



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:58 AM UTC

PDB ID : 4YZF / pdb_00004yzf
Title : Crystal structure of the anion exchanger domain of human erythrocyte Band 3
Authors : Alguel, Y.; Arakawa, T.; Yugiri, T.K.; Iwanari, H.; Hatae, H.; Iwata, M.; Abe, Y.; Hino, T.; Suno, C.I.; Kuma, H.; Kang, D.; Murata, T.; Hamakubo, T.; Cameron, A.D.; Kobayashi, T.; Hamasaki, N.; Iwata, S.
Deposited on : 2015-03-25
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](#) ①) 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

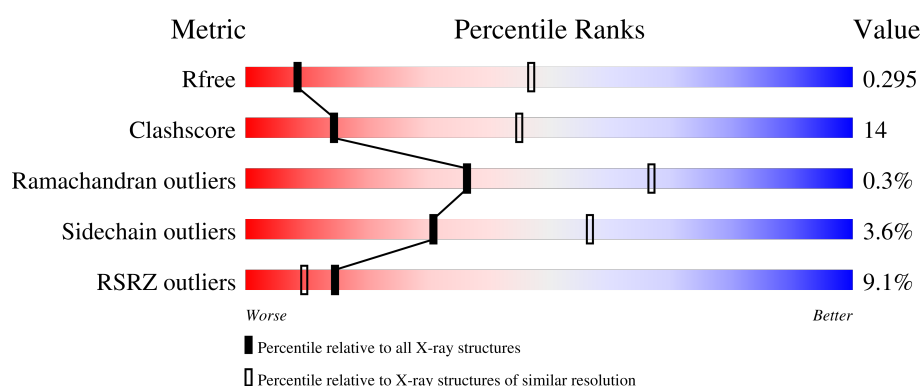
1 Overall quality at a glance

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	911	3% 30% 20% . 48%
1	B	911	4% 31% 19% . 48%
1	C	911	4% 30% 20% . 48%
1	D	911	6% 31% 20% . 48%
2	E	223	7% 72% 23% 5%

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Mol	Chain	Length	Quality of chain
2	G	223	8% 83% 16%
2	I	223	25% 67% 29%
2	K	223	8% 80% 19%
3	F	218	3% 77% 23%
3	H	218	8% 83% 16%
3	J	218	13% 74% 24%
3	L	218	8% 84% 15%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28724 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 Band 3 anion transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	0	0
			3769	2535	598	619	17			
1	B	475	Total	C	N	O	S	0	0	0
			3769	2535	598	619	17			
1	C	475	Total	C	N	O	S	0	0	0
			3769	2535	598	619	17			
1	D	475	Total	C	N	O	S	0	0	0
			3769	2535	598	619	17			

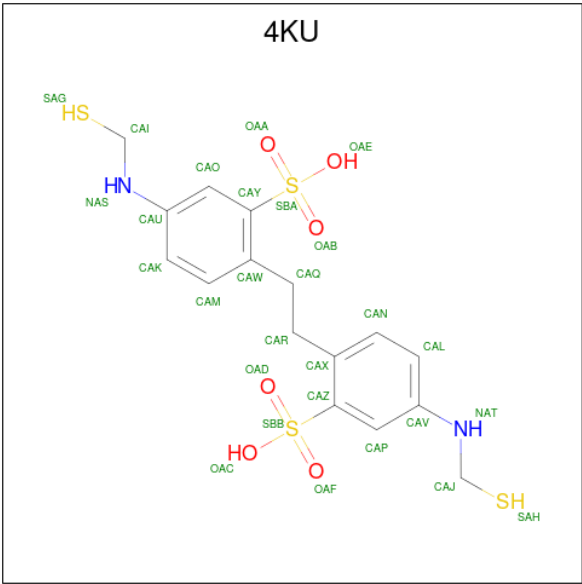
- Molecule 2 is a protein called FAB fragment of Immunoglobulin (IgG) molecule.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	223	Total	C	N	O	S	0	0	0
			1690	1077	274	334	5			
2	G	223	Total	C	N	O	S	0	0	0
			1690	1077	274	334	5			
2	I	223	Total	C	N	O	S	0	0	0
			1690	1077	274	334	5			
2	K	223	Total	C	N	O	S	0	0	0
			1690	1077	274	334	5			

- Molecule 3 is a protein called FAB fragment of Immunoglobulin (IgG) molecule.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	218	Total	C	N	O	S	0	0	0
			1694	1055	285	346	8			
3	H	218	Total	C	N	O	S	0	0	0
			1694	1055	285	346	8			
3	J	218	Total	C	N	O	S	0	0	0
			1694	1055	285	346	8			
3	L	218	Total	C	N	O	S	0	0	0
			1694	1055	285	346	8			

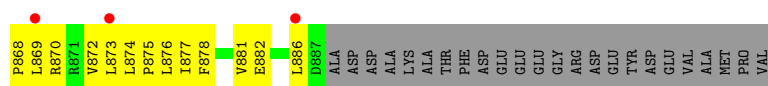
- Molecule 4 is 2,2'-ethane-1,2-diylbis{5-[(sulfanylmethyl)amino]benzenesulfonic acid} (CCD ID: 4KU) (formula: C₁₆H₂₀N₂O₆S₄).



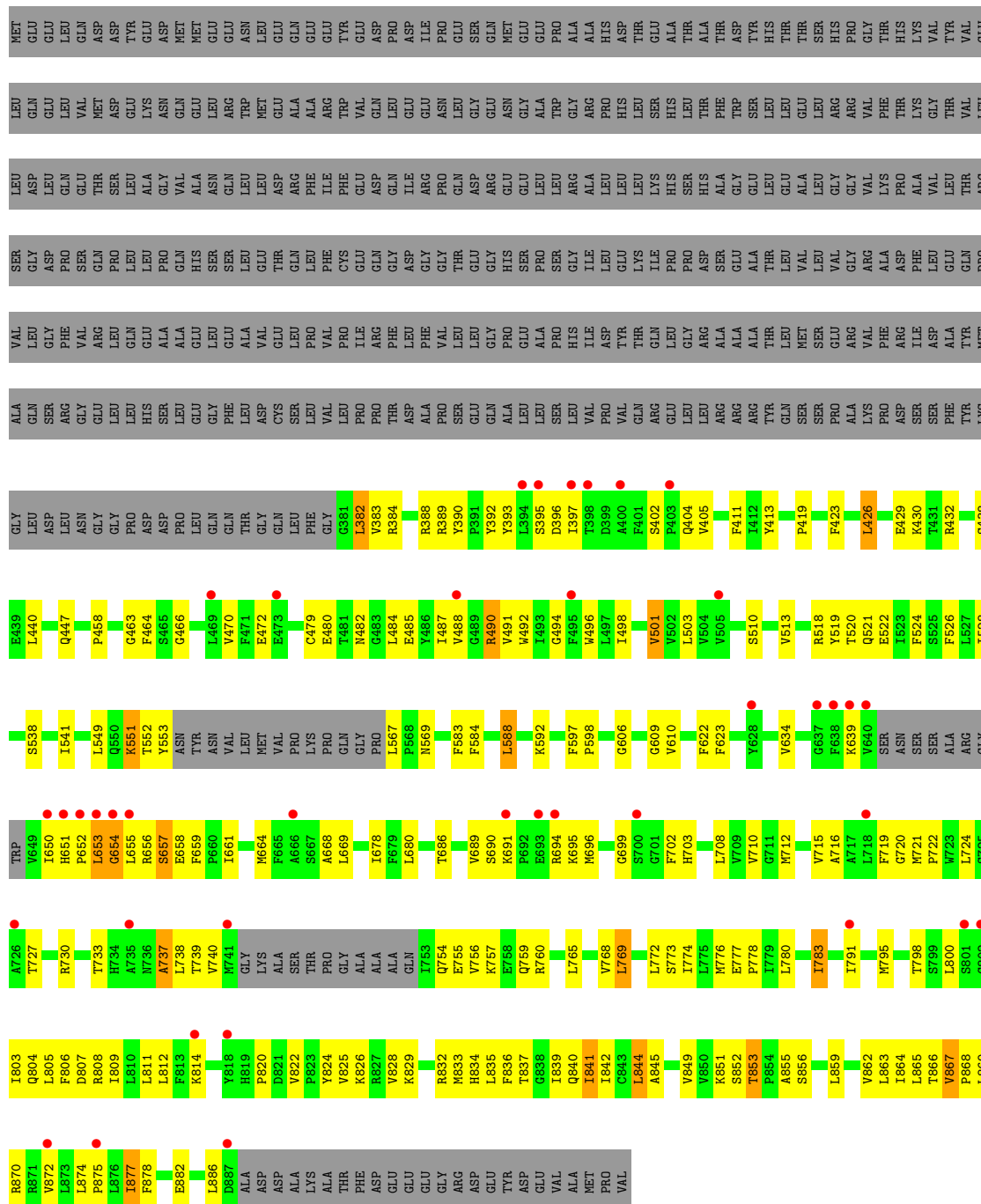
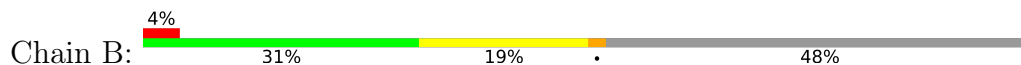
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			28	16	2	6	4		
4	B	1	Total	C	N	O	S	0	0
			28	16	2	6	4		
4	C	1	Total	C	N	O	S	0	0
			28	16	2	6	4		
4	D	1	Total	C	N	O	S	0	0
			28	16	2	6	4		

- Molecule 1: Band 3 anion transport protein

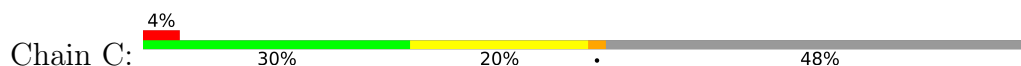


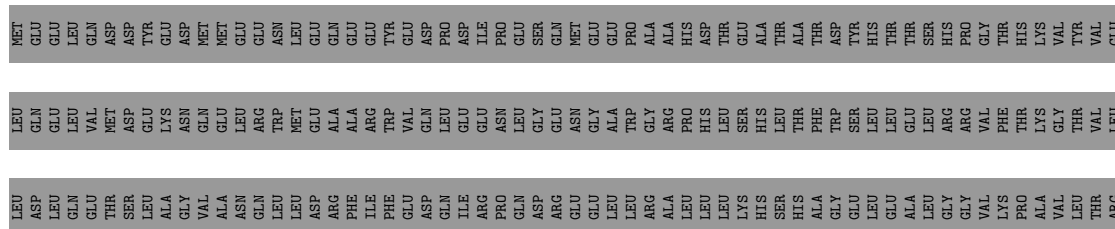
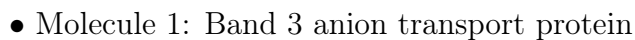


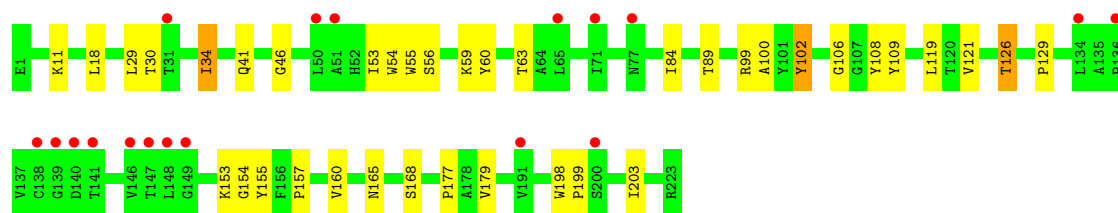
• Molecule 1: Band 3 anion transport protein



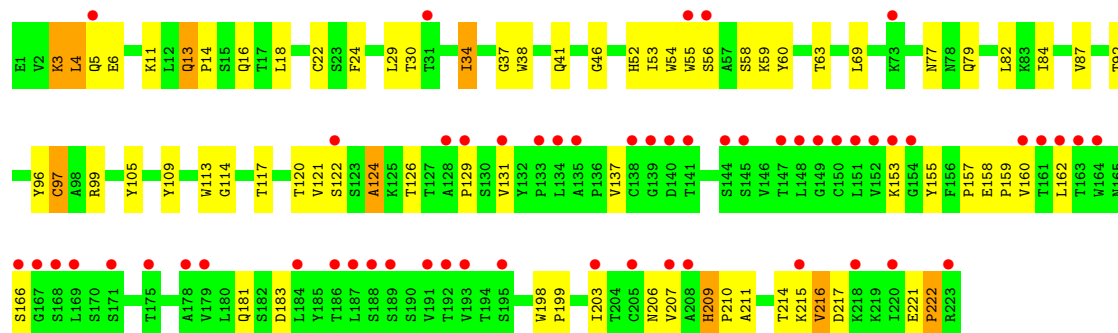
• Molecule 1: Band 3 anion transport protein



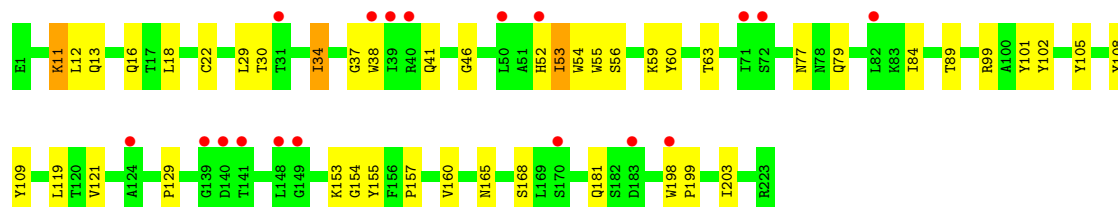
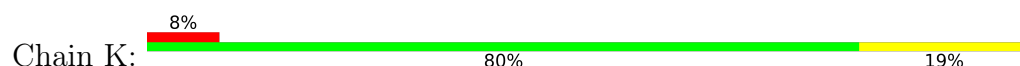




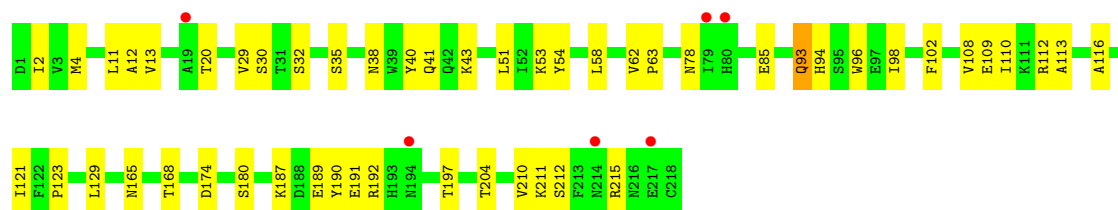
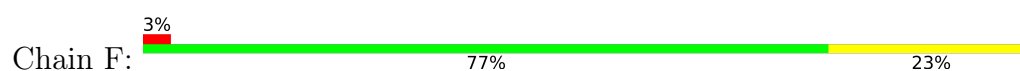
- Molecule 2: FAB fragment of Immunoglobulin (IgG) molecule



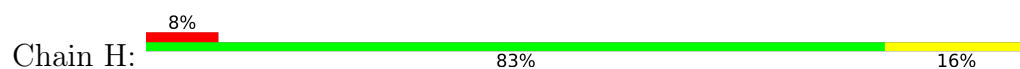
- Molecule 2: FAB fragment of Immunoglobulin (IgG) molecule



- Molecule 3: FAB fragment of Immunoglobulin (IgG) molecule

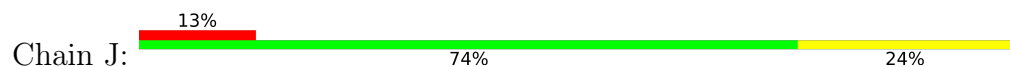


- Molecule 3: FAB fragment of Immunoglobulin (IgG) molecule

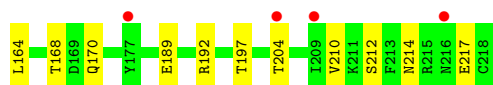
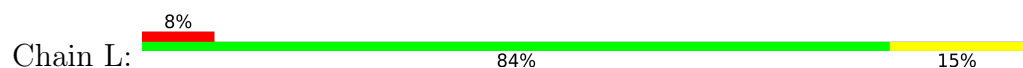




- Molecule 3: FAB fragment of Immunoglobulin (IgG) molecule



- Molecule 3: FAB fragment of Immunoglobulin (IgG) molecule



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	152.82Å 171.96Å 271.70Å 90.00° 101.16° 90.00°	Depositor
Resolution (Å)	37.72 – 3.50 37.72 – 3.50	Depositor EDS
% Data completeness (in resolution range)	94.6 (37.72-3.50) 94.8 (37.72-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1951)	Depositor
R, R_{free}	0.274 , 0.290 0.277 , 0.295	Depositor DCC
R_{free} test set	4135 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	115.1	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 86.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	28724	wwPDB-VP
Average B, all atoms (Å ²)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.75 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.3662e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 4KU

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	0.56	0/3862	1.00	22/5246 (0.4%)
1	B	0.49	0/3862	0.97	14/5246 (0.3%)
1	C	0.53	0/3862	0.98	18/5246 (0.3%)
1	D	0.49	0/3862	0.94	14/5246 (0.3%)
2	E	0.59	0/1737	1.32	18/2377 (0.8%)
2	G	0.48	0/1737	0.93	3/2377 (0.1%)
2	I	0.55	0/1737	1.20	15/2377 (0.6%)
2	K	0.47	0/1737	0.92	3/2377 (0.1%)
3	F	0.55	0/1736	0.93	2/2360 (0.1%)
3	H	0.47	1/1736 (0.1%)	0.84	1/2360 (0.0%)
3	J	0.48	0/1736	0.92	3/2360 (0.1%)
3	L	0.44	0/1736	0.82	1/2360 (0.0%)
All	All	0.51	1/29340 (0.0%)	0.99	114/39932 (0.3%)

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
3	H	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	112	ARG	CA-C	5.01	1.59	1.52

