



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:00 PM UTC

PDB ID : 1NYQ / pdb_00001nyq
Title : Structure of Staphylococcus aureus threonyl-tRNA synthetase complexed with an analogue of threonyl adenylate
Authors : Torres-Larios, A.; Sankaranarayanan, R.; Rees, B.; Dock-Bregeon, A.C.; Moras, D.
Deposited on : 2003-02-13
Resolution : 3.20 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

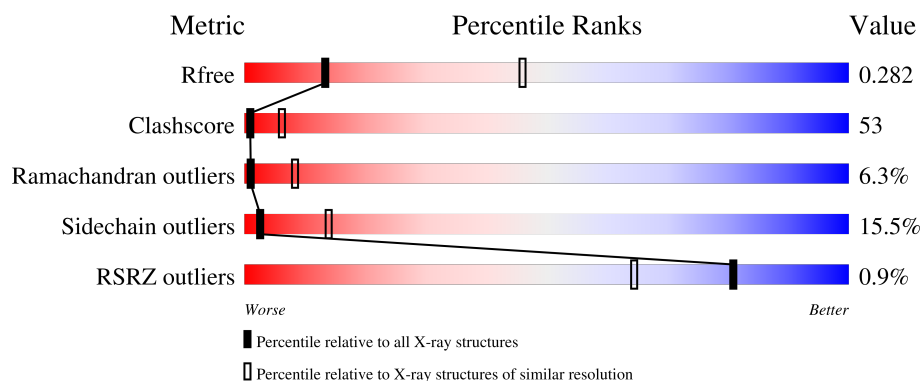
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	645	30% 51% 17%
1	B	645	30% 50% 18%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10663 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.

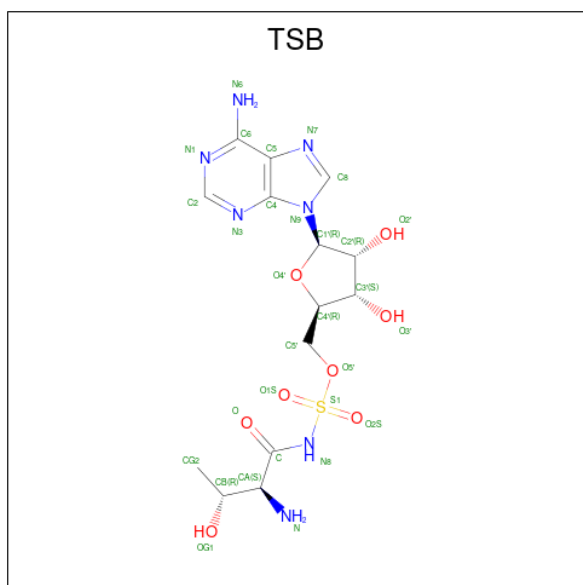
- Molecule 1 is a protein called threonyl-tRNA synthetase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	0	0
			5216	3296	894	1003	23			
1	B	645	Total	C	N	O	S	0	0	0
			5242	3311	898	1009	24			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 5'-O-(N-(L-THREONYL)-SULFAMOYL)ADENOSINE (CCD ID: TSB) (formula: C₁₄H₂₁N₇O₈S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			30	14	7	8	1		
3	B	1	Total	C	N	O	S	0	0
			30	14	7	8	1		

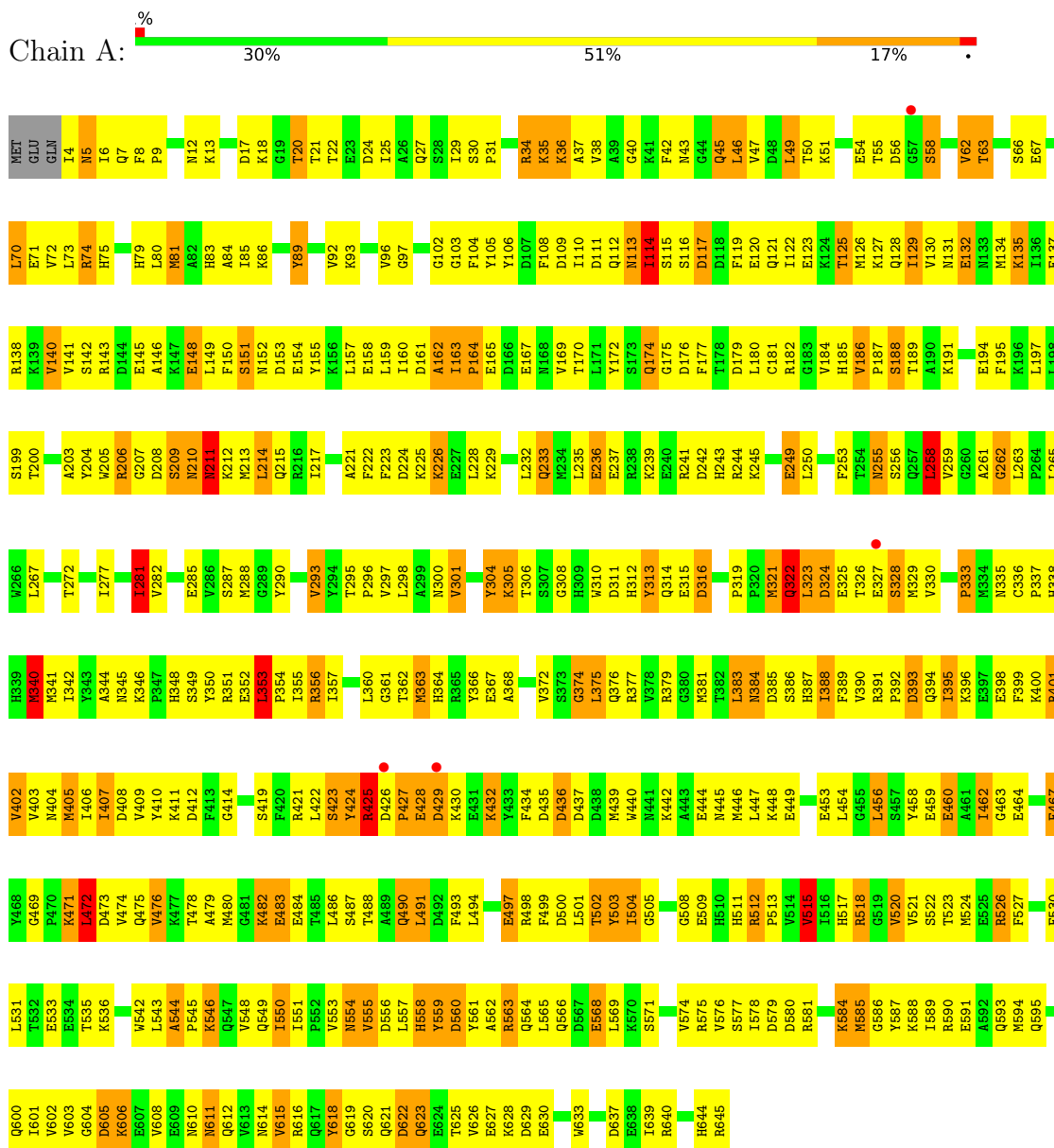
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	75	Total	O	0	0
			75	75		
4	B	68	Total	O	0	0
			68	68		

3 Residue-property plots [i](#)

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

• Molecule 1: threonyl-tRNA synthetase 1



• Molecule 1: threonyl-tRNA synthetase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.28Å 122.73Å 149.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.20 15.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.3 (15.00-3.20) 94.5 (15.00-3.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.19 (at 3.15Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.285 0.204 , 0.282	Depositor DCC
R_{free} test set	3182 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å ²)	78.4	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10663	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: TSB, ZN

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	0.76	2/5325 (0.0%)	1.24	49/7182 (0.7%)
1	B	0.68	1/5351 (0.0%)	1.20	58/7216 (0.8%)
All	All	0.72	3/10676 (0.0%)	1.22	107/14398 (0.7%)

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	3
1	B	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	480	MET	SD-CE	6.17	1.95	1.79
1	A	462	ILE	CA-CB	6.17	1.61	1.54
1	A	281	ILE	CA-CB	5.02	1.59	1.54

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	LEU	CA-C-N	-18.96	96.14	119.84
1	A	353	LEU	C-N-CA	-18.96	96.14	119.84
1	B	353	LEU	CA-C-N	-13.67	103.45	121.91
1	B	353	LEU	C-N-CA	-13.67	103.45	121.91
1	B	361	GLY	N-CA-C	10.82	130.20	111.15
1	B	424	TYR	N-CA-C	10.68	125.09	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	233	GLN	N-CA-C	-10.52	99.90	111.36
1	B	77	THR	N-CA-C	-10.26	101.08	114.31
1	B	376	GLN	N-CA-C	10.08	122.02	111.14
1	A	460	GLU	N-CA-C	-9.15	98.19	110.55
1	B	111	ASP	N-CA-C	-8.90	102.83	114.31
1	B	565	LEU	N-CA-C	-8.70	101.77	111.07
1	A	111	ASP	N-CA-C	-8.40	102.08	111.07
1	A	360	LEU	N-CA-C	-8.38	97.06	109.62
1	A	333	PRO	N-CA-C	-8.21	105.15	114.92
1	A	184	VAL	N-CA-C	7.94	120.08	109.37
1	A	361	GLY	N-CA-C	7.90	124.05	111.64
1	A	515	VAL	N-CA-C	7.89	119.22	108.17
1	A	584	LYS	N-CA-C	7.87	120.49	109.15
1	B	353	LEU	N-CA-C	7.59	126.59	109.81
1	B	119	PHE	N-CA-C	-7.52	103.10	111.82
1	A	424	TYR	N-CA-C	7.43	121.76	109.95
1	B	479	ALA	N-CA-C	-7.19	101.02	111.30
1	A	353	LEU	N-CA-C	7.18	125.68	109.81
1	B	523	THR	N-CA-C	-7.01	99.18	110.32
1	B	248	LYS	N-CA-C	-6.99	102.22	111.24
1	B	78	ALA	N-CA-C	-6.98	103.60	111.07
1	B	547	GLN	N-CA-C	6.91	119.83	111.82
1	A	322	GLN	N-CA-C	6.91	125.51	110.80
1	A	233	GLN	N-CA-C	-6.81	103.79	111.14
1	A	262	GLY	N-CA-C	-6.79	105.70	115.27
1	B	193	LYS	N-CA-C	6.74	118.51	111.03
1	B	480	MET	N-CA-C	-6.70	103.83	113.21
1	A	606	LYS	N-CA-C	-6.66	103.28	111.33
1	A	67	GLU	N-CA-C	-6.65	104.11	111.36
1	A	295	THR	CA-C-N	6.64	128.14	119.84
1	A	295	THR	C-N-CA	6.64	128.14	119.84
1	A	22	THR	N-CA-C	-6.57	103.38	111.33
1	A	305	LYS	N-CA-C	-6.54	103.84	110.97
1	B	377	ARG	N-CA-C	-6.53	96.39	108.02
1	B	644	HIS	N-CA-C	-6.52	105.95	114.04
1	B	190	ALA	N-CA-C	-6.45	106.04	114.04
1	B	435	ASP	N-CA-C	-6.45	105.37	113.23
1	A	384	ASN	N-CA-C	-6.40	99.21	109.39
1	A	618	TYR	N-CA-C	-6.38	104.42	111.82
1	A	520	VAL	N-CA-C	6.34	116.45	110.30
1	B	127	LYS	N-CA-C	-6.34	106.25	112.97
1	B	125	THR	N-CA-C	-6.25	104.71	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	433	TYR	N-CA-C	-6.25	102.36	111.30
1	B	437	ASP	N-CA-C	-6.25	104.92	112.54
1	A	301	VAL	N-CA-C	6.23	117.73	110.62
1	B	494	LEU	N-CA-C	6.23	117.94	111.03
1	B	288	MET	N-CA-C	-6.21	106.06	113.21
1	A	161	ASP	N-CA-C	6.21	119.22	109.96
1	B	121	GLN	N-CA-C	-6.14	104.52	112.68
1	B	239	LYS	N-CA-C	-6.13	105.45	113.12
1	A	505	GLY	N-CA-C	6.05	121.77	112.51
1	A	503	TYR	N-CA-C	-6.00	101.05	109.69
1	B	273	ILE	N-CA-C	-5.99	104.49	110.30
1	B	390	VAL	N-CA-C	5.96	118.57	108.86
1	B	519	GLY	N-CA-C	-5.96	99.07	113.18
1	B	60	GLU	N-CA-C	-5.95	97.77	108.48
1	B	185	HIS	N-CA-C	5.90	118.82	109.50
1	A	237	GLU	N-CA-C	-5.85	104.91	111.28
1	B	356	ARG	N-CA-C	5.83	118.22	107.73
1	A	103	GLY	N-CA-C	5.83	118.96	110.63
1	A	425	ARG	N-CA-C	5.82	123.19	110.80
1	A	383	LEU	N-CA-C	5.81	119.11	109.46
1	A	615	VAL	N-CA-C	5.81	117.97	108.97
1	B	384	ASN	N-CA-C	-5.76	100.98	109.62
1	B	59	ILE	N-CA-C	5.72	117.99	109.17
1	A	258	LEU	N-CA-C	-5.67	105.86	112.89
1	B	45	GLN	N-CA-C	-5.64	99.41	108.55
1	B	405	MET	N-CA-C	-5.58	105.10	111.07
1	A	504	ILE	N-CA-C	5.58	115.92	108.11
1	A	393	ASP	N-CA-C	5.57	119.33	112.54
1	B	550	ILE	CB-CA-C	-5.56	103.04	111.33
1	A	411	LYS	N-CA-C	-5.54	105.24	111.28
1	B	258	LEU	N-CA-C	-5.52	106.04	112.89
1	A	89	TYR	N-CA-C	5.50	118.95	110.42
1	B	324	ASP	CA-C-O	5.50	121.80	118.33
1	B	332	ARG	N-CA-C	5.43	117.30	109.48
1	B	515	VAL	N-CA-C	5.41	115.68	108.11
1	B	148	GLU	N-CA-C	5.35	116.92	111.14
1	B	59	ILE	CB-CA-C	-5.33	103.91	111.38
1	A	546	LYS	N-CA-C	-5.33	99.76	108.76
1	A	340	MET	N-CA-C	-5.30	105.20	110.97
1	B	222	PHE	N-CA-C	5.28	116.31	108.86
1	A	558	HIS	N-CA-C	5.26	119.54	113.18
1	B	452	ASP	N-CA-C	5.25	116.81	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	544	ALA	CA-C-N	5.24	125.29	119.32
1	A	544	ALA	C-N-CA	5.24	125.29	119.32
1	A	593	GLN	N-CA-C	-5.24	106.15	112.54
1	B	102	GLY	N-CA-C	-5.21	107.61	114.95
1	A	121	GLN	N-CA-C	-5.20	106.02	112.93
1	B	364	HIS	N-CA-C	5.19	117.37	108.90
1	B	541	THR	N-CA-C	5.19	121.86	110.80
1	B	342	ILE	N-CA-C	-5.19	105.65	110.53
1	A	354	PRO	N-CA-C	-5.14	101.87	112.47
1	B	297	VAL	N-CA-C	-5.12	106.91	112.80
1	A	472	LEU	N-CA-C	-5.11	97.55	107.62
1	A	132	GLU	N-CA-C	-5.09	105.86	111.71
1	B	84	ALA	N-CA-C	-5.08	106.92	113.23
1	A	148	GLU	N-CA-C	-5.03	105.71	111.14
1	B	49	LEU	N-CA-C	5.03	116.45	111.07
1	B	380	GLY	N-CA-C	-5.03	101.27	113.18
1	B	55	THR	N-CA-C	5.02	115.00	108.07

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	290	TYR	Sidechain
1	A	304	TYR	Sidechain
1	A	350	TYR	Sidechain
1	B	304	TYR	Sidechain

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	5216	0	5105	523	0
1	B	5242	0	5131	586	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	30	0	20	3	0
3	B	30	0	20	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	75	0	0	19	0
4	B	68	0	0	21	0
All	All	10663	0	10276	1093	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 53.

