



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:42 PM EDT

PDB ID : 5D12 / pdb_00005d12
Title : Kinase domain of cSrc in complex with RL40
Authors : Becker, C.; Richters, A.; Engel, J.; Rauh, D.
Deposited on : 2015-08-03
Resolution : 3.00 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

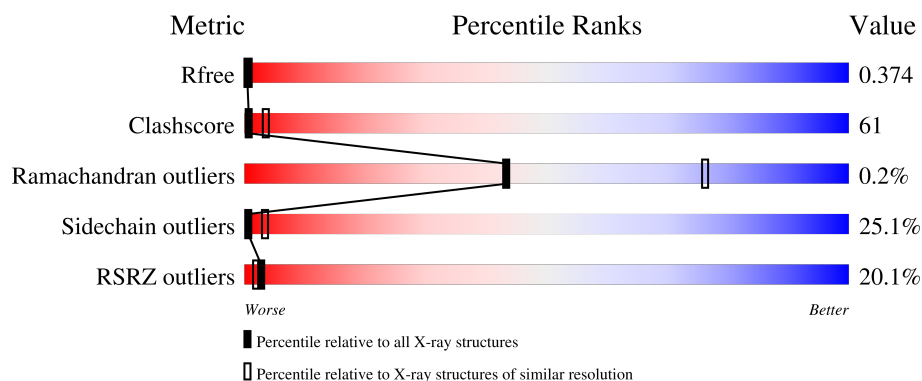
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	286	
1	B	286	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4158 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.

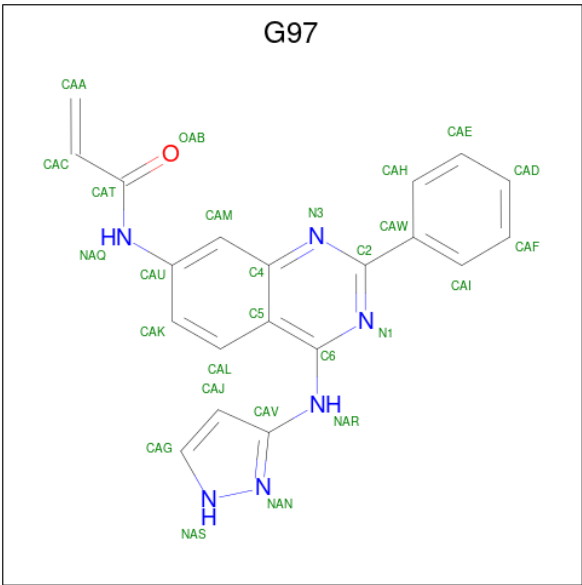
- Molecule 1 is a protein called Proto-oncogene tyrosine-protein kinase Src.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	1	0
			2091	1344	351	379	17			
1	B	253	Total	C	N	O	S	0	2	0
			2013	1294	336	367	16			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	GLY	-	expression tag	UNP P00523
A	249	HIS	-	expression tag	UNP P00523
A	250	MET	-	expression tag	UNP P00523
A	338	MET	THR	engineered mutation	UNP P00523
A	345	CYS	SER	engineered mutation	UNP P00523
B	248	GLY	-	expression tag	UNP P00523
B	249	HIS	-	expression tag	UNP P00523
B	250	MET	-	expression tag	UNP P00523
B	338	MET	THR	engineered mutation	UNP P00523
B	345	CYS	SER	engineered mutation	UNP P00523

- Molecule 2 is N-[2-phenyl-4-(1H-pyrazol-3-ylamino)quinazolin-7-yl]prop-2-enamide (CCD ID: G97) (formula: C₂₀H₁₆N₆O).