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	867	VAL	CA-C-N	-9.20	110.80	119.82
1	A	867	VAL	C-N-CA	-9.20	110.80	119.82
2	E	96	TYR	N-CA-C	8.99	123.26	108.96
2	E	97	CYS	N-CA-C	-8.58	96.64	110.20
1	C	659	PHE	CA-C-N	8.56	128.63	119.90
1	C	659	PHE	C-N-CA	8.56	128.63	119.90
2	E	13	GLN	N-CA-C	-8.55	99.30	110.07
2	I	97	CYS	N-CA-C	-8.53	96.72	110.20
2	I	96	TYR	N-CA-C	8.43	122.37	108.96
2	E	214	THR	N-CA-C	8.14	121.68	108.41
1	B	867	VAL	CA-C-N	-8.09	111.90	119.82
1	B	867	VAL	C-N-CA	-8.09	111.90	119.82
1	B	737	ALA	N-CA-C	8.01	121.17	111.40
1	D	867	VAL	CA-C-N	-7.95	112.03	119.82
1	D	867	VAL	C-N-CA	-7.95	112.03	119.82
1	C	867	VAL	CA-C-N	-7.92	112.06	119.82
1	C	867	VAL	C-N-CA	-7.92	112.06	119.82
1	A	737	ALA	CA-C-N	7.83	135.79	121.70
1	A	737	ALA	C-N-CA	7.83	135.79	121.70
1	C	657	SER	N-CA-C	-7.81	98.45	109.69
1	D	737	ALA	N-CA-C	7.79	120.90	111.40
1	C	737	ALA	CA-C-N	7.75	135.64	121.70
1	C	737	ALA	C-N-CA	7.75	135.64	121.70
2	I	215	LYS	N-CA-C	-7.66	95.81	108.76
1	C	737	ALA	N-CA-C	7.62	120.69	111.40
1	A	567	LEU	CA-C-N	-7.43	113.16	120.52
1	A	567	LEU	C-N-CA	-7.43	113.16	120.52
1	B	737	ALA	CA-C-N	7.30	134.84	121.70
1	B	737	ALA	C-N-CA	7.30	134.84	121.70
1	D	737	ALA	CA-C-N	7.21	134.67	121.70
1	D	737	ALA	C-N-CA	7.21	134.67	121.70
1	B	657	SER	CA-C-N	7.04	134.37	121.70
1	B	657	SER	C-N-CA	7.04	134.37	121.70
1	A	657	SER	CA-C-N	6.99	134.28	121.70
1	A	657	SER	C-N-CA	6.99	134.28	121.70
3	H	112	ARG	N-CA-C	6.95	119.50	109.14
2	I	209	HIS	CA-C-N	6.91	128.48	119.84
2	I	209	HIS	C-N-CA	6.91	128.48	119.84
2	E	215	LYS	N-CA-C	-6.88	97.13	108.76
3	J	7	SER	N-CA-C	6.87	114.19	108.07
1	C	436	GLY	N-CA-C	6.83	122.23	112.81
1	D	657	SER	CA-C-N	6.80	133.94	121.70
1	D	657	SER	C-N-CA	6.80	133.94	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	659	PHE	CA-C-N	6.76	127.17	119.93
1	B	659	PHE	C-N-CA	6.76	127.17	119.93
2	E	6	GLU	CB-CA-C	-6.70	100.85	111.17
1	A	737	ALA	N-CA-C	6.64	119.50	111.40
1	B	567	LEU	CA-C-N	-6.60	113.99	120.52
1	B	567	LEU	C-N-CA	-6.60	113.99	120.52
2	E	53	ILE	N-CA-C	6.59	118.28	108.46
1	A	659	PHE	CA-C-N	6.53	126.92	119.93
1	A	659	PHE	C-N-CA	6.53	126.92	119.93
2	E	158	GLU	C-N-CD	-6.51	106.27	120.60
1	D	659	PHE	CA-C-N	6.43	126.46	119.90
1	D	659	PHE	C-N-CA	6.43	126.46	119.90
2	I	13	GLN	CA-C-N	-6.43	113.36	119.85
2	I	13	GLN	C-N-CA	-6.43	113.36	119.85
1	A	657	SER	N-CA-C	-6.39	100.49	109.69
2	K	102	TYR	CA-C-N	6.38	126.16	120.10
2	K	102	TYR	C-N-CA	6.38	126.16	120.10
1	C	657	SER	CA-C-N	6.31	133.06	121.70
1	C	657	SER	C-N-CA	6.31	133.06	121.70
2	I	3	LYS	N-CA-C	6.24	118.68	108.52
2	G	102	TYR	CA-C-N	6.22	126.01	120.10
2	G	102	TYR	C-N-CA	6.22	126.01	120.10
2	I	216	VAL	N-CA-C	6.18	118.28	108.89
2	E	216	VAL	N-CA-C	6.15	118.24	108.89
2	K	53	ILE	N-CA-C	6.07	117.50	108.46
2	I	214	THR	N-CA-C	6.06	118.78	108.90
2	E	24	PHE	N-CA-C	6.01	118.31	109.24
2	I	124	ALA	N-CA-C	5.92	119.05	110.28
2	E	221	GLU	CA-C-N	5.90	125.81	119.85
2	E	221	GLU	C-N-CA	5.90	125.81	119.85
1	C	872	VAL	N-CA-C	-5.85	107.21	112.12
1	D	657	SER	N-CA-C	-5.81	101.32	109.69
2	I	158	GLU	C-N-CD	-5.73	107.99	120.60
1	C	595	SER	N-CA-C	5.68	117.47	111.28
1	D	881	VAL	N-CA-C	-5.68	106.27	111.67
2	G	53	ILE	N-CA-C	5.68	116.92	108.46
2	I	53	ILE	N-CA-C	5.68	116.92	108.46
2	I	117	THR	N-CA-C	-5.66	100.91	109.85
1	A	651	HIS	CA-C-N	5.52	125.23	119.82
1	A	651	HIS	C-N-CA	5.52	125.23	119.82
1	B	783	ILE	N-CA-C	5.51	112.57	107.56
1	B	657	SER	N-CA-C	-5.50	101.76	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	853	THR	CA-C-N	-5.50	114.01	120.12
1	A	853	THR	C-N-CA	-5.50	114.01	120.12
1	A	595	SER	N-CA-C	5.44	117.21	111.28
2	E	207	VAL	N-CA-C	5.40	115.64	107.75
1	A	436	GLY	N-CA-C	5.38	120.23	112.81
2	E	209	HIS	CA-C-N	5.37	126.56	119.84
2	E	209	HIS	C-N-CA	5.37	126.56	119.84
2	E	114	GLY	N-CA-C	-5.31	104.38	112.51
1	D	567	LEU	CA-C-N	-5.30	115.27	120.52
1	D	567	LEU	C-N-CA	-5.30	115.27	120.52
1	C	651	HIS	CA-C-N	5.29	125.01	119.82
1	C	651	HIS	C-N-CA	5.29	125.01	119.82
2	E	93	ALA	N-CA-C	5.25	114.76	107.73
1	A	881	VAL	N-CA-C	-5.24	106.69	111.67
3	J	108	VAL	CA-C-N	5.22	131.01	122.81
3	J	108	VAL	C-N-CA	5.22	131.01	122.81
1	C	567	LEU	CA-C-N	-5.21	115.37	120.52
1	C	567	LEU	C-N-CA	-5.21	115.37	120.52
2	E	5	GLN	N-CA-C	5.18	117.52	108.76
3	L	110	ILE	N-CA-C	5.17	115.71	108.89
1	B	654	GLY	N-CA-C	5.16	116.86	111.95
2	I	4	LEU	N-CA-C	-5.16	100.99	109.40
1	A	610	VAL	CA-C-N	-5.15	113.62	119.28
1	A	610	VAL	C-N-CA	-5.15	113.62	119.28
3	F	108	VAL	CA-C-N	5.13	130.87	122.81
3	F	108	VAL	C-N-CA	5.13	130.87	122.81
1	A	657	SER	CA-C-O	-5.11	115.41	121.60
1	D	508	GLU	N-CA-C	5.05	118.29	111.17
1	C	657	SER	CA-C-O	-5.05	115.49	121.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	111	LYS	Mainchain