All (1093) 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:593:GLN:NE2	1:B:616:ARG:HH21	1.41	1.18
1:B:395:ILE:HD11	1:B:514:VAL:HG21	1.28	1.15
1:B:478:THR:HG22	1:B:479:ALA:H	1.08	1.13
1:A:426:ASP:HB3	1:A:427:PRO:HD2	1.31	1.10
1:B:74:ARG:HG2	1:B:221:ALA:HB3	1.28	1.08
1:B:135:LYS:HG2	1:B:136:ILE:H	1.19	1.08
1:B:322:GLN:HA	1:B:328:SER:HA	1.34	1.05
1:A:113:ASN:HA	1:A:215:GLN:HE22	1.25	1.01
1:B:593:GLN:HE21	1:B:616:ARG:NH2	1.58	1.00
1:B:27:GLN:NE2	1:B:34:ARG:HH11	1.59	1.00
1:A:20:THR:HG23	1:A:24:ASP:HB2	1.46	0.96
1:A:482:LYS:HZ2	1:A:483:GLU:H	1.08	0.96
1:B:132:GLU:HB2	1:B:134:MET:HE2	1.47	0.95
1:A:384:ASN:HD22	1:A:521:VAL:H	0.97	0.95
1:B:580:ASP:HB3	4:B:2024:HOH:O	1.66	0.95
1:B:554:ASN:HB3	1:B:557:LEU:HB3	1.48	0.94
1:B:43:ASN:HD21	1:B:57:GLY:HA3	1.34	0.93
1:B:170:THR:HG23	1:B:182:ARG:NH1	1.85	0.92
1:B:303:LEU:HD21	1:B:337:PRO:HB2	1.50	0.92
1:A:554:ASN:ND2	1:A:556:ASP:H	1.69	0.91
1:B:27:GLN:HE22	1:B:34:ARG:HH11	1.16	0.91
1:A:18:LYS:HE2	1:A:54:GLU:HG3	1.50	0.90
1:B:601:ILE:HD11	1:B:615:VAL:HG12	1.54	0.90
1:A:554:ASN:C	1:A:554:ASN:HD22	1.78	0.90
1:B:170:THR:HG23	1:B:182:ARG:HH11	1.37	0.89
1:B:593:GLN:HE21	1:B:616:ARG:HH21	0.94	0.89
1:A:531:LEU:O	1:A:535:THR:HG22	1.69	0.89
1:B:4:ILE:HG23	1:B:5:ASN:N	1.88	0.89
1:A:74:ARG:NH2	1:A:102:GLY:HA2	1.87	0.88
1:A:384:ASN:ND2	1:A:521:VAL:H	1.71	0.88
1:B:4:ILE:HG12	1:B:5:ASN:H	1.35	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:THR:HG22	1:A:480:MET:H	1.37	0.88
1:A:482:LYS:HZ2	1:A:483:GLU:N	1.71	0.88
1:A:550:ILE:HD13	1:A:565:LEU:HD23	1.56	0.88
1:B:550:ILE:HG23	1:B:601:ILE:HG22	1.55	0.87
1:B:471:LYS:HG3	1:B:473:ASP:OD1	1.75	0.87
1:A:478:THR:HG21	1:A:480:MET:HG2	1.56	0.87
1:B:478:THR:HG22	1:B:479:ALA:N	1.90	0.86
1:A:256:SER:HB3	1:A:259:VAL:HG23	1.55	0.86
1:B:4:ILE:HD11	1:B:55:THR:O	1.74	0.86
1:B:497:GLU:HA	1:B:512:ARG:HE	1.39	0.85
1:B:163:ILE:N	1:B:164:PRO:HD3	1.92	0.85
1:A:312:HIS:NE2	1:A:429:ASP:HB2	1.93	0.83
1:B:6:ILE:O	1:B:13:LYS:HB2	1.79	0.83
1:A:406:ILE:HD13	1:A:487:SER:HB3	1.60	0.83
1:B:85:ILE:HG13	1:B:108:PHE:CZ	2.14	0.83
1:B:123:GLU:HB2	1:B:197:LEU:HD12	1.60	0.83
1:A:614:ASN:HD21	1:A:623:GLN:HG3	1.44	0.82
1:B:593:GLN:NE2	1:B:616:ARG:NH2	2.18	0.82
1:B:471:LYS:CB	1:B:490:GLN:HG2	2.09	0.82
1:B:43:ASN:ND2	1:B:57:GLY:HA3	1.94	0.82
1:B:494:LEU:HD11	4:B:2005:HOH:O	1.78	0.82
1:A:204:TYR:HE1	1:A:207:GLY:HA2	1.46	0.81
1:A:440:TRP:O	1:A:444:GLU:HG3	1.81	0.81
1:B:156:LYS:HG2	1:B:180:LEU:HD12	1.62	0.81
1:B:430:LYS:HD2	1:B:436:ASP:OD2	1.80	0.81
1:A:566:GLN:HE21	1:A:577:SER:HA	1.46	0.81
1:B:521:VAL:HG22	1:B:527:PHE:CE1	2.15	0.81
1:A:616:ARG:HH21	1:A:623:GLN:HE22	1.28	0.81
1:A:553:VAL:HB	1:A:558:HIS:CE1	2.16	0.81
1:A:304:TYR:HE1	1:A:337:PRO:HG3	1.44	0.80
1:A:85:ILE:HG13	1:A:108:PHE:CE2	2.17	0.80
1:A:518:ARG:O	1:A:518:ARG:HD3	1.81	0.80
1:A:553:VAL:HB	1:A:558:HIS:ND1	1.97	0.80
1:A:482:LYS:NZ	1:A:483:GLU:H	1.79	0.80
1:A:544:ALA:O	1:A:575:ARG:NH1	2.15	0.80
1:B:563:ARG:O	1:B:563:ARG:HD3	1.81	0.79
1:B:353:LEU:HD13	1:B:390:VAL:HA	1.63	0.79
1:B:27:GLN:NE2	1:B:34:ARG:HD3	1.96	0.79
1:B:27:GLN:HE22	1:B:34:ARG:NH1	1.79	0.79
1:B:48:ASP:HB2	1:B:138:ARG:NH1	1.97	0.79
1:B:471:LYS:HB2	1:B:490:GLN:HG2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:MET:O	1:A:322:GLN:HB2	1.79	0.79
1:B:421:ARG:HH21	1:B:464:GLU:HB3	1.45	0.79
1:A:445:ASN:O	1:A:449:GLU:HG3	1.83	0.79
1:B:160:ILE:HD11	1:B:180:LEU:CD1	2.13	0.79
1:A:426:ASP:HB3	1:A:427:PRO:CD	2.13	0.78
1:B:140:VAL:HA	1:B:170:THR:HG22	1.64	0.78
1:B:46:LEU:O	1:B:184:VAL:HG11	1.84	0.78
1:B:615:VAL:HG23	1:B:623:GLN:HB3	1.63	0.78
1:A:140:VAL:HG13	1:A:170:THR:HG22	1.63	0.78
1:B:92:VAL:HB	1:B:109:ASP:HB2	1.66	0.78
1:A:612:GLN:NE2	1:A:625:THR:HG21	1.98	0.77
1:B:399:PHE:O	1:B:403:VAL:HG23	1.84	0.77
1:A:400:LYS:HG2	1:A:454:LEU:HD13	1.66	0.77
1:A:480:MET:HE3	1:A:482:LYS:HG3	1.67	0.77
1:A:204:TYR:CD2	1:A:209:SER:HA	2.20	0.77
1:B:395:ILE:CD1	1:B:514:VAL:HG21	2.13	0.77
1:B:421:ARG:NH2	1:B:464:GLU:HB3	1.99	0.77
1:B:395:ILE:CG2	1:B:491:LEU:HD11	2.14	0.76
1:B:627:GLU:HG3	1:B:630:GLU:H	1.50	0.76
1:B:126:MET:HE1	1:B:197:LEU:HD21	1.68	0.76
1:A:163:ILE:N	1:A:164:PRO:HD3	1.99	0.76
1:A:113:ASN:HA	1:A:215:GLN:NE2	2.00	0.76
1:B:353:LEU:CD1	1:B:390:VAL:HA	2.15	0.76
1:B:454:LEU:HB3	1:B:456:LEU:HD13	1.67	0.76
1:A:185:HIS:CE1	4:A:1003:HOH:O	2.38	0.76
1:A:604:GLY:O	1:A:608:VAL:HG23	1.86	0.76
1:B:490:GLN:HB2	1:B:517:HIS:HB2	1.68	0.76
1:A:618:TYR:O	1:A:620:SER:N	2.18	0.75
1:A:616:ARG:HH21	1:A:623:GLN:NE2	1.84	0.75
1:B:43:ASN:HD21	1:B:57:GLY:CA	1.98	0.75
1:B:323:LEU:HD12	1:B:324:ASP:H	1.52	0.75
1:B:521:VAL:HG22	1:B:527:PHE:CZ	2.21	0.75
1:A:554:ASN:HD22	1:A:556:ASP:H	1.33	0.75
1:B:478:THR:CG2	1:B:479:ALA:H	1.92	0.75
1:A:113:ASN:CA	1:A:215:GLN:HE22	1.99	0.74
1:B:223:PHE:O	1:B:224:ASP:HB3	1.88	0.74
1:B:18:LYS:HE3	1:B:54:GLU:OE1	1.87	0.73
1:B:143:ARG:HG2	1:B:167:GLU:OE2	1.85	0.73
1:B:353:LEU:HD13	1:B:353:LEU:O	1.88	0.73
1:B:477:LYS:HG3	1:B:483:GLU:HG2	1.70	0.73
1:A:20:THR:HG23	1:A:24:ASP:CB	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:ILE:HG22	1:B:16:PHE:H	1.54	0.73
1:B:384:ASN:HD22	1:B:521:VAL:H	1.36	0.73
1:A:589:ILE:HG23	1:A:600:GLN:HE22	1.54	0.72
1:B:312:HIS:CE1	1:B:429:ASP:HB2	2.23	0.72
1:A:262:GLY:O	1:A:263:LEU:HD23	1.90	0.72
1:A:128:GLN:HA	1:A:131:ASN:ND2	2.04	0.71
1:B:110:ILE:HB	1:B:215:GLN:HG2	1.70	0.71
1:A:256:SER:HB3	1:A:259:VAL:CG2	2.20	0.71
1:B:540:PRO:HG2	1:B:543:LEU:HD12	1.72	0.71
1:B:477:LYS:HE3	1:B:483:GLU:OE2	1.89	0.71
1:A:478:THR:CG2	1:A:480:MET:HG2	2.19	0.71
1:B:84:ALA:HB2	1:B:126:MET:HG2	1.72	0.71
1:A:591:GLU:O	1:A:595:GLN:HG3	1.91	0.71
1:A:5:ASN:O	1:A:56:ASP:HB2	1.90	0.70
1:B:340:MET:HE3	1:B:495:LEU:CD2	2.21	0.70
1:B:85:ILE:HD11	1:B:122:ILE:HD13	1.73	0.70
1:B:428:GLU:HG2	1:B:440:TRP:HE1	1.56	0.70
1:B:135:LYS:HG2	1:B:136:ILE:N	1.97	0.70
1:B:174:GLN:HG3	1:B:189:THR:HG21	1.74	0.70
1:A:132:GLU:OE1	1:A:134:MET:HE2	1.92	0.70
1:B:22:THR:HB	1:B:49:LEU:HD23	1.73	0.70
1:B:261:ALA:HB3	1:B:379:ARG:NH2	2.07	0.70
1:A:601:ILE:HD12	1:A:615:VAL:HG22	1.74	0.70
1:B:563:ARG:HA	1:B:578:ILE:HD11	1.74	0.70
1:A:89:TYR:HB2	1:A:92:VAL:CG2	2.22	0.70
1:A:114:ILE:HD11	1:A:215:GLN:CB	2.21	0.69
1:B:141:VAL:CG1	1:B:145:GLU:HB3	2.21	0.69
1:B:83:HIS:CD2	1:B:177:PHE:HB2	2.27	0.69
1:B:231:HIS:O	1:B:232:LEU:HD23	1.92	0.69
1:A:301:VAL:HG23	1:A:328:SER:O	1.91	0.69
1:B:340:MET:HE3	1:B:495:LEU:HD22	1.73	0.69
1:B:431:GLU:O	1:B:431:GLU:HG2	1.92	0.69
1:A:424:TYR:OH	1:A:448:LYS:HE3	1.92	0.69
1:A:589:ILE:HG23	1:A:600:GLN:NE2	2.07	0.69
1:A:478:THR:HG22	1:A:479:ALA:N	2.05	0.69
1:A:114:ILE:HD11	1:A:215:GLN:HB2	1.74	0.69
1:A:384:ASN:HD22	1:A:521:VAL:N	1.82	0.69
1:A:18:LYS:CE	1:A:54:GLU:HG3	2.23	0.68
1:A:449:GLU:O	1:A:453:GLU:HG3	1.93	0.68
1:B:156:LYS:CG	1:B:180:LEU:HD12	2.22	0.68
1:A:298:LEU:HD23	1:B:331:LEU:HD11	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:ILE:CG2	1:B:16:PHE:H	2.05	0.68
1:B:490:GLN:N	1:B:517:HIS:O	2.22	0.68
1:A:488:THR:O	1:A:518:ARG:HA	1.94	0.68
1:B:110:ILE:HB	1:B:215:GLN:HE21	1.59	0.68
1:B:274:ARG:O	1:B:278:GLU:HG3	1.93	0.68
1:A:616:ARG:NH2	1:A:623:GLN:HE22	1.90	0.68
1:B:351:ARG:HG3	1:B:351:ARG:HH11	1.59	0.68
1:B:160:ILE:HD11	1:B:180:LEU:HD11	1.73	0.68
1:B:518:ARG:O	1:B:518:ARG:HD3	1.93	0.68
1:A:322:GLN:OE1	1:A:323:LEU:HD12	1.94	0.68
1:A:396:LYS:HG3	1:A:446:MET:HE2	1.75	0.68
1:A:410:TYR:OH	1:A:486:LEU:HD23	1.94	0.68
1:B:287:SER:C	1:B:289:GLY:H	1.99	0.68
1:B:645:ARG:HD3	1:B:645:ARG:C	2.19	0.67
1:B:512:ARG:HG3	1:B:512:ARG:HH11	1.58	0.67
1:A:467:PHE:CD1	1:A:467:PHE:C	2.72	0.67
1:B:353:LEU:HD12	1:B:391:ARG:N	2.09	0.67
1:A:185:HIS:NE2	4:A:1003:HOH:O	2.27	0.67
1:A:8:PHE:CD2	1:A:9:PRO:HD2	2.29	0.67
1:B:74:ARG:HD2	1:B:103:GLY:HA2	1.77	0.67
1:B:494:LEU:CD2	1:B:498:ARG:HD2	2.25	0.67
1:A:340:MET:HE3	1:A:389:PHE:CZ	2.30	0.67
1:A:406:ILE:HD13	1:A:487:SER:CB	2.24	0.67
1:A:526:ARG:HH11	1:A:526:ARG:HB2	1.60	0.67
1:A:473:ASP:HB3	1:A:475:GLN:NE2	2.10	0.66
1:B:480:MET:C	1:B:482:LYS:H	2.03	0.66
1:B:612:GLN:HG2	1:B:627:GLU:HA	1.78	0.66
1:A:174:GLN:HE22	1:A:189:THR:HG21	1.60	0.66
1:B:143:ARG:HG2	1:B:143:ARG:HH11	1.59	0.66
1:B:214:LEU:HD13	1:B:214:LEU:N	2.10	0.66
1:A:319:PRO:HG2	1:B:321:MET:HB2	1.77	0.66
1:A:8:PHE:CE2	1:A:29:ILE:HD11	2.30	0.66
1:A:113:ASN:O	1:A:114:ILE:HG23	1.96	0.66
1:B:488:THR:O	1:B:518:ARG:HA	1.95	0.66
1:B:428:GLU:HG2	1:B:440:TRP:NE1	2.10	0.66
1:B:476:VAL:HG21	1:B:530:PHE:CZ	2.30	0.66
1:B:518:ARG:HD3	1:B:518:ARG:C	2.21	0.66
1:B:587:TYR:C	1:B:589:ILE:H	2.04	0.66
1:A:204:TYR:CE2	1:A:209:SER:HA	2.30	0.65
1:B:48:ASP:HB2	1:B:138:ARG:HH11	1.57	0.65
1:A:304:TYR:CE1	1:A:337:PRO:HG3	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:ILE:HG21	1:B:16:PHE:O	1.97	0.65
1:B:303:LEU:CD2	1:B:337:PRO:HB2	2.24	0.65
1:A:80:LEU:HG	1:A:126:MET:HB2	1.77	0.65
1:A:75:HIS:NE2	4:A:1003:HOH:O	2.30	0.65
1:A:323:LEU:HD13	1:A:323:LEU:O	1.95	0.65
1:B:75:HIS:CE1	1:B:181:CYS:SG	2.90	0.65
1:B:428:GLU:OE1	1:B:435:ASP:HA	1.97	0.65
1:B:497:GLU:HA	1:B:512:ARG:NE	2.10	0.65
1:A:36:LYS:HB2	1:A:36:LYS:NZ	2.12	0.65
1:A:323:LEU:HG	1:B:366:TYR:OH	1.96	0.65
1:A:454:LEU:HB3	1:A:456:LEU:CD1	2.27	0.65
1:B:579:ASP:OD2	1:B:581:ARG:NH2	2.29	0.65
1:A:146:ALA:O	1:A:149:LEU:HB3	1.96	0.65
1:A:281:ILE:CG2	1:A:282:VAL:N	2.60	0.65
1:B:160:ILE:HD11	1:B:180:LEU:HD13	1.78	0.65
1:A:8:PHE:CB	1:A:9:PRO:HD2	2.27	0.64
1:A:312:HIS:CE1	1:A:429:ASP:HB2	2.33	0.64
1:A:353:LEU:O	1:A:355:ILE:N	2.30	0.64
1:B:75:HIS:CE1	1:B:181:CYS:HG	2.15	0.64
1:A:403:VAL:HG12	1:A:407:ILE:CD1	2.28	0.64
1:A:403:VAL:HG12	1:A:407:ILE:HD12	1.80	0.64
1:B:89:TYR:OH	1:B:114:ILE:HG22	1.97	0.64
1:A:170:THR:OG1	1:A:182:ARG:HG2	1.97	0.64
1:A:305:LYS:HD3	1:A:310:TRP:CG	2.33	0.64
1:A:621:GLN:HG2	1:A:622:ASP:N	2.13	0.64
1:B:406:ILE:HD13	1:B:487:SER:HB2	1.78	0.64
1:A:323:LEU:HD11	1:A:326:THR:HG21	1.79	0.64
1:B:376:GLN:NE2	4:B:2055:HOH:O	2.31	0.64
1:B:156:LYS:CB	1:B:180:LEU:HD12	2.28	0.64
1:B:392:PRO:HA	1:B:395:ILE:HG13	1.79	0.63
1:B:213:MET:HE3	1:B:213:MET:O	1.98	0.63
1:A:478:THR:CG2	1:A:479:ALA:N	2.62	0.63
1:B:429:ASP:N	4:B:2005:HOH:O	2.32	0.63
1:B:604:GLY:O	1:B:608:VAL:HG23	1.98	0.63
1:A:194:GLU:HG3	1:A:225:LYS:HA	1.81	0.63
1:A:353:LEU:O	1:A:353:LEU:HD13	1.99	0.63
1:A:517:HIS:HB3	3:A:1002:TSB:OG1	1.99	0.63
1:B:126:MET:O	1:B:130:VAL:HG23	1.99	0.63
1:A:258:LEU:HD23	1:A:258:LEU:O	1.99	0.63
1:B:171:LEU:HD22	1:B:178:THR:CG2	2.28	0.63
1:B:25:ILE:HG21	1:B:59:ILE:CD1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:LEU:HD12	1:B:324:ASP:N	2.14	0.62
1:B:601:ILE:HG22	1:B:601:ILE:O	1.97	0.62
1:A:391:ARG:NH1	1:A:393:ASP:OD1	2.32	0.62
1:A:621:GLN:HG2	1:A:622:ASP:H	1.64	0.62
1:A:522:SER:OG	1:A:523:THR:N	2.31	0.62
1:A:110:ILE:HG22	1:A:112:GLN:H	1.65	0.62
1:A:482:LYS:NZ	1:A:482:LYS:HA	2.14	0.62
1:B:606:LYS:H	1:B:606:LYS:HD2	1.64	0.62
1:A:323:LEU:HD13	1:A:326:THR:OG1	2.00	0.62
1:A:554:ASN:ND2	1:A:554:ASN:C	2.51	0.62
1:A:621:GLN:HG2	1:A:622:ASP:CG	2.25	0.62
1:B:4:ILE:HG12	1:B:5:ASN:N	2.12	0.62
1:B:417:ASP:OD1	1:B:417:ASP:N	2.26	0.62
1:B:604:GLY:N	1:B:607:GLU:OE1	2.31	0.62
1:B:215:GLN:N	1:B:215:GLN:OE1	2.33	0.62
1:A:143:ARG:HH11	1:A:163:ILE:HA	1.63	0.62
1:A:160:ILE:HD13	1:A:180:LEU:HD11	1.81	0.62
1:A:566:GLN:HB2	1:A:578:ILE:HD11	1.81	0.62
1:A:423:SER:HB2	1:A:464:GLU:C	2.25	0.61
1:B:9:PRO:HD3	1:B:59:ILE:O	2.00	0.61
1:A:8:PHE:CG	1:A:9:PRO:HD2	2.34	0.61
1:A:115:SER:C	1:A:117:ASP:H	2.09	0.61
1:A:129:ILE:HD12	1:A:129:ILE:O	2.01	0.61
1:B:471:LYS:HB3	1:B:490:GLN:HG2	1.82	0.61
1:B:130:VAL:O	1:B:132:GLU:N	2.34	0.61
1:A:584:LYS:O	1:A:587:TYR:N	2.34	0.61
1:B:488:THR:O	1:B:488:THR:HG23	2.01	0.61
1:A:143:ARG:NH1	1:A:163:ILE:HA	2.16	0.61
1:A:645:ARG:O	1:A:645:ARG:HG2	2.00	0.61
1:A:222:PHE:HD2	1:A:228:LEU:HD12	1.64	0.61
1:A:326:THR:HG22	1:A:327:GLU:HG3	1.82	0.61
1:A:42:PHE:O	1:A:43:ASN:HB2	2.01	0.60
1:A:31:PRO:HA	1:A:34:ARG:HG2	1.83	0.60
1:A:224:ASP:HB2	4:A:1043:HOH:O	2.00	0.60
