:O	1:B:323:PHE:CD2	2.67	0.44
1:B:551:PHE:CD1	1:B:551:PHE:C	2.95	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:B:599:TYR:C	1:B:599:TYR:CD2	2.94	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:413:ILE:HG22	1:B:578:MET:HE2	1.99	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:A:708:LEU:HD12	1:A:885:MET:HE2	1.99	0.44
1:B:398:LEU:HD23	1:B:398:LEU:C	2.43	0.44
1:B:819:LEU:C	1:B:819:LEU:HD23	2.43	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:315:GLN:C	1:B:322:ARG:HH21	2.14	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:822:ILE:HD11	3:A:1951:X6K:H162	1.99	0.43
1:B:332:LEU:O	1:B:336:LEU:HD22	2.17	0.43
1:B:777:TYR:C	1:B:779:ILE:H	2.26	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:B:317:LEU:HD13	1:B:317:LEU:C	2.44	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: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:715:LEU:C	1:A:715:LEU:HD23	2.44	0.43
1:A:819:LEU:C	1:A:819:LEU:CD2	2.89	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:551:PHE:C	1:B:551:PHE:HD1	2.26	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:A:885:MET:HE3	1:A:888:ALA:HB1	2.01	0.42
1:A:835:MET:C	1:A:836:PRO:O	2.58	0.42
1:B:329:LYS:O	1:B:332:LEU:HB3	2.18	0.42
1:A:559:VAL:O	1:A:560:GLU:C	2.62	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: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:549:ASN:C	1:A:549:ASN:HD22	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:805:ASP:CG	1:A:805:ASP:O	2.63	0.42
1:B:712:MET:CE	1:B:712:MET:CA	2.80	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
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:A:819:LEU:HD11	1:A:845:MET:HE3	2.01	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: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:A:806:ARG:NH2	1:A:810:ASN:CG	2.78	0.41
1:B:590:GLY:O	1:B:595:ARG:NE	2.53	0.41
1:A:369:LEU:O	1:A:370:SER:C	2.63	0.41
1:A:580:LEU:HD22	1:A:584:LEU:HD11	2.02	0.41
1:A:823:ASP:CG	1:A:823:ASP:O	2.63	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:782:GLU:CD	1:A:782:GLU:N	2.78	0.41
1:B:569:ASP:OD1	1:B:570:GLU:N	2.54	0.41
1:B:598:PHE:C	1:B:598:PHE:HD2	2.24	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
1:A:647:THR:C	1:A:664:LYS:HB3	2.44	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:737:THR:O	1:A:738:SER:C	2.63	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:A:948:ARG:HH11	1:A:948:ARG:C	2.29	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:555:LEU:HD22	1:B:555:LEU:HA	1.92	0.41
1:A:357:TRP:CD1	1:A:357:TRP:C	2.99	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:B:633:GLN:NE2	1:B:668:MET:C	2.79	0.40
1:A:405:LEU:HD23	1:A:533:LEU:CD2	2.50	0.40
1:A:610:GLU:CD	1:A:643:LYS:HB2	2.47	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:614:LEU:C	1:A:614:LEU:CD1	2.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:LYS:C	1:B:685:VAL:HG22	2.45	0.40
1:B:945:GLN:O	1:B:946:TYR:C	2.64	0.40
1:A:566:ARG:C	1:A:567:LYS:HG2	2.46	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:B:332:LEU:HD13	1:B:357:TRP:CG	2.56	0.40
1:B:397:TYR:C	1:B:401:LEU:HD11	2.46	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
1:B:600:ASN:ND2	1:B:782:GLU:OE2[8_565]	2.11	0.09

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	546/696 (78%)	507 (93%)	34 (6%)	5 (1%)	14	47
1	B	544/696 (78%)	519 (95%)	16 (3%)	9 (2%)	7	35
All	All	1090/1392 (78%)	1026 (94%)	50 (5%)	14 (1%)	9	39

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

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Mol	Chain	Res	Type
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%)	371 (75%)	124 (25%)	0	4
1	B	494/612 (81%)	380 (77%)	114 (23%)	1	5
All	All	989/1224 (81%)	751 (76%)	238 (24%)	1	4