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3769	0	3990	154	0
1	B	3769	0	3990	144	0
1	C	3769	0	3988	141	0
1	D	3769	0	3989	144	0
2	E	1690	0	1645	40	0
2	G	1690	0	1645	28	0
2	I	1690	0	1645	46	0
2	K	1690	0	1645	32	0
3	F	1694	0	1609	34	0
3	H	1694	0	1609	29	0
3	J	1694	0	1609	40	0
3	L	1694	0	1609	27	0
4	A	28	0	15	1	0
4	B	28	0	14	2	0
4	C	28	0	15	3	0
4	D	28	0	15	2	0
All	All	28724	0	29032	811	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (811) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:828:VAL:HG23	1:A:829:LYS:HG3	1.48	0.94
1:D:851:LYS:HE3	1:D:859:LEU:HD22	1.51	0.92
1:C:828:VAL:HG23	1:C:829:LYS:HG3	1.49	0.92
1:D:828:VAL:HG23	1:D:829:LYS:HG3	1.54	0.90
1:D:737:ALA:HB3	1:D:738:LEU:HB2	1.55	0.89
1:B:737:ALA:HB3	1:B:738:LEU:HB2	1.55	0.89
2:I:124:ALA:HB2	2:I:183:ASP:HB3	1.53	0.89
1:C:851:LYS:HE3	1:C:859:LEU:HD22	1.52	0.89
1:D:592:LYS:HB2	1:D:606:GLY:HA3	1.56	0.88
1:C:592:LYS:HB2	1:C:606:GLY:HA3	1.55	0.88
1:C:737:ALA:HB3	1:C:738:LEU:HB2	1.55	0.87
2:K:30:THR:HA	2:K:55:TRP:HD1	1.38	0.87
1:A:851:LYS:HE3	1:A:859:LEU:HD22	1.57	0.86
1:A:737:ALA:HB3	1:A:738:LEU:HB2	1.54	0.86
1:B:592:LYS:HB2	1:B:606:GLY:HA3	1.58	0.85
3:F:112:ARG:NH1	3:F:174:ASP:O	2.09	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:828:VAL:HG23	1:B:829:LYS:HG3	1.57	0.85
1:A:592:LYS:HB2	1:A:606:GLY:HA3	1.58	0.83
2:E:30:THR:HA	2:E:55:TRP:CD1	2.16	0.81
2:I:30:THR:HA	2:I:55:TRP:CD1	2.16	0.80
2:E:30:THR:HA	2:E:55:TRP:HD1	1.47	0.80
1:B:501:VAL:HG21	1:B:710:VAL:HB	1.64	0.79
2:G:30:THR:HA	2:G:55:TRP:HD1	1.47	0.79
1:D:501:VAL:HG21	1:D:710:VAL:HB	1.64	0.79
1:A:549:LEU:HD22	1:B:569:ASN:HD21	1.47	0.79
1:B:851:LYS:HE3	1:B:859:LEU:HD22	1.63	0.78
1:C:518:ARG:NH1	1:C:804:GLN:OE1	2.17	0.78
1:A:610:VAL:HG13	1:A:791:ILE:HD12	1.65	0.77
3:H:29:VAL:HG23	3:H:96:TRP:HB2	1.66	0.77
1:A:518:ARG:NH1	1:A:804:GLN:OE1	2.18	0.77
1:D:519:TYR:HD2	1:D:867:VAL:HG13	1.49	0.77
1:C:501:VAL:HG21	1:C:710:VAL:HB	1.66	0.76
1:C:809:ILE:HG12	1:C:841:ILE:HD11	1.66	0.76
1:C:829:LYS:HB3	1:C:833:MET:N	2.00	0.76
1:C:610:VAL:HG13	1:C:791:ILE:HD12	1.68	0.76
2:G:11:LYS:HE3	2:G:126:THR:HG23	1.67	0.76
3:H:41:GLN:HB2	3:H:51:LEU:HD11	1.66	0.75
1:A:389:ARG:NH1	1:A:699:GLY:O	2.19	0.75
3:L:41:GLN:HB2	3:L:51:LEU:HD11	1.68	0.75
1:C:389:ARG:NH1	1:C:699:GLY:O	2.21	0.74
2:E:124:ALA:HB2	2:E:183:ASP:HB3	1.68	0.74
1:B:389:ARG:NH1	1:B:699:GLY:O	2.20	0.74
1:A:501:VAL:HG21	1:A:710:VAL:HB	1.69	0.74
1:B:829:LYS:HB3	1:B:833:MET:N	2.03	0.74
2:K:30:THR:HA	2:K:55:TRP:CD1	2.22	0.73
1:D:829:LYS:HB3	1:D:833:MET:N	2.04	0.73
1:D:518:ARG:NH1	1:D:804:GLN:OE1	2.22	0.73
2:E:13:GLN:HB2	2:E:16:GLN:CD	2.14	0.73
1:B:519:TYR:HD2	1:B:867:VAL:HG13	1.54	0.72
3:J:4:MET:HE1	3:J:93:GLN:HA	1.70	0.72
3:J:112:ARG:NH1	3:J:174:ASP:O	2.20	0.72
2:I:30:THR:HA	2:I:55:TRP:HD1	1.54	0.72
1:A:680:LEU:HD21	1:A:863:LEU:HD23	1.72	0.71
1:B:829:LYS:HB3	1:B:833:MET:H	1.56	0.71
1:D:389:ARG:NH2	1:D:396:ASP:OD2	2.18	0.71
1:C:680:LEU:HD21	1:C:863:LEU:HD23	1.72	0.70
1:D:610:VAL:HG13	1:D:791:ILE:HD12	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:109:GLU:OE2	3:J:177:TYR:OH	2.06	0.70
3:L:29:VAL:HG23	3:L:96:TRP:HB2	1.72	0.70
1:C:829:LYS:HB3	1:C:833:MET:H	1.56	0.70
1:A:829:LYS:HB3	1:A:833:MET:N	2.05	0.70
1:D:389:ARG:NH1	1:D:699:GLY:O	2.25	0.70
2:G:30:THR:HA	2:G:55:TRP:CD1	2.26	0.70
2:G:165:ASN:O	2:G:168:SER:OG	2.09	0.70
1:C:488:VAL:HG21	1:C:654:GLY:HA2	1.74	0.69
1:A:851:LYS:HB2	1:A:859:LEU:HD13	1.74	0.69
1:C:522:GLU:OE1	1:C:805:LEU:N	2.22	0.69
3:J:112:ARG:HH12	3:J:174:ASP:HB2	1.58	0.69
1:C:812:LEU:HA	1:C:834:HIS:CE1	2.28	0.68
3:F:29:VAL:HG23	3:F:96:TRP:HB2	1.76	0.68
1:A:812:LEU:HA	1:A:834:HIS:CE1	2.28	0.68
1:A:522:GLU:OE1	1:A:805:LEU:N	2.23	0.68
1:C:447:GLN:HG2	1:C:712:MET:HB3	1.74	0.68
3:J:29:VAL:HG23	3:J:96:TRP:HB2	1.74	0.68
1:B:520:THR:OG1	1:B:521:GLN:N	2.24	0.68
1:B:480:GLU:O	2:G:108:TYR:OH	2.09	0.68
1:A:829:LYS:HB3	1:A:833:MET:H	1.60	0.67
1:B:526:PHE:CD2	1:B:844:LEU:HD21	2.29	0.67
1:B:610:VAL:HG13	1:B:791:ILE:HD12	1.74	0.67
2:G:60:TYR:CD1	3:H:98:ILE:HG21	2.29	0.67
1:A:520:THR:HG22	1:A:867:VAL:HG11	1.75	0.67
1:D:708:LEU:O	1:D:712:MET:HG2	1.95	0.67
1:B:661:ILE:HG13	1:B:664:MET:HE2	1.77	0.67
2:E:13:GLN:HB2	2:E:16:GLN:NE2	2.10	0.67
1:A:526:PHE:CD2	1:A:844:LEU:HD21	2.30	0.67
1:B:809:ILE:HG12	1:B:841:ILE:HD11	1.76	0.67
1:D:809:ILE:HG12	1:D:841:ILE:HD11	1.77	0.66
1:D:829:LYS:HB3	1:D:833:MET:H	1.59	0.66
3:H:197:THR:OG1	3:H:212:SER:OG	2.14	0.66
1:C:803:ILE:HG22	1:C:806:PHE:H	1.59	0.66
2:E:54:TRP:CH2	2:E:60:TYR:HD2	2.14	0.66
3:H:84:GLU:HA	3:H:110:ILE:HD11	1.75	0.66
3:J:189:GLU:HA	3:J:192:ARG:HG3	1.77	0.66
1:D:480:GLU:O	2:K:108:TYR:OH	2.10	0.66
1:C:526:PHE:CD2	1:C:844:LEU:HD21	2.31	0.66
1:B:588:LEU:HD12	1:B:609:GLY:HA2	1.78	0.65
1:A:519:TYR:HD2	1:A:867:VAL:HG13	1.62	0.65
3:L:197:THR:HG1	3:L:212:SER:HG	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:522:GLU:OE1	1:D:805:LEU:N	2.24	0.65
1:A:447:GLN:HG2	1:A:712:MET:HB3	1.78	0.65
1:B:689:VAL:HG12	1:B:696:MET:HE1	1.79	0.65
1:C:520:THR:OG1	1:C:521:GLN:N	2.28	0.65
1:D:520:THR:OG1	1:D:521:GLN:N	2.23	0.64
3:H:51:LEU:HA	3:H:62:VAL:HG21	1.79	0.64
2:I:129:PRO:HB3	2:I:155:TYR:HB3	1.79	0.64
1:A:488:VAL:HG21	1:A:654:GLY:HA2	1.79	0.64
1:A:413:TYR:CD1	1:A:769:LEU:HB3	2.32	0.64
1:C:708:LEU:O	1:C:712:MET:HG2	1.97	0.64
2:K:60:TYR:CD1	3:L:98:ILE:HG21	2.32	0.64
1:B:820:PRO:HD3	1:B:826:LYS:HD2	1.78	0.64
1:A:818:TYR:O	1:A:826:LYS:NZ	2.28	0.64
2:E:6:GLU:O	2:E:117:THR:HB	1.98	0.64
1:C:482:ASN:HB3	2:I:56:SER:OG	1.97	0.64
1:D:680:LEU:HD21	1:D:863:LEU:HD23	1.80	0.64
1:A:803:ILE:HG22	1:A:806:PHE:H	1.62	0.63
1:A:809:ILE:HG12	1:A:841:ILE:HD11	1.81	0.63
1:B:413:TYR:CD1	1:B:769:LEU:HB3	2.33	0.63
1:D:867:VAL:HB	1:D:868:PRO:HD3	1.80	0.63
1:C:689:VAL:HG12	1:C:696:MET:HE1	1.79	0.63
1:D:832:ARG:HD3	1:D:835:LEU:HD12	1.80	0.63
3:J:40:TYR:HE2	3:J:93:GLN:HG2	1.64	0.63
1:B:806:PHE:HA	1:B:809:ILE:HD12	1.81	0.62
1:B:488:VAL:HG21	1:B:654:GLY:HA2	1.80	0.62
1:C:658:GLU:HG2	2:I:59:LYS:CG	2.30	0.62
1:D:526:PHE:CD2	1:D:844:LEU:HD21	2.34	0.62
1:A:492:TRP:CD2	1:A:664:MET:HB2	2.35	0.62
1:A:520:THR:OG1	1:A:521:GLN:N	2.31	0.62
2:I:34:ILE:HG23	2:I:99:ARG:HD2	1.81	0.62
1:A:824:TYR:O	1:A:828:VAL:HG22	2.00	0.62
1:D:432:ARG:HG2	3:L:96:TRP:CZ3	2.35	0.62
1:B:867:VAL:HB	1:B:868:PRO:HD3	1.81	0.62
1:C:588:LEU:HD12	1:C:609:GLY:HA2	1.82	0.61
1:C:824:TYR:O	1:C:828:VAL:HG22	2.00	0.61
1:D:661:ILE:HG13	1:D:664:MET:HE2	1.81	0.61
3:F:112:ARG:HH12	3:F:174:ASP:HB2	1.64	0.61
3:F:197:THR:OG1	3:F:212:SER:OG	2.17	0.61
1:B:518:ARG:NH1	1:B:804:GLN:OE1	2.34	0.61
1:D:851:LYS:HA	1:D:856:SER:HB2	1.83	0.61
1:C:413:TYR:CD1	1:C:769:LEU:HB3	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:519:TYR:HD2	1:C:867:VAL:HG13	1.66	0.61
1:C:867:VAL:HB	1:C:868:PRO:HD3	1.82	0.61
1:A:820:PRO:HD3	1:A:826:LYS:HD2	1.83	0.61
1:B:447:GLN:HG2	1:B:712:MET:HB3	1.83	0.61
1:D:689:VAL:HG12	1:D:696:MET:HE1	1.82	0.61
1:D:808:ARG:NH2	1:D:840:GLN:HG3	2.14	0.61
1:A:651:HIS:CD2	1:A:653:LEU:HB2	2.34	0.61
1:D:757:LYS:HB3	1:D:759:GLN:HE22	1.66	0.61
1:C:658:GLU:HG2	2:I:59:LYS:HG2	1.82	0.61
1:C:820:PRO:HD3	1:C:826:LYS:HD2	1.83	0.61
1:C:484:LEU:HD13	1:C:663:MET:HG2	1.83	0.60
1:C:691:LYS:HE2	1:C:694:ARG:HE	1.64	0.60
1:D:820:PRO:HD3	1:D:826:LYS:HD2	1.82	0.60
1:B:832:ARG:HD3	1:B:835:LEU:HD12	1.82	0.60
1:B:824:TYR:O	1:B:828:VAL:HG22	2.02	0.60
1:C:780:LEU:HA	1:C:783:ILE:HD12	1.83	0.60
4:C:1000:4KU:H18	4:C:1000:4KU:SAH	2.41	0.60
1:D:824:TYR:O	1:D:828:VAL:HG22	2.02	0.60
1:A:716:ALA:HB1	1:A:721:MET:HB2	1.84	0.60
1:B:836:PHE:CD2	1:B:886:LEU:HD13	2.37	0.60
1:C:851:LYS:HB2	1:C:859:LEU:HD13	1.84	0.60
1:C:520:THR:HG22	1:C:867:VAL:HG11	1.84	0.60
1:C:492:TRP:CE2	1:C:664:MET:HB2	2.37	0.60
1:C:716:ALA:HB1	1:C:721:MET:HB2	1.82	0.60
3:H:189:GLU:HA	3:H:192:ARG:HG3	1.85	0.59
2:I:198:TRP:CH2	2:I:222:PRO:HG3	2.38	0.59
1:A:584:PHE:HE2	1:A:616:ILE:HG21	1.67	0.59
1:B:389:ARG:NH2	1:B:396:ASP:OD2	2.24	0.59
1:B:466:GLY:O	1:B:470:VAL:HG23	2.02	0.59
1:A:867:VAL:HB	1:A:868:PRO:HD3	1.84	0.59
1:C:492:TRP:CD2	1:C:664:MET:HB2	2.37	0.59
4:A:1000:4KU:H18	4:A:1000:4KU:SAH	2.42	0.59
1:D:447:GLN:HG2	1:D:712:MET:HB3	1.84	0.59
1:B:426:LEU:O	1:B:430:LYS:HG2	2.03	0.59
1:B:661:ILE:O	1:B:664:MET:HG2	2.03	0.59
1:C:389:ARG:NH2	1:C:396:ASP:OD2	2.21	0.59
1:C:866:THR:O	1:C:870:ARG:HB2	2.02	0.58
3:F:12:ALA:HA	3:F:109:GLU:O	2.03	0.58
2:K:165:ASN:O	2:K:168:SER:OG	2.21	0.58
1:C:851:LYS:HA	1:C:856:SER:HB2	1.84	0.58
1:D:696:MET:HB2	1:D:756:VAL:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:811:LEU:HD22	1:D:826:LYS:HZ3	1.68	0.58
1:B:686:THR:O	1:B:690:SER:OG	2.22	0.58
1:A:484:LEU:HD23	2:E:58:SER:HB2	1.84	0.58
1:D:864:ILE:O	1:D:868:PRO:HD2	2.03	0.58
1:A:708:LEU:O	1:A:712:MET:HG2	2.03	0.58
2:I:60:TYR:CD1	3:J:98:ILE:HG21	2.38	0.58
3:L:40:TYR:HE2	3:L:93:GLN:HG2	1.69	0.58
1:B:811:LEU:HD22	1:B:826:LYS:HZ1	1.69	0.57
2:E:60:TYR:CD1	3:F:98:ILE:HG21	2.38	0.57
1:D:413:TYR:CD1	1:D:769:LEU:HB3	2.39	0.57
1:C:411:PHE:CD1	1:C:610:VAL:HG11	2.39	0.57
3:L:189:GLU:HA	3:L:192:ARG:HG3	1.87	0.57
3:J:41:GLN:HB2	3:J:51:LEU:HD11	1.86	0.57
1:B:696:MET:HB2	1:B:756:VAL:HG22	1.85	0.57
1:D:588:LEU:HD12	1:D:609:GLY:HA2	1.87	0.57
1:A:472:GLU:OE1	1:A:490:ARG:NH1	2.38	0.57
1:B:808:ARG:NH2	1:B:840:GLN:HG3	2.19	0.57
3:L:4:MET:HE1	3:L:93:GLN:HA	1.85	0.57
2:G:177:PRO:O	3:H:166:SER:OG	2.19	0.56
1:A:866:THR:O	1:A:870:ARG:HB2	2.05	0.56
1:B:807:ASP:O	1:B:811:LEU:HG	2.06	0.56
1:D:432:ARG:HH22	1:D:480:GLU:CD	2.14	0.56
2:K:34:ILE:HG23	2:K:99:ARG:HD2	1.87	0.56
2:E:6:GLU:HG3	2:E:97:CYS:HB2	1.87	0.56
2:E:6:GLU:OE2	2:E:114:GLY:HA3	2.06	0.56
1:A:822:VAL:O	1:A:825:VAL:HG22	2.05	0.56
1:B:708:LEU:O	1:B:712:MET:HG2	2.05	0.56
2:K:11:LYS:HG3	2:K:12:LEU:N	2.20	0.56
3:L:197:THR:OG1	3:L:212:SER:OG	2.17	0.56
1:A:492:TRP:CE2	1:A:664:MET:HB2	2.40	0.56
1:B:658:GLU:HG2	2:G:59:LYS:HG2	1.88	0.56
3:H:84:GLU:HA	3:H:110:ILE:CD1	2.35	0.56
1:B:864:ILE:O	1:B:868:PRO:HD2	2.06	0.56
1:B:680:LEU:HD21	1:B:863:LEU:HD23	1.88	0.56
1:D:488:VAL:HG21	1:D:654:GLY:HA2	1.87	0.56
1:D:492:TRP:CE2	1:D:664:MET:HB2	2.41	0.56
3:H:4:MET:HE1	3:H:93:GLN:HA	1.88	0.56
1:A:411:PHE:CD1	1:A:610:VAL:HG11	2.40	0.55
1:D:661:ILE:O	1:D:664:MET:HG2	2.06	0.55
1:B:472:GLU:OE1	1:B:490:ARG:NH1	2.40	0.55
1:C:865:LEU:O	1:C:869:LEU:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:412:ILE:HG13	1:D:734:HIS:HD2	1.70	0.55
1:B:845:ALA:O	1:B:849:VAL:HG23	2.06	0.55
1:C:820:PRO:HG2	1:C:822:VAL:O	2.05	0.55
1:B:853:THR:O	1:B:856:SER:HB3	2.07	0.55
1:C:496:TRP:CE2	1:C:668:ALA:HB2	2.41	0.55
1:D:757:LYS:HB3	1:D:759:GLN:NE2	2.21	0.55
1:B:402:SER:HB2	1:B:405:VAL:HG23	1.89	0.55
3:F:112:ARG:HG2	3:F:113:ALA:N	2.22	0.55
1:A:819:HIS:HA	1:A:826:LYS:HD2	1.89	0.55
1:B:733:THR:HG21	1:B:795:MET:HG2	1.87	0.55
1:A:544:PHE:HZ	1:A:572:LEU:HD23	1.71	0.55
1:C:490:ARG:NH2	1:C:722:PRO:HA	2.21	0.55
2:E:27:PHE:CZ	2:E:99:ARG:HD3	2.42	0.55
1:B:522:GLU:OE1	1:B:805:LEU:N	2.31	0.55
1:C:862:VAL:HA	1:C:865:LEU:HB3	1.87	0.55
2:I:18:LEU:HD23	2:I:84:ILE:HD12	1.89	0.55
1:C:733:THR:HG21	1:C:795:MET:HG2	1.88	0.55
1:C:853:THR:O	1:C:856:SER:HB3	2.07	0.55
1:D:807:ASP:O	1:D:811:LEU:HG	2.07	0.55
3:F:2:ILE:HB	3:F:94:HIS:NE2	2.22	0.55
1:A:496:TRP:CE2	1:A:668:ALA:HB2	2.41	0.54
1:D:737:ALA:CB	1:D:738:LEU:HB2	2.33	0.54
3:J:197:THR:OG1	3:J:212:SER:OG	2.15	0.54
2:K:13:GLN:HB2	2:K:16:GLN:NE2	2.22	0.54
1:A:806:PHE:HA	1:A:809:ILE:HD12	1.88	0.54
1:C:549:LEU:HD22	1:D:569:ASN:HD21	1.72	0.54
1:D:695:LYS:HG2	1:D:755:GLU:HA	1.88	0.54
1:A:658:GLU:HG2	2:E:59:LYS:HD2	1.90	0.54
1:B:490:ARG:NH2	1:B:722:PRO:HA	2.22	0.54
1:C:432:ARG:HG2	3:J:96:TRP:CZ3	2.42	0.54
1:C:432:ARG:HH22	1:C:480:GLU:CD	2.15	0.54
1:D:658:GLU:HG2	2:K:59:LYS:HG2	1.89	0.54
1:D:806:PHE:HA	1:D:809:ILE:HD12	1.88	0.54
2:E:34:ILE:HG23	2:E:99:ARG:HD2	1.88	0.54
1:D:432:ARG:HG2	3:L:96:TRP:CH2	2.42	0.54
2:G:54:TRP:CH2	2:G:60:TYR:HD2	2.26	0.54
1:B:651:HIS:CD2	1:B:653:LEU:HB2	2.43	0.54
1:D:829:LYS:HE2	1:D:878:PHE:CD2	2.42	0.54
1:C:829:LYS:HE2	1:C:878:PHE:CD2	2.42	0.54
2:I:29:LEU:O	2:I:55:TRP:HB2	2.06	0.54