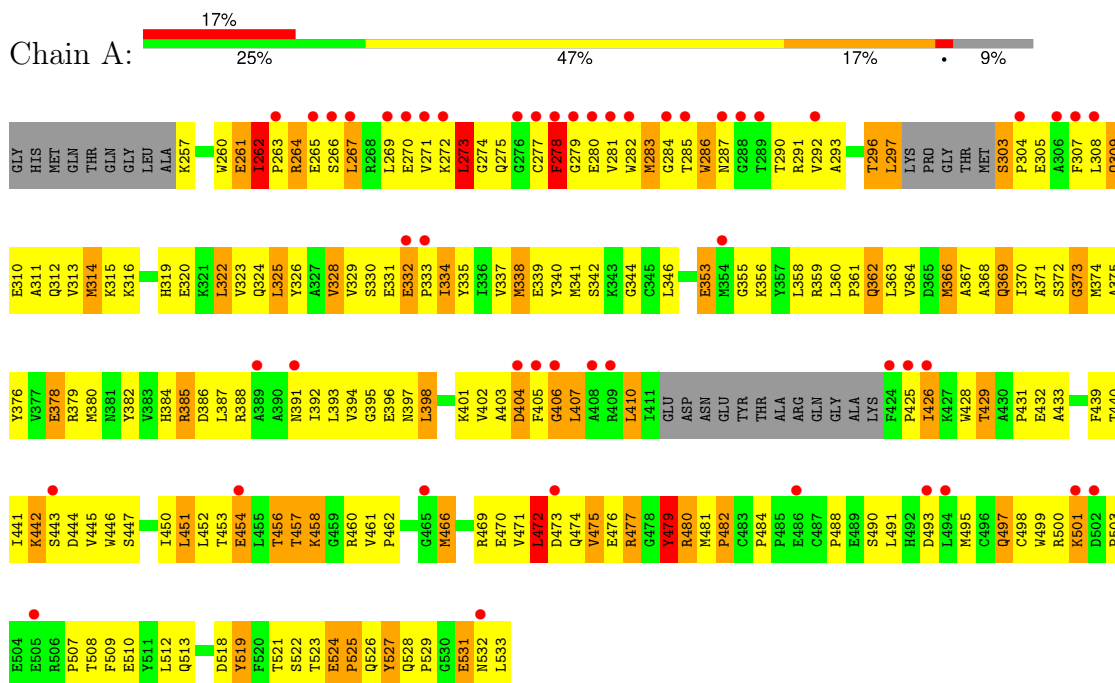


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			27	20	6	1		
2	B	1	Total	C	N	O	0	0
			27	20	6	1		

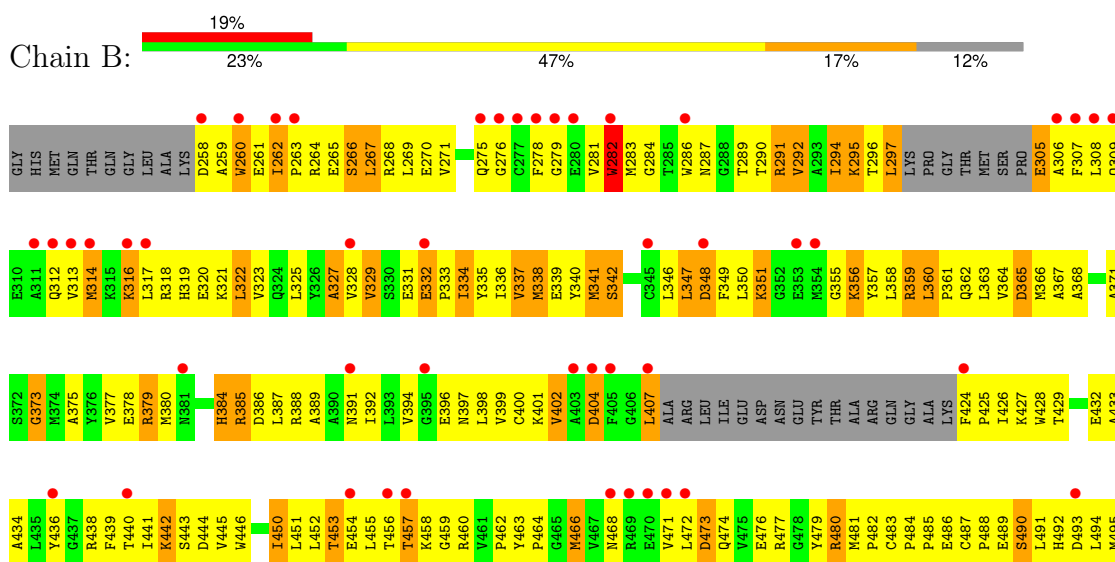
3 Residue-property plots

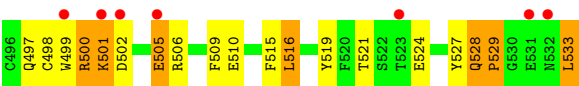
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Proto-oncogene tyrosine-protein kinase Src



• Molecule 1: Proto-oncogene tyrosine-protein kinase Src





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	42.27Å 63.79Å 74.97Å 101.56° 89.91° 89.98°	Depositor
Resolution (Å)	43.49 – 3.00 43.49 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.7 (43.49-3.00) 94.7 (43.49-3.00)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.21 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.290 , 0.376 0.294 , 0.374	Depositor DCC
R_{free} test set	728 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.001 for h,-k,-l	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	4158	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.63% 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: G97

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	0.91	2/2144 (0.1%)	1.32	20/2903 (0.7%)
1	B	0.91	1/2066 (0.0%)	1.29	22/2801 (0.8%)
All	All	0.91	3/4210 (0.1%)	1.31	42/5704 (0.7%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	502	ASP	N-CA	-5.68	1.38	1.46
1	A	482	PRO	N-CA	-5.31	1.41	1.46
1	A	525	PRO	CA-C	5.30	1.59	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	524	GLU	CA-C-N	12.58	134.41	120.45
1	A	524	GLU	C-N-CA	12.58	134.41	120.45
1	A	406	GLY	N-CA-C	-9.82	99.27	112.82
1	A	525	PRO	CA-C-N	9.19	136.87	122.26
1	A	525	PRO	C-N-CA	9.19	136.87	122.26
1	A	472	LEU	N-CA-C	8.10	119.73	111.07