All (238) 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	309	VAL
1	A	313	GLU
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	341	TRP
1	A	342	LYS

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Mol	Chain	Res	Type
1	A	344	GLU
1	A	345	ASP
1	A	347	VAL
1	A	353	MET
1	A	354	LEU
1	A	363	GLU
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	395	LEU
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
1	A	540	ARG
1	A	544	ASN
1	A	546	THR
1	A	547	LEU
1	A	549	ASN
1	A	552	TYR
1	A	559	VAL
1	A	560	GLU
1	A	563	GLU
1	A	565	VAL
1	A	568	GLN
1	A	573	HIS
1	A	578	MET
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

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Mol	Chain	Res	Type
1	A	618	VAL
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	674	LYS
1	A	677	LEU
1	A	678	MET
1	A	682	LEU
1	A	683	THR
1	A	685	VAL
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	720	LEU
1	A	722	ARG
1	A	725	LEU
1	A	727	LEU
1	A	734	VAL
1	A	737	THR
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	752	VAL
1	A	758	ARG
1	A	765	PHE
1	A	774	ASN
1	A	782	GLU
1	A	786	THR
1	A	790	SER
1	A	791	CYS
1	A	803	VAL

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Mol	Chain	Res	Type
1	A	811	LEU
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	841	LEU
1	A	855	GLU
1	A	859	GLU
1	A	881	LEU
1	A	886	VAL
1	A	893	ILE
1	A	896	GLU
1	A	908	LEU
1	A	912	LEU
1	A	913	THR
1	A	914	ASP
1	A	919	GLN
1	A	930	THR
1	A	938	GLU
1	A	940	ILE
1	A	942	ARG
1	A	944	THR
1	A	948	ARG
1	B	299	THR
1	B	300	ILE
1	B	301	VAL
1	B	302	TYR
1	B	307	THR
1	B	308	TYR
1	B	309	VAL
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

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Mol	Chain	Res	Type
1	B	328	HIS
1	B	329	LYS
1	B	333	THR
1	B	335	PHE
1	B	336	LEU
1	B	339	ILE
1	B	342	LYS
1	B	344	GLU
1	B	351	LEU
1	B	360	MET
1	B	370	SER
1	B	372	THR
1	B	373	PHE
1	B	378	VAL
1	B	391	ASP
1	B	392	GLU
1	B	394	LEU
1	B	396	LEU
1	B	398	LEU
1	B	402	VAL
1	B	419	CYS
1	B	533	LEU
1	B	535	THR
1	B	536	PHE
1	B	539	GLN
1	B	546	THR
1	B	547	LEU
1	B	549	ASN
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
1	B	605	ARG
1	B	611	LEU
1	B	614	LEU
1	B	627	LYS
1	B	634	LYS
1	B	638	GLU
1	B	643	LYS

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Mol	Chain	Res	Type
1	B	645	ASN
1	B	647	THR
1	B	651	PRO
1	B	652	ILE
1	B	660	ILE
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	725	LEU
1	B	727	LEU
1	B	729	LEU
1	B	734	VAL
1	B	746	TYR
1	B	747	VAL
1	B	748	ASP
1	B	750	CYS
1	B	758	ARG
1	B	762	ILE
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	813	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
1	B	858	HIS
1	B	862	LYS

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Mol	Chain	Res	Type
1	B	866	THR
1	B	876	ASN
1	B	877	VAL
1	B	881	LEU
1	B	883	SER
1	B	889	THR
1	B	893	ILE
1	B	906	GLU
1	B	908	LEU
1	B	909	GLN
1	B	930	THR
1	B	937	VAL
1	B	940	ILE
1	B	941	HIS
1	B	944	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) 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	573	HIS
1	A	691	HIS
1	A	707	GLN
1	A	764	ASN
1	A	769	HIS
1	A	810	ASN
1	A	863	GLN
1	A	870	HIS
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