1:A:527:LEU:HD11	1:A:848:TRP:HD1	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:LYS:HE2	1:A:878:PHE:CD2	2.43	0.54
3:F:41:GLN:HB2	3:F:51:LEU:HD11	1.90	0.54
1:A:482:ASN:HB3	2:E:56:SER:OG	2.07	0.54
3:L:84:GLU:HA	3:L:110:ILE:HD13	1.90	0.54
1:A:851:LYS:CE	1:A:859:LEU:HD22	2.34	0.54
1:B:829:LYS:HE2	1:B:878:PHE:CD2	2.42	0.54
1:C:472:GLU:OE1	1:C:490:ARG:NH1	2.40	0.54
3:F:2:ILE:HD12	3:F:94:HIS:CE1	2.42	0.54
2:I:87:VAL:HG12	2:I:121:VAL:HG11	1.89	0.54
1:B:820:PRO:HG2	1:B:822:VAL:O	2.09	0.53
1:D:845:ALA:O	1:D:849:VAL:HG23	2.09	0.53
2:I:126:THR:HG23	2:I:157:PRO:HD3	1.90	0.53
1:B:716:ALA:HB1	1:B:721:MET:HB2	1.90	0.53
1:B:737:ALA:CB	1:B:738:LEU:HB2	2.34	0.53
1:D:657:SER:HB2	1:D:658:GLU:O	2.09	0.53
1:B:851:LYS:HA	1:B:856:SER:HB2	1.91	0.53
1:C:768:VAL:O	1:C:772:LEU:HG	2.08	0.53
1:D:466:GLY:O	1:D:470:VAL:HG23	2.08	0.53
1:D:866:THR:O	1:D:870:ARG:HB2	2.08	0.53
3:J:12:ALA:HA	3:J:109:GLU:O	2.08	0.53
1:C:397:ILE:HG23	1:C:761:ILE:HD11	1.89	0.53
1:A:657:SER:HB2	1:A:658:GLU:C	2.34	0.53
1:A:661:ILE:O	1:A:664:MET:HG2	2.09	0.53
1:D:426:LEU:O	1:D:430:LYS:HG2	2.08	0.53
1:A:651:HIS:CD2	1:A:653:LEU:H	2.27	0.53
1:C:657:SER:HB2	1:C:658:GLU:O	2.08	0.53
3:J:40:TYR:HE2	3:J:93:GLN:CG	2.21	0.53
2:G:18:LEU:HD23	2:G:84:ILE:HD12	1.90	0.53
1:B:773:SER:HA	1:B:776:MET:HG3	1.91	0.53
1:C:773:SER:HA	1:C:776:MET:HG3	1.90	0.53
1:D:490:ARG:NH2	1:D:722:PRO:HA	2.23	0.53
1:D:851:LYS:HB2	1:D:859:LEU:HD13	1.91	0.53
1:B:519:TYR:CD2	1:B:867:VAL:HG13	2.39	0.52
1:C:808:ARG:NH2	1:C:840:GLN:HG3	2.25	0.52
3:H:112:ARG:HG3	3:H:113:ALA:N	2.24	0.52
1:B:440:LEU:HD11	1:B:464:PHE:HB2	1.91	0.52
2:K:18:LEU:HD23	2:K:84:ILE:HD12	1.91	0.52
1:D:412:ILE:HG13	1:D:734:HIS:CD2	2.44	0.52
1:D:716:ALA:HB1	1:D:721:MET:HB2	1.90	0.52
1:A:440:LEU:HD11	1:A:464:PHE:HB2	1.90	0.52
1:B:520:THR:HG22	1:B:867:VAL:HG11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:39:TRP:HB2	3:H:52:ILE:HB	1.92	0.52
1:A:526:PHE:HD2	1:A:844:LEU:HD21	1.74	0.52
1:B:419:PRO:O	1:B:423:PHE:HB2	2.09	0.52
1:C:811:LEU:HD23	1:C:814:LYS:HD2	1.91	0.52
1:D:773:SER:HA	1:D:776:MET:HG3	1.92	0.52
1:D:853:THR:O	1:D:856:SER:HB3	2.10	0.52
3:H:110:ILE:N	3:H:170:GLN:OE1	2.38	0.52
2:I:4:LEU:HD13	2:I:24:PHE:HB3	1.92	0.52
1:A:757:LYS:HB3	1:A:759:GLN:NE2	2.25	0.52
1:C:811:LEU:HD22	1:C:826:LYS:HZ1	1.75	0.52
1:B:657:SER:HB2	1:B:658:GLU:C	2.35	0.52
1:C:832:ARG:HD3	1:C:835:LEU:HD12	1.92	0.52
1:A:597:PHE:HB3	1:A:602:ARG:HB2	1.91	0.51
1:B:878:PHE:HD2	1:B:882:GLU:HB3	1.74	0.51
1:C:552:THR:HB	1:C:553:TYR:HB3	1.93	0.51
1:D:836:PHE:CD2	1:D:886:LEU:HD13	2.45	0.51
2:K:54:TRP:CH2	2:K:60:TYR:HD2	2.28	0.51
1:A:426:LEU:O	1:A:430:LYS:HG2	2.10	0.51
3:J:3:VAL:HB	3:J:26:SER:HB3	1.92	0.51
1:B:811:LEU:HD23	1:B:814:LYS:HD2	1.91	0.51
1:C:551:LYS:O	1:C:552:THR:OG1	2.25	0.51
2:E:162:LEU:HD12	2:E:207:VAL:HG22	1.92	0.51
3:F:40:TYR:HE2	3:F:93:GLN:HG2	1.75	0.51
2:I:6:GLU:HG3	2:I:97:CYS:HB2	1.92	0.51
3:J:52:ILE:CD1	3:J:58:LEU:HG	2.40	0.51
1:A:590:LYS:O	1:A:594:SER:N	2.42	0.51
1:C:443:SER:OG	1:C:447:GLN:NE2	2.43	0.51
1:D:438:SER:OG	1:D:639:LYS:O	2.27	0.51
1:D:696:MET:HB2	1:D:756:VAL:CG2	2.41	0.51
3:H:110:ILE:O	3:H:170:GLN:NE2	2.32	0.51
1:A:520:THR:HG22	1:A:867:VAL:CG1	2.40	0.51
1:B:526:PHE:HD2	1:B:844:LEU:HD21	1.75	0.51
1:B:803:ILE:HG22	1:B:806:PHE:H	1.74	0.51
1:D:803:ILE:HG22	1:D:806:PHE:H	1.74	0.51
1:A:657:SER:HB2	1:A:658:GLU:O	2.10	0.51
1:C:581:THR:HG21	1:C:787:VAL:HG13	1.92	0.51
1:D:811:LEU:HD22	1:D:826:LYS:NZ	2.24	0.51
1:B:739:THR:HG23	1:B:756:VAL:HG12	1.92	0.51
2:E:158:GLU:HG3	2:E:159:PRO:HA	1.92	0.51
1:A:811:LEU:HD22	1:A:826:LYS:HZ1	1.75	0.51
1:C:739:THR:HG23	1:C:756:VAL:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:822:VAL:O	1:C:825:VAL:HG22	2.11	0.51
1:A:524:PHE:CZ	1:A:528:ILE:HD11	2.46	0.51
1:A:691:LYS:HD2	1:A:693:GLU:OE1	2.11	0.51
1:A:739:THR:HG23	1:A:756:VAL:HG12	1.92	0.51
2:E:2:VAL:HG11	2:E:112:TYR:CD1	2.46	0.51
3:L:40:TYR:HE2	3:L:93:GLN:CG	2.24	0.51
1:A:540:LEU:HD22	1:A:578:MET:SD	2.51	0.51
1:D:411:PHE:CD1	1:D:610:VAL:HG11	2.46	0.51
2:E:87:VAL:HG12	2:E:121:VAL:HG11	1.93	0.51
1:B:658:GLU:HG2	2:G:59:LYS:CG	2.41	0.50
1:C:487:ILE:HG13	1:C:650:ILE:HD13	1.93	0.50
1:C:864:ILE:O	1:C:868:PRO:HD2	2.10	0.50
1:D:482:ASN:HB3	2:K:56:SER:OG	2.11	0.50
1:D:520:THR:HG22	1:D:867:VAL:HG11	1.92	0.50
1:C:455:GLY:O	1:C:760:ARG:NH1	2.45	0.50
1:A:689:VAL:HG12	1:A:696:MET:HE1	1.93	0.50
1:A:811:LEU:HD23	1:A:814:LYS:HD2	1.93	0.50
1:D:552:THR:HB	1:D:553:TYR:HB3	1.93	0.50
2:K:109:TYR:CZ	3:L:53:LYS:HD2	2.46	0.50
1:C:651:HIS:CD2	1:C:653:LEU:HB2	2.46	0.50
1:C:657:SER:HB2	1:C:658:GLU:C	2.37	0.50
1:C:661:ILE:O	1:C:664:MET:HG2	2.11	0.50
1:B:432:ARG:HG2	3:H:96:TRP:CZ3	2.47	0.50
1:B:696:MET:HB2	1:B:756:VAL:CG2	2.42	0.50
2:I:206:ASN:ND2	2:I:217:ASP:OD1	2.42	0.50
3:L:58:LEU:HD21	3:L:66:PHE:O	2.12	0.50
1:B:661:ILE:HA	1:B:664:MET:SD	2.52	0.50
1:C:447:GLN:HE22	1:C:724:LEU:HG	1.76	0.50
1:D:472:GLU:OE1	1:D:490:ARG:NH1	2.45	0.50
1:D:492:TRP:CD2	1:D:664:MET:HB2	2.47	0.50
1:C:660:PRO:HD3	2:I:58:SER:HA	1.94	0.50
1:D:820:PRO:HG2	1:D:822:VAL:O	2.12	0.50
1:A:584:PHE:CE2	1:A:616:ILE:HG21	2.46	0.50
1:C:426:LEU:O	1:C:430:LYS:HG2	2.12	0.50
1:C:737:ALA:CB	1:C:738:LEU:HB2	2.35	0.50
1:D:808:ARG:HH22	1:D:840:GLN:HG3	1.77	0.50
1:D:837:THR:O	1:D:840:GLN:HB2	2.12	0.50
1:B:866:THR:O	1:B:870:ARG:HB2	2.12	0.49
2:I:162:LEU:HD12	2:I:207:VAL:HG22	1.94	0.49
1:B:432:ARG:HH22	1:B:480:GLU:CD	2.20	0.49
1:B:551:LYS:O	1:B:552:THR:OG1	2.22	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:812:LEU:HA	1:C:834:HIS:HE1	1.77	0.49
1:D:657:SER:HB2	1:D:658:GLU:C	2.37	0.49
1:D:590:LYS:O	1:D:594:SER:N	2.46	0.49
1:A:634:VAL:HG12	1:A:774:ILE:HD13	1.95	0.49
1:B:492:TRP:CE2	1:B:664:MET:HB2	2.48	0.49
1:D:519:TYR:CD2	1:D:867:VAL:HG13	2.37	0.49
1:A:820:PRO:HG2	1:A:822:VAL:O	2.12	0.49
1:A:839:ILE:O	1:A:842:ILE:HG22	2.13	0.49
1:B:384:ARG:O	1:B:388:ARG:HG3	2.12	0.49
1:B:757:LYS:HB3	1:B:759:GLN:NE2	2.27	0.49
2:E:129:PRO:HB3	2:E:155:TYR:HB3	1.95	0.49
1:C:526:PHE:HD2	1:C:844:LEU:HD21	1.77	0.49
2:I:77:ASN:O	2:I:79:GLN:HG3	2.13	0.49
3:J:121:ILE:HG22	3:J:211:LYS:HE2	1.95	0.49
1:A:397:ILE:HG23	1:A:761:ILE:HD11	1.94	0.49
1:D:768:VAL:O	1:D:772:LEU:HG	2.12	0.49
2:G:34:ILE:HG23	2:G:99:ARG:HD2	1.94	0.49
3:J:117:PRO:HG3	3:J:148:ILE:HD11	1.94	0.49
1:C:651:HIS:CD2	1:C:653:LEU:H	2.31	0.49
1:D:686:THR:O	1:D:690:SER:OG	2.28	0.49
1:A:490:ARG:NH2	1:A:722:PRO:HA	2.28	0.49
1:D:658:GLU:HG2	2:K:59:LYS:CG	2.42	0.49
1:A:808:ARG:NH2	1:A:840:GLN:HG3	2.28	0.48
2:K:13:GLN:HB2	2:K:16:GLN:CD	2.38	0.48
2:K:198:TRP:CG	2:K:199:PRO:HA	2.48	0.48
3:L:84:GLU:HA	3:L:110:ILE:CD1	2.43	0.48
1:C:757:LYS:HB3	1:C:759:GLN:NE2	2.27	0.48
1:D:496:TRP:CE2	1:D:668:ALA:HB2	2.48	0.48
1:A:389:ARG:NH2	1:A:396:ASP:OD2	2.28	0.48
1:A:581:THR:HG21	1:A:787:VAL:HG13	1.95	0.48
1:B:382:LEU:HB2	1:B:703:HIS:HB3	1.95	0.48
1:C:487:ILE:O	1:C:491:VAL:HG23	2.13	0.48
1:D:811:LEU:HD13	1:D:826:LYS:HE3	1.95	0.48
1:B:413:TYR:CE1	1:B:769:LEU:HB3	2.49	0.48
1:A:466:GLY:O	1:A:470:VAL:HG23	2.14	0.48
1:A:864:ILE:O	1:A:868:PRO:HD2	2.14	0.48
1:B:837:THR:O	1:B:840:GLN:HB2	2.13	0.48
1:D:780:LEU:HA	1:D:783:ILE:HD12	1.94	0.48
2:E:181:GLN:O	2:E:181:GLN:HG3	2.14	0.48
1:A:853:THR:O	1:A:856:SER:HB3	2.13	0.48
1:C:786:ALA:O	1:C:789:PHE:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:811:LEU:HD23	1:D:814:LYS:HD2	1.94	0.48
2:E:137:VAL:HG22	3:F:123:PRO:HD3	1.95	0.48
1:C:590:LYS:O	1:C:594:SER:N	2.47	0.48
1:D:447:GLN:HE21	1:D:712:MET:HB2	1.78	0.48
1:D:453:LEU:O	1:D:760:ARG:NH1	2.47	0.48
1:D:865:LEU:O	1:D:869:LEU:HB3	2.14	0.48
2:I:54:TRP:CH2	2:I:60:TYR:HD2	2.31	0.48
2:K:89:THR:HA	2:K:121:VAL:HB	1.95	0.48
1:A:520:THR:CG2	1:A:867:VAL:HG11	2.44	0.48
1:A:865:LEU:O	1:A:869:LEU:HB3	2.13	0.48
1:C:818:TYR:O	1:C:826:LYS:NZ	2.39	0.48
3:F:11:LEU:HG	3:F:13:VAL:HG23	1.95	0.48
2:I:37:GLY:HA3	2:I:52:HIS:CG	2.49	0.48
3:L:110:ILE:O	3:L:170:GLN:NE2	2.43	0.48
1:A:527:LEU:CD1	1:A:848:TRP:HD1	2.27	0.48
1:B:411:PHE:CD1	1:B:610:VAL:HG11	2.48	0.48
1:D:862:VAL:HA	1:D:865:LEU:HB3	1.95	0.48
3:J:214:ASN:HB2	3:J:217:GLU:HB3	1.96	0.48
1:A:737:ALA:CB	1:A:738:LEU:HB2	2.34	0.47
1:A:836:PHE:CD2	1:A:886:LEU:HD13	2.49	0.47
1:A:569:ASN:HD21	1:B:549:LEU:HD22	1.79	0.47
1:C:440:LEU:HD11	1:C:464:PHE:HB2	1.95	0.47
3:F:30:SER:HB3	3:F:35:SER:HA	1.95	0.47
1:A:757:LYS:HB3	1:A:759:GLN:HE22	1.79	0.47
1:A:847:LEU:HD21	1:A:863:LEU:HA	1.97	0.47
1:B:634:VAL:HG12	1:B:774:ILE:HD13	1.96	0.47
1:C:819:HIS:HA	1:C:826:LYS:HD2	1.97	0.47
2:G:109:TYR:CZ	3:H:53:LYS:HD2	2.50	0.47
2:K:129:PRO:HB3	2:K:155:TYR:HB3	1.95	0.47
1:A:544:PHE:CZ	1:A:572:LEU:HD23	2.49	0.47
1:D:808:ARG:HH21	1:D:837:THR:HA	1.79	0.47
2:E:109:TYR:CZ	3:F:53:LYS:HD2	2.50	0.47
1:B:657:SER:HB2	1:B:658:GLU:O	2.14	0.47
1:C:520:THR:HG22	1:C:867:VAL:CG1	2.44	0.47
1:A:519:TYR:CD2	1:A:867:VAL:HG13	2.47	0.47
1:A:818:TYR:C	1:A:826:LYS:HZ3	2.16	0.47
1:B:479:CYS:HA	1:B:484:LEU:HD12	1.97	0.47
4:B:1000:4KU:H11	4:B:1000:4KU:H7	1.43	0.47
1:C:777:GLU:HB3	1:C:778:PRO:HD3	1.96	0.47
1:D:390:TYR:O	1:D:393:TYR:HB3	2.15	0.47
1:D:733:THR:HG21	1:D:795:MET:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:878:PHE:HD2	1:D:882:GLU:HB3	1.79	0.47
3:J:112:ARG:HG2	3:J:113:ALA:N	2.30	0.47
1:A:588:LEU:HD12	1:A:609:GLY:HA2	1.96	0.47
1:B:392:TYR:O	1:B:395:SER:OG	2.22	0.47
1:B:404:GLN:HG2	1:B:738:LEU:H	1.80	0.47
1:B:865:LEU:O	1:B:869:LEU:HB3	2.15	0.47
1:C:519:TYR:CD2	1:C:867:VAL:HG13	2.47	0.47
3:F:116:ALA:HA	3:F:204:THR:HG21	1.97	0.47
2:I:13:GLN:HB2	2:I:16:GLN:CD	2.40	0.47
2:I:92:THR:HG23	2:I:120:THR:HA	1.97	0.47
2:K:153:LYS:HG2	2:K:154:GLY:N	2.30	0.47
3:F:4:MET:HB2	3:F:4:MET:HE3	1.58	0.47
3:J:39:TRP:CZ3	3:J:92:CYS:HB3	2.49	0.47
1:C:597:PHE:HB3	1:C:602:ARG:HB2	1.95	0.47
2:K:41:GLN:HG3	2:K:46:GLY:O	2.15	0.47
1:A:686:THR:O	1:A:690:SER:OG	2.33	0.46
1:B:812:LEU:HA	1:B:834:HIS:CE1	2.50	0.46
3:F:189:GLU:HA	3:F:192:ARG:HG3	1.97	0.46
1:A:443:SER:O	1:A:447:GLN:HB2	2.16	0.46
1:B:780:LEU:HA	1:B:783:ILE:HD12	1.97	0.46
1:C:630:GLN:HB3	1:C:785:LEU:HD12	1.97	0.46
1:A:678:ILE:HG12	1:A:725:SER:HB3	1.95	0.46
1:C:402:SER:HB2	1:C:405:VAL:HG23	1.98	0.46
1:C:432:ARG:O	1:C:433:ASN:HB2	2.15	0.46
1:C:485:GLU:OE2	1:C:655:LEU:HB2	2.14	0.46
3:H:40:TYR:HE2	3:H:93:GLN:HG2	1.80	0.46
3:J:112:ARG:NH1	3:J:174:ASP:HB2	2.26	0.46
1:B:538:SER:HA	1:B:541:ILE:HG22	1.98	0.46
1:D:715:VAL:O	1:D:719:PHE:HD1	1.97	0.46
2:I:131:VAL:HB	2:I:216:VAL:HG11	1.98	0.46
1:A:863:LEU:O	1:A:867:VAL:HG23	2.16	0.46
1:C:839:ILE:O	1:C:842:ILE:HG22	2.16	0.46
1:D:547:HIS:ND1	1:D:567:LEU:HA	2.30	0.46
2:E:77:ASN:O	2:E:79:GLN:HG3	2.16	0.46
2:G:179:VAL:HG21	3:H:165:ASN:O	2.15	0.46
2:I:5:GLN:O	2:I:22:CYS:HA	2.14	0.46
1:B:808:ARG:HH22	1:B:840:GLN:HG3	1.80	0.46
1:C:878:PHE:HD2	1:C:882:GLU:HB3	1.80	0.46
1:D:513:VAL:HG11	1:D:702:PHE:CE2	2.50	0.46
2:G:11:LYS:HB2	2:G:157:PRO:HG3	1.97	0.46
3:J:29:VAL:HG21	3:J:94:HIS:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:164:LEU:O	3:H:164:LEU:HD12	2.16	0.46
1:A:768:VAL:O	1:A:772:LEU:HG	2.16	0.46
1:D:487:ILE:HG13	1:D:650:ILE:HD13	1.98	0.46
2:G:102:TYR:CZ	2:G:106:GLY:HA2	2.51	0.46
1:B:862:VAL:HA	1:B:865:LEU:HB3	1.97	0.46
1:D:584:PHE:CE2	1:D:616:ILE:HG21	2.51	0.46
1:D:777:GLU:HB3	1:D:778:PRO:HD3	1.97	0.46
2:K:53:ILE:HD12	2:K:59:LYS:HE2	1.98	0.46
1:B:872:VAL:O	1:B:875:PRO:HD2	2.15	0.45
2:K:101:TYR:O	2:K:108:TYR:HA	2.16	0.45
1:A:812:LEU:HA	1:A:834:HIS:HE1	1.78	0.45
1:A:851:LYS:HA	1:A:856:SER:HB2	1.98	0.45
1:B:513:VAL:HG11	1:B:702:PHE:CE2	2.51	0.45
1:C:414:PHE:CE1	1:C:783:ILE:HD13	2.51	0.45
3:J:7:SER:HB2	3:J:8:PRO:HA	1.97	0.45
3:L:51:LEU:HA	3:L:62:VAL:HG21	1.98	0.45
1:A:440:LEU:HA	1:A:722:PRO:HG3	1.97	0.45
1:A:738:LEU:O	1:A:756:VAL:HB	2.16	0.45
1:A:873:LEU:O	1:A:876:LEU:HB3	2.17	0.45
1:B:768:VAL:O	1:B:772:LEU:HG	2.16	0.45
1:B:808:ARG:HH21	1:B:837:THR:HA	1.80	0.45
1:B:835:LEU:O	1:B:839:ILE:HG13	2.17	0.45
1:C:738:LEU:O	1:C:756:VAL:HB	2.15	0.45
1:D:419:PRO:O	1:D:423:PHE:HB2	2.15	0.45
2:E:4:LEU:HD13	2:E:24:PHE:HB3	1.98	0.45
3:L:93:GLN:HB3	3:L:102:PHE:CD2	2.51	0.45
1:A:845:ALA:O	1:A:849:VAL:HG23	2.17	0.45
1:B:757:LYS:HB3	1:B:759:GLN:HE22	1.80	0.45