1:B:234:MET:SD	1:B:234:MET:C	2.85	0.60
1:B:621:GLN:O	1:B:623:GLN:N	2.35	0.60
1:A:321:MET:HE3	1:B:321:MET:SD	2.42	0.60
1:A:336:CYS:HB2	1:A:337:PRO:CD	2.31	0.60
1:A:340:MET:HE1	1:A:515:VAL:HG21	1.82	0.60
1:A:478:THR:HG22	1:A:480:MET:N	2.13	0.60
1:B:95:GLY:HA2	1:B:155:TYR:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ILE:HB	1:B:215:GLN:CG	2.31	0.60
1:B:404:ASN:HA	1:B:407:ILE:HD12	1.83	0.60
1:B:241:ARG:HG3	1:B:536:LYS:HG2	1.83	0.60
1:A:390:VAL:HB	1:A:394:GLN:HG3	1.83	0.60
1:B:554:ASN:HB3	1:B:557:LEU:CB	2.25	0.60
3:A:1002:TSB:H4'	4:A:1040:HOH:O	2.01	0.60
1:B:66:SER:HB3	1:B:69:ALA:HB3	1.82	0.60
1:B:304:TYR:HE1	1:B:337:PRO:HG3	1.66	0.60
1:B:545:PRO:O	1:B:575:ARG:HD2	2.01	0.60
1:A:105:TYR:HA	1:A:217:ILE:O	2.02	0.60
1:B:391:ARG:HB3	1:B:503:TYR:CZ	2.37	0.60
1:B:388:ILE:O	1:B:515:VAL:HA	2.01	0.60
1:B:186:VAL:CG1	1:B:191:LYS:HB3	2.31	0.59
1:B:326:THR:HB	4:B:2069:HOH:O	2.02	0.59
1:A:21:THR:HG22	1:A:50:THR:O	2.03	0.59
1:A:403:VAL:O	1:A:407:ILE:HD12	2.01	0.59
1:A:473:ASP:HB3	1:A:475:GLN:HE21	1.67	0.59
1:B:141:VAL:HG11	1:B:145:GLU:HB3	1.84	0.59
1:B:234:MET:SD	1:B:235:LEU:HD23	2.42	0.59
1:B:353:LEU:HD12	1:B:391:ARG:H	1.67	0.59
1:A:323:LEU:HD13	1:A:326:THR:CB	2.32	0.59
1:A:584:LYS:O	1:A:585:MET:C	2.46	0.59
1:A:524:MET:HE3	1:A:524:MET:HA	1.83	0.59
1:B:171:LEU:HD22	1:B:178:THR:HG22	1.83	0.59
1:A:73:LEU:HD22	1:A:223:PHE:CE1	2.37	0.59
1:B:41:LYS:HA	1:B:45:GLN:O	2.03	0.59
1:A:20:THR:HG21	1:A:25:ILE:HG13	1.83	0.59
1:A:324:ASP:C	1:A:326:THR:H	2.10	0.59
1:B:134:MET:HE3	1:B:174:GLN:OE1	2.02	0.59
1:B:322:GLN:HB3	1:B:328:SER:HB3	1.83	0.59
1:B:612:GLN:HA	1:B:628:LYS:H	1.68	0.59
1:A:181:CYS:HB3	4:A:1003:HOH:O	2.02	0.59
1:A:285:GLU:OE2	1:A:518:ARG:NH2	2.36	0.58
1:B:27:GLN:HA	1:B:27:GLN:HE21	1.68	0.58
1:A:235:LEU:O	1:A:239:LYS:HG3	2.03	0.58
1:B:81:MET:HA	1:B:126:MET:SD	2.43	0.58
1:B:83:HIS:NE2	1:B:177:PHE:HB2	2.19	0.58
1:A:115:SER:C	1:A:117:ASP:N	2.61	0.58
1:A:316:ASP:N	1:A:316:ASP:OD1	2.36	0.58
1:A:398:GLU:O	1:A:402:VAL:HG23	2.03	0.58
1:A:551:ILE:HG23	1:A:588:LYS:HD3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:582:ASN:O	1:B:583:GLU:HG2	2.04	0.58
1:A:388:ILE:N	1:A:388:ILE:HD12	2.17	0.58
1:B:4:ILE:CG2	1:B:16:PHE:O	2.52	0.58
1:B:579:ASP:OD1	1:B:581:ARG:NE	2.36	0.58
1:A:306:THR:O	1:A:498:ARG:HB3	2.04	0.58
1:A:308:GLY:O	1:A:312:HIS:HD2	1.87	0.58
1:B:422:LEU:HG	1:B:447:LEU:HD11	1.86	0.58
1:B:550:ILE:HG23	1:B:601:ILE:CG2	2.30	0.58
1:A:322:GLN:HG2	1:A:329:MET:HG2	1.84	0.57
1:B:565:LEU:CD2	1:B:601:ILE:HG21	2.34	0.57
1:A:554:ASN:CG	1:A:557:LEU:HB2	2.28	0.57
1:A:601:ILE:CD1	1:A:615:VAL:HG22	2.33	0.57
1:B:336:CYS:N	1:B:337:PRO:HD2	2.19	0.57
1:B:383:LEU:HD22	3:B:2002:TSB:H5'1	1.85	0.57
1:A:612:GLN:HE22	1:A:625:THR:HG21	1.67	0.57
1:B:422:LEU:HG	1:B:447:LEU:CD1	2.35	0.57
1:B:428:GLU:CG	1:B:440:TRP:HE1	2.16	0.57
1:B:471:LYS:NZ	1:B:473:ASP:OD2	2.37	0.57
1:A:242:ASP:OD1	1:A:244:ARG:HB2	2.04	0.57
1:B:110:ILE:HB	1:B:215:GLN:NE2	2.19	0.57
1:B:136:ILE:C	1:B:136:ILE:HD12	2.29	0.57
1:B:198:LEU:HG	1:B:219:GLY:HA2	1.86	0.57
1:A:186:VAL:HG13	1:A:188:SER:H	1.69	0.57
1:B:194:GLU:HG3	1:B:225:LYS:N	2.19	0.57
1:A:8:PHE:HE2	1:A:29:ILE:HD11	1.69	0.57
1:A:342:ILE:HD13	1:B:267:LEU:HD23	1.87	0.57
1:A:366:TYR:CE2	1:B:323:LEU:HB2	2.40	0.57
1:A:410:TYR:CZ	1:A:486:LEU:HD23	2.39	0.57
1:A:559:TYR:O	1:A:562:ALA:N	2.37	0.57
1:A:563:ARG:HG3	1:A:563:ARG:HH11	1.69	0.57
1:B:125:THR:O	1:B:129:ILE:HG13	2.04	0.57
1:B:553:VAL:HG23	1:B:603:VAL:O	2.04	0.57
1:A:618:TYR:C	1:A:620:SER:H	2.12	0.57
1:B:134:MET:HB2	1:B:174:GLN:OE1	2.04	0.57
1:B:521:VAL:HG13	1:B:521:VAL:O	2.05	0.57
1:B:585:MET:HA	1:B:588:LYS:HB2	1.85	0.57
1:A:4:ILE:HD13	1:A:18:LYS:HA	1.86	0.57
1:A:163:ILE:HG22	1:A:163:ILE:O	2.04	0.57
1:B:82:ALA:HB2	1:B:106:TYR:CD2	2.39	0.57
1:B:139:LYS:HE3	1:B:141:VAL:HG21	1.86	0.57
1:A:157:LEU:O	1:A:160:ILE:HG22	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:ASN:HD22	1:A:555:VAL:N	2.02	0.57
1:B:570:LYS:C	1:B:572:GLN:N	2.61	0.57
1:A:89:TYR:HB2	1:A:92:VAL:HG21	1.86	0.57
1:A:424:TYR:O	1:A:462:ILE:HD12	2.05	0.57
1:B:5:ASN:HB3	1:B:56:ASP:OD1	2.03	0.57
1:B:569:LEU:CD2	1:B:632:ILE:HG13	2.35	0.57
1:A:324:ASP:O	1:A:326:THR:N	2.37	0.56
1:A:554:ASN:ND2	1:A:557:LEU:H	2.03	0.56
1:B:66:SER:HB3	1:B:69:ALA:CB	2.34	0.56
1:B:137:GLU:O	1:B:137:GLU:HG3	2.03	0.56
1:A:288:MET:SD	1:A:405:MET:CE	2.93	0.56
1:A:454:LEU:HB3	1:A:456:LEU:HD13	1.85	0.56
1:A:518:ARG:HD3	1:A:518:ARG:C	2.27	0.56
1:A:313:TYR:CE1	1:A:316:ASP:HB2	2.41	0.56
1:B:139:LYS:HE3	1:B:141:VAL:CG2	2.36	0.56
1:B:570:LYS:C	1:B:572:GLN:H	2.13	0.56
1:A:259:VAL:O	1:B:299:ALA:HA	2.05	0.56
1:A:456:LEU:CD1	1:A:456:LEU:N	2.69	0.56
1:A:323:LEU:CD1	1:A:326:THR:CB	2.83	0.56
1:B:148:GLU:O	1:B:150:PHE:N	2.38	0.56
1:B:162:ALA:HB1	1:B:164:PRO:HD3	1.87	0.56
1:A:353:LEU:O	1:A:389:PHE:O	2.23	0.56
1:B:49:LEU:HD12	1:B:187:PRO:HG3	1.86	0.56
1:A:80:LEU:HG	1:A:126:MET:HE3	1.88	0.56
1:A:439:MET:HE1	1:A:494:LEU:HD12	1.88	0.56
1:B:322:GLN:CA	1:B:328:SER:HA	2.23	0.56
1:A:336:CYS:N	1:A:337:PRO:HD2	2.21	0.55
1:A:637:ASP:OD2	1:A:640:ARG:NH2	2.37	0.55
1:B:114:ILE:HD11	1:B:200:THR:HG21	1.88	0.55
1:B:327:GLU:OE1	1:B:327:GLU:HA	2.05	0.55
1:B:390:VAL:HB	1:B:394:GLN:OE1	2.05	0.55
1:B:473:ASP:HB3	1:B:485:THR:HG23	1.87	0.55
1:A:130:VAL:HG13	1:A:189:THR:O	2.07	0.55
1:B:188:SER:C	1:B:190:ALA:H	2.14	0.55
1:B:351:ARG:HG3	1:B:351:ARG:NH1	2.21	0.55
1:B:543:LEU:O	1:B:544:ALA:C	2.48	0.55
1:A:34:ARG:HG3	1:A:35:LYS:N	2.21	0.55
1:A:288:MET:SD	1:A:405:MET:HE3	2.46	0.55
1:B:459:GLU:O	1:B:460:GLU:C	2.49	0.55
1:A:204:TYR:CE1	1:A:207:GLY:HA2	2.35	0.55
1:A:409:VAL:O	1:A:412:ASP:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:LEU:HD21	1:B:222:PHE:O	2.06	0.55
1:A:119:PHE:O	1:A:123:GLU:HB2	2.07	0.55
1:B:193:LYS:N	1:B:193:LYS:HD2	2.22	0.55
1:A:579:ASP:OD1	1:A:588:LYS:HE2	2.07	0.55
1:A:384:ASN:ND2	1:A:521:VAL:HG12	2.22	0.55
1:A:428:GLU:CB	1:A:440:TRP:HE1	2.19	0.55
1:B:282:VAL:HG13	1:B:292:HIS:CE1	2.41	0.55
1:A:4:ILE:O	1:A:6:ILE:HG13	2.07	0.55
1:A:162:ALA:HB3	1:A:167:GLU:OE2	2.06	0.55
1:A:376:GLN:NE2	1:A:484:GLU:OE1	2.40	0.55
1:B:6:ILE:HD13	1:B:25:ILE:HD13	1.88	0.55
1:A:340:MET:HG3	1:A:501:LEU:HD11	1.88	0.55
1:A:45:GLN:NE2	4:A:1062:HOH:O	2.40	0.54
1:A:163:ILE:N	1:A:164:PRO:CD	2.69	0.54
1:A:561:TYR:O	1:A:564:GLN:HB3	2.07	0.54
1:B:430:LYS:CG	1:B:431:GLU:H	2.20	0.54
1:B:478:THR:HG21	1:B:480:MET:HE2	1.89	0.54
1:B:556:ASP:HB2	4:B:2033:HOH:O	2.07	0.54
1:A:425:ARG:NH2	1:A:437:ASP:HA	2.23	0.54
1:B:5:ASN:HB3	1:B:56:ASP:CG	2.32	0.54
1:A:568:GLU:O	1:A:571:SER:OG	2.25	0.54
1:B:136:ILE:HG13	1:B:136:ILE:O	2.05	0.54
1:B:83:HIS:CE1	1:B:177:PHE:HB2	2.42	0.54
1:B:143:ARG:O	1:B:147:LYS:HB2	2.07	0.54
1:A:4:ILE:C	1:A:56:ASP:HB3	2.32	0.54
1:A:29:ILE:O	1:A:30:SER:HB3	2.08	0.54
1:A:323:LEU:CD1	1:A:326:THR:HB	2.37	0.54
1:B:149:LEU:HG	1:B:150:PHE:CD1	2.42	0.54
1:B:214:LEU:HD13	1:B:214:LEU:H	1.71	0.54
1:B:423:SER:HB3	1:B:465:ALA:N	2.22	0.54
1:B:448:LYS:O	1:B:451:ALA:HB3	2.08	0.54
1:A:181:CYS:SG	4:A:1003:HOH:O	2.59	0.54
1:B:8:PHE:CE1	1:B:59:ILE:HD11	2.43	0.54
1:B:449:GLU:O	1:B:453:GLU:HG3	2.08	0.54
1:A:155:TYR:CD1	1:A:205:TRP:CZ3	2.96	0.54
1:A:429:ASP:O	1:A:494:LEU:HD11	2.08	0.54
1:B:210:ASN:O	1:B:211:ASN:CG	2.51	0.54
1:B:428:GLU:CB	1:B:440:TRP:HE1	2.21	0.54
1:B:644:HIS:N	1:B:644:HIS:CD2	2.74	0.54
1:A:344:ALA:O	1:A:346:LYS:N	2.41	0.53
1:B:147:LYS:HA	1:B:160:ILE:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:LEU:HD11	1:B:595:GLN:HA	1.89	0.53
1:B:445:ASN:O	1:B:449:GLU:HG3	2.08	0.53
1:A:174:GLN:O	1:A:176:ASP:N	2.38	0.53
1:A:490:GLN:CG	1:A:517:HIS:HB2	2.38	0.53
1:B:163:ILE:N	1:B:164:PRO:CD	2.68	0.53
1:B:231:HIS:O	1:B:231:HIS:ND1	2.41	0.53
1:B:244:ARG:HB3	4:B:2015:HOH:O	2.07	0.53
1:A:342:ILE:CD1	1:B:267:LEU:HD23	2.38	0.53
1:A:467:PHE:HD1	1:A:467:PHE:O	1.92	0.53
1:A:590:ARG:HG2	1:A:590:ARG:HH11	1.74	0.53
1:B:148:GLU:O	1:B:149:LEU:C	2.51	0.53
1:B:547:GLN:HG3	1:B:575:ARG:HB2	1.90	0.53
1:A:85:ILE:HG13	1:A:108:PHE:CZ	2.43	0.53
1:B:87:ARG:HD2	1:B:125:THR:HG23	1.90	0.53
1:B:287:SER:C	1:B:289:GLY:N	2.66	0.53
1:B:522:SER:OG	1:B:523:THR:N	2.39	0.53
1:A:20:THR:CG2	1:A:21:THR:N	2.70	0.53
1:A:566:GLN:NE2	1:A:578:ILE:HD12	2.24	0.53
1:B:558:HIS:NE2	1:B:604:GLY:C	2.67	0.53
1:A:21:THR:CG2	1:A:50:THR:O	2.57	0.53
1:A:212:LYS:HG3	1:A:213:MET:N	2.24	0.53
1:A:367:GLU:OE1	1:A:377:ARG:HD2	2.09	0.53
1:A:590:ARG:HG2	1:A:590:ARG:NH1	2.23	0.53
1:B:494:LEU:HD22	1:B:498:ARG:HD2	1.91	0.53
1:B:593:GLN:O	1:B:594:MET:C	2.51	0.53
1:A:391:ARG:HD3	1:A:503:TYR:CE1	2.43	0.53
1:B:475:GLN:NE2	1:B:485:THR:HG23	2.23	0.53
1:B:590:ARG:O	1:B:594:MET:HG3	2.08	0.53
1:A:37:ALA:HB3	1:A:49:LEU:HD11	1.89	0.53
1:A:340:MET:HE3	1:A:389:PHE:CE2	2.43	0.53
1:B:313:TYR:O	1:B:314:GLN:C	2.52	0.53
1:B:354:PRO:HA	1:B:390:VAL:HG12	1.91	0.53
1:A:176:ASP:C	1:A:176:ASP:OD1	2.52	0.52
1:B:105:TYR:HA	1:B:217:ILE:O	2.09	0.52
1:B:402:VAL:O	1:B:406:ILE:HG13	2.09	0.52
1:A:253:PHE:CE2	1:A:375:LEU:HG	2.45	0.52
1:A:526:ARG:HH11	1:A:526:ARG:CB	2.20	0.52
1:B:21:THR:HG22	1:B:52:PRO:HA	1.91	0.52
1:B:130:VAL:C	1:B:132:GLU:N	2.67	0.52
1:A:115:SER:O	1:A:117:ASP:N	2.42	0.52
1:A:428:GLU:OE2	1:A:435:ASP:C	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:ALA:O	1:B:480:MET:HG3	2.09	0.52
1:A:70:LEU:HD23	1:A:74:ARG:CZ	2.40	0.52
1:B:298:LEU:CD2	1:B:331:LEU:HD23	2.39	0.52
1:B:631:PHE:HD2	1:B:632:ILE:HD12	1.74	0.52
1:B:579:ASP:CG	1:B:581:ARG:HH21	2.17	0.52
1:A:245:LYS:O	1:A:249:GLU:HB2	2.10	0.52
1:A:135:LYS:HE2	1:A:137:GLU:HG2	1.92	0.52
1:B:21:THR:O	1:B:25:ILE:HG13	2.09	0.52
1:B:22:THR:HB	1:B:49:LEU:CD2	2.38	0.52
1:A:20:THR:CG2	1:A:25:ILE:HG13	2.40	0.52
1:A:337:PRO:O	1:A:340:MET:HB2	2.10	0.52
1:A:526:ARG:HH11	1:A:526:ARG:CG	2.23	0.52
1:B:223:PHE:O	1:B:224:ASP:CB	2.57	0.52
1:B:561:TYR:CD2	1:B:608:VAL:HG22	2.45	0.52
1:A:186:VAL:HG13	1:A:188:SER:O	2.09	0.52
1:A:281:ILE:HG23	1:A:282:VAL:N	2.24	0.52
1:A:388:ILE:N	1:A:388:ILE:CD1	2.72	0.52
1:A:612:GLN:NE2	1:A:625:THR:CG2	2.69	0.52
1:B:542:TRP:CZ2	1:B:543:LEU:HD21	2.45	0.52
1:B:598:PRO:HB2	1:B:599:TYR:HD1	1.75	0.52
1:A:79:HIS:CD2	1:A:185:HIS:NE2	2.78	0.52
1:A:243:HIS:HB3	1:A:533:GLU:HG3	1.92	0.52
1:A:262:GLY:C	1:A:263:LEU:HD23	2.35	0.52
1:A:322:GLN:CB	1:A:327:GLU:O	2.58	0.52
1:B:174:GLN:CG	1:B:189:THR:HG21	2.40	0.52
1:B:246:ILE:HG21	1:B:532:THR:CG2	2.40	0.52
1:B:429:ASP:O	1:B:430:LYS:HB2	2.09	0.52
1:B:434:PHE:HE2	1:B:438:ASP:OD1	1.92	0.52
1:A:298:LEU:C	1:A:298:LEU:HD12	2.35	0.51
1:B:224:ASP:OD2	1:B:226:LYS:HB3	2.10	0.51
1:A:4:ILE:HG23	1:A:18:LYS:HB2	1.91	0.51
1:A:392:PRO:HG3	4:A:1075:HOH:O	2.09	0.51
1:A:426:ASP:OD1	1:A:463:GLY:HA2	2.09	0.51
1:A:515:VAL:HG12	1:A:517:HIS:CD2	2.45	0.51
1:B:563:ARG:HG3	1:B:563:ARG:HH11	1.75	0.51
1:B:95:GLY:O	1:B:155:TYR:HB2	2.11	0.51
1:B:481:GLY:O	1:B:483:GLU:N	2.43	0.51
1:A:157:LEU:HA	1:A:160:ILE:HG22	1.92	0.51
1:A:384:ASN:HD21	1:A:520:VAL:HB	1.75	0.51
1:B:565:LEU:HD21	1:B:601:ILE:HG21	1.93	0.51
1:B:606:LYS:HD3	1:B:607:GLU:CD	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LEU:HD21	1:B:303:LEU:HA	1.93	0.51
1:B:392:PRO:HA	1:B:395:ILE:CD1	2.40	0.51
1:A:114:ILE:HD11	1:A:215:GLN:HB3	1.91	0.51
1:A:125:THR:C	1:A:127:LYS:N	2.66	0.51
1:A:321:MET:O	1:A:328:SER:HA	2.11	0.51
1:B:261:ALA:HB3	1:B:379:ARG:HH21	1.73	0.51
1:B:458:TYR:CD1	1:B:458:TYR:N	2.79	0.51
1:B:477:LYS:CE	1:B:483:GLU:OE2	2.59	0.51
1:B:615:VAL:HG23	1:B:623:GLN:CB	2.37	0.51
1:A:554:ASN:OD1	1:A:557:LEU:HB2	2.11	0.51
1:A:591:GLU:HG2	1:A:595:GLN:NE2	2.26	0.51
1:B:8:PHE:C	1:B:10:ASP:H	2.19	0.51
1:B:83:HIS:CE1	1:B:174:GLN:HE21	2.29	0.51
1:B:186:VAL:O	1:B:188:SER:N	2.44	0.51
1:A:73:LEU:HD22	1:A:223:PHE:CD1	2.46	0.51
1:A:419:SER:O	1:A:475:GLN:N	2.40	0.51
1:A:336:CYS:HA	1:A:387:HIS:CE1	2.46	0.51
1:B:42:PHE:H	1:B:47:VAL:CG1	2.24	0.51
1:B:84:ALA:HA	1:B:129:ILE:CD1	2.41	0.51
1:A:113:ASN:C	1:A:215:GLN:HE22	2.18	0.50
1:A:422:LEU:HD22	1:A:447:LEU:HD21	1.93	0.50
1:A:426:ASP:O	1:A:428:GLU:N	2.44	0.50