1	B	306	ALA	N-CA-C	7.59	123.45	108.18
1	B	270	GLU	N-CA-C	7.49	119.52	111.36
1	B	524	GLU	CA-C-N	7.07	126.56	118.85
1	B	524	GLU	C-N-CA	7.07	126.56	118.85
1	A	369	GLN	N-CA-C	-6.72	103.96	111.28
1	A	273	LEU	N-CA-C	6.68	121.10	112.41
1	B	348	ASP	N-CA-C	-6.54	103.26	111.11
1	A	479	TYR	N-CA-C	6.34	118.96	109.25
1	B	329	VAL	N-CA-C	-6.33	98.62	107.80
1	A	461	VAL	N-CA-C	-6.32	102.76	108.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	347	LEU	CA-C-N	6.27	129.01	120.54
1	B	347	LEU	C-N-CA	6.27	129.01	120.54
1	B	510	GLU	N-CA-C	-6.18	104.45	111.07
1	A	262	ILE	N-CA-C	6.11	114.20	109.19
1	A	519	TYR	N-CA-C	6.09	117.92	111.28
1	B	373	GLY	N-CA-C	-6.02	105.21	112.49
1	B	342	SER	N-CA-C	5.79	119.61	112.54
1	B	529	PRO	N-CA-C	5.72	120.00	111.41
1	B	500	ARG	N-CA-C	-5.63	101.72	110.10
1	B	365	ASP	N-CA-C	-5.55	105.13	111.07
1	A	353	GLU	N-CA-C	5.49	117.97	111.33
1	B	490	SER	N-CA-C	-5.46	105.33	111.28
1	A	334	ILE	CB-CA-C	-5.32	103.17	111.26
1	B	459	GLY	N-CA-C	5.28	122.60	115.32
1	B	347	LEU	O-C-N	5.27	127.50	122.07
1	A	373	GLY	N-CA-C	-5.26	106.04	112.77
1	B	347	LEU	N-CA-C	-5.21	105.50	111.07
1	A	525	PRO	N-CA-C	5.19	120.84	114.35
1	B	282	TRP	N-CA-C	5.18	117.07	109.24
1	B	340	TYR	N-CA-C	5.14	117.10	108.73
1	A	371	ALA	N-CA-C	-5.12	105.59	111.07
1	B	327	ALA	N-CA-C	5.11	116.58	108.96
1	B	292	VAL	N-CA-C	-5.09	100.96	108.23
1	A	458	LYS	N-CA-C	-5.08	106.38	112.58
1	A	286	TRP	N-CA-C	5.07	117.51	109.50
1	A	493	ASP	N-CA-C	-5.02	105.94	111.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2091	0	2062	261	0
1	B	2013	0	1967	234	1
2	A	27	0	16	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	27	0	16	2	0
All	All	4158	0	4061	498	1

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 61.