1:D:526:PHE:HD2	1:D:844:LEU:HD21	1.80	0.45
2:G:129:PRO:HB3	2:G:155:TYR:HB3	1.98	0.45
2:I:3:LYS:HA	2:I:3:LYS:HD3	1.79	0.45
3:J:129:LEU:O	3:J:187:LYS:HD2	2.16	0.45
1:A:412:ILE:HA	1:A:415:ALA:HB3	1.97	0.45
1:A:651:HIS:HA	1:A:652:PRO:HD2	1.82	0.45
1:A:439:GLU:OE2	1:A:640:VAL:HG13	2.17	0.45
1:A:596:TYR:O	1:A:602:ARG:HD2	2.17	0.45
1:B:485:GLU:OE2	1:B:655:LEU:HB2	2.17	0.45
1:C:849:VAL:O	1:C:852:SER:HB3	2.17	0.45
1:D:384:ARG:O	1:D:388:ARG:HG3	2.15	0.45
3:J:51:LEU:HA	3:J:62:VAL:HG21	1.99	0.45
3:L:164:LEU:HD12	3:L:164:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:VAL:O	1:B:719:PHE:HD1	2.00	0.45
1:C:439:GLU:OE2	1:C:640:VAL:HG13	2.17	0.45
3:J:2:ILE:HD12	3:J:94:HIS:CE1	2.52	0.45
1:A:849:VAL:O	1:A:852:SER:HB3	2.17	0.45
1:B:822:VAL:O	1:B:825:VAL:HG22	2.16	0.45
1:C:629:THR:HB	1:C:631:LYS:HE2	1.99	0.45
1:C:695:LYS:HB3	1:C:755:GLU:HA	1.98	0.45
1:C:845:ALA:O	1:C:849:VAL:HG23	2.16	0.45
1:D:468:LEU:O	1:D:472:GLU:HG2	2.17	0.45
1:D:842:ILE:O	1:D:846:VAL:HG23	2.17	0.45
4:D:1000:4KU:H7	4:D:1000:4KU:H11	1.45	0.45
2:I:69:LEU:CD2	2:I:84:ILE:HG12	2.47	0.45
1:A:733:THR:HG21	1:A:795:MET:HG2	1.99	0.45
1:B:482:ASN:HB3	2:G:56:SER:OG	2.17	0.45
1:B:839:ILE:O	1:B:842:ILE:HG22	2.17	0.45
1:B:877:ILE:HD13	1:B:877:ILE:HA	1.81	0.45
1:C:870:ARG:O	1:C:874:LEU:N	2.50	0.45
2:I:162:LEU:HA	2:I:206:ASN:O	2.16	0.45
1:A:878:PHE:HD2	1:A:882:GLU:HB3	1.82	0.44
1:C:696:MET:HB2	1:C:756:VAL:HG22	1.97	0.44
1:D:487:ILE:O	1:D:491:VAL:HG23	2.16	0.44
2:I:38:TRP:CD1	2:I:82:LEU:HB2	2.52	0.44
3:L:39:TRP:HB2	3:L:52:ILE:HB	1.99	0.44
1:D:765:LEU:O	1:D:769:LEU:HB2	2.17	0.44
3:J:119:VAL:HA	3:J:139:PHE:O	2.18	0.44
3:J:191:GLU:HA	3:J:215:ARG:CD	2.47	0.44
1:A:658:GLU:HG2	2:E:59:LYS:CG	2.47	0.44
1:A:808:ARG:HH21	1:A:837:THR:HA	1.83	0.44
3:H:116:ALA:HA	3:H:204:THR:HG21	1.98	0.44
1:A:389:ARG:HA	1:A:389:ARG:HD2	1.74	0.44
1:A:551:LYS:HB3	1:A:551:LYS:HE2	1.65	0.44
1:B:583:PHE:HD2	1:B:584:PHE:HD1	1.64	0.44
1:B:727:THR:HG21	1:B:730:ARG:NH2	2.32	0.44
1:C:524:PHE:CZ	1:C:528:ILE:HD11	2.52	0.44
1:D:494:GLY:O	1:D:498:ILE:HG13	2.16	0.44
1:A:382:LEU:HA	1:A:703:HIS:ND1	2.32	0.44
1:A:455:GLY:O	1:A:760:ARG:NH1	2.50	0.44
1:A:777:GLU:HB3	1:A:778:PRO:HD3	1.98	0.44
1:A:780:LEU:HA	1:A:783:ILE:HD12	2.00	0.44
1:D:404:GLN:HG2	1:D:738:LEU:H	1.82	0.44
1:D:443:SER:HB2	1:D:721:MET:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:651:HIS:CD2	1:D:653:LEU:HB2	2.52	0.44
2:E:69:LEU:HD22	2:E:82:LEU:HD11	2.00	0.44
3:F:121:ILE:HG22	3:F:211:LYS:HE2	2.00	0.44
2:G:29:LEU:O	2:G:55:TRP:HB2	2.18	0.44
1:B:458:PRO:HB3	1:B:760:ARG:HD3	2.00	0.44
2:G:41:GLN:HG3	2:G:46:GLY:O	2.17	0.44
2:K:11:LYS:HB3	2:K:157:PRO:HG3	1.98	0.44
2:K:109:TYR:HB3	3:L:38:ASN:ND2	2.32	0.44
2:K:153:LYS:HG2	2:K:154:GLY:H	1.82	0.44
1:B:485:GLU:CD	1:B:656:ARG:H	2.25	0.44
1:B:695:LYS:HG2	1:B:755:GLU:HA	2.00	0.44
1:B:777:GLU:HB3	1:B:778:PRO:HD3	1.99	0.44
1:B:849:VAL:O	1:B:852:SER:HB3	2.18	0.44
1:B:853:THR:HB	1:B:855:ALA:HB3	2.00	0.44
1:C:551:LYS:HB3	1:C:551:LYS:HE2	1.67	0.44
1:C:740:VAL:HB	1:C:754:GLN:HB3	2.00	0.44
1:D:634:VAL:HG12	1:D:774:ILE:HD13	1.99	0.44
1:D:691:LYS:HE2	1:D:694:ARG:HE	1.82	0.44
1:C:877:ILE:HD13	1:C:877:ILE:HA	1.82	0.44
1:D:822:VAL:O	1:D:825:VAL:HG22	2.17	0.44
2:G:198:TRP:CG	2:G:199:PRO:HA	2.52	0.44
2:I:14:PRO:HD3	2:I:122:SER:C	2.43	0.44
2:K:105:TYR:HB2	3:L:54:TYR:CE1	2.53	0.44
1:A:414:PHE:CE1	1:A:783:ILE:HD13	2.52	0.44
1:C:678:ILE:HG12	1:C:725:SER:HB3	1.99	0.44
1:D:551:LYS:O	1:D:552:THR:OG1	2.26	0.44
3:F:165:ASN:HA	3:F:180:SER:O	2.18	0.44
3:F:190:TYR:CZ	3:F:215:ARG:HG3	2.53	0.44
2:I:41:GLN:HG3	2:I:46:GLY:O	2.17	0.44
1:D:389:ARG:HG3	1:D:760:ARG:NH2	2.33	0.43
1:D:839:ILE:O	1:D:842:ILE:HG22	2.18	0.43
3:J:116:ALA:HA	3:J:204:THR:HG21	2.00	0.43
1:B:447:GLN:HE21	1:B:712:MET:HB2	1.83	0.43
1:B:552:THR:HB	1:B:553:TYR:HB3	1.99	0.43
2:G:153:LYS:HG2	2:G:154:GLY:N	2.33	0.43
3:J:13:VAL:CG1	3:J:17:GLN:HB3	2.48	0.43
3:J:29:VAL:CG2	3:J:96:TRP:HB2	2.45	0.43
1:B:487:ILE:O	1:B:491:VAL:HG23	2.17	0.43
1:A:581:THR:OG1	1:A:617:MET:HG3	2.18	0.43
1:A:660:PRO:HD3	2:E:58:SER:HA	1.99	0.43
1:A:661:ILE:HG13	1:A:664:MET:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:ALA:HA	1:C:730:ARG:HD3	2.00	0.43
1:A:487:ILE:O	1:A:491:VAL:HG23	2.18	0.43
1:A:735:ALA:C	1:A:737:ALA:H	2.25	0.43
1:D:551:LYS:HE2	1:D:551:LYS:HB3	1.64	0.43
1:A:820:PRO:HD3	1:A:826:LYS:CD	2.46	0.43
1:B:510:SER:O	1:B:513:VAL:HB	2.18	0.43
1:B:872:VAL:C	1:B:875:PRO:HD2	2.43	0.43
1:C:658:GLU:HG2	2:I:59:LYS:HD2	2.00	0.43
1:D:443:SER:O	1:D:447:GLN:HB2	2.19	0.43
2:E:34:ILE:CG2	2:E:99:ARG:HD2	2.49	0.43
2:E:109:TYR:HB3	3:F:38:ASN:ND2	2.33	0.43
2:E:158:GLU:HG3	2:E:159:PRO:CA	2.49	0.43
3:F:129:LEU:O	3:F:187:LYS:HD2	2.19	0.43
2:K:181:GLN:O	2:K:181:GLN:HG3	2.19	0.43
1:A:429:GLU:OE2	3:F:32:SER:HB3	2.18	0.43
1:A:547:HIS:ND1	1:A:567:LEU:HA	2.34	0.43
1:C:753:ILE:HD12	1:C:753:ILE:N	2.33	0.43
2:G:18:LEU:HD13	2:G:119:LEU:HD13	2.01	0.43
2:I:137:VAL:HG22	3:J:123:PRO:HD3	2.00	0.43
2:K:29:LEU:O	2:K:55:TRP:HB2	2.19	0.43
1:A:715:VAL:O	1:A:718:LEU:HB3	2.19	0.43
1:B:389:ARG:HG3	1:B:760:ARG:NH2	2.34	0.43
3:F:40:TYR:HE2	3:F:93:GLN:CG	2.31	0.43
2:G:89:THR:HA	2:G:121:VAL:HB	2.00	0.43
3:H:153:LYS:HB2	3:H:197:THR:HB	2.01	0.43
1:A:837:THR:O	1:A:840:GLN:HB2	2.19	0.43
1:A:853:THR:HB	1:A:855:ALA:HB3	2.00	0.43
1:B:851:LYS:HB2	1:B:859:LEU:HD13	2.01	0.43
1:C:806:PHE:HA	1:C:809:ILE:HD12	2.00	0.43
1:D:413:TYR:CE1	1:D:769:LEU:HB3	2.54	0.43
1:D:740:VAL:HB	1:D:754:GLN:HB3	2.01	0.43
2:G:153:LYS:HG2	2:G:154:GLY:H	1.84	0.43
3:H:117:PRO:HG3	3:H:148:ILE:HD11	2.01	0.43
1:B:429:GLU:OE1	3:H:31:THR:HB	2.19	0.43
1:A:484:LEU:HD13	1:A:663:MET:HG2	2.01	0.42
1:B:496:TRP:CE2	1:B:668:ALA:HB2	2.54	0.42
2:E:198:TRP:CG	2:E:199:PRO:HA	2.53	0.42
3:F:20:THR:HG22	3:F:78:ASN:OD1	2.18	0.42
3:F:191:GLU:HA	3:F:215:ARG:CD	2.49	0.42
2:I:198:TRP:CG	2:I:199:PRO:HA	2.53	0.42
3:L:40:TYR:CE2	3:L:93:GLN:HG2	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:812:LEU:HD22	1:A:834:HIS:ND1	2.34	0.42
1:B:487:ILE:HD11	1:B:720:GLY:HA2	2.00	0.42
1:D:526:PHE:CE1	1:D:800:LEU:HD11	2.54	0.42
3:L:112:ARG:HG3	3:L:113:ALA:N	2.34	0.42
1:B:754:GLN:HG3	1:B:755:GLU:OE1	2.19	0.42
3:F:62:VAL:HA	3:F:63:PRO:HD3	1.84	0.42
2:I:6:GLU:OE2	2:I:114:GLY:HA3	2.19	0.42
2:I:60:TYR:CD2	3:J:98:ILE:HG12	2.53	0.42
2:I:209:HIS:CE1	2:I:211:ALA:HB3	2.53	0.42
1:A:432:ARG:HG2	3:F:96:TRP:CZ3	2.54	0.42
1:A:482:ASN:HB3	2:E:56:SER:HG	1.82	0.42
1:C:405:VAL:HG22	1:C:759:GLN:NE2	2.34	0.42
2:E:22:CYS:HB2	2:E:38:TRP:CZ2	2.55	0.42
2:G:109:TYR:HB3	3:H:38:ASN:ND2	2.34	0.42
1:D:440:LEU:HD11	1:D:464:PHE:HB2	2.00	0.42
1:D:597:PHE:HB3	1:D:602:ARG:HB2	2.01	0.42
1:D:651:HIS:NE2	1:D:653:LEU:HB2	2.35	0.42
3:F:43:LYS:HE2	3:F:85:GLU:O	2.18	0.42
1:A:678:ILE:HG21	1:A:710:VAL:HG22	2.01	0.42
1:B:812:LEU:HD22	1:B:834:HIS:ND1	2.35	0.42
1:C:660:PRO:HG3	2:I:58:SER:HB2	2.02	0.42
2:I:113:TRP:CE3	3:J:48:PRO:HD2	2.55	0.42
1:A:487:ILE:HD11	1:A:720:GLY:HA2	2.02	0.42
1:A:862:VAL:HA	1:A:865:LEU:HB3	2.01	0.42
1:B:494:GLY:O	1:B:498:ILE:HG13	2.19	0.42
1:B:622:PHE:HD1	1:B:623:PHE:CD1	2.38	0.42
2:K:18:LEU:HD13	2:K:119:LEU:HD13	2.01	0.42
2:K:37:GLY:HA3	2:K:52:HIS:CG	2.55	0.42
1:A:458:PRO:HB3	1:A:760:ARG:HD3	2.02	0.42
1:B:432:ARG:HG2	3:H:96:TRP:CH2	2.54	0.42
1:C:510:SER:O	1:C:513:VAL:HB	2.20	0.42
1:D:629:THR:HB	1:D:631:LYS:HE2	2.01	0.42
3:H:52:ILE:HD13	3:H:58:LEU:HA	2.02	0.42
1:A:665:PHE:HD1	1:A:665:PHE:HA	1.71	0.42
1:C:820:PRO:HD3	1:C:826:LYS:CD	2.48	0.42
3:F:93:GLN:HE21	3:F:93:GLN:HB2	1.61	0.42
3:J:40:TYR:CE2	3:J:93:GLN:HG2	2.50	0.42
1:A:485:GLU:OE2	1:A:655:LEU:HB2	2.19	0.42
1:A:616:ILE:O	1:A:620:VAL:HG23	2.20	0.42
1:B:804:GLN:HG2	1:B:808:ARG:HH11	1.85	0.42
1:C:432:ARG:HG2	3:J:96:TRP:CH2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:678:ILE:HG21	1:C:710:VAL:HG22	2.00	0.42
1:D:389:ARG:HD2	1:D:389:ARG:HA	1.72	0.42
1:D:870:ARG:O	1:D:874:LEU:N	2.53	0.42
3:F:93:GLN:HB3	3:F:102:PHE:CD2	2.55	0.42
2:I:157:PRO:HD2	2:I:211:ALA:CB	2.50	0.42
2:I:221:GLU:HA	2:I:222:PRO:HD3	1.92	0.42
3:L:214:ASN:HB2	3:L:217:GLU:HB3	2.02	0.42
1:A:382:LEU:HB2	1:A:703:HIS:HB3	2.02	0.41
1:B:870:ARG:O	1:B:874:LEU:N	2.53	0.41
1:B:382:LEU:HA	1:B:703:HIS:ND1	2.35	0.41
1:C:466:GLY:O	1:C:470:VAL:HG23	2.20	0.41
1:C:836:PHE:CD2	1:C:886:LEU:HD13	2.55	0.41
2:I:181:GLN:O	2:I:181:GLN:HG3	2.20	0.41
3:L:24:ARG:HA	3:L:73:THR:O	2.20	0.41
1:A:450:LEU:HD23	1:A:450:LEU:HA	1.86	0.41
1:C:510:SER:HG	1:C:703:HIS:HE2	1.67	0.41
2:G:126:THR:HG22	2:G:157:PRO:HD3	2.02	0.41
1:C:520:THR:CG2	1:C:867:VAL:HG11	2.49	0.41
2:I:153:LYS:NZ	3:J:184:THR:HG21	2.35	0.41
1:B:492:TRP:CD2	1:B:664:MET:HB2	2.55	0.41
1:B:678:ILE:HG21	1:B:710:VAL:HG22	2.02	0.41
1:C:810:LEU:HB3	1:C:814:LYS:HE2	2.01	0.41
1:D:584:PHE:HE2	1:D:616:ILE:HG21	1.85	0.41
1:D:851:LYS:HE2	4:D:1000:4KU:H2	1.73	0.41
3:L:116:ALA:HA	3:L:204:THR:HG21	2.02	0.41
1:A:413:TYR:CE1	1:A:769:LEU:HB3	2.56	0.41
1:A:653:LEU:HA	1:A:653:LEU:HD13	1.66	0.41
1:B:487:ILE:HG13	1:B:650:ILE:HD13	2.03	0.41
1:B:524:PHE:CZ	1:B:528:ILE:HD11	2.55	0.41
1:B:851:LYS:HE2	4:B:1000:4KU:H2	1.77	0.41
3:H:40:TYR:HE2	3:H:93:GLN:CG	2.33	0.41
3:H:93:GLN:HB3	3:H:102:PHE:CD2	2.56	0.41
1:B:526:PHE:CE1	1:B:800:LEU:HD11	2.55	0.41
1:C:457:GLN:HG3	1:C:460:LEU:HG	2.02	0.41
1:D:583:PHE:HD2	1:D:584:PHE:HD1	1.67	0.41
2:I:105:TYR:HD2	3:J:54:TYR:CE2	2.39	0.41
2:I:109:TYR:CZ	3:J:53:LYS:HD2	2.56	0.41
1:A:870:ARG:O	1:A:874:LEU:N	2.53	0.41
1:B:390:TYR:O	1:B:393:TYR:HB3	2.21	0.41
1:B:765:LEU:O	1:B:769:LEU:HB2	2.21	0.41
1:B:820:PRO:HD3	1:B:826:LYS:CD	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:583:PHE:HD2	1:C:584:PHE:HD1	1.68	0.41
1:C:808:ARG:HH21	1:C:837:THR:HA	1.86	0.41
1:D:393:TYR:HD1	1:D:760:ARG:NE	2.18	0.41
1:D:439:GLU:OE2	1:D:640:VAL:HG13	2.19	0.41
2:E:105:TYR:HB2	3:F:54:TYR:CE1	2.56	0.41
1:B:438:SER:OG	1:B:639:LYS:O	2.33	0.41
1:C:715:VAL:O	1:C:718:LEU:HB3	2.21	0.41
1:D:432:ARG:NH2	1:D:480:GLU:OE1	2.53	0.41
1:D:518:ARG:HB3	1:D:887:ASP:HB2	2.03	0.41
1:D:661:ILE:HA	1:D:664:MET:SD	2.61	0.41
1:D:812:LEU:HD22	1:D:834:HIS:ND1	2.36	0.41
1:D:849:VAL:O	1:D:852:SER:HB3	2.21	0.41
3:J:16:GLY:HA2	3:J:81:PRO:HB2	2.03	0.41
2:K:22:CYS:HB2	2:K:38:TRP:CZ2	2.56	0.41
1:A:583:PHE:HD2	1:A:584:PHE:HD1	1.68	0.41
1:A:872:VAL:C	1:A:875:PRO:HD2	2.46	0.41
1:B:389:ARG:HD2	1:B:389:ARG:HA	1.73	0.41
1:B:463:GLY:HA2	1:B:724:LEU:HD13	2.02	0.41
1:B:691:LYS:HE2	1:B:694:ARG:HE	1.86	0.41
1:C:807:ASP:O	1:C:811:LEU:HG	2.20	0.41
4:C:1000:4KU:SAG	4:C:1000:4KU:H6	2.61	0.41
1:D:494:GLY:O	1:D:497:LEU:HB2	2.21	0.41
1:D:524:PHE:CZ	1:D:528:ILE:HD11	2.56	0.41
1:A:675:PHE:HD2	1:A:676:ILE:HD13	1.85	0.40
4:C:1000:4KU:H11	4:C:1000:4KU:H7	1.49	0.40
2:E:18:LEU:HD23	2:E:84:ILE:HD12	2.03	0.40
3:F:40:TYR:CE2	3:F:93:GLN:HG2	2.56	0.40
2:K:77:ASN:O	2:K:79:GLN:HG3	2.21	0.40
1:A:635:PRO:HG2	1:A:774:ILE:HD11	2.03	0.40
1:C:393:TYR:HD1	1:C:760:ARG:NE	2.19	0.40
1:C:476:PHE:CD1	1:C:476:PHE:C	2.99	0.40
1:C:735:ALA:C	1:C:737:ALA:H	2.29	0.40
1:C:811:LEU:HD22	1:C:826:LYS:NZ	2.37	0.40
1:C:872:VAL:C	1:C:875:PRO:HD2	2.46	0.40
1:D:808:ARG:HH22	1:D:840:GLN:NE2	2.19	0.40
1:A:551:LYS:O	1:A:552:THR:OG1	2.30	0.40
1:A:683:GLN:OE1	1:A:702:PHE:HD2	2.05	0.40
1:A:695:LYS:HB3	1:A:755:GLU:HA	2.03	0.40
1:B:740:VAL:HB	1:B:754:GLN:HB3	2.03	0.40
1:C:510:SER:HG	1:C:703:HIS:CD2	2.38	0.40
1:C:527:LEU:HD11	1:C:848:TRP:HD1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:815:PRO:HG2	1:D:818:TYR:HD2	1.86	0.40
1:A:696:MET:HB2	1:A:756:VAL:HG22	2.02	0.40
1:C:468:LEU:O	1:C:472:GLU:HG2	2.20	0.40
1:D:393:TYR:HD1	1:D:760:ARG:CZ	2.34	0.40
1:D:539:LYS:O	1:D:542:LYS:HB3	2.22	0.40
2:E:3:LYS:HB2	2:E:25:SER:OG	2.22	0.40
1:A:447:GLN:HE21	1:A:712:MET:HB2	1.87	0.40
1:A:484:LEU:HD21	2:E:56:SER:HB3	2.03	0.40
1:B:651:HIS:HA	1:B:652:PRO:HD2	1.94	0.40
1:C:634:VAL:HG12	1:C:774:ILE:HD13	2.03	0.40
1:D:628:TYR:OH	1:D:630:GLN:HG2	2.21	0.40
1:D:874:LEU:HD23	1:D:874:LEU:HA	1.92	0.40
2:E:29:LEU:O	2:E:55:TRP:HB2	2.22	0.40
2:E:221:GLU:HA	2:E:222:PRO:HD3	1.86	0.40
2:G:99:ARG:HG3	2:G:100:ALA:N	2.36	0.40
3:H:121:ILE:HG22	3:H:211:LYS:HE2	2.03	0.40