1:A:482:LYS:HA	1:A:482:LYS:HZ3	1.75	0.50
1:B:643:LYS:C	1:B:644:HIS:HD2	2.18	0.50
1:A:132:GLU:OE1	1:A:134:MET:CE	2.59	0.50
1:B:97:GLY:HA3	1:B:106:TYR:CD1	2.45	0.50
1:B:449:GLU:O	1:B:453:GLU:CG	2.60	0.50
1:B:467:PHE:C	1:B:467:PHE:CD1	2.88	0.50
1:A:21:THR:H	1:A:24:ASP:HB2	1.76	0.50
1:A:154:GLU:O	1:A:158:GLU:HG2	2.11	0.50
1:B:13:LYS:HD3	1:B:13:LYS:O	2.12	0.50
1:B:114:ILE:O	1:B:115:SER:HB3	2.11	0.50
1:A:428:GLU:HB3	1:A:440:TRP:HE1	1.75	0.50
1:B:1:MET:O	1:B:1:MET:HG2	2.11	0.50
1:A:322:GLN:OE1	1:A:323:LEU:CD1	2.59	0.50
1:B:139:LYS:HG2	1:B:141:VAL:HG23	1.93	0.50
1:B:383:LEU:HD12	1:B:384:ASN:H	1.77	0.50
1:B:392:PRO:HA	1:B:395:ILE:CG1	2.42	0.50
1:A:261:ALA:O	1:A:379:ARG:HD2	2.11	0.50
1:B:131:ASN:H	1:B:131:ASN:ND2	2.10	0.50
1:B:249:GLU:O	1:B:595:GLN:NE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:GLN:HG2	4:B:2059:HOH:O	2.10	0.50
1:B:439:MET:O	1:B:442:LYS:HB3	2.12	0.50
1:A:181:CYS:CB	4:A:1003:HOH:O	2.60	0.50
1:A:630:GLU:O	1:A:633:TRP:HB3	2.10	0.50
1:A:313:TYR:CD1	1:A:316:ASP:HB2	2.47	0.50
1:A:480:MET:HE3	1:A:482:LYS:CG	2.38	0.50
1:A:555:VAL:CG2	1:A:555:VAL:O	2.59	0.50
1:B:303:LEU:HD23	1:B:304:TYR:CZ	2.46	0.50
1:A:8:PHE:HB3	1:A:9:PRO:HD2	1.92	0.50
1:A:84:ALA:HB2	1:A:126:MET:HB3	1.94	0.49
1:B:129:ILE:O	1:B:129:ILE:HG22	2.12	0.49
1:B:428:GLU:OE1	1:B:435:ASP:CA	2.60	0.49
1:A:242:ASP:OD1	1:A:244:ARG:N	2.35	0.49
1:B:66:SER:O	1:B:67:GLU:C	2.54	0.49
1:B:130:VAL:C	1:B:132:GLU:H	2.20	0.49
1:B:83:HIS:HE1	1:B:174:GLN:HE21	1.58	0.49
1:B:135:LYS:CG	1:B:136:ILE:H	2.04	0.49
1:B:422:LEU:N	1:B:422:LEU:CD1	2.75	0.49
1:B:444:GLU:HG2	1:B:470:PRO:HB3	1.94	0.49
1:A:439:MET:HE1	1:A:494:LEU:CD1	2.42	0.49
1:A:566:GLN:CD	1:A:578:ILE:HD12	2.37	0.49
1:B:139:LYS:HG2	1:B:141:VAL:CG2	2.42	0.49
1:B:470:PRO:HD2	1:B:491:LEU:O	2.11	0.49
1:B:500:ASP:HA	1:B:512:ARG:NH2	2.26	0.49
1:A:110:ILE:HB	1:A:112:GLN:O	2.13	0.49
1:A:383:LEU:HD23	1:A:385:ASP:HB2	1.94	0.49
1:B:163:ILE:H	1:B:164:PRO:HD3	1.71	0.49
1:B:569:LEU:HD21	1:B:632:ILE:HG13	1.93	0.49
1:B:641:LEU:O	1:B:642:LYS:C	2.52	0.49
1:A:490:GLN:HG2	1:A:517:HIS:HB2	1.94	0.49
1:A:7:GLN:HG2	1:A:13:LYS:HG2	1.95	0.49
1:A:155:TYR:HB3	1:A:205:TRP:CZ3	2.48	0.49
1:A:174:GLN:NE2	1:A:189:THR:HG21	2.28	0.49
1:A:621:GLN:CG	1:A:622:ASP:H	2.21	0.49
1:B:452:ASP:C	1:B:454:LEU:N	2.70	0.49
1:A:5:ASN:HB3	1:A:56:ASP:OD2	2.13	0.49
1:A:322:GLN:HB3	1:A:327:GLU:O	2.13	0.49
1:A:500:ASP:HA	1:A:512:ARG:NH1	2.27	0.49
1:B:27:GLN:HE21	1:B:34:ARG:HD3	1.76	0.49
1:B:137:GLU:HG2	4:B:2021:HOH:O	2.12	0.49
1:B:187:PRO:HA	4:B:2045:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:LEU:N	1:B:422:LEU:HD12	2.27	0.49
1:B:195:PHE:CD1	1:B:195:PHE:N	2.81	0.49
1:B:318:PHE:HE1	1:B:365:ARG:O	1.96	0.49
1:B:323:LEU:HD13	1:B:324:ASP:OD2	2.12	0.49
1:B:480:MET:O	1:B:482:LYS:N	2.40	0.49
1:B:583:GLU:O	1:B:588:LYS:HE2	2.11	0.49
1:A:428:GLU:CG	1:A:440:TRP:HE1	2.26	0.49
1:A:569:LEU:HB3	1:A:574:VAL:HB	1.94	0.49
1:B:16:PHE:O	1:B:17:ASP:C	2.55	0.49
1:B:325:GLU:O	1:B:327:GLU:HG2	2.12	0.49
1:A:313:TYR:O	1:A:315:GLU:N	2.45	0.48
1:A:432:LYS:O	1:A:434:PHE:CD2	2.66	0.48
1:B:2:GLU:HA	1:B:17:ASP:HB3	1.95	0.48
1:A:554:ASN:HD21	1:A:556:ASP:HB2	1.79	0.48
1:A:602:VAL:O	1:A:614:ASN:HB3	2.12	0.48
1:B:395:ILE:HD11	1:B:514:VAL:CG2	2.20	0.48
1:B:397:GLU:OE1	1:B:398:GLU:N	2.46	0.48
1:A:399:PHE:HE2	1:A:472:LEU:HD12	1.79	0.48
1:B:355:ILE:N	4:B:2048:HOH:O	2.45	0.48
1:B:593:GLN:O	1:B:596:LYS:N	2.46	0.48
1:B:601:ILE:CD1	1:B:615:VAL:HG12	2.36	0.48
1:A:122:ILE:O	1:A:126:MET:HG2	2.13	0.48
1:B:312:HIS:HE1	1:B:429:ASP:HB2	1.75	0.48
1:A:353:LEU:CD1	1:A:390:VAL:C	2.87	0.48
1:A:486:LEU:O	1:A:522:SER:HB2	2.13	0.48
1:A:531:LEU:O	1:A:535:THR:CG2	2.54	0.48
1:B:140:VAL:HG22	1:B:170:THR:CG2	2.44	0.48
1:B:203:ALA:O	1:B:214:LEU:HD22	2.13	0.48
1:B:210:ASN:O	1:B:211:ASN:ND2	2.46	0.48
1:B:353:LEU:C	1:B:355:ILE:H	2.21	0.48
1:B:410:TYR:H	1:B:410:TYR:HD1	1.61	0.48
1:B:473:ASP:HB3	1:B:475:GLN:HE21	1.77	0.48
1:A:169:VAL:HG23	1:A:169:VAL:O	2.13	0.48
1:A:187:PRO:O	1:A:188:SER:HB2	2.13	0.48
1:A:194:GLU:HG3	1:A:225:LYS:CA	2.44	0.48
1:A:288:MET:SD	1:A:405:MET:HE1	2.54	0.48
1:A:458:TYR:N	1:A:458:TYR:CD1	2.81	0.48
1:A:555:VAL:O	1:A:555:VAL:HG23	2.13	0.48
1:B:277:ILE:O	1:B:280:TYR:HB3	2.14	0.48
1:B:598:PRO:C	1:B:599:TYR:CD1	2.91	0.48
1:A:281:ILE:HG22	1:A:282:VAL:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ARG:NH1	1:A:398:GLU:OE2	2.46	0.48
1:A:395:ILE:HG21	1:A:491:LEU:HD21	1.95	0.48
1:B:281:ILE:HG23	1:B:282:VAL:N	2.29	0.48
1:A:210:ASN:O	1:A:211:ASN:O	2.32	0.48
1:A:337:PRO:O	1:A:338:HIS:C	2.57	0.48
1:B:96:VAL:HG23	1:B:107:ASP:OD2	2.14	0.48
1:A:49:LEU:HD23	1:A:49:LEU:HA	1.73	0.48
1:A:138:ARG:HD2	1:A:138:ARG:C	2.39	0.48
1:B:132:GLU:O	1:B:133:ASN:C	2.56	0.48
1:B:392:PRO:O	1:B:395:ILE:HG13	2.14	0.48
1:B:479:ALA:C	1:B:480:MET:HG3	2.38	0.48
1:B:587:TYR:HA	1:B:590:ARG:HG2	1.96	0.48
1:B:46:LEU:O	1:B:184:VAL:CG1	2.58	0.47
1:B:389:PHE:HE2	1:B:501:LEU:HD13	1.78	0.47
1:A:79:HIS:O	1:A:80:LEU:C	2.56	0.47
1:A:74:ARG:HH22	1:A:102:GLY:HA2	1.77	0.47
1:B:394:GLN:O	1:B:396:LYS:N	2.48	0.47
1:B:502:THR:HA	1:B:513:PRO:HD3	1.96	0.47
1:B:595:GLN:O	1:B:597:ILE:HG13	2.15	0.47
1:A:81:MET:HE2	1:A:104:PHE:HE2	1.80	0.47
1:A:374:GLY:C	1:A:376:GLN:H	2.23	0.47
1:B:55:THR:HB	1:B:56:ASP:H	1.58	0.47
1:B:110:ILE:CB	1:B:215:GLN:HE21	2.26	0.47
1:A:321:MET:HE3	1:B:321:MET:CE	2.45	0.47
1:A:410:TYR:HH	1:A:487:SER:HG	1.56	0.47
1:B:85:ILE:CD1	1:B:122:ILE:HD13	2.44	0.47
1:B:172:TYR:CD1	1:B:173:SER:N	2.82	0.47
1:B:473:ASP:HB3	1:B:475:GLN:NE2	2.29	0.47
1:B:574:VAL:HG12	1:B:575:ARG:N	2.30	0.47
1:A:253:PHE:HA	1:A:267:LEU:HG	1.95	0.47
1:A:349:SER:O	1:A:352:GLU:HG2	2.13	0.47
1:B:561:TYR:HE2	1:B:603:VAL:HG11	1.78	0.47
1:A:277:ILE:CG2	1:A:524:MET:HE1	2.45	0.47
1:A:399:PHE:CE2	1:A:472:LEU:HD12	2.49	0.47
1:A:425:ARG:HA	1:A:440:TRP:CZ3	2.50	0.47
1:A:471:LYS:HA	1:A:490:GLN:HA	1.97	0.47
1:A:500:ASP:HA	1:A:512:ARG:HH12	1.79	0.47
1:A:549:GLN:HA	1:A:549:GLN:OE1	2.14	0.47
1:A:602:VAL:HG23	4:A:1019:HOH:O	2.13	0.47
1:A:605:ASP:O	1:A:606:LYS:C	2.55	0.47
1:B:93:LYS:HB2	1:B:93:LYS:NZ	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:VAL:HG22	4:B:2004:HOH:O	2.14	0.47
1:B:410:TYR:N	1:B:410:TYR:CD1	2.81	0.47
1:A:423:SER:HB3	1:A:464:GLU:CB	2.44	0.47
1:A:610:ASN:HB3	4:A:1004:HOH:O	2.15	0.47
1:B:46:LEU:HG	1:B:184:VAL:HG11	1.97	0.47
1:B:130:VAL:HG13	1:B:190:ALA:HA	1.97	0.47
1:B:155:TYR:CZ	1:B:159:LEU:HD22	2.50	0.47
1:B:174:GLN:O	1:B:174:GLN:NE2	2.47	0.47
1:B:587:TYR:C	1:B:589:ILE:N	2.67	0.47
1:A:71:GLU:HB3	4:A:1068:HOH:O	2.15	0.47
1:A:391:ARG:H	1:A:394:GLN:CG	2.28	0.47
1:A:625:THR:CG2	1:A:626:VAL:N	2.78	0.47
1:B:19:GLY:O	1:B:20:THR:C	2.58	0.47
1:A:611:ASN:HD22	1:A:611:ASN:HA	1.56	0.47
1:B:123:GLU:HB2	1:B:197:LEU:CD1	2.37	0.47
1:A:46:LEU:HG	4:A:1021:HOH:O	2.14	0.46
1:A:297:VAL:HG23	1:A:362:THR:O	2.14	0.46
1:A:386:SER:HB3	1:A:518:ARG:HD2	1.97	0.46
1:A:399:PHE:O	1:A:403:VAL:HG23	2.15	0.46
1:A:627:GLU:O	1:A:628:LYS:C	2.54	0.46
1:B:194:GLU:CD	1:B:225:LYS:HG2	2.40	0.46
1:B:633:TRP:CD1	1:B:633:TRP:C	2.93	0.46
1:A:205:TRP:O	1:A:207:GLY:N	2.47	0.46
1:A:323:LEU:O	1:A:324:ASP:O	2.33	0.46
1:A:502:THR:HA	1:A:513:PRO:HD3	1.96	0.46
1:B:395:ILE:HG23	1:B:491:LEU:HD11	1.96	0.46
1:A:72:VAL:O	1:A:73:LEU:C	2.58	0.46
1:A:447:LEU:HD11	1:A:471:LYS:C	2.40	0.46
1:B:202:GLY:O	1:B:203:ALA:HB2	2.15	0.46
1:B:340:MET:HE3	1:B:495:LEU:HD23	1.97	0.46
1:B:423:SER:HB3	1:B:464:GLU:C	2.40	0.46
1:A:8:PHE:CZ	1:A:29:ILE:HD11	2.51	0.46
1:A:191:LYS:HE3	4:A:1007:HOH:O	2.14	0.46
1:A:454:LEU:HB3	1:A:456:LEU:HD11	1.97	0.46
1:B:222:PHE:CD2	1:B:228:LEU:HD13	2.51	0.46
1:B:459:GLU:O	1:B:460:GLU:O	2.33	0.46
1:A:34:ARG:O	1:A:36:LYS:N	2.47	0.46
1:B:140:VAL:HG22	1:B:170:THR:HG22	1.98	0.46
1:B:388:ILE:HG21	1:B:398:GLU:HG2	1.97	0.46
1:B:467:PHE:CD1	1:B:468:TYR:N	2.84	0.46
1:A:406:ILE:HG21	1:A:474:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:LYS:NZ	1:A:473:ASP:OD2	2.48	0.46
1:A:476:VAL:HG13	1:A:530:PHE:CE1	2.50	0.46
1:B:87:ARG:O	1:B:88:LEU:HB2	2.15	0.46
1:A:157:LEU:O	1:A:160:ILE:CG2	2.64	0.46
1:A:469:GLY:HA3	1:A:491:LEU:O	2.16	0.46
1:A:150:PHE:O	1:A:157:LEU:HD21	2.15	0.46
1:A:177:PHE:CZ	1:A:179:ASP:HB2	2.51	0.46
1:A:581:ARG:O	1:A:588:LYS:NZ	2.45	0.46
1:B:396:LYS:HG3	1:B:397:GLU:N	2.31	0.46
1:A:38:VAL:O	1:A:187:PRO:HD3	2.16	0.46
1:A:109:ASP:OD2	1:A:155:TYR:OH	2.26	0.46
1:B:39:ALA:O	1:B:62:VAL:HB	2.16	0.46
1:B:236:GLU:O	1:B:240:GLU:HG2	2.16	0.46
1:B:478:THR:CG2	1:B:479:ALA:N	2.62	0.46
1:B:550:ILE:HG21	1:B:562:ALA:HB1	1.97	0.46
1:B:27:GLN:NE2	1:B:27:GLN:HA	2.29	0.46
1:B:105:TYR:CD1	1:B:105:TYR:C	2.93	0.46
1:B:156:LYS:HB3	1:B:180:LEU:HD12	1.96	0.46
1:A:125:THR:O	1:A:129:ILE:HG23	2.17	0.45
1:A:323:LEU:CG	1:B:366:TYR:OH	2.63	0.45
1:A:471:LYS:HG2	1:A:490:GLN:HB3	1.96	0.45
1:A:478:THR:CG2	1:A:479:ALA:H	2.29	0.45
1:A:499:PHE:O	1:A:500:ASP:C	2.59	0.45
1:B:426:ASP:O	1:B:427:PRO:C	2.59	0.45
1:B:605:ASP:O	1:B:609:GLU:HB2	2.16	0.45
1:A:73:LEU:HB2	1:A:223:PHE:CZ	2.50	0.45
1:A:335:ASN:HB2	1:A:385:ASP:OD2	2.16	0.45
1:B:70:LEU:HD22	1:B:74:ARG:CZ	2.46	0.45
1:B:383:LEU:HA	1:B:523:THR:HA	1.98	0.45
1:B:623:GLN:O	1:B:624:GLU:C	2.59	0.45
1:A:186:VAL:HG22	1:A:187:PRO:HD2	1.98	0.45
1:A:298:LEU:CD2	1:B:331:LEU:HD11	2.44	0.45
1:B:544:ALA:O	1:B:545:PRO:C	2.59	0.45
1:B:547:GLN:OE1	1:B:574:VAL:HG13	2.16	0.45
1:A:435:ASP:O	1:A:436:ASP:C	2.60	0.45
1:B:17:ASP:OD1	1:B:17:ASP:N	2.50	0.45
1:B:73:LEU:HD22	1:B:223:PHE:CD1	2.51	0.45
1:B:124:LYS:O	1:B:128:GLN:HB2	2.17	0.45
1:B:636:VAL:HA	1:B:639:ILE:HD12	1.98	0.45
1:A:195:PHE:HA	1:A:221:ALA:HA	1.98	0.45
1:A:203:ALA:O	1:A:214:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:TYR:CE2	1:A:511:HIS:HB3	2.51	0.45
1:B:234:MET:SD	1:B:235:LEU:N	2.90	0.45
1:B:622:ASP:O	1:B:623:GLN:C	2.60	0.45
1:A:40:GLY:HA2	1:A:62:VAL:HG23	1.98	0.45
1:A:93:LYS:HB3	1:A:153:ASP:OD1	2.16	0.45
1:A:97:GLY:HA3	1:A:106:TYR:CE2	2.52	0.45
1:B:303:LEU:HD23	1:B:304:TYR:CE1	2.51	0.45
1:B:501:LEU:O	1:B:513:PRO:HD2	2.16	0.45
1:A:521:VAL:HG22	1:A:527:PHE:CE1	2.52	0.45
1:B:83:HIS:CE1	1:B:174:GLN:NE2	2.84	0.45
1:B:99:VAL:HG12	1:B:104:PHE:HB3	1.97	0.45
1:B:614:ASN:HB2	1:B:625:THR:HG22	1.98	0.45
1:A:428:GLU:HG2	1:A:429:ASP:N	2.32	0.45
1:B:425:ARG:NH1	4:B:2003:HOH:O	2.49	0.45
1:B:430:LYS:CG	1:B:431:GLU:N	2.79	0.45
1:B:487:SER:HB3	1:B:520:VAL:O	2.16	0.45
1:B:512:ARG:HG3	1:B:512:ARG:NH1	2.27	0.45
1:B:602:VAL:O	1:B:614:ASN:HB3	2.17	0.45
1:B:614:ASN:HA	1:B:625:THR:HA	1.99	0.45
1:A:5:ASN:C	1:A:56:ASP:HB2	2.41	0.45
1:A:388:ILE:HG21	1:A:398:GLU:HG2	1.98	0.45
1:A:589:ILE:O	1:A:589:ILE:HG22	2.16	0.45
1:B:62:VAL:HG13	1:B:69:ALA:HB2	1.98	0.45
1:B:93:LYS:HB2	1:B:93:LYS:HZ2	1.82	0.45
1:B:143:ARG:HH11	1:B:143:ARG:CG	2.27	0.45
1:B:421:ARG:C	1:B:422:LEU:HD12	2.42	0.45
1:B:435:ASP:O	1:B:436:ASP:C	2.60	0.45
1:B:75:HIS:O	1:B:78:ALA:HB3	2.17	0.45
1:B:298:LEU:HD23	1:B:331:LEU:HD23	1.97	0.45
1:B:422:LEU:HD13	1:B:458:TYR:HB3	1.99	0.45
1:A:353:LEU:CD1	1:A:390:VAL:HA	2.47	0.44
1:A:404:ASN:O	1:A:408:ASP:N	2.42	0.44
1:A:521:VAL:HG22	1:A:527:PHE:CD1	2.52	0.44
1:B:27:GLN:HE21	1:B:27:GLN:CA	2.26	0.44
1:B:222:PHE:HD2	1:B:228:LEU:HD13	1.82	0.44
1:B:473:ASP:HB3	1:B:485:THR:CG2	2.47	0.44
1:A:114:ILE:HG12	1:A:215:GLN:NE2	2.32	0.44
1:A:123:GLU:HA	1:A:126:MET:HG2	1.98	0.44
1:A:249:GLU:HB3	1:A:250:LEU:HD13	2.00	0.44
1:A:398:GLU:HA	1:A:401:ARG:HH21	1.81	0.44
1:A:458:TYR:C	1:A:459:GLU:HG2	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:MET:O	1:A:586:GLY:C	2.58	0.44
1:B:43:ASN:ND2	1:B:57:GLY:CA	2.69	0.44
1:B:167:GLU:O	1:B:167:GLU:CG	2.65	0.44
1:B:428:GLU:OE1	1:B:428:GLU:C	2.60	0.44
1:B:428:GLU:CD	1:B:435:ASP:HB3	2.42	0.44
1:B:585:MET:O	1:B:586:GLY:C	2.58	0.44
1:A:180:LEU:HD23	1:A:180:LEU:O	2.18	0.44
1:A:349:SER:C	1:A:351:ARG:N	2.72	0.44
1:B:313:TYR:O	1:B:315:GLU:N	2.50	0.44
1:B:315:GLU:H	1:B:315:GLU:HG2	1.48	0.44
1:B:388:ILE:HG22	1:B:390:VAL:HG13	1.98	0.44