All (498) 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:471:VAL:O	1:A:475:VAL:CG2	1.66	1.43
1:A:426:ILE:HD13	1:A:472:LEU:CD1	1.51	1.41
1:A:426:ILE:CD1	1:A:472:LEU:CD1	1.98	1.40
1:A:426:ILE:CD1	1:A:472:LEU:HD13	1.53	1.35
1:B:329:VAL:O	1:B:334:ILE:CG2	1.71	1.34
1:B:428:TRP:CZ2	1:B:454:GLU:OE1	1.85	1.29
1:B:428:TRP:CE2	1:B:454:GLU:OE1	1.87	1.25
1:A:471:VAL:O	1:A:475:VAL:HG22	1.29	1.21
1:B:329:VAL:O	1:B:334:ILE:HG23	1.31	1.20
1:B:286:TRP:HB2	1:B:292:VAL:HG21	1.24	1.17
1:B:314:MET:HE2	1:B:325:LEU:HB2	1.20	1.16
1:B:296:THR:HG21	1:B:335:TYR:CE1	1.80	1.16
1:B:428:TRP:NE1	1:B:454:GLU:OE1	1.77	1.14
1:B:325:LEU:HD12	1:B:337:VAL:O	1.44	1.12
1:B:296:THR:CG2	1:B:335:TYR:CD1	2.33	1.12
1:A:271:VAL:O	1:A:282:TRP:HB3	1.52	1.08
1:A:384:HIS:O	1:A:444:ASP:OD1	1.70	1.08
1:B:296:THR:HG21	1:B:335:TYR:CD1	1.89	1.08
1:A:385:ARG:HB2	1:A:407:LEU:HD13	1.07	1.04
1:A:385:ARG:HB2	1:A:407:LEU:CD1	1.86	1.04
1:A:471:VAL:O	1:A:475:VAL:HG23	1.56	1.03
1:A:519:TYR:CE1	1:A:523:THR:HG21	1.95	1.01
1:A:426:ILE:HD12	1:A:472:LEU:CD1	1.87	1.00
1:B:331:GLU:O	1:B:333:PRO:O	1.80	1.00
1:A:508:THR:O	1:A:512:LEU:HG	1.62	0.99
1:B:329:VAL:O	1:B:334:ILE:HG22	1.61	0.98
1:A:425:PRO:O	1:A:429:THR:OG1	1.81	0.97
1:A:334:ILE:O	1:A:335:TYR:CD2	2.17	0.96
1:B:428:TRP:HZ2	1:B:454:GLU:OE1	1.48	0.96
1:B:269:LEU:HD21	1:B:335:TYR:HE1	1.31	0.95
1:A:272:LYS:NZ	1:A:275:GLN:OE1	2.00	0.94
1:B:427:LYS:HE2	1:B:463:TYR:HB2	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:THR:HB	1:A:335:TYR:CE2	2.02	0.94
1:A:325:LEU:HD12	1:A:337:VAL:O	1.64	0.94
1:A:378:GLU:OE2	1:A:508:THR:OG1	1.86	0.94
1:A:426:ILE:HD12	1:A:472:LEU:HD12	1.49	0.94
1:A:519:TYR:CD1	1:A:523:THR:HG21	2.02	0.94
1:B:450:ILE:O	1:B:453:THR:OG1	1.85	0.94
1:A:453:THR:O	1:A:457:THR:OG1	1.85	0.94
1:A:426:ILE:CD1	1:A:472:LEU:HD12	1.96	0.93
1:B:314:MET:CE	1:B:325:LEU:HB2	1.99	0.93
1:A:370:ILE:HD11	1:A:392:ILE:HG21	1.51	0.92
1:A:385:ARG:CB	1:A:407:LEU:HD13	1.98	0.92
1:B:346:LEU:HD11	1:B:366:MET:HE1	1.50	0.92
1:B:362:GLN:O	1:B:366:MET:HG3	1.69	0.92
1:A:286:TRP:N	1:A:290:THR:O	2.03	0.91
1:B:309:GLN:NE2	1:B:312:GLN:CB	2.33	0.91
1:A:279:GLY:HA2	1:A:297:LEU:HA	1.53	0.90
1:A:275:GLN:HG3	1:A:279:GLY:O	1.72	0.89
1:A:426:ILE:HD13	1:A:472:LEU:HD13	0.91	0.89
1:A:495:MET:O	1:A:498:CYS:HB2	1.70	0.89
1:A:497:GLN:HG2	1:A:500:ARG:NH1	1.89	0.87
1:B:314:MET:HE2	1:B:325:LEU:CB	2.03	0.87
1:B:473:ASP:O	1:B:477:ARG:HG3	1.73	0.87
1:B:320:GLU:O	1:B:401:LYS:HE2	1.73	0.87