There are no symmetry-related clashes.

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	467/911 (51%)	435 (93%)	31 (7%)	1 (0%)	43	74
1	B	467/911 (51%)	436 (93%)	30 (6%)	1 (0%)	43	74
1	C	467/911 (51%)	436 (93%)	30 (6%)	1 (0%)	43	74
1	D	467/911 (51%)	436 (93%)	30 (6%)	1 (0%)	43	74
2	E	221/223 (99%)	211 (96%)	7 (3%)	3 (1%)	9	38
2	G	221/223 (99%)	214 (97%)	7 (3%)	0	100	100
2	I	221/223 (99%)	212 (96%)	6 (3%)	3 (1%)	9	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	221/223 (99%)	213 (96%)	8 (4%)	0	100	100
3	F	216/218 (99%)	208 (96%)	8 (4%)	0	100	100
3	H	216/218 (99%)	209 (97%)	7 (3%)	0	100	100
3	J	216/218 (99%)	209 (97%)	7 (3%)	0	100	100
3	L	216/218 (99%)	211 (98%)	5 (2%)	0	100	100
All	All	3616/5408 (67%)	3430 (95%)	176 (5%)	10 (0%)	36	67

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	166	SER
2	I	166	SER
2	E	159	PRO
2	I	159	PRO
2	E	210	PRO
2	I	210	PRO
1	B	598	PRO
1	C	598	PRO
1	A	598	PRO
1	D	598	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	417/786 (53%)	396 (95%)	21 (5%)	22	48
1	B	417/786 (53%)	399 (96%)	18 (4%)	26	51
1	C	417/786 (53%)	398 (95%)	19 (5%)	24	50
1	D	417/786 (53%)	399 (96%)	18 (4%)	26	51
2	E	190/190 (100%)	184 (97%)	6 (3%)	34	59
2	G	190/190 (100%)	185 (97%)	5 (3%)	40	62
2	I	190/190 (100%)	184 (97%)	6 (3%)	34	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	190/190 (100%)	185 (97%)	5 (3%)	40	62
3	F	193/193 (100%)	188 (97%)	5 (3%)	40	62
3	H	193/193 (100%)	189 (98%)	4 (2%)	47	66
3	J	193/193 (100%)	188 (97%)	5 (3%)	40	62
3	L	193/193 (100%)	189 (98%)	4 (2%)	47	66
All	All	3200/4676 (68%)	3084 (96%)	116 (4%)	31	57

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	382	LEU
1	A	383	VAL
1	A	426	LEU
1	A	490	ARG
1	A	501	VAL
1	A	503	LEU
1	A	551	LYS
1	A	581	THR
1	A	588	LEU
1	A	597	PHE
1	A	633	SER
1	A	653	LEU
1	A	669	LEU
1	A	730	ARG
1	A	769	LEU
1	A	775	LEU
1	A	798	THR
1	A	841	ILE
1	A	844	LEU
1	A	866	THR
1	A	877	ILE
1	B	382	LEU
1	B	383	VAL
1	B	397	ILE
1	B	426	LEU
1	B	490	ARG
1	B	501	VAL
1	B	503	LEU
1	B	551	LYS
1	B	588	LEU

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Mol	Chain	Res	Type
1	B	597	PHE
1	B	653	LEU
1	B	669	LEU
1	B	769	LEU
1	B	798	THR
1	B	841	ILE
1	B	844	LEU
1	B	853	THR
1	B	877	ILE
1	C	382	LEU
1	C	383	VAL
1	C	426	LEU
1	C	490	ARG
1	C	501	VAL
1	C	503	LEU
1	C	512	LEU
1	C	551	LYS
1	C	581	THR
1	C	588	LEU
1	C	597	PHE
1	C	653	LEU
1	C	669	LEU
1	C	775	LEU
1	C	798	THR
1	C	841	ILE
1	C	844	LEU
1	C	866	THR
1	C	877	ILE
1	D	382	LEU
1	D	383	VAL
1	D	397	ILE
1	D	490	ARG
1	D	501	VAL
1	D	503	LEU
1	D	512	LEU
1	D	551	LYS
1	D	581	THR
1	D	588	LEU
1	D	597	PHE
1	D	653	LEU
1	D	669	LEU
1	D	769	LEU

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Mol	Chain	Res	Type
1	D	798	THR
1	D	841	ILE
1	D	844	LEU
1	D	877	ILE
2	E	11	LYS
2	E	34	ILE
2	E	63	THR
2	E	160	VAL
2	E	203	ILE
2	E	222	PRO
3	F	58	LEU
3	F	93	GLN
3	F	110	ILE
3	F	168	THR
3	F	210	VAL
2	G	34	ILE
2	G	63	THR
2	G	126	THR
2	G	160	VAL
2	G	203	ILE
3	H	58	LEU
3	H	93	GLN
3	H	168	THR
3	H	210	VAL
2	I	11	LYS
2	I	34	ILE
2	I	63	THR
2	I	160	VAL
2	I	203	ILE
2	I	222	PRO
3	J	58	LEU
3	J	93	GLN
3	J	110	ILE
3	J	168	THR
3	J	210	VAL
2	K	11	LYS
2	K	34	ILE
2	K	63	THR
2	K	160	VAL
2	K	203	ILE
3	L	58	LEU
3	L	93	GLN

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Mol	Chain	Res	Type
3	L	168	THR
3	L	210	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	545	GLN
1	A	651	HIS
1	A	834	HIS
1	B	569	ASN
1	B	651	HIS
1	B	834	HIS
1	B	840	GLN
1	C	447	GLN
1	C	651	HIS
1	C	834	HIS
1	D	569	ASN
1	D	834	HIS
1	D	840	GLN
3	F	38	ASN
3	F	80	HIS
3	F	93	GLN
3	F	142	ASN
3	F	149	ASN
2	G	41	GLN
2	G	79	GLN
2	G	115	GLN
3	H	38	ASN
3	H	42	GLN
3	H	57	ASN
3	H	80	HIS
3	H	93	GLN
3	H	142	ASN
3	H	149	ASN
2	I	79	GLN
2	I	174	HIS
3	J	80	HIS
2	K	13	GLN
2	K	16	GLN
2	K	79	GLN
3	L	38	ASN
3	L	41	GLN

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Mol	Chain	Res	Type
3	L	57	ASN
3	L	80	HIS
3	L	93	GLN
3	L	149	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
4	4KU	D	1000	1	29,29,29	1.74	3 (10%)	36,42,42	2.58	14 (38%)
4	4KU	B	1000	1	29,29,29	1.72	4 (13%)	36,42,42	2.78	14 (38%)
4	4KU	C	1000	1	29,29,29	1.71	4 (13%)	36,42,42	2.77	14 (38%)
4	4KU	A	1000	1	29,29,29	1.75	4 (13%)	36,42,42	3.24	16 (44%)

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
4	4KU	D	1000	1	-	6/21/23/23	0/2/2/2
4	4KU	B	1000	1	-	7/21/23/23	0/2/2/2
4	4KU	C	1000	1	-	6/21/23/23	0/2/2/2
4	4KU	A	1000	1	-	2/21/23/23	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1000	4KU	CAI-SAG	-6.35	1.66	1.81
4	D	1000	4KU	CAI-SAG	-6.18	1.66	1.81
4	C	1000	4KU	CAI-SAG	-6.06	1.66	1.81
4	B	1000	4KU	CAI-SAG	-5.97	1.67	1.81
4	D	1000	4KU	CAJ-SAH	-5.95	1.67	1.81
4	B	1000	4KU	CAJ-SAH	-5.82	1.67	1.81
4	C	1000	4KU	CAJ-SAH	-5.81	1.67	1.81
4	A	1000	4KU	CAJ-SAH	-5.61	1.67	1.81
4	D	1000	4KU	CAV-NAT	2.19	1.44	1.38
4	B	1000	4KU	CAV-NAT	2.19	1.44	1.38
4	B	1000	4KU	CAU-NAS	2.13	1.44	1.38
4	A	1000	4KU	CAU-NAS	2.11	1.44	1.38
4	C	1000	4KU	CAU-NAS	2.06	1.44	1.38
4	A	1000	4KU	CAV-NAT	2.03	1.44	1.38
4	C	1000	4KU	CAV-NAT	2.02	1.44	1.38

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1000	4KU	CAR-CAX-CAZ	-9.97	115.58	125.37
4	A	1000	4KU	CAR-CAQ-CAW	-7.99	99.98	112.76
4	B	1000	4KU	CAR-CAX-CAZ	-7.82	117.69	125.37
4	C	1000	4KU	CAR-CAX-CAZ	-7.65	117.86	125.37
4	D	1000	4KU	CAR-CAX-CAZ	-7.48	118.03	125.37
4	C	1000	4KU	CAQ-CAW-CAY	-6.67	118.82	125.37
4	B	1000	4KU	CAQ-CAW-CAY	-6.09	119.39	125.37
4	D	1000	4KU	CAQ-CAW-CAY	-5.14	120.32	125.37
4	A	1000	4KU	CAO-CAY-CAW	-5.10	117.80	121.84
4	D	1000	4KU	OAC-SBB-CAZ	4.96	115.76	106.12
4	A	1000	4KU	OAB-SBA-CAY	4.84	117.69	106.52
4	B	1000	4KU	OAC-SBB-CAZ	4.65	115.16	106.12
4	A	1000	4KU	OAD-SBB-CAZ	4.62	117.18	106.52
4	C	1000	4KU	CAR-CAQ-CAW	-4.61	105.39	112.76
4	C	1000	4KU	OAE-SBA-CAY	4.59	115.04	106.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1000	4KU	CAO-CAY-CAW	-4.52	118.25	121.84
4	B	1000	4KU	CAR-CAQ-CAW	-4.33	105.83	112.76
4	A	1000	4KU	CAQ-CAW-CAY	-4.31	121.14	125.37
4	A	1000	4KU	OAE-SBA-CAY	4.29	114.45	106.12
4	D	1000	4KU	CAR-CAQ-CAW	-4.27	105.94	112.76
4	B	1000	4KU	OAB-SBA-CAY	4.09	115.97	106.52
4	C	1000	4KU	CAO-CAY-CAW	-3.98	118.68	121.84
4	A	1000	4KU	CAN-CAX-CAZ	3.90	121.79	116.44
4	A	1000	4KU	CAP-CAZ-CAX	-3.85	118.78	121.84
4	C	1000	4KU	OAD-SBB-CAZ	3.83	115.36	106.52
4	A	1000	4KU	OAC-SBB-CAZ	3.81	113.53	106.12
4	C	1000	4KU	OAC-SBB-CAZ	3.80	113.50	106.12
4	B	1000	4KU	OAF-SBB-CAZ	3.70	115.06	106.52
4	B	1000	4KU	OAE-SBA-CAY	3.69	113.28	106.12
4	D	1000	4KU	OAA-SBA-CAY	3.64	114.93	106.52
4	C	1000	4KU	OAB-SBA-CAY	3.57	114.77	106.52
4	D	1000	4KU	OAB-SBA-CAY	3.56	114.73	106.52
4	B	1000	4KU	OAA-SBA-CAY	3.50	114.60	106.52
4	C	1000	4KU	CAN-CAX-CAZ	3.41	121.12	116.44
4	D	1000	4KU	CAO-CAY-CAW	-3.40	119.14	121.84
4	D	1000	4KU	OAF-SBB-CAZ	3.33	114.21	106.52
4	D	1000	4KU	OAE-SBA-CAY	3.32	112.57	106.12
4	C	1000	4KU	CAM-CAW-CAY	3.21	120.83	116.44
4	B	1000	4KU	CAN-CAX-CAZ	3.18	120.80	116.44
4	C	1000	4KU	CAP-CAZ-CAX	-3.05	119.42	121.84
4	D	1000	4KU	CAN-CAX-CAZ	2.95	120.48	116.44
4	B	1000	4KU	CAM-CAW-CAY	2.95	120.48	116.44
4	A	1000	4KU	CAL-CAN-CAX	-2.73	117.82	121.39
4	B	1000	4KU	CAP-CAZ-CAX	-2.73	119.68	121.84
4	A	1000	4KU	CAM-CAW-CAY	2.69	120.13	116.44
4	D	1000	4KU	OAD-SBB-CAZ	2.68	112.70	106.52
4	A	1000	4KU	OAF-SBB-CAZ	2.66	112.65	106.52
4	C	1000	4KU	OAA-SBA-CAY	2.61	112.54	106.52
4	C	1000	4KU	OAF-SBB-CAZ	2.52	112.33	106.52
4	C	1000	4KU	CAL-CAN-CAX	-2.44	118.21	121.39
4	D	1000	4KU	CAP-CAZ-CAX	-2.41	119.93	121.84
4	B	1000	4KU	CAL-CAN-CAX	-2.38	118.28	121.39
4	D	1000	4KU	CAM-CAW-CAY	2.37	119.69	116.44
4	B	1000	4KU	OAD-SBB-CAZ	2.37	111.98	106.52
4	D	1000	4KU	CAL-CAN-CAX	-2.35	118.31	121.39
4	A	1000	4KU	CAQ-CAR-CAX	2.23	116.33	112.76
4	A	1000	4KU	CAW-CAY-SBA	2.13	123.19	121.36

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	1000	4KU	OAA-SBA-CAY	2.02	111.17	106.52

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1000	4KU	CAW-CAQ-CAR-CAX
4	B	1000	4KU	CAW-CAQ-CAR-CAX
4	A	1000	4KU	CAR-CAQ-CAW-CAY
4	B	1000	4KU	CAQ-CAR-CAX-CAZ
4	B	1000	4KU	CAL-CAV-NAT-CAJ
4	C	1000	4KU	CAW-CAQ-CAR-CAX
4	A	1000	4KU	CAR-CAQ-CAW-CAM
4	B	1000	4KU	CAQ-CAR-CAX-CAN
4	C	1000	4KU	CAQ-CAR-CAX-CAN
4	D	1000	4KU	CAQ-CAR-CAX-CAN
4	C	1000	4KU	CAR-CAQ-CAW-CAM
4	B	1000	4KU	CAO-CAU-NAS-CAI
4	D	1000	4KU	CAL-CAV-NAT-CAJ
4	C	1000	4KU	CAR-CAQ-CAW-CAY
4	C	1000	4KU	CAQ-CAR-CAX-CAZ
4	D	1000	4KU	CAQ-CAR-CAX-CAZ
4	B	1000	4KU	CAP-CAV-NAT-CAJ
4	B	1000	4KU	CAK-CAU-NAS-CAI
4	D	1000	4KU	CAP-CAV-NAT-CAJ
4	C	1000	4KU	CAL-CAV-NAT-CAJ
4	D	1000	4KU	CAO-CAU-NAS-CAI

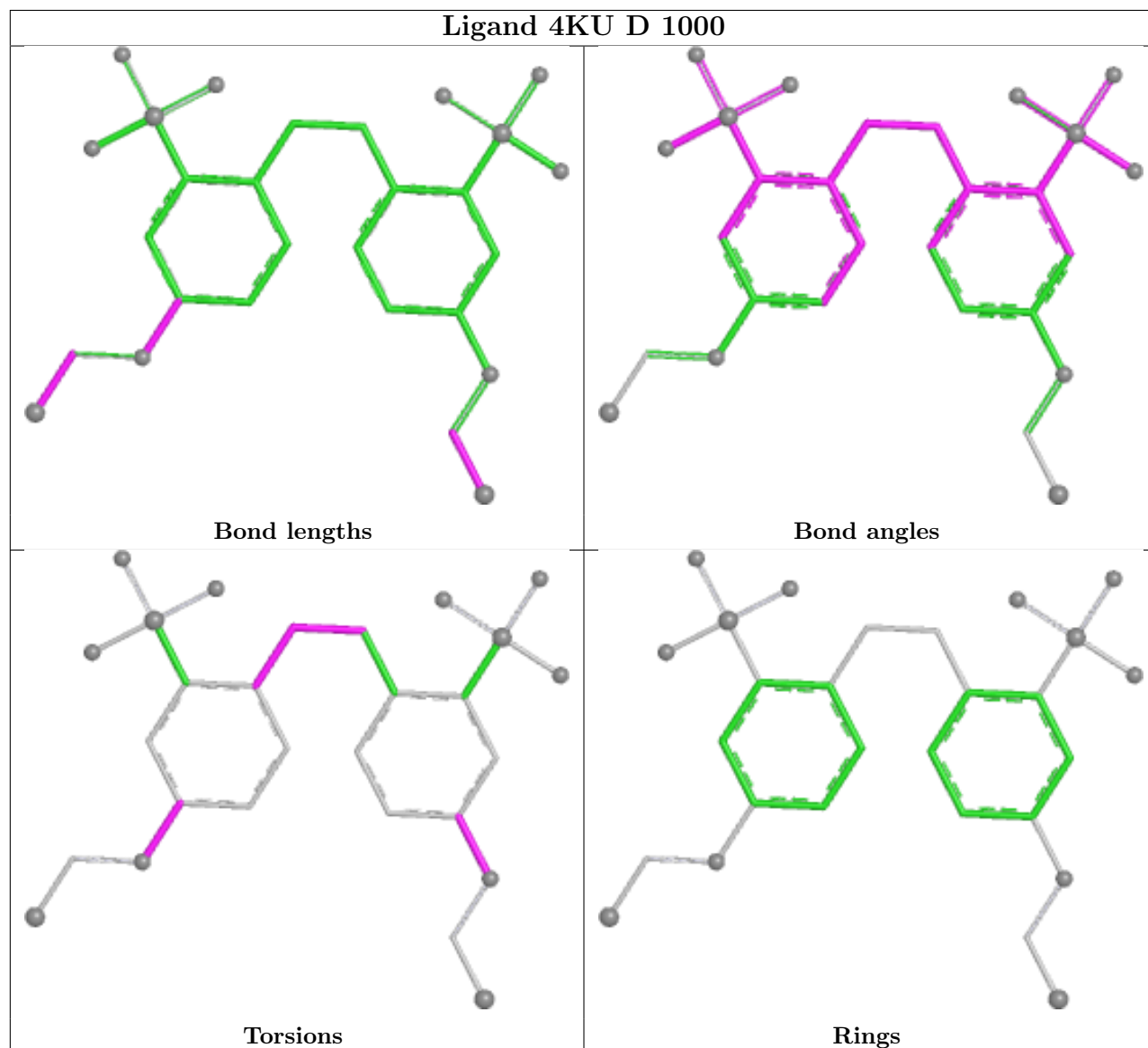
There are no ring outliers.