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Mol	Chain	Res	Type
1	B	810	ASN
1	B	857	HIS
1	B	858	HIS
1	B	870	HIS
1	B	876	ASN
1	B	880	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
3	X6K	A	1951	-	29,30,30	2.72	9 (31%)	35,43,43	1.91	8 (22%)
2	SO4	A	1949	-	4,4,4	0.24	0	6,6,6	0.17	0
3	X6K	B	1950	-	29,30,30	2.67	8 (27%)	35,43,43	2.03	9 (25%)
2	SO4	B	1951	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	A	1950	-	4,4,4	0.35	0	6,6,6	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	X6K	A	1951	-	-	1/8/16/16	0/5/5/5
3	X6K	B	1950	-	-	1/8/16/16	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1951	X6K	C06-N01	6.08	1.45	1.32
3	B	1950	X6K	O07-C06	6.07	1.45	1.38
3	A	1951	X6K	O07-C06	6.02	1.45	1.38
3	B	1950	X6K	C06-N01	5.97	1.44	1.32
3	A	1951	X6K	C26-C20	5.72	1.49	1.39
3	B	1950	X6K	C26-C20	5.63	1.49	1.39
3	B	1950	X6K	C19-N10	4.61	1.44	1.34
3	A	1951	X6K	C19-N10	4.59	1.44	1.34
3	B	1950	X6K	O07-C08	4.33	1.45	1.38
3	B	1950	X6K	C22-C23	4.19	1.46	1.38
3	A	1951	X6K	O07-C08	4.17	1.45	1.38
3	A	1951	X6K	C22-C23	3.97	1.45	1.38
3	A	1951	X6K	C05-C09	3.54	1.52	1.46
3	A	1951	X6K	C11-N12	3.51	1.46	1.37
3	B	1950	X6K	C05-C09	3.18	1.51	1.46
3	B	1950	X6K	C11-N12	3.05	1.45	1.37
3	A	1951	X6K	C05-C06	-2.12	1.35	1.42

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1950	X6K	O07-C08-C11	6.37	132.83	126.48
3	A	1951	X6K	O07-C08-C11	6.31	132.77	126.48
3	B	1950	X6K	C17-N12-C13	4.83	122.44	111.57
3	A	1951	X6K	C17-N12-C13	3.21	118.79	111.57
3	A	1951	X6K	C17-N12-C11	3.15	129.60	118.92
3	A	1951	X6K	O07-C06-N01	3.09	132.19	123.39
3	B	1950	X6K	C13-N12-C11	-3.07	108.52	118.92
3	B	1950	X6K	C17-N12-C11	2.99	129.05	118.92
3	B	1950	X6K	O07-C06-N01	2.99	131.89	123.39
3	A	1951	X6K	N18-C19-N10	-2.95	120.28	125.13
3	B	1950	X6K	N18-C19-N10	-2.89	120.37	125.13
3	B	1950	X6K	C20-C19-N18	2.56	121.62	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1951	X6K	C08-O07-C06	2.46	108.76	105.66
3	A	1951	X6K	C13-N12-C11	-2.16	111.61	118.92
3	B	1950	X6K	C03-C02-N01	-2.13	120.05	123.42
3	B	1950	X6K	C08-O07-C06	2.06	108.26	105.66
3	A	1951	X6K	C08-C11-N18	-2.06	119.38	123.81

There are no chirality outliers.

All (2) torsion outliers are listed below:

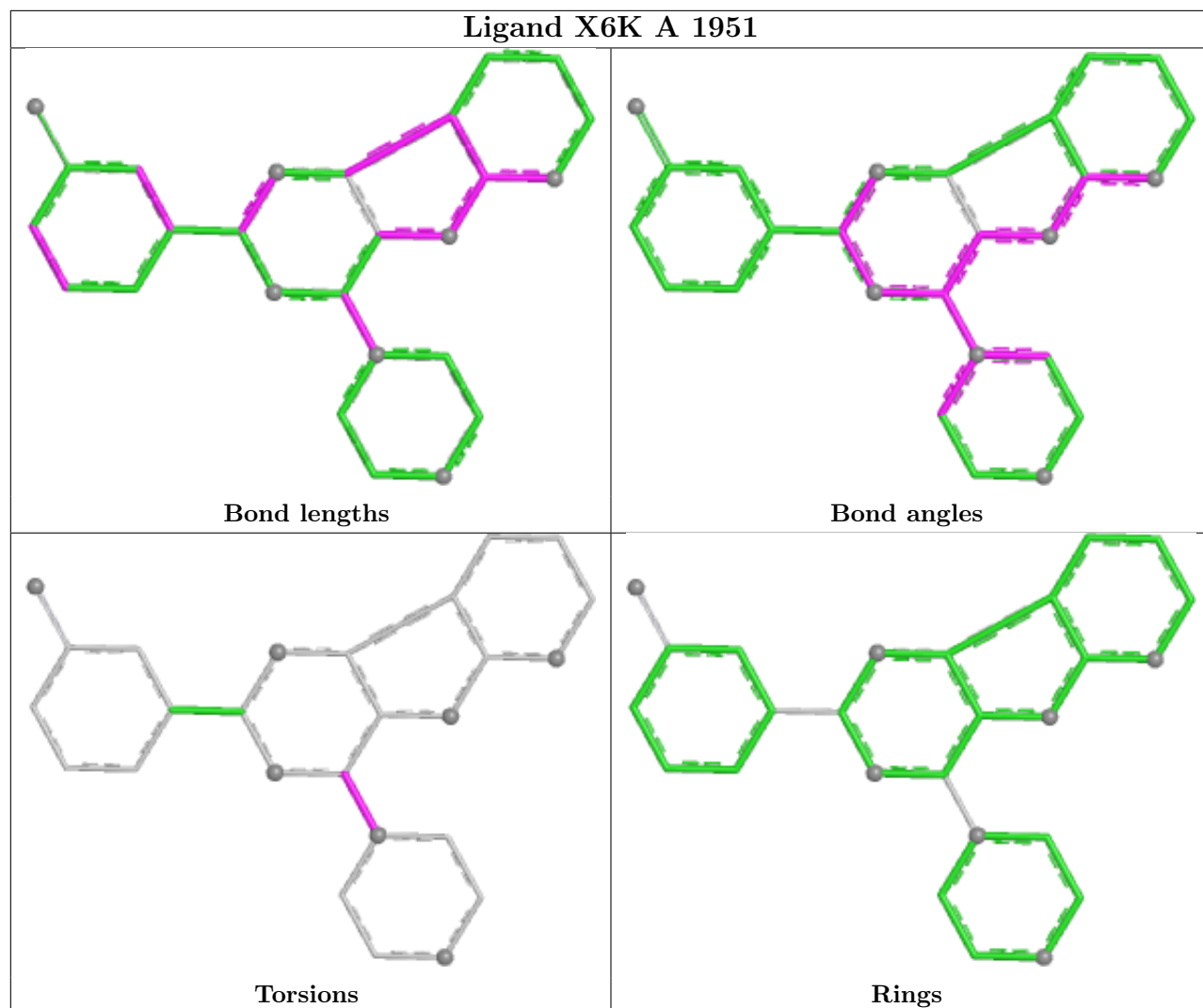
Mol	Chain	Res	Type	Atoms
3	B	1950	X6K	N10-C19-C20-C21
3	A	1951	X6K	N18-C11-N12-C13