1:B:612:GLN:HB3	1:B:626:VAL:O	2.17	0.44
1:A:36:LYS:HB2	1:A:36:LYS:HZ2	1.81	0.44
1:A:157:LEU:HA	1:A:160:ILE:CG2	2.47	0.44
1:A:181:CYS:SG	1:A:182:ARG:N	2.90	0.44
1:A:205:TRP:NE1	1:A:206:ARG:HG3	2.33	0.44
1:A:296:PRO:HG3	4:B:2009:HOH:O	2.16	0.44
1:A:326:THR:O	1:A:327:GLU:CG	2.65	0.44
1:A:589:ILE:O	1:A:589:ILE:CG2	2.66	0.44
1:B:126:MET:C	1:B:128:GLN:H	2.24	0.44
1:B:147:LYS:CA	1:B:160:ILE:HG21	2.47	0.44
1:B:268:PRO:O	1:B:269:ASN:C	2.60	0.44
1:A:548:VAL:O	1:A:576:VAL:HA	2.17	0.44
1:B:79:HIS:CD2	1:B:172:TYR:OH	2.71	0.44
1:B:84:ALA:HB2	1:B:126:MET:CG	2.44	0.44
1:B:202:GLY:HA2	1:B:214:LEU:O	2.17	0.44
1:B:283:ASP:HB2	4:B:2026:HOH:O	2.18	0.44
1:B:350:TYR:CE2	1:B:506:GLN:HA	2.53	0.44
1:B:378:VAL:HG23	1:B:379:ARG:N	2.33	0.44
1:B:379:ARG:NH2	4:B:2038:HOH:O	2.31	0.44
1:B:534:GLU:OE1	1:B:534:GLU:HA	2.18	0.44
1:A:84:ALA:HB1	1:A:125:THR:HG22	1.97	0.44
1:A:561:TYR:CD2	1:A:608:VAL:HG22	2.53	0.44
1:B:410:TYR:HD1	1:B:410:TYR:N	2.16	0.44
1:B:434:PHE:O	1:B:435:ASP:HB2	2.17	0.44
1:B:554:ASN:O	1:B:557:LEU:N	2.47	0.44
1:B:561:TYR:CE2	1:B:603:VAL:HG11	2.53	0.44
1:B:597:ILE:HA	1:B:598:PRO:HD2	1.74	0.44
1:B:602:VAL:HG23	1:B:614:ASN:OD1	2.18	0.44
1:A:323:LEU:O	1:A:323:LEU:CD1	2.66	0.44
1:A:559:TYR:O	1:A:560:ASP:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:ILE:HG21	1:A:616:ARG:HH12	1.83	0.44
1:A:612:GLN:HB2	1:A:626:VAL:O	2.18	0.44
1:B:8:PHE:O	1:B:10:ASP:N	2.51	0.44
1:B:42:PHE:HD1	1:B:59:ILE:HG23	1.83	0.44
1:B:261:ALA:N	4:B:2038:HOH:O	2.48	0.44
1:B:434:PHE:O	1:B:434:PHE:CD1	2.71	0.44
1:B:540:PRO:CG	1:B:543:LEU:HD12	2.45	0.44
1:A:323:LEU:HD13	1:A:326:THR:HB	1.99	0.44
1:A:558:HIS:NE2	1:A:605:ASP:OD1	2.43	0.44
1:B:131:ASN:ND2	1:B:131:ASN:N	2.64	0.44
1:B:297:VAL:O	1:B:332:ARG:HG2	2.18	0.44
1:B:331:LEU:HB3	4:B:2032:HOH:O	2.18	0.44
1:B:377:ARG:HA	3:B:2002:TSB:N1	2.32	0.44
1:B:422:LEU:HD13	1:B:458:TYR:CB	2.48	0.44
1:B:638:GLU:O	1:B:638:GLU:HG2	2.18	0.44
1:B:172:TYR:O	1:B:178:THR:HG23	2.17	0.44
1:B:186:VAL:O	1:B:187:PRO:C	2.59	0.44
1:B:186:VAL:HG11	1:B:191:LYS:HB3	2.00	0.44
1:B:267:LEU:O	1:B:268:PRO:C	2.61	0.44
1:B:621:GLN:H	1:B:621:GLN:CD	2.26	0.44
1:A:34:ARG:HG3	1:A:35:LYS:H	1.83	0.43
1:A:186:VAL:CG1	1:A:188:SER:O	2.66	0.43
1:B:163:ILE:HG22	1:B:163:ILE:O	2.18	0.43
1:B:322:GLN:OE1	1:B:322:GLN:N	2.51	0.43
1:B:598:PRO:O	1:B:617:GLN:HA	2.18	0.43
1:A:80:LEU:CG	1:A:126:MET:HB2	2.48	0.43
1:A:259:VAL:O	1:B:300:ASN:N	2.46	0.43
1:A:338:HIS:O	1:A:341:MET:HB2	2.19	0.43
1:A:639:ILE:O	1:A:640:ARG:C	2.61	0.43
1:B:458:TYR:HD2	1:B:460:GLU:HG3	1.83	0.43
1:A:142:SER:O	1:A:143:ARG:C	2.62	0.43
1:A:499:PHE:HB2	1:A:501:LEU:HG	2.00	0.43
1:B:42:PHE:H	1:B:47:VAL:HG13	1.83	0.43
1:B:250:LEU:HD13	1:B:250:LEU:HA	1.66	0.43
1:B:452:ASP:O	1:B:453:GLU:C	2.61	0.43
1:B:569:LEU:HD23	1:B:632:ILE:HG13	1.99	0.43
1:B:595:GLN:O	1:B:596:LYS:C	2.61	0.43
1:B:606:LYS:HD3	1:B:607:GLU:OE2	2.17	0.43
1:A:224:ASP:OD1	1:A:226:LYS:HB2	2.19	0.43
1:A:250:LEU:CD1	1:A:250:LEU:N	2.81	0.43
1:A:410:TYR:OH	1:A:486:LEU:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:LYS:HE3	1:A:493:PHE:CE1	2.53	0.43
1:A:494:LEU:O	1:A:497:GLU:HB2	2.19	0.43
1:B:422:LEU:HD21	1:B:451:ALA:CB	2.48	0.43
1:B:450:ALA:HA	1:B:453:GLU:HG3	2.00	0.43
1:B:559:TYR:CE2	1:B:563:ARG:HG3	2.53	0.43
1:A:145:GLU:H	1:A:145:GLU:CD	2.27	0.43
1:A:374:GLY:O	1:A:376:GLN:N	2.47	0.43
1:A:423:SER:HB3	1:A:464:GLU:HB2	2.01	0.43
1:B:42:PHE:CD1	1:B:53:LEU:HD13	2.53	0.43
1:B:343:TYR:O	1:B:348:HIS:NE2	2.48	0.43
1:B:613:VAL:HG13	1:B:628:LYS:HA	2.00	0.43
1:A:47:VAL:HB	1:A:51:LYS:HG2	2.01	0.43
1:A:229:LYS:O	1:A:233:GLN:HG3	2.18	0.43
1:B:204:TYR:HA	1:B:213:MET:HA	1.99	0.43
1:B:243:HIS:HB3	1:B:533:GLU:HG3	1.99	0.43
1:B:480:MET:C	1:B:482:LYS:N	2.72	0.43
1:B:486:LEU:HD12	1:B:486:LEU:HA	1.82	0.43
1:A:34:ARG:C	1:A:36:LYS:H	2.25	0.43
1:A:80:LEU:CD1	1:A:129:ILE:HG12	2.49	0.43
1:A:110:ILE:HG22	1:A:112:GLN:N	2.32	0.43
1:A:526:ARG:CG	1:A:526:ARG:NH1	2.81	0.43
1:A:106:TYR:CD1	1:A:108:PHE:CE1	3.06	0.43
1:A:311:ASP:HB2	1:A:312:HIS:CD2	2.54	0.43
1:B:292:HIS:HA	1:B:358:ALA:O	2.19	0.43
1:A:155:TYR:O	1:A:159:LEU:HD13	2.18	0.43
1:A:236:GLU:OE2	1:A:239:LYS:HD2	2.19	0.43
1:A:340:MET:HE3	1:A:389:PHE:HZ	1.80	0.43
1:B:45:GLN:HB3	1:B:47:VAL:HG12	1.99	0.43
1:B:72:VAL:HG22	1:B:184:VAL:HG22	2.00	0.43
1:B:119:PHE:O	1:B:123:GLU:N	2.48	0.43
1:B:298:LEU:HD21	1:B:331:LEU:HD23	2.01	0.43
1:A:109:ASP:C	1:A:109:ASP:OD1	2.62	0.43
1:A:376:GLN:O	1:A:526:ARG:NH1	2.52	0.43
1:B:48:ASP:OD1	1:B:49:LEU:N	2.52	0.43
1:B:167:GLU:O	1:B:167:GLU:HG2	2.19	0.43
1:B:281:ILE:CG2	1:B:282:VAL:N	2.82	0.43
1:A:128:GLN:HA	1:A:131:ASN:HD22	1.81	0.42
1:A:151:SER:O	1:A:153:ASP:N	2.52	0.42
1:A:353:LEU:HD22	1:A:353:LEU:HA	1.78	0.42
1:A:385:ASP:OD1	1:A:386:SER:N	2.52	0.42
1:A:391:ARG:O	1:A:392:PRO:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:ASN:ND2	1:A:556:ASP:N	2.51	0.42
1:B:165:GLU:O	1:B:166:ASP:HB3	2.19	0.42
1:B:458:TYR:CD2	1:B:460:GLU:HG3	2.54	0.42
1:B:631:PHE:CD2	1:B:632:ILE:HD12	2.54	0.42
1:A:157:LEU:CA	1:A:160:ILE:HG22	2.49	0.42
1:A:326:THR:O	1:A:327:GLU:HG2	2.20	0.42
1:B:42:PHE:CB	1:B:47:VAL:HG11	2.49	0.42
1:B:87:ARG:HH12	1:B:128:GLN:HG3	1.83	0.42
1:B:231:HIS:O	1:B:231:HIS:CG	2.71	0.42
1:B:384:ASN:ND2	1:B:521:VAL:H	2.12	0.42
1:B:428:GLU:OE2	1:B:435:ASP:HB3	2.18	0.42
1:A:6:ILE:HD13	1:A:25:ILE:HD11	2.02	0.42
1:A:162:ALA:O	1:A:167:GLU:OE1	2.38	0.42
1:A:265:LEU:HD23	1:B:296:PRO:CD	2.49	0.42
1:A:300:ASN:HD22	1:A:327:GLU:HB3	1.84	0.42
1:B:49:LEU:HD23	1:B:49:LEU:HA	1.86	0.42
1:B:186:VAL:HA	1:B:187:PRO:HD2	1.76	0.42
1:B:494:LEU:HD21	1:B:498:ARG:HD2	1.99	0.42
1:A:20:THR:HG22	1:A:21:THR:N	2.33	0.42
1:A:367:GLU:O	1:A:368:ALA:C	2.62	0.42
1:B:336:CYS:HA	1:B:387:HIS:CE1	2.55	0.42
1:B:391:ARG:HB3	1:B:503:TYR:OH	2.19	0.42
1:A:108:PHE:O	1:A:214:LEU:HG	2.19	0.42
1:A:155:TYR:HB3	1:A:205:TRP:HZ3	1.84	0.42
1:A:281:ILE:HD12	1:A:281:ILE:HA	1.74	0.42
1:B:353:LEU:C	1:B:355:ILE:N	2.78	0.42
1:A:255:ASN:ND2	1:A:255:ASN:N	2.64	0.42
1:A:580:ASP:OD1	1:A:580:ASP:C	2.63	0.42
1:A:625:THR:HG22	1:A:626:VAL:N	2.35	0.42
1:B:51:LYS:HA	1:B:52:PRO:HD3	1.87	0.42
1:B:74:ARG:CG	1:B:221:ALA:HB3	2.20	0.42
1:B:81:MET:O	1:B:85:ILE:HG12	2.20	0.42
1:B:471:LYS:HB2	1:B:490:GLN:CG	2.41	0.42
1:A:79:HIS:NE2	4:A:1003:HOH:O	2.11	0.42
1:A:162:ALA:C	1:A:164:PRO:HD3	2.42	0.42
1:A:563:ARG:HH11	1:A:563:ARG:CG	2.31	0.42
1:B:71:GLU:O	1:B:75:HIS:N	2.43	0.42
1:B:205:TRP:HB2	1:B:211:ASN:ND2	2.35	0.42
1:A:258:LEU:O	1:A:258:LEU:CD2	2.67	0.42
1:A:353:LEU:HD12	1:A:391:ARG:N	2.34	0.42
1:A:566:GLN:NE2	1:A:577:SER:HA	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ASP:HB2	1:B:156:LYS:HD2	2.01	0.42
1:A:125:THR:C	1:A:127:LYS:H	2.28	0.42
1:A:265:LEU:HD23	1:B:296:PRO:HD3	2.02	0.42
1:A:335:ASN:O	1:A:336:CYS:C	2.63	0.42
1:A:363:MET:O	1:A:381:MET:HG2	2.20	0.42
1:B:352:GLU:O	1:B:355:ILE:HG13	2.19	0.42
1:B:553:VAL:HG21	1:B:604:GLY:HA3	2.02	0.42
1:A:256:SER:OG	1:B:341:MET:HE2	2.20	0.42
1:A:460:GLU:OE1	1:A:460:GLU:HA	2.20	0.42
1:A:471:LYS:NZ	1:A:473:ASP:CG	2.77	0.42
1:A:546:LYS:HE2	1:A:577:SER:OG	2.20	0.42
1:B:85:ILE:HG13	1:B:108:PHE:CE2	2.54	0.42
1:B:92:VAL:HB	1:B:109:ASP:CB	2.44	0.42
1:B:135:LYS:O	1:B:174:GLN:HG2	2.19	0.42
1:B:409:VAL:O	1:B:410:TYR:C	2.63	0.42
1:A:34:ARG:NH2	4:A:1045:HOH:O	2.48	0.41
1:A:277:ILE:HG21	1:A:524:MET:HE1	2.02	0.41
1:A:363:MET:HE3	1:A:363:MET:HB2	1.76	0.41
1:A:589:ILE:CG2	1:A:616:ARG:NH1	2.83	0.41
1:B:8:PHE:HB3	1:B:10:ASP:OD1	2.20	0.41
1:A:400:LYS:CG	1:A:454:LEU:HD13	2.43	0.41
1:A:644:HIS:ND1	1:A:645:ARG:N	2.68	0.41
1:B:334:MET:SD	3:B:2002:TSB:N	2.83	0.41
1:B:448:LYS:HD3	1:B:460:GLU:OE2	2.19	0.41
1:B:545:PRO:HB2	4:B:2012:HOH:O	2.19	0.41
1:A:364:HIS:HA	1:A:379:ARG:O	2.20	0.41
1:B:33:LEU:O	1:B:37:ALA:N	2.42	0.41
1:B:107:ASP:OD1	1:B:216:ARG:HB2	2.20	0.41
1:A:70:LEU:CD2	1:A:74:ARG:CZ	2.99	0.41
1:A:637:ASP:CG	1:A:640:ARG:NH2	2.78	0.41
1:A:645:ARG:O	1:A:645:ARG:CG	2.62	0.41
1:B:94:PHE:CE2	1:B:108:PHE:HE1	2.39	0.41
1:B:430:LYS:HG2	1:B:431:GLU:H	1.85	0.41
1:A:114:ILE:HG12	1:A:215:GLN:CD	2.46	0.41
1:A:447:LEU:C	1:A:447:LEU:HD23	2.46	0.41
1:A:490:GLN:HG2	1:A:490:GLN:H	1.55	0.41
1:A:566:GLN:CD	1:A:578:ILE:CD1	2.93	0.41
1:B:82:ALA:HB1	1:B:94:PHE:CD2	2.55	0.41
1:B:114:ILE:HG13	1:B:115:SER:N	2.35	0.41
1:B:402:VAL:HG22	1:B:403:VAL:N	2.34	0.41
1:A:8:PHE:CB	1:A:9:PRO:CD	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLN:OE1	1:A:27:GLN:HA	2.21	0.41
1:A:83:HIS:ND1	1:A:177:PHE:HB3	2.36	0.41
1:B:23:GLU:O	1:B:26:ALA:HB3	2.21	0.41
1:B:203:ALA:O	1:B:214:LEU:CD2	2.69	0.41
1:B:636:VAL:O	1:B:639:ILE:HB	2.20	0.41
1:A:36:LYS:HE3	1:A:63:THR:OG1	2.21	0.41
1:A:204:TYR:HE1	1:A:207:GLY:CA	2.25	0.41
1:A:340:MET:CE	1:A:389:PHE:CE2	3.04	0.41
1:A:414:GLY:HA3	1:A:644:HIS:CE1	2.55	0.41
1:A:480:MET:HE3	1:A:482:LYS:HB2	2.02	0.41
1:B:72:VAL:HG22	1:B:184:VAL:CG2	2.50	0.41
1:B:252:LEU:HD22	1:B:270:GLY:HA2	2.03	0.41
1:B:422:LEU:HD21	1:B:451:ALA:HB2	2.03	0.41
1:A:7:GLN:O	1:A:58:SER:HA	2.20	0.41
1:A:45:GLN:O	1:A:47:VAL:HG13	2.21	0.41
1:A:428:GLU:CD	1:A:428:GLU:C	2.88	0.41
1:A:480:MET:HE3	1:A:482:LYS:CB	2.51	0.41
1:A:584:LYS:O	1:A:587:TYR:HB3	2.21	0.41
1:B:143:ARG:HG2	1:B:143:ARG:NH1	2.31	0.41
1:B:143:ARG:NH2	1:B:160:ILE:O	2.54	0.41
1:B:174:GLN:HE21	1:B:174:GLN:HB3	1.64	0.41
1:B:267:LEU:HB3	4:B:2014:HOH:O	2.20	0.41
1:B:304:TYR:OH	1:B:332:ARG:HB3	2.21	0.41
1:B:521:VAL:CG2	1:B:527:PHE:CE1	2.97	0.41
1:A:348:HIS:HA	1:A:352:GLU:OE2	2.21	0.41
1:A:353:LEU:HD13	1:A:390:VAL:HA	2.03	0.41
1:A:521:VAL:CG2	1:A:527:PHE:CE1	3.03	0.41
1:B:45:GLN:C	1:B:47:VAL:H	2.28	0.41
1:B:94:PHE:HE2	1:B:108:PHE:HE1	1.69	0.41
1:B:100:ILE:HB	1:B:101:GLU:H	1.49	0.41
1:B:349:SER:C	1:B:351:ARG:N	2.77	0.41
1:B:440:TRP:O	1:B:441:ASN:C	2.63	0.41
1:B:581:ARG:HE	1:B:581:ARG:HB2	1.75	0.41
1:B:585:MET:CE	1:B:602:VAL:HG11	2.51	0.41
1:B:628:LYS:O	1:B:632:ILE:HD13	2.21	0.41
1:A:482:LYS:HZ2	1:A:482:LYS:CA	2.34	0.41
1:A:501:LEU:C	1:A:502:THR:HG22	2.45	0.41
1:A:542:TRP:CE2	1:A:543:LEU:HG	2.55	0.41
1:B:129:ILE:HG23	1:B:134:MET:HE1	2.03	0.41
1:B:172:TYR:CD1	1:B:172:TYR:C	2.99	0.41
1:B:424:TYR:O	1:B:465:ALA:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:MET:SD	1:A:197:LEU:HD21	2.61	0.40
1:A:293:VAL:HB	1:B:266:TRP:O	2.20	0.40
1:A:349:SER:C	1:A:351:ARG:H	2.29	0.40
1:B:83:HIS:CG	1:B:177:PHE:HB2	2.55	0.40
1:B:131:ASN:N	1:B:131:ASN:HD22	2.18	0.40
1:B:155:TYR:OH	1:B:159:LEU:HD22	2.21	0.40
1:B:268:PRO:N	4:B:2014:HOH:O	2.53	0.40
1:B:336:CYS:HB2	1:B:337:PRO:CD	2.50	0.40
1:B:454:LEU:HB3	1:B:456:LEU:CD1	2.44	0.40
1:B:85:ILE:O	1:B:85:ILE:HG22	2.21	0.40
1:A:30:SER:HA	1:A:31:PRO:HD3	1.88	0.40
1:A:113:ASN:C	1:A:114:ILE:HG12	2.47	0.40
1:A:405:MET:SD	1:A:520:VAL:HG21	2.61	0.40
1:A:498:ARG:H	1:A:498:ARG:HG2	1.69	0.40
1:A:612:GLN:HB3	4:A:1004:HOH:O	2.22	0.40
1:B:135:LYS:HZ3	1:B:137:GLU:HB3	1.85	0.40
1:B:143:ARG:CG	1:B:143:ARG:NH1	2.83	0.40
1:B:499:PHE:HB2	1:B:501:LEU:HG	2.03	0.40
1:A:191:LYS:CE	4:A:1007:HOH:O	2.70	0.40
1:A:353:LEU:HD12	1:A:390:VAL:C	2.45	0.40
1:A:357:ILE:N	1:A:357:ILE:HD13	2.37	0.40
1:A:526:ARG:NH1	3:A:1002:TSB:N3	2.69	0.40
1:B:4:ILE:HG22	1:B:16:PHE:N	2.29	0.40
1:B:68:GLU:H	1:B:68:GLU:HG2	1.74	0.40
1:B:93:LYS:H	1:B:109:ASP:HB2	1.86	0.40
1:B:343:TYR:CG	1:B:389:PHE:CD2	3.10	0.40
1:B:474:VAL:HB	1:B:487:SER:OG	2.21	0.40
1:A:120:GLU:O	1:A:120:GLU:HG2	2.20	0.40
1:A:386:SER:HB3	1:A:518:ARG:NH1	2.37	0.40
1:A:430:LYS:HB3	1:A:434:PHE:O	2.21	0.40
1:A:627:GLU:HG3	1:A:629:ASP:HB2	2.03	0.40
1:B:83:HIS:HE1	1:B:174:GLN:NE2	2.19	0.40
1:B:89:TYR:CD1	1:B:89:TYR:C	3.00	0.40
1:B:326:THR:HG22	1:B:326:THR:O	2.21	0.40
1:B:392:PRO:HA	1:B:395:ILE:HD11	2.03	0.40
1:B:396:LYS:HD3	1:B:400:LYS:NZ	2.36	0.40
1:B:477:LYS:HB3	1:B:481:GLY:HA2	2.04	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	640/645 (99%)	525 (82%)	81 (13%)	34 (5%)	1	12
1	B	643/645 (100%)	471 (73%)	125 (19%)	47 (7%)	1	6
All	All	1283/1290 (100%)	996 (78%)	206 (16%)	81 (6%)	1	8