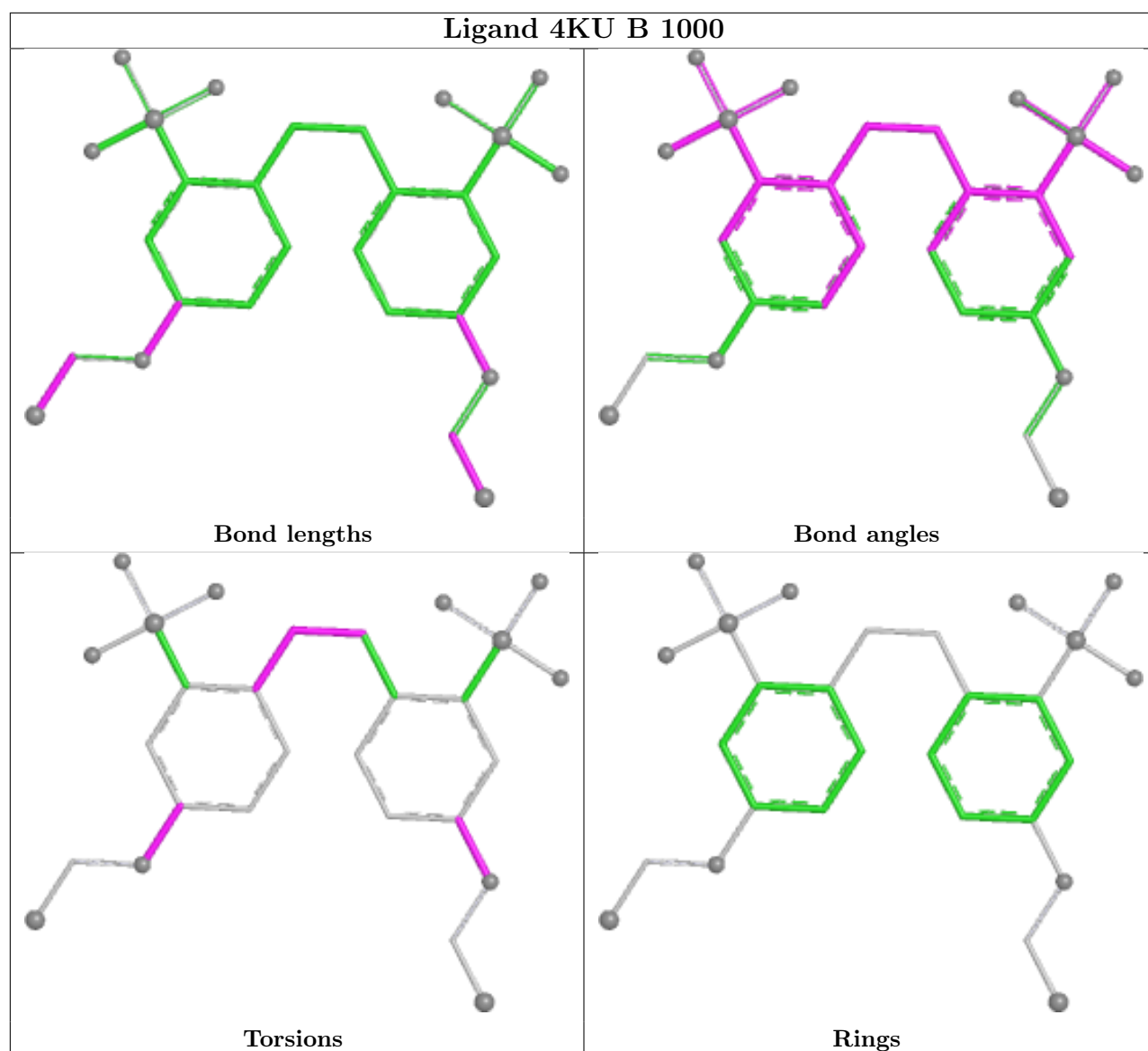
4 monomers are involved in 8 short contacts:

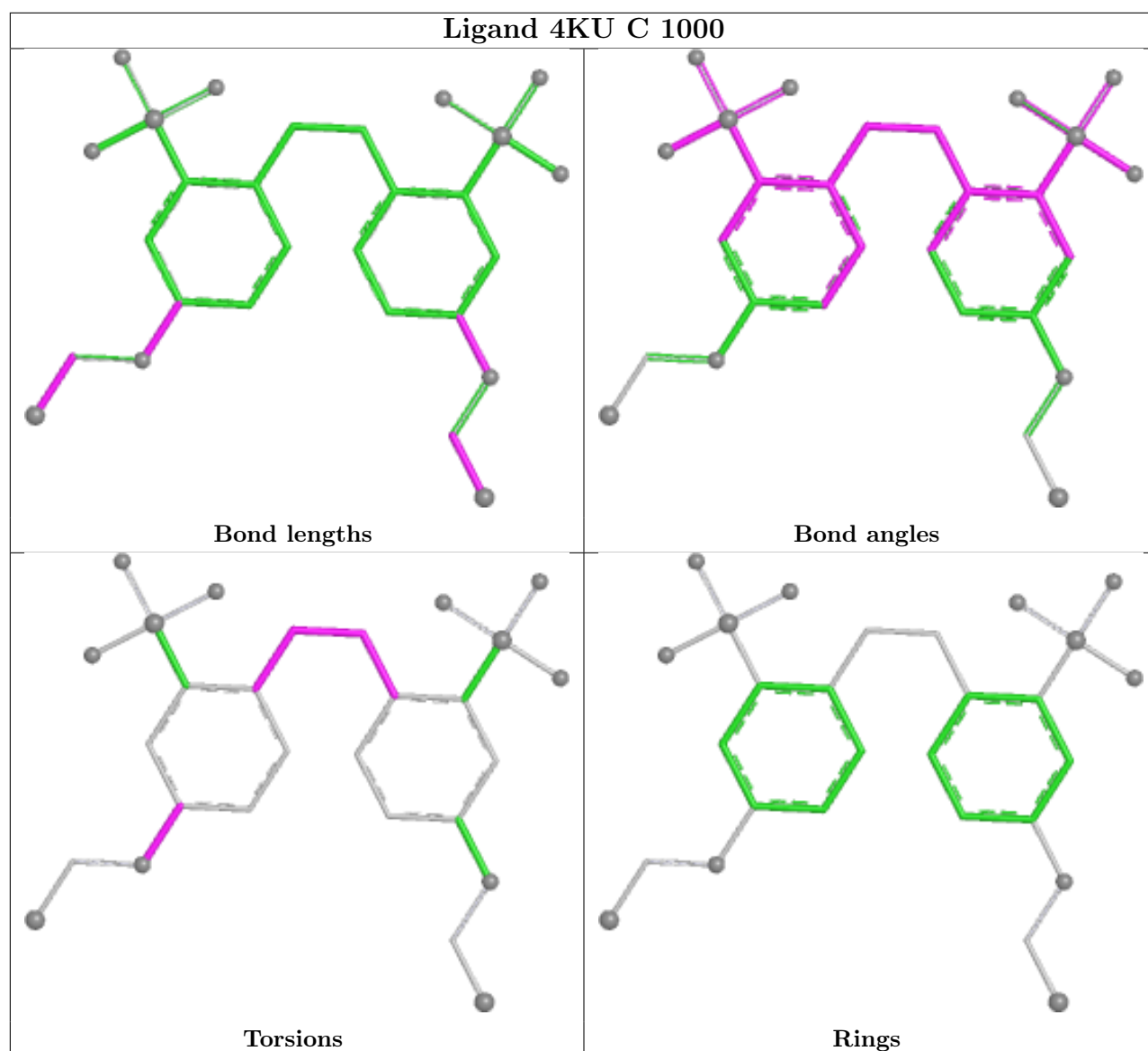
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1000	4KU	2	0
4	B	1000	4KU	2	0
4	C	1000	4KU	3	0
4	A	1000	4KU	1	0

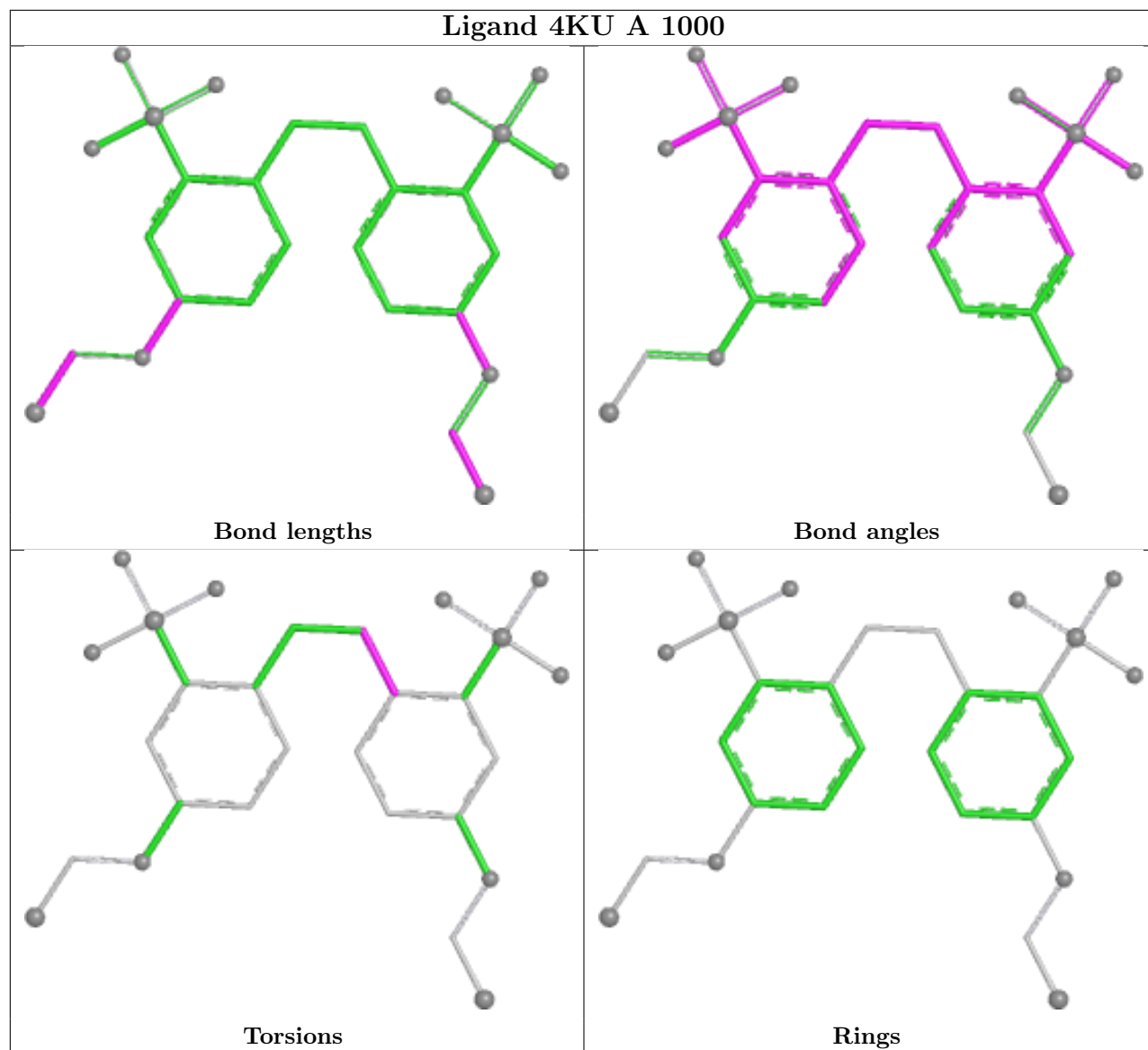
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	475/911 (52%)	0.29	31 (6%) 25 15	71, 103, 169, 208	0
1	B	475/911 (52%)	0.50	39 (8%) 17 11	90, 142, 202, 249	0
1	C	475/911 (52%)	0.27	32 (6%) 24 15	79, 114, 184, 226	0
1	D	475/911 (52%)	0.66	57 (12%) 9 6	103, 151, 219, 259	0
2	E	223/223 (100%)	0.49	16 (7%) 21 14	79, 105, 150, 177	0
2	G	223/223 (100%)	0.46	18 (8%) 18 12	124, 152, 211, 250	0
2	I	223/223 (100%)	1.06	56 (25%) 1 2	79, 112, 310, 355	0
2	K	223/223 (100%)	0.51	18 (8%) 18 12	126, 152, 209, 248	0
3	F	218/218 (100%)	0.32	6 (2%) 55 32	81, 111, 141, 179	0
3	H	218/218 (100%)	0.55	17 (7%) 19 12	125, 181, 255, 268	0
3	J	218/218 (100%)	0.84	28 (12%) 7 6	90, 164, 292, 310	0
3	L	218/218 (100%)	0.44	17 (7%) 19 12	127, 169, 242, 253	0
All	All	3664/5408 (67%)	0.50	335 (9%) 15 10	71, 139, 238, 355	0

All (335) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	802	GLY	8.9
2	K	141	THR	7.8
2	K	140	ASP	6.5
2	G	148	LEU	6.4
3	F	194	ASN	6.4
1	D	700	SER	6.4
1	B	473	GLU	6.1
1	B	694	ARG	6.0
3	L	146	LYS	5.9
2	E	107	GLY	5.7
1	D	473	GLU	5.5