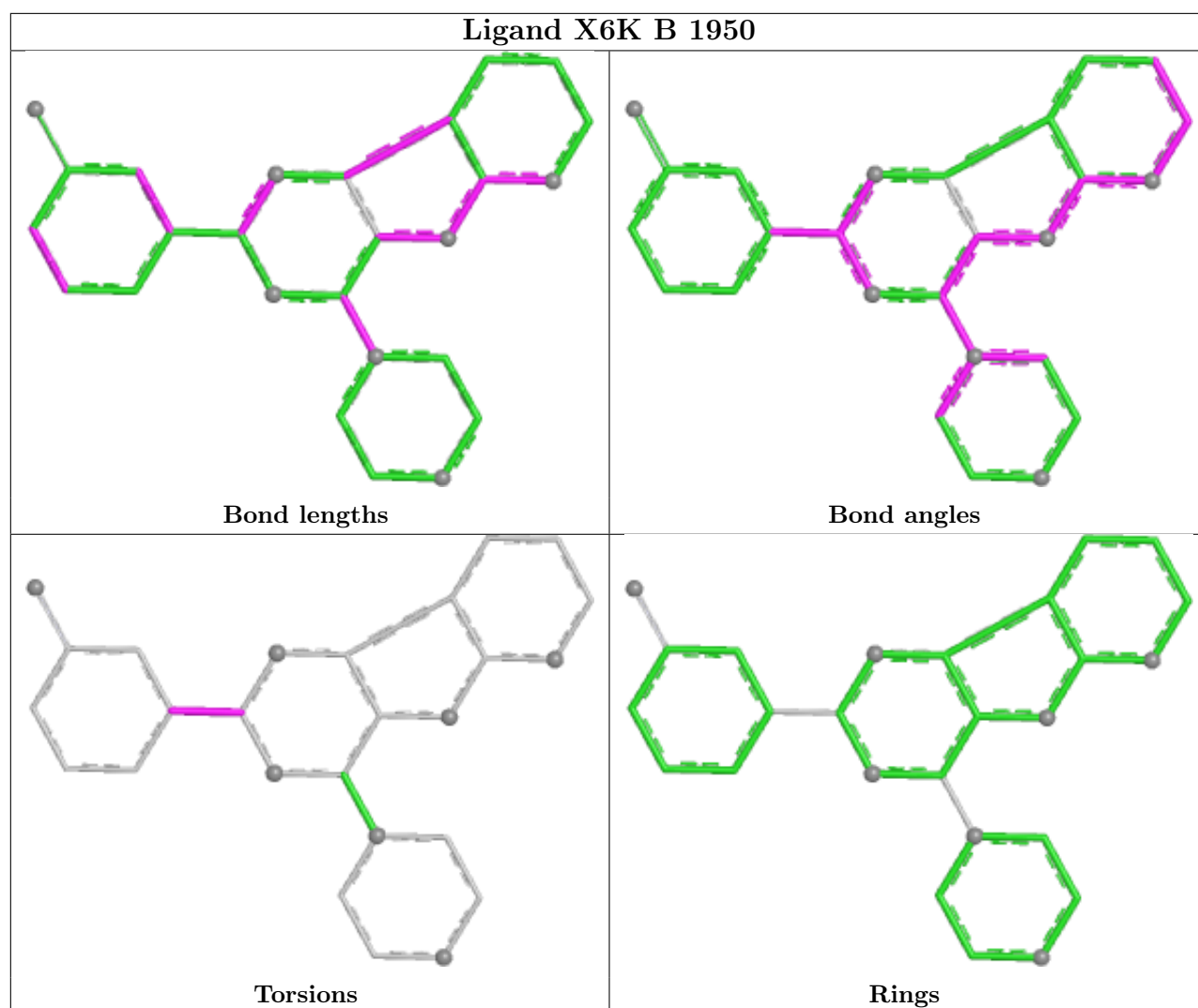
There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1951	X6K	3	0
2	A	1949	SO4	1	0
3	B	1950	X6K	9	0
2	B	1951	SO4	1	0
2	A	1950	SO4	1	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, 95th 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 ²)	Q<0.9
1	A	550/696 (79%)	0.01	4 (0%) 84 63	18, 62, 117, 129	0
1	B	550/696 (79%)	-0.05	9 (1%) 70 45	48, 75, 126, 135	0
All	All	1100/1392 (79%)	-0.02	13 (1%) 76 52	18, 69, 121, 135	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	690	HIS	4.3
1	A	322	ARG	3.5
1	A	306	PRO	3.0
1	A	324	TYR	2.9
1	B	298	HIS	2.8
1	A	887	ASP	2.4
1	B	693	TYR	2.4
1	B	322	ARG	2.4
1	B	331	ALA	2.2
1	B	531	ALA	2.2
1	B	533	LEU	2.2
1	B	324	TYR	2.1
1	B	318	VAL	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