All (81) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	113	ASN
1	A	114	ILE
1	A	206	ARG
1	A	211	ASN
1	A	322	GLN
1	A	324	ASP
1	A	325	GLU
1	A	345	ASN
1	A	425	ARG
1	A	436	ASP
1	A	619	GLY
1	B	4	ILE
1	B	88	LEU
1	B	131	ASN
1	B	149	LEU
1	B	210	ASN
1	B	224	ASP
1	B	430	LYS
1	B	460	GLU
1	B	478	THR
1	B	482	LYS
1	B	555	VAL
1	B	596	LYS
1	B	622	ASP

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Mol	Chain	Res	Type
1	A	35	LYS
1	A	151	SER
1	A	152	ASN
1	A	162	ALA
1	A	164	PRO
1	A	175	GLY
1	A	188	SER
1	A	314	GLN
1	A	374	GLY
1	A	375	LEU
1	A	395	ILE
1	A	536	LYS
1	B	187	PRO
1	B	205	TRP
1	B	206	ARG
1	B	211	ASN
1	B	314	GLN
1	B	621	GLN
1	B	635	LEU
1	A	116	SER
1	A	427	PRO
1	A	508	GLY
1	A	559	TYR
1	B	100	ILE
1	B	352	GLU
1	B	436	ASP
1	B	544	ALA
1	B	642	LYS
1	A	62	VAL
1	A	209	SER
1	A	560	ASP
1	A	585	MET
1	B	9	PRO
1	B	115	SER
1	B	166	ASP
1	B	203	ALA
1	B	426	ASP
1	B	624	GLU
1	B	37	ALA
1	B	97	GLY
1	B	114	ILE
1	B	201	ALA