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Mol	Chain	Res	Type	RSRZ
1	D	652	PRO	5.4
1	B	653	LEU	5.4
1	D	694	ARG	5.4
3	J	137	VAL	5.3
2	I	161	THR	5.3
2	I	139	GLY	5.2
2	I	193	VAL	5.1
1	C	398	THR	5.0
2	I	167	GLY	5.0
2	I	187	LEU	5.0
1	A	819	HIS	4.9
3	H	216	ASN	4.9
3	J	97	GLU	4.7
1	A	830	THR	4.7
2	I	150	CYS	4.6
1	A	832	ARG	4.6
3	L	216	ASN	4.6
1	D	469	LEU	4.6
1	B	652	PRO	4.6
2	K	39	ILE	4.6
1	C	818	TYR	4.6
2	I	144	SER	4.5
1	D	874	LEU	4.5
3	L	131	SER	4.5
1	A	831	TRP	4.4
2	K	139	GLY	4.4
2	K	71	ILE	4.3
1	D	430	LYS	4.2
2	E	90	ALA	4.2
2	K	148	LEU	4.2
1	D	412	ILE	4.1
2	I	149	GLY	4.1
2	I	135	ALA	4.1
1	D	386	ILE	4.1
3	H	191	GLU	4.0
1	B	654	GLY	4.0
2	G	149	GLY	4.0
1	A	584	PHE	4.0
1	D	653	LEU	4.0
1	D	398	THR	4.0
2	I	163	THR	4.0
2	I	203	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
3	J	135	SER	4.0
2	I	175	THR	4.0
1	B	875	PRO	4.0
1	A	834	HIS	4.0
3	J	16	GLY	3.9
2	I	152	VAL	3.9
1	C	427	LEU	3.9
3	H	60	SER	3.9
2	I	160	VAL	3.9
1	B	801	SER	3.9
3	J	99	PRO	3.9
1	C	884	GLN	3.9
2	I	138	CYS	3.8
3	L	155	ASP	3.8
2	I	223	ARG	3.8
2	G	134	LEU	3.8
3	L	147	ASP	3.8
1	D	395	SER	3.7
2	I	134	LEU	3.7
3	H	19	ALA	3.7
1	A	398	THR	3.7
1	D	693	GLU	3.7
2	G	51	ALA	3.6
1	D	834	HIS	3.6
2	I	133	PRO	3.6
1	B	469	LEU	3.6
1	A	681	GLU	3.6
1	B	691	LYS	3.6
2	I	128	ALA	3.6
2	I	208	ALA	3.6
1	D	699	GLY	3.6
3	H	174	ASP	3.6
2	G	200	SER	3.5
2	G	50	LEU	3.5
2	E	137	VAL	3.5
3	J	184	THR	3.5
2	I	195	SER	3.5
1	D	731	SER	3.5
2	I	56	SER	3.5
3	J	98	ILE	3.4
1	D	822	VAL	3.4
3	H	63	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	617	MET	3.4
2	I	169	LEU	3.4
1	B	818	TYR	3.4
1	D	470	VAL	3.4
2	I	154	GLY	3.4
1	B	398	THR	3.4
2	I	148	LEU	3.3
2	G	77	ASN	3.3
3	L	132	GLY	3.3
1	D	690	SER	3.3
2	I	166	SER	3.3
2	K	38	TRP	3.2
1	D	651	HIS	3.2
1	C	384	ARG	3.2
3	H	218	CYS	3.2
1	D	654	GLY	3.2
1	D	471	PHE	3.2
1	D	825	VAL	3.2
2	I	191	VAL	3.2
1	C	799	SER	3.2
2	G	139	GLY	3.2
2	I	131	VAL	3.2
1	D	655	LEU	3.2
2	K	149	GLY	3.1
3	H	169	ASP	3.1
1	D	451	PHE	3.1
2	K	52	HIS	3.1
2	I	164	TRP	3.1
1	A	656	ARG	3.1
1	C	707	LEU	3.1
1	D	886	LEU	3.1
2	G	65	LEU	3.1
2	G	146	VAL	3.1
1	D	460	LEU	3.1
3	J	110	ILE	3.0
1	C	835	LEU	3.0
2	I	188	SER	3.0
2	E	108	TYR	3.0
2	I	55	TRP	3.0
1	B	638	PHE	3.0
1	B	394	LEU	3.0
2	E	143	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	460	LEU	3.0
2	I	151	LEU	3.0
3	J	136	VAL	3.0
1	A	553	TYR	2.9
2	G	140	ASP	2.9
3	J	162	GLY	2.9
3	L	19	ALA	2.9
1	B	639	LYS	2.9
3	H	187	LYS	2.9
1	C	753	ILE	2.9
3	F	217	GLU	2.9
1	C	509	GLY	2.9
2	I	168	SER	2.9
1	D	392	TYR	2.9
1	D	403	PRO	2.9
2	I	145	SER	2.9
1	D	639	LYS	2.9
2	I	215	LYS	2.9
3	J	200	ALA	2.9
1	A	821	ASP	2.9
1	B	640	VAL	2.9
1	B	814	LYS	2.9
3	J	175	SER	2.8
1	A	835	LEU	2.8
2	E	138	CYS	2.8
3	J	11	LEU	2.8
1	A	728	THR	2.8
1	D	735	ALA	2.8
1	B	650	ILE	2.8
3	H	61	GLY	2.8
1	A	886	LEU	2.8
2	I	129	PRO	2.8
1	D	414	PHE	2.8
2	E	31	THR	2.8
1	C	819	HIS	2.7
2	I	192	THR	2.7
1	D	704	LEU	2.7
2	I	162	LEU	2.7
1	B	791	ILE	2.7
1	B	651	HIS	2.7
2	K	72	SER	2.7
2	G	147	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	640	VAL	2.7
1	A	869	LEU	2.7
1	C	820	PRO	2.7
2	I	31	THR	2.7
3	L	37	MET	2.7
1	B	488	VAL	2.7
2	I	189	SER	2.7
3	L	63	PRO	2.6
3	H	20	THR	2.6
1	D	847	LEU	2.6
2	I	171	SER	2.6
2	K	170	SER	2.6
1	A	519	TYR	2.6
1	D	887	ASP	2.6
1	A	459	LEU	2.6
1	D	734	HIS	2.6
1	A	873	LEU	2.6
2	K	183	ASP	2.6
3	J	138	CYS	2.6
1	B	655	LEU	2.6
1	A	685	THR	2.6
2	I	220	ILE	2.6
2	I	153	LYS	2.6
1	D	512	LEU	2.6
3	F	80	HIS	2.6
2	G	141	THR	2.6
3	J	210	VAL	2.5
2	E	220	ILE	2.5
2	E	53	ILE	2.5
3	H	207	SER	2.5
2	I	73	LYS	2.5
2	G	31	THR	2.5
1	C	512	LEU	2.5
1	D	394	LEU	2.5
2	E	195	SER	2.5
1	D	697	VAL	2.5
1	D	709	VAL	2.5
1	B	726	ALA	2.5
2	E	223	ARG	2.5
3	H	205	SER	2.5
3	J	193	HIS	2.5
3	L	154	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	816	PRO	2.5
1	B	637	GLY	2.5
3	J	95	SER	2.5
2	E	36	VAL	2.5
2	E	136	PRO	2.4
1	A	822	VAL	2.4
3	J	150	VAL	2.4
1	B	735	ALA	2.4
1	D	589	ARG	2.4
2	I	207	VAL	2.4
1	D	736	ASN	2.4
1	B	403	PRO	2.4
1	B	741	MET	2.4
1	A	829	LYS	2.4
1	C	567	LEU	2.4
2	K	50	LEU	2.4
3	L	158	GLU	2.4
2	I	178	ALA	2.4
1	C	831	TRP	2.4
1	C	391	PRO	2.4
1	C	687	LEU	2.4
1	D	835	LEU	2.4
1	B	718	LEU	2.4
1	D	501	VAL	2.4
2	I	141	THR	2.4
1	D	567	LEU	2.4
2	I	184	LEU	2.4
1	D	459	LEU	2.3
1	A	825	VAL	2.3
2	I	140	ASP	2.3
1	B	666	ALA	2.3
2	K	124	ALA	2.3
2	K	198	TRP	2.3
1	C	726	ALA	2.3
3	L	55	ALA	2.3
1	C	584	PHE	2.3
1	A	384	ARG	2.3
1	C	656	ARG	2.3
2	G	138	CYS	2.3
1	A	616	ILE	2.3
1	D	605	ILE	2.3
3	F	79	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	832	ARG	2.3
1	B	397	ILE	2.3
1	B	628	TYR	2.3
3	J	209	ILE	2.3
1	B	887	ASP	2.3
1	B	505	VAL	2.3
2	E	89	THR	2.3
1	D	573	LEU	2.3
2	I	179	VAL	2.3
3	H	146	LYS	2.3
1	A	387	ARG	2.3
3	F	214	ASN	2.2
3	L	204	THR	2.2
3	J	139	PHE	2.2
1	C	553	TYR	2.2
2	G	136	PRO	2.2
1	D	650	ILE	2.2
1	D	839	ILE	2.2
2	I	218	LYS	2.2
1	C	436	GLY	2.2
1	D	870	ARG	2.2
3	J	81	PRO	2.2
3	L	1	ASP	2.2
1	A	682	SER	2.2
1	C	682	SER	2.2
1	C	869	LEU	2.2
1	B	400	ALA	2.2
3	H	12	ALA	2.2
1	C	460	LEU	2.2
3	J	67	SER	2.2
1	B	872	VAL	2.2
2	I	147	THR	2.2
2	E	196	SER	2.2
3	J	120	SER	2.2
3	L	177	TYR	2.2
1	C	834	HIS	2.1
2	I	5	GLN	2.1
1	D	624	ILE	2.1
1	B	693	GLU	2.1
2	K	31	THR	2.1
3	J	100	TRP	2.1
1	A	840	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	397	ILE	2.1
3	L	209	ILE	2.1
3	J	117	PRO	2.1
1	C	844	LEU	2.1
1	D	798	THR	2.1
2	E	141	THR	2.1
3	H	125	SER	2.1
1	D	500	LEU	2.1
2	I	186	THR	2.1
3	J	176	THR	2.1
3	F	19	ALA	2.1
1	D	679	PHE	2.1
1	D	604	VAL	2.1
2	G	191	VAL	2.1
3	J	183	LEU	2.1
1	C	728	THR	2.0
2	K	40	ARG	2.0
3	H	98	ILE	2.0
1	B	700	SER	2.0
2	I	122	SER	2.0
3	J	202	HIS	2.0
3	L	117	PRO	2.0
1	A	523	ILE	2.0
1	B	395	SER	2.0
1	B	495	PHE	2.0
2	I	205	CYS	2.0
1	C	854	PRO	2.0
2	G	71	ILE	2.0
1	C	507	PHE	2.0
2	K	82	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

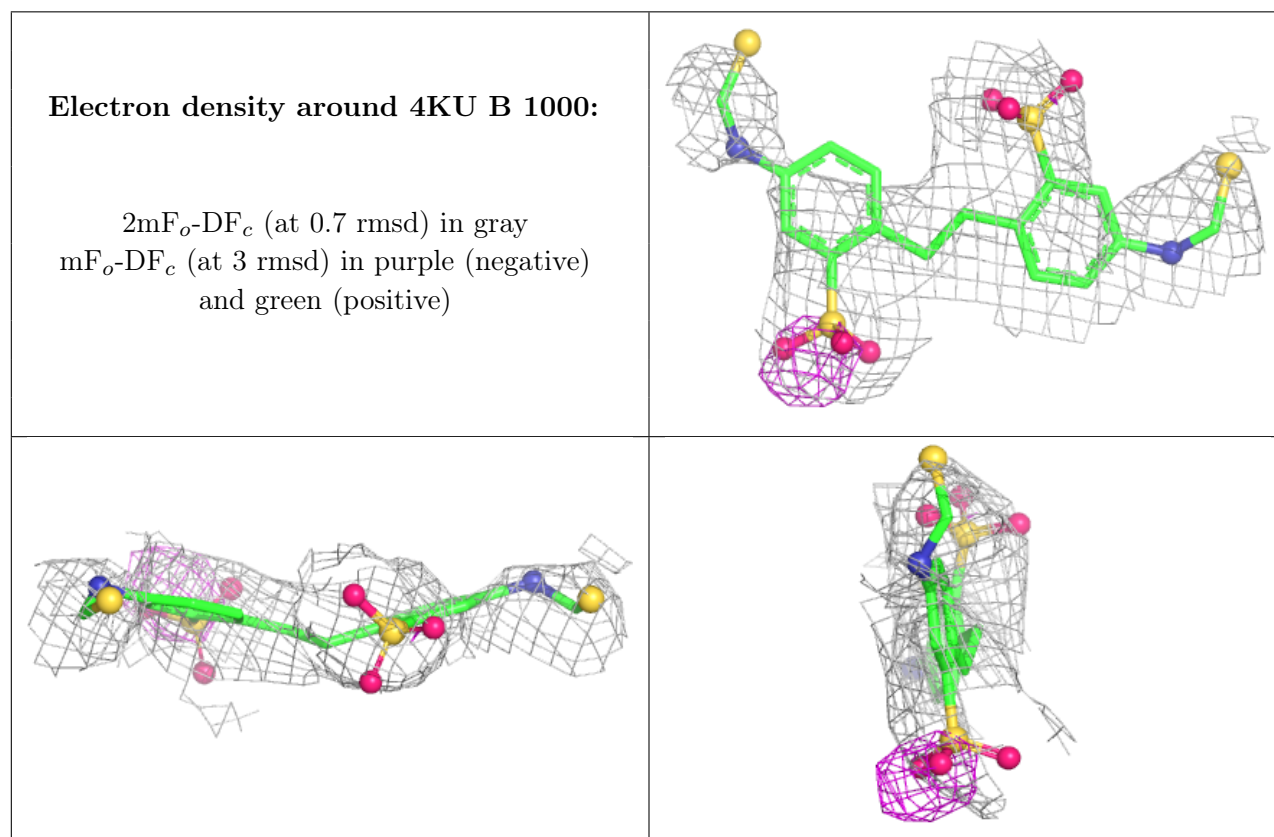
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

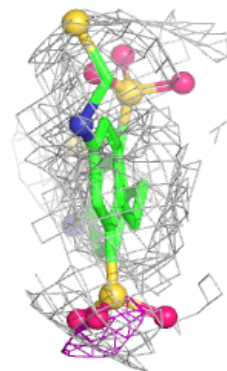
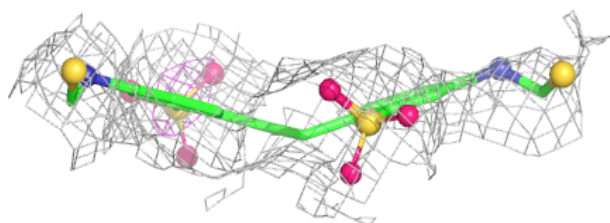
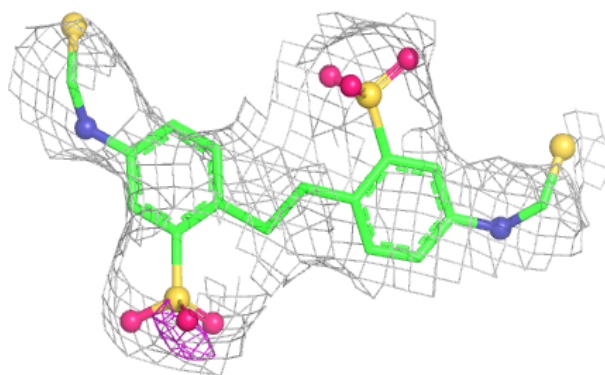
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	4KU	B	1000	28/28	0.68	0.13	143,146,152,155	0
4	4KU	D	1000	28/28	0.77	0.11	148,152,159,163	0
4	4KU	A	1000	28/28	0.80	0.15	105,108,112,114	0
4	4KU	C	1000	28/28	0.84	0.12	113,118,123,125	0

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.

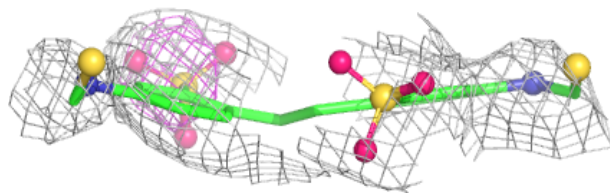
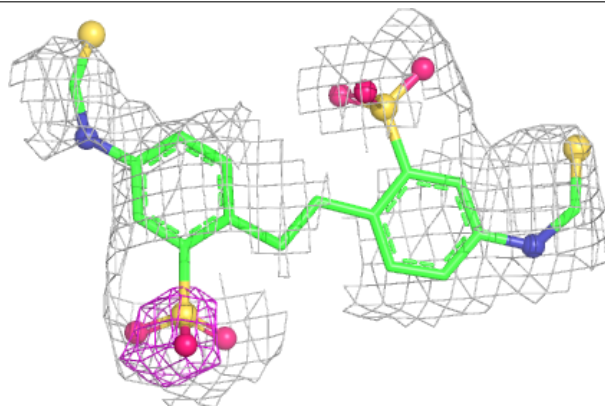


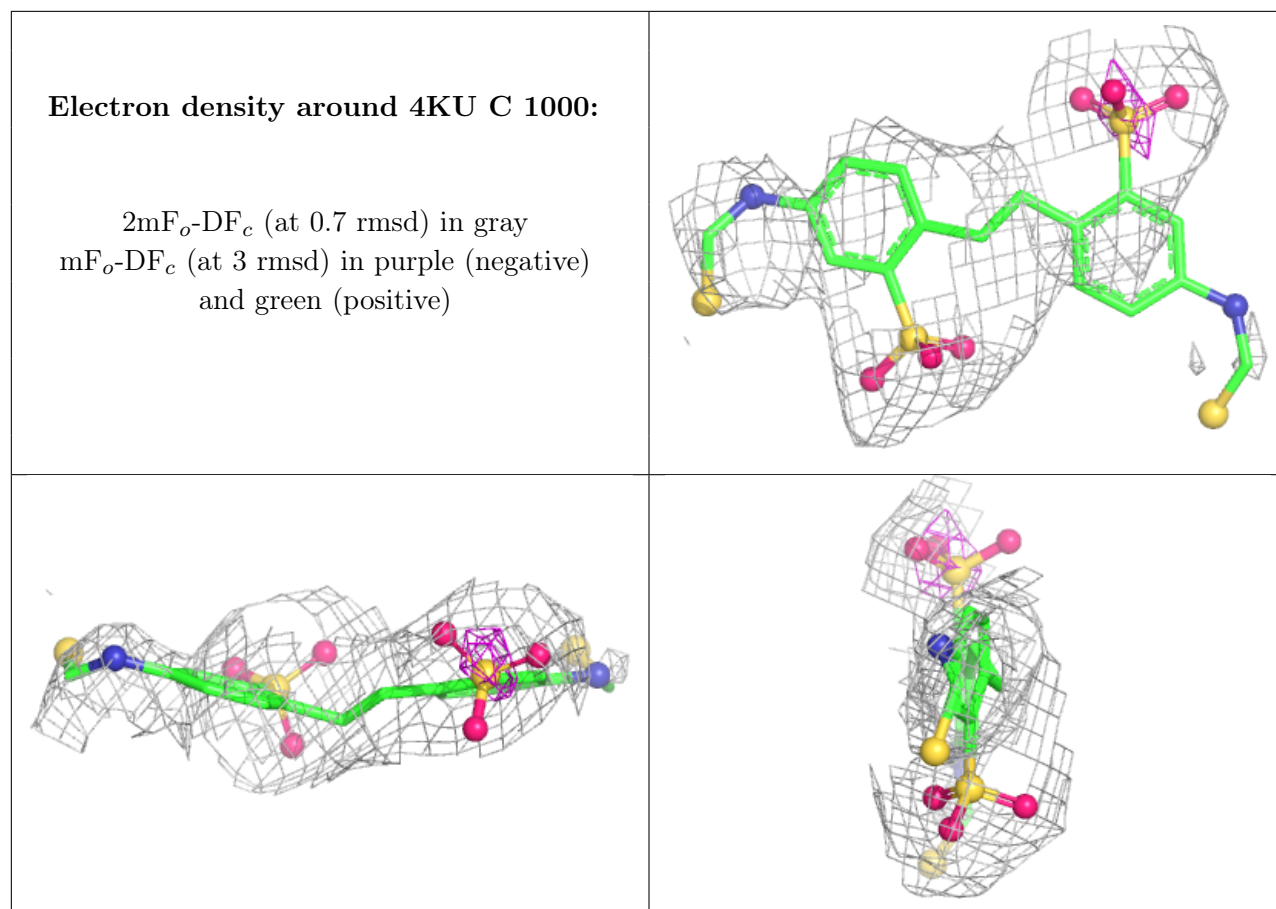
Electron density around 4KU D 1000:

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

**Electron density around 4KU A 1000:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.