1:B:296:THR:HG22	1:B:335:TYR:CD1	2.08	0.86
1:A:338:MET:HE1	2:A:601:G97:HAG	1.58	0.86
1:B:286:TRP:HB2	1:B:292:VAL:CG2	2.04	0.86
1:A:378:GLU:CD	1:A:508:THR:HG1	1.83	0.85
1:A:450:ILE:HD13	1:A:499:TRP:CZ2	2.11	0.85
1:B:480:ARG:HG2	1:B:480:ARG:HH11	1.41	0.84
1:A:279:GLY:C	1:A:280:GLU:HG3	2.00	0.84
1:A:283:MET:HG3	1:A:340:TYR:CE1	2.14	0.82
1:A:519:TYR:CE1	1:A:523:THR:CG2	2.63	0.82
1:A:297:LEU:CD2	1:A:307:PHE:CG	2.62	0.82
1:B:307:PHE:HZ	1:B:336:ILE:HG13	1.44	0.82
1:B:264:ARG:NH2	1:B:331:GLU:O	2.12	0.81
1:A:311:ALA:O	1:A:315:LYS:HG3	1.80	0.81
1:A:378:GLU:CD	1:A:508:THR:OG1	2.24	0.80
1:A:277:CYS:C	1:A:278:PHE:CD2	2.60	0.80
1:A:296:THR:HB	1:A:335:TYR:HE2	1.46	0.79
1:A:426:ILE:HD13	1:A:472:LEU:HD11	1.64	0.79
1:B:325:LEU:CD1	1:B:337:VAL:O	2.29	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:ARG:O	1:B:363:LEU:HG	1.80	0.79
1:A:462:PRO:HB3	1:A:481:MET:HE1	1.65	0.79
1:B:494:LEU:HD22	1:B:515:PHE:CE1	2.17	0.79
1:A:314:MET:HG3	1:A:405:PHE:CD2	2.18	0.78
1:B:497:GLN:O	1:B:500:ARG:HG3	1.83	0.78
1:A:270:GLU:HB2	1:A:284:GLY:HA2	1.66	0.78
1:B:424:PHE:CB	1:B:425:PRO:HA	2.12	0.78
1:A:440:THR:OG1	1:A:442:LYS:HB2	1.85	0.77
1:B:379:ARG:HG3	1:B:379:ARG:HH11	1.50	0.77
1:A:322:LEU:CD2	1:A:405:PHE:HZ	1.98	0.77
1:B:286:TRP:CB	1:B:292:VAL:HG21	2.13	0.77
1:B:346:LEU:HD11	1:B:366:MET:CE	2.14	0.76
1:A:286:TRP:CE2	1:A:287:ASN:HB2	2.21	0.76
1:A:454:GLU:HA	1:A:457:THR:OG1	1.84	0.76
1:A:325:LEU:CD1	1:A:337:VAL:O	2.34	0.75
1:A:453:THR:C	1:A:457:THR:HG1	1.94	0.75
1:A:332:GLU:HA	1:A:334:ILE:N	2.00	0.75
1:B:262:ILE:HD13	1:B:286:TRP:HE1	1.50	0.75
1:B:297:LEU:HD12	1:B:334:ILE:O	1.86	0.75
1:A:271:VAL:O	1:A:282:TRP:CB	2.31	0.75
1:B:269:LEU:HD21	1:B:335:TYR:CE1	2.19	0.75
1:B:505:GLU:N	1:B:505:GLU:OE2	2.20	0.75
1:B:346:LEU:CD1	1:B:366:MET:HE1	2.16	0.74
1:B:263:PRO:O	1:B:266:SER:OG	2.04	0.74
1:A:261:GLU:OE2	1:A:331:GLU:OE2	2.06	0.73
1:A:325:LEU:HD12	1:A:326:TYR:H	1.53	0.73
1:A:262:ILE:HG13	1:A:263:PRO:CD	2.18	0.73
1:A:279:GLY:O	1:A:280:GLU:CG	2.37	0.73
1:A:262:ILE:HG13	1:A:263:PRO:HD2	1.70	0.72
1:A:286:TRP:HB3	1:A:290:THR:HG23	1.71	0.72
1:B:307:PHE:CZ	1:B:336:ILE:HG13	2.24	0.72
1:B:356:LYS:HB3	1:B:357:TYR:CD1	2.25	0.72
1:A:353:GLU:O	1:A:356:LYS:HG3	1.88	0.72
1:A:453:THR:C	1:A:457:THR:OG1	2.32	0.72
1:B:440:THR:HG22	1:B:441:ILE:HG22	1.72	0.71
1:A:387:LEU:C	1:A:388:ARG:HG3	2.13	0.71
1:A:362:GLN:O	1:A:366:MET:HG3	1.90	0.71
1:A:441:ILE:O	1:A:445:VAL:HG23	1.90	0.71
1:A:531:GLU:HG3	1:A:532:ASN:N	2.05	0.71
1:A:279:GLY:O	1:A:280:GLU:HG3	1.91	0.71