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Mol	Chain	Res	Type
1	B	588	LYS
1	B	64	PRO
1	B	133	ASN
1	B	268	PRO
1	B	481	GLY
1	B	545	PRO
1	A	372	VAL
1	B	395	ILE
1	B	427	PRO
1	B	44	GLY
1	B	508	GLY
1	A	163	ILE
1	B	30	SER
1	B	636	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	567/570 (100%)	470 (83%)	97 (17%)	2	11
1	B	570/570 (100%)	491 (86%)	79 (14%)	3	17
All	All	1137/1140 (100%)	961 (84%)	176 (16%)	2	14

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	17	ASP
1	A	20	THR
1	A	34	ARG
1	A	36	LYS
1	A	45	GLN
1	A	46	LEU
1	A	49	LEU
1	A	55	THR

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Mol	Chain	Res	Type
1	A	58	SER
1	A	63	THR
1	A	66	SER
1	A	70	LEU
1	A	74	ARG
1	A	81	MET
1	A	86	LYS
1	A	96	VAL
1	A	114	ILE
1	A	117	ASP
1	A	125	THR
1	A	129	ILE
1	A	135	LYS
1	A	140	VAL
1	A	141	VAL
1	A	148	GLU
1	A	165	GLU
1	A	172	TYR
1	A	174	GLN
1	A	186	VAL
1	A	199	SER
1	A	200	THR
1	A	208	ASP
1	A	210	ASN
1	A	211	ASN
1	A	214	LEU
1	A	226	LYS
1	A	232	LEU
1	A	236	GLU
1	A	241	ARG
1	A	249	GLU
1	A	255	ASN
1	A	258	LEU
1	A	272	THR
1	A	281	ILE
1	A	287	SER
1	A	293	VAL
1	A	313	TYR
1	A	316	ASP
1	A	321	MET
1	A	323	LEU
1	A	328	SER

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Mol	Chain	Res	Type
1	A	330	VAL
1	A	333	PRO
1	A	340	MET
1	A	353	LEU
1	A	356	ARG
1	A	363	MET
1	A	388	ILE
1	A	401	ARG
1	A	402	VAL
1	A	405	MET
1	A	407	ILE
1	A	421	ARG
1	A	423	SER
1	A	425	ARG
1	A	428	GLU
1	A	429	ASP
1	A	432	LYS
1	A	456	LEU
1	A	467	PHE
1	A	471	LYS
1	A	472	LEU
1	A	476	VAL
1	A	482	LYS
1	A	483	GLU
1	A	490	GLN
1	A	491	LEU
1	A	497	GLU
1	A	502	THR
1	A	504	ILE
1	A	509	GLU
1	A	512	ARG
1	A	515	VAL
1	A	518	ARG
1	A	526	ARG
1	A	545	PRO
1	A	550	ILE
1	A	554	ASN
1	A	555	VAL
1	A	563	ARG
1	A	568	GLU
1	A	594	MET
1	A	603	VAL