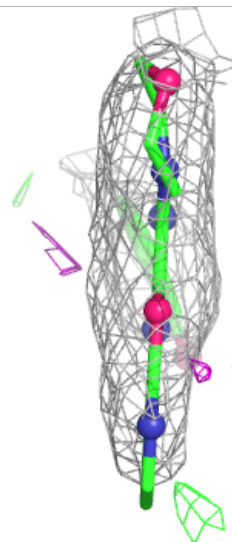
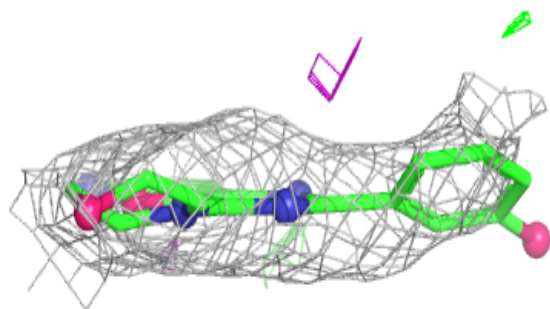
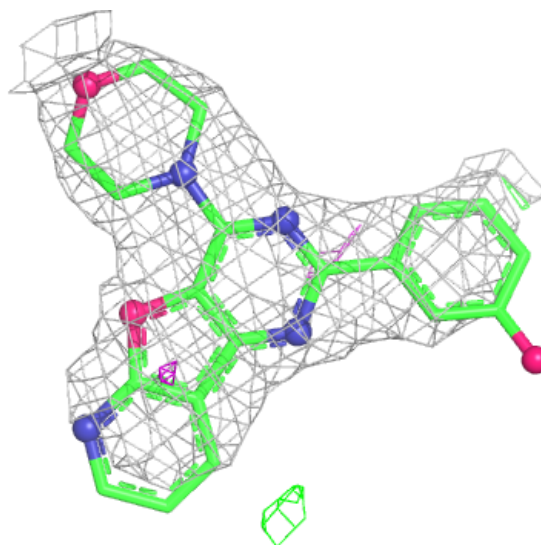
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.66	0.09	194,194,194,194	0
2	SO4	A	1950	5/5	0.79	0.12	146,147,147,147	0
3	X6K	B	1950	26/26	0.85	0.17	113,121,125,125	0
3	X6K	A	1951	26/26	0.89	0.18	114,119,123,123	0
2	SO4	A	1949	5/5	0.89	0.11	145,145,145,146	0

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

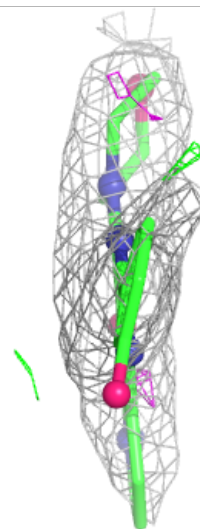
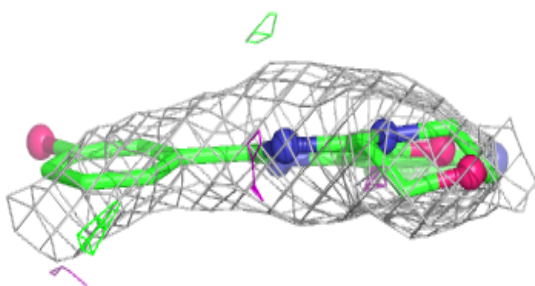
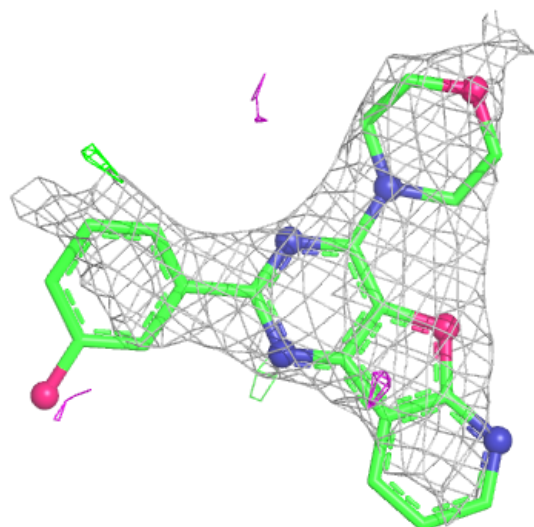
Electron density around X6K B 1950:

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



Electron density around X6K A 1951:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.