1:B:359:ARG:C	1:B:363:LEU:HG	2.16	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:GLY:HA3	2:A:601:G97:HAF	1.72	0.70
1:B:262:ILE:CD1	1:B:267:LEU:HD22	2.22	0.70
1:B:360:LEU:HB3	1:B:361:PRO:HD3	1.74	0.70
1:B:296:THR:HB	1:B:297:LEU:HD13	1.75	0.69
1:A:382:TYR:CE1	1:A:410:LEU:HD13	2.28	0.69
1:A:261:GLU:OE1	1:A:262:ILE:N	2.25	0.69
1:A:519:TYR:CD1	1:A:523:THR:CG2	2.76	0.69
1:A:474:GLN:O	1:A:477:ARG:HB3	1.92	0.69
1:B:258:ASP:OD1	1:B:259:ALA:N	2.25	0.69
1:A:262:ILE:HG13	1:A:263:PRO:N	2.06	0.68
1:A:277:CYS:O	1:A:278:PHE:CD2	2.47	0.68
1:A:519:TYR:O	1:A:523:THR:HB	1.92	0.68
1:A:346:LEU:HD11	1:A:366:MET:HE1	1.75	0.67
1:A:453:THR:HG23	1:A:484:PRO:HG3	1.75	0.67
1:A:466:MET:HE3	1:A:474:GLN:HG3	1.75	0.67
1:B:275:GLN:HG3	1:B:276:GLY:H	1.59	0.67
1:A:277:CYS:O	1:A:278:PHE:HD2	1.77	0.67
1:B:267:LEU:HD23	1:B:267:LEU:H	1.59	0.67
1:A:378:GLU:OE1	1:A:508:THR:OG1	2.13	0.66
1:A:286:TRP:CD2	1:A:287:ASN:HB2	2.30	0.66
1:A:322:LEU:HD21	1:A:405:PHE:HZ	1.60	0.66
1:A:532:ASN:O	1:A:533:LEU:HD23	1.96	0.66
1:B:500:ARG:HD2	1:B:505:GLU:HB3	1.77	0.65
1:B:378:GLU:HG3	1:B:441:ILE:HG12	1.77	0.65
2:A:601:G97:HAJ	2:A:601:G97:N1	2.12	0.65
1:B:359:ARG:O	1:B:363:LEU:N	2.26	0.65
1:B:494:LEU:HD22	1:B:515:PHE:CD1	2.31	0.65
1:A:264:ARG:HB2	1:A:264:ARG:CZ	2.27	0.65
1:A:426:ILE:CD1	1:A:472:LEU:HD11	2.20	0.65
1:B:384:HIS:O	1:B:444:ASP:OD1	2.15	0.65
1:A:370:ILE:HD11	1:A:392:ILE:CG2	2.26	0.64
1:B:373:GLY:O	1:B:377:VAL:HG23	1.96	0.64
1:B:314:MET:SD	1:B:404:ASP:OD2	2.55	0.64
1:A:406:GLY:O	1:A:407:LEU:HB2	1.96	0.64
1:A:338:MET:HE1	2:A:601:G97:CAG	2.27	0.64
1:B:358:LEU:O	1:B:359:ARG:NH1	2.31	0.64
1:B:360:LEU:HB3	1:B:361:PRO:CD	2.28	0.64
1:A:346:LEU:CD1	1:A:366:MET:HE1	2.27	0.64
1:B:480:ARG:HH11	1:B:480:ARG:CG	2.11	0.63
1:A:385:ARG:HG3	1:A:407:LEU:O	1.99	0.63
1:A:275:GLN:O	1:A:275:GLN:HG2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:GLY:C	1:A:280:GLU:CG	2.71	0.63
1:A:457:THR:O	1:A:458:LYS:HB2	1.97	0.63
1:B:296:THR:HG22	1:B:335:TYR:CG	2.34	0.62
2:A:601:G97:N1	2:A:601:G97:CAJ	2.59	0.62
1:B:450:ILE:HG23	1:B:481:MET:HE1	1.81	0.62
1:A:386:ASP:HB2	1:A:407:LEU:HD12	1.82	0.62
1:A:264:ARG:HB2	1:A:264:ARG:NH1	2.14	0.62
1:A:260:TRP:HZ3	1:A:326:TYR:O	1.82	0.62
1:B:275:GLN:HG3	1:B:276:GLY:N	2.15	0.62
1:B:359:ARG:HG3	1:B:359:ARG:HH11	1.64	0.62
1:A:303:SER:N	1:A:304:PRO:CD	2.63	0.62
1:A:356:LYS:O	1:A:359:ARG:NH2	2.32	0.62
1:A:297:LEU:HD22	1:A:307:PHE:CG	2.34	0.61
1:A:319:HIS:HD2	1:A:376:TYR:CD1	2.18	0.61