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Mol	Chain	Res	Type
1	A	605	ASP
1	A	611	ASN
1	A	622	ASP
1	A	623	GLN
1	B	2	GLU
1	B	6	ILE
1	B	13	LYS
1	B	17	ASP
1	B	45	GLN
1	B	47	VAL
1	B	49	LEU
1	B	63	THR
1	B	67	GLU
1	B	70	LEU
1	B	71	GLU
1	B	79	HIS
1	B	93	LYS
1	B	94	PHE
1	B	99	VAL
1	B	100	ILE
1	B	106	TYR
1	B	109	ASP
1	B	110	ILE
1	B	111	ASP
1	B	128	GLN
1	B	131	ASN
1	B	136	ILE
1	B	143	ARG
1	B	144	ASP
1	B	167	GLU
1	B	174	GLN
1	B	176	ASP
1	B	179	ASP
1	B	184	VAL
1	B	195	PHE
1	B	200	THR
1	B	214	LEU
1	B	233	GLN
1	B	234	MET
1	B	235	LEU
1	B	250	LEU
1	B	254	THR

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Mol	Chain	Res	Type
1	B	268	PRO
1	B	284	LYS
1	B	292	HIS
1	B	315	GLU
1	B	323	LEU
1	B	328	SER
1	B	336	CYS
1	B	342	ILE
1	B	353	LEU
1	B	372	VAL
1	B	402	VAL
1	B	406	ILE
1	B	416	GLU
1	B	417	ASP
1	B	428	GLU
1	B	431	GLU
1	B	436	ASP
1	B	453	GLU
1	B	458	TYR
1	B	471	LYS
1	B	472	LEU
1	B	494	LEU
1	B	497	GLU
1	B	512	ARG
1	B	518	ARG
1	B	521	VAL
1	B	545	PRO
1	B	550	ILE
1	B	555	VAL
1	B	563	ARG
1	B	585	MET
1	B	595	GLN
1	B	601	ILE
1	B	602	VAL
1	B	606	LYS
1	B	610	ASN
1	B	611	ASN
1	B	621	GLN
1	B	625	THR
1	B	628	LYS
1	B	645	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	7	GLN
1	A	128	GLN
1	A	131	ASN
1	A	168	ASN
1	A	174	GLN
1	A	210	ASN
1	A	215	GLN
1	A	231	HIS
1	A	255	ASN
1	A	335	ASN
1	A	384	ASN
1	A	441	ASN
1	A	475	GLN
1	A	554	ASN
1	A	564	GLN
1	A	566	GLN
1	A	582	ASN
1	A	595	GLN
1	A	600	GLN
1	A	610	ASN
1	A	611	ASN
1	A	612	GLN
1	A	623	GLN
1	B	7	GLN
1	B	27	GLN
1	B	79	HIS
1	B	83	HIS
1	B	131	ASN
1	B	133	ASN
1	B	185	HIS
1	B	211	ASN
1	B	233	GLN
1	B	269	ASN
1	B	376	GLN
1	B	384	ASN
1	B	404	ASN
1	B	445	ASN
1	B	475	GLN
1	B	511	HIS
1	B	582	ASN
1	B	593	GLN

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Mol	Chain	Res	Type
1	B	595	GLN
1	B	611	ASN
1	B	612	GLN
1	B	617	GLN
1	B	623	GLN
1	B	644	HIS

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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	TSB	A	1002	2	32,32,32	2.04	3 (9%)	46,48,48	0.89	2 (4%)
3	TSB	B	2002	2	32,32,32	1.93	3 (9%)	46,48,48	0.86	1 (2%)

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	TSB	A	1002	2	-	0/22/39/39	0/3/3/3
3	TSB	B	2002	2	-	1/22/39/39	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	TSB	O2S-S1	8.53	1.49	1.42
3	B	2002	TSB	O2S-S1	7.96	1.49	1.42
3	A	1002	TSB	O1S-S1	6.57	1.48	1.42
3	B	2002	TSB	O1S-S1	6.30	1.48	1.42
3	A	1002	TSB	C-N8	-3.15	1.32	1.37
3	B	2002	TSB	C-N8	-2.97	1.32	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2002	TSB	C-CA-N	3.65	115.67	110.31
3	A	1002	TSB	C-CA-N	3.17	114.97	110.31
3	A	1002	TSB	C5'-O5'-S1	2.56	122.35	116.97

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2002	TSB	C4'-C5'-O5'-S1

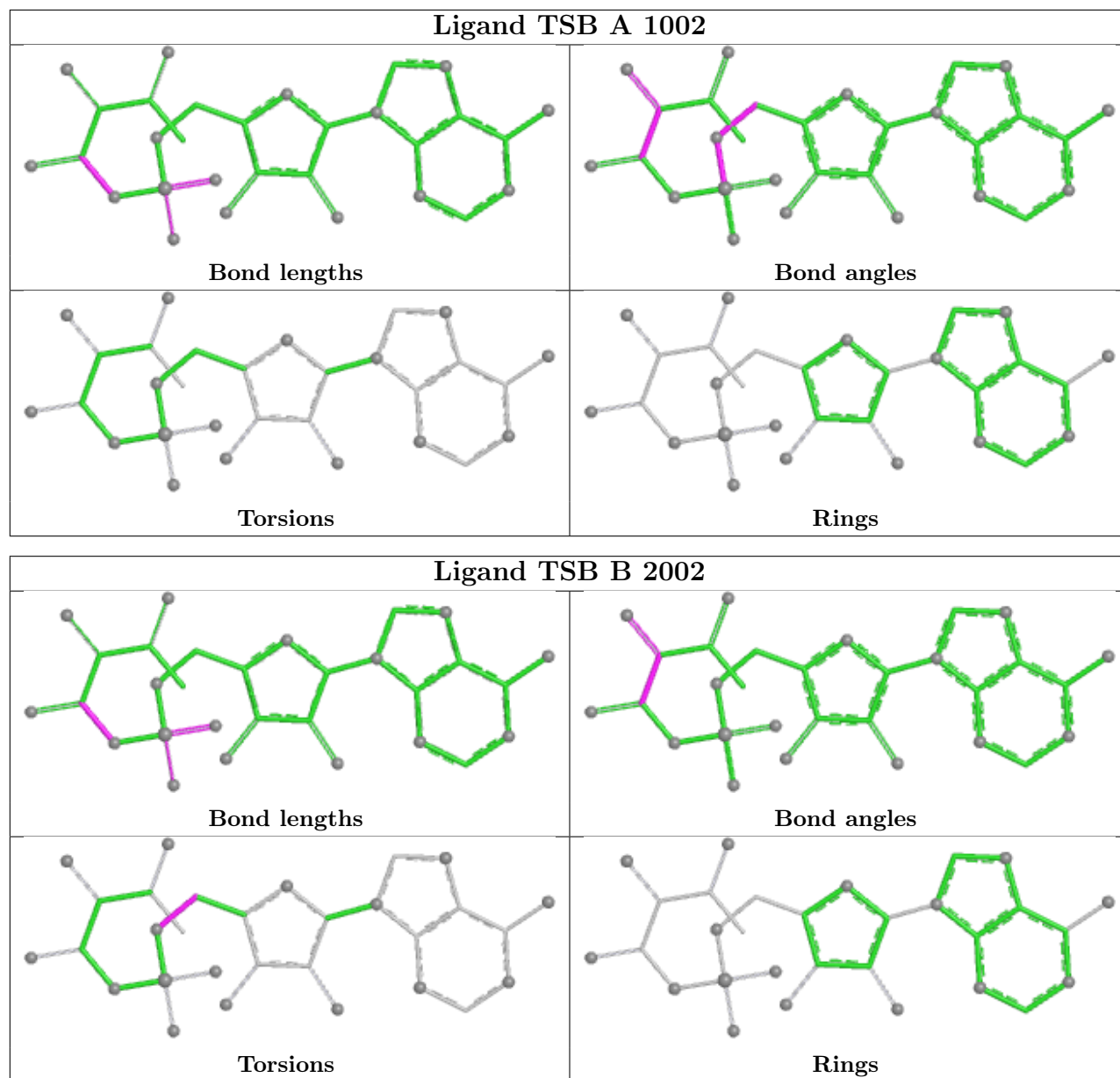
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	TSB	3	0
3	B	2002	TSB	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	642/645 (99%)	-0.63	4 (0%) 85 73	19, 54, 113, 144	0
1	B	645/645 (100%)	-0.39	7 (1%) 78 61	24, 71, 156, 182	0
All	All	1287/1290 (99%)	-0.51	11 (0%) 81 64	19, 61, 144, 182	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	161	ASP	4.5
1	B	169	VAL	3.8
1	B	211	ASN	3.2
1	B	172	TYR	3.2
1	A	426	ASP	3.0
1	B	427	PRO	2.8
1	A	429	ASP	2.3
1	B	162	ALA	2.3
1	A	57	GLY	2.2
1	A	327	GLU	2.1
1	B	160	ILE	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](#)

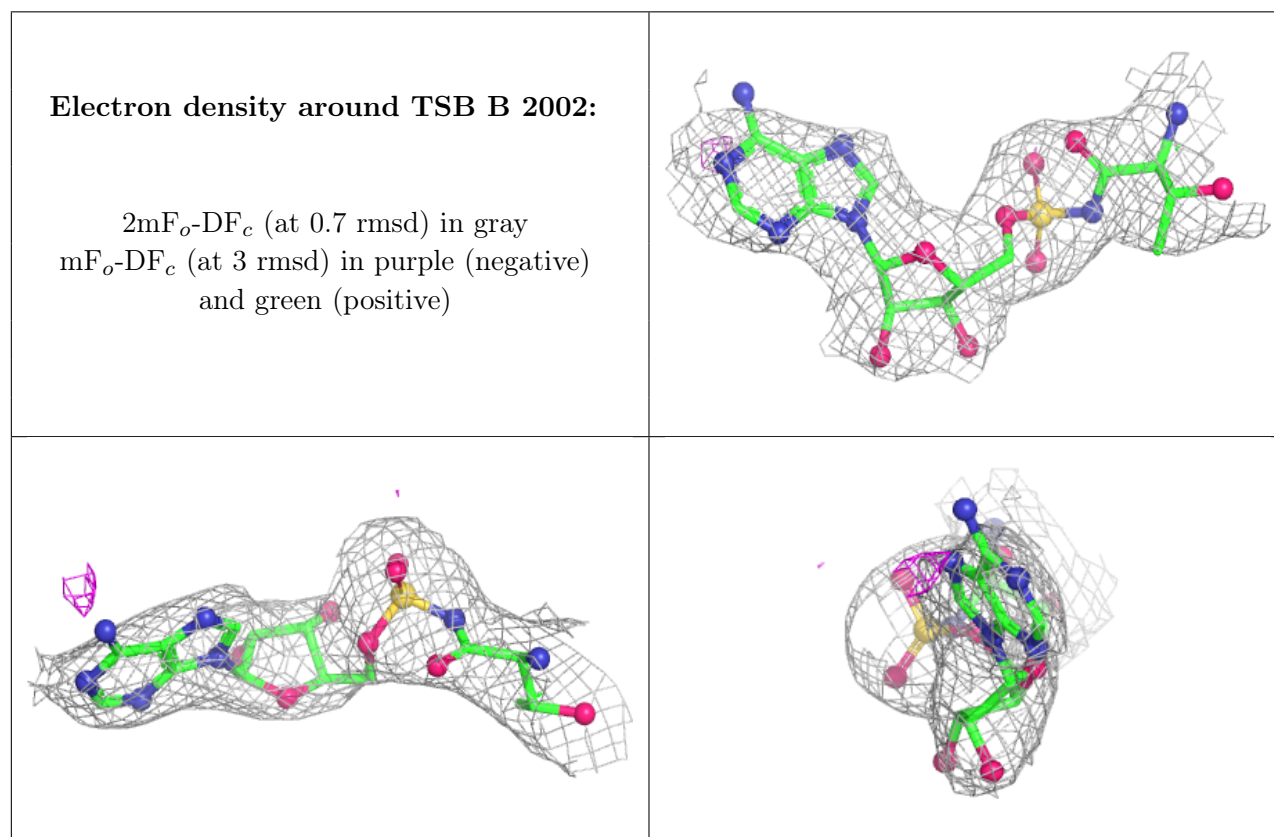
There are no oligosaccharides in this entry.

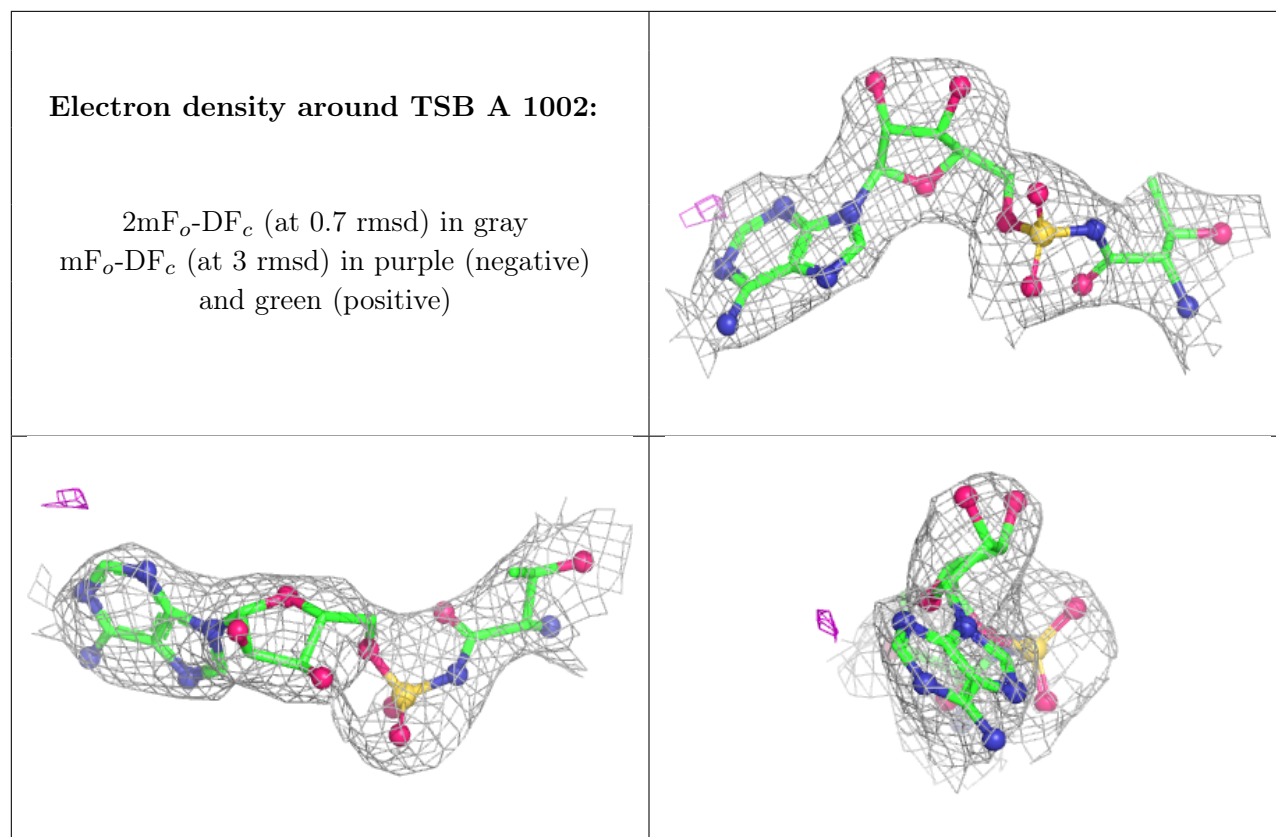
6.4 Ligands [i](#)

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
3	TSB	B	2002	30/30	0.96	0.07	41,48,50,51	0
3	TSB	A	1002	30/30	0.99	0.05	33,37,41,41	0
2	ZN	A	1001	1/1	1.00	0.03	40,40,40,40	0
2	ZN	B	2001	1/1	1.00	0.02	52,52,52,52	0

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





6.5 Other polymers [i](#)

There are no such residues in this entry.