1:B:346:LEU:CD1	1:B:366:MET:CE	2.76	0.61
1:B:488:PRO:O	1:B:491:LEU:N	2.29	0.61
1:A:397:ASN:O	1:A:398:LEU:HB2	2.01	0.61
1:B:494:LEU:HD22	1:B:515:PHE:HE1	1.66	0.61
1:A:265:GLU:CD	1:A:266:SER:H	2.08	0.61
1:A:497:GLN:HG2	1:A:500:ARG:HH12	1.66	0.61
1:A:507:PRO:HB2	1:A:512:LEU:HD21	1.82	0.61
1:A:322:LEU:HD23	1:A:405:PHE:HZ	1.65	0.61
1:A:273:LEU:HD12	1:A:281:VAL:HG12	1.82	0.61
1:A:518:ASP:OD2	1:B:460:ARG:NE	2.34	0.61
1:B:262:ILE:CD1	1:B:286:TRP:HE1	2.14	0.60
1:B:432:GLU:HG2	1:B:438:ARG:HB2	1.82	0.60
1:A:265:GLU:O	1:A:266:SER:HB3	2.00	0.60
1:B:278:PHE:CE1	1:B:407:LEU:HD22	2.36	0.60
1:A:451:LEU:HA	1:A:454:GLU:OE2	2.02	0.60
1:B:500:ARG:HB2	1:B:506:ARG:HG3	1.83	0.60
1:A:355:GLY:HA2	1:A:358:LEU:HD12	1.84	0.59
1:A:378:GLU:HG3	1:A:441:ILE:HG12	1.84	0.59
1:B:295:LYS:HZ3	1:B:295:LYS:HB2	1.67	0.59
1:A:322:LEU:HD23	1:A:405:PHE:CZ	2.37	0.59
1:A:362:GLN:O	1:A:366:MET:CG	2.51	0.59
1:B:360:LEU:CD1	1:B:533:LEU:HD13	2.32	0.59
1:A:271:VAL:HG12	1:A:272:LYS:N	2.18	0.59
1:A:332:GLU:HA	1:A:333:PRO:C	2.26	0.59
1:B:440:THR:HG22	1:B:441:ILE:N	2.18	0.59
1:B:295:LYS:HB2	1:B:295:LYS:NZ	2.18	0.59
2:B:601:G97:HAJ	2:B:601:G97:N1	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:THR:O	1:A:297:LEU:HB3	2.02	0.58
1:A:384:HIS:CE1	1:A:404:ASP:O	2.56	0.58
1:B:267:LEU:HD23	1:B:267:LEU:N	2.18	0.58
1:B:307:PHE:CZ	1:B:336:ILE:CG1	2.86	0.58
1:B:466:MET:CE	1:B:471:VAL:HA	2.33	0.58
1:B:436:TYR:HB2	1:B:438:ARG:HD2	1.85	0.58
1:B:275:GLN:O	1:B:279:GLY:O	2.21	0.58
1:A:322:LEU:CD2	1:A:405:PHE:CZ	2.85	0.58
1:A:286:TRP:CB	1:A:290:THR:HG23	2.31	0.58
1:A:319:HIS:CD2	1:A:376:TYR:CD1	2.91	0.58
1:B:313:VAL:O	1:B:317:LEU:HD23	2.04	0.58
1:B:307:PHE:CE2	1:B:336:ILE:HD11	2.39	0.57
1:B:313:VAL:HG23	1:B:314:MET:H	1.70	0.57
1:B:264:ARG:CZ	1:B:329:VAL:HG11	2.34	0.57
1:A:339:GLU:O	1:A:339:GLU:HG3	2.03	0.57
1:B:313:VAL:HG23	1:B:314:MET:N	2.18	0.57
1:B:440:THR:HG22	1:B:441:ILE:H	1.69	0.57
1:A:479:TYR:C	1:A:479:TYR:CD2	2.82	0.56
1:A:479:TYR:O	1:A:480:ARG:NH1	2.38	0.56
1:A:264:ARG:O	1:A:267:LEU:CD1	2.54	0.56
1:A:311:ALA:HA	1:A:314:MET:HB2	1.88	0.56
1:B:482:PRO:O	1:B:484:PRO:HD3	2.04	0.56
1:A:297:LEU:HD22	1:A:307:PHE:CD1	2.41	0.56
1:A:329:VAL:HG12	1:A:329:VAL:O	2.05	0.56
1:B:262:ILE:CD1	1:B:267:LEU:CD2	2.84	0.56
1:A:428:TRP:O	1:A:447:SER:OG	2.17	0.56
1:B:258:ASP:N	1:B:261:GLU:OE1	2.39	0.56
1:A:428:TRP:CH2	1:A:462:PRO:HD3	2.41	0.55
1:B:359:ARG:NH1	1:B:359:ARG:HG3	2.21	0.55
1:A:273:LEU:HD12	1:A:281:VAL:O	2.06	0.55
1:A:324:GLN:HG3	1:A:325:LEU:O	2.07	0.55
1:A:426:ILE:HD11	1:A:472:LEU:HD13	1.73	0.55
1:A:528:GLN:HG3	1:A:529:PRO:HD2	1.88	0.55
1:A:406:GLY:O	1:A:407:LEU:CB	2.54	0.55
1:B:332:GLU:HA	1:B:333:PRO:C	2.31	0.55
1:B:384:HIS:CD2	1:B:386:ASP:H	2.25	0.55
1:B:396:GLU:O	1:B:399:VAL:HG23	2.07	0.55
2:B:601:G97:N1	2:B:601:G97:CAJ	2.67	0.55
1:A:309:GLN:O	1:A:313:VAL:HG23	2.07	0.55
1:A:479:TYR:CD2	1:A:479:TYR:O	2.60	0.54
1:B:356:LYS:HB3	1:B:357:TYR:CE1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:LEU:HD13	1:B:533:LEU:HD13	1.89	0.54
1:A:290:THR:O	1:A:290:THR:HG23	2.08	0.54
1:B:319:HIS:CD2	1:B:321:LYS:H	2.25	0.54
1:B:491:LEU:O	1:B:494:LEU:HB3	2.07	0.54
1:B:441:ILE:O	1:B:445:VAL:HG23	2.07	0.54
1:B:329:VAL:C	1:B:334:ILE:HG23	2.22	0.54
1:B:428:TRP:HE1	1:B:454:GLU:CD	2.15	0.54
1:B:388:ARG:HB2	1:B:391:ASN:HD22	1.72	0.54
1:A:271:VAL:O	1:A:282:TRP:CE3	2.61	0.54
1:B:355:GLY:HA2	1:B:358:LEU:HB2	1.90	0.54
1:A:384:HIS:HE1	1:A:404:ASP:O	1.90	0.54
1:B:446:TRP:CD1	1:B:446:TRP:C	2.85	0.54
1:A:273:LEU:CD1	1:A:281:VAL:HG12	2.37	0.54
1:A:501:LYS:O	1:A:503:PRO:HD3	2.07	0.54
1:B:363:LEU:HD12	1:B:533:LEU:HD21	1.90	0.54
1:B:462:PRO:HB2	1:B:463:TYR:CD1	2.43	0.54
1:A:454:GLU:CA	1:A:457:THR:OG1	2.53	0.53
1:B:493:ASP:O	1:B:497:GLN:HG3	2.08	0.53
1:A:440:THR:OG1	1:A:443:SER:N	2.42	0.53
1:A:470:GLU:O	1:A:474:GLN:CG	2.56	0.53
1:A:479:TYR:C	1:A:480:ARG:NH1	2.67	0.53
1:B:363:LEU:CD1	1:B:533:LEU:HD21	2.38	0.53
1:A:308:LEU:O	1:A:312:GLN:HG2	2.09	0.53
1:A:394:VAL:HG12	1:A:395:GLY:N	2.24	0.53
1:A:491:LEU:O	1:A:495:MET:HG3	2.08	0.53
1:A:384:HIS:O	1:A:444:ASP:CG	2.49	0.53
1:B:305:GLU:HA	1:B:305:GLU:OE1	2.09	0.53
1:B:528:GLN:NE2	1:B:529:PRO:HD2	2.24	0.53
1:B:527:TYR:C	1:B:527:TYR:CD2	2.87	0.53
1:A:527:TYR:C	1:A:527:TYR:CD2	2.87	0.52
1:A:374:MET:HE1	1:A:444:ASP:OD2	2.09	0.52
1:B:441:ILE:O	1:B:444:ASP:HB2	2.09	0.52
1:B:286:TRP:CZ2	1:B:327:ALA:HB2	2.45	0.52
1:A:257:LYS:HD3	1:A:331:GLU:OE1	2.09	0.52
1:B:282:TRP:CD1	1:B:282:TRP:N	2.78	0.52
1:B:428:TRP:HZ2	1:B:454:GLU:CD	2.17	0.52
1:B:463:TYR:N	1:B:464:PRO:CD	2.72	0.52
1:A:373:GLY:O	1:A:376:TYR:HB3	2.09	0.52
1:A:279:GLY:O	1:A:280:GLU:HG2	2.10	0.52
1:A:519:TYR:OH	1:A:524:GLU:HG3	2.10	0.52
1:A:260:TRP:CZ3	1:A:326:TYR:O	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:LEU:CD2	1:B:335:TYR:HE1	2.13	0.51
1:B:497:GLN:O	1:B:500:ARG:CG	2.56	0.51
1:B:500:ARG:CD	1:B:505:GLU:HB3	2.40	0.51
1:A:314:MET:CG	1:A:405:PHE:CD2	2.92	0.51
1:B:363:LEU:HD12	1:B:533:LEU:CD2	2.40	0.51
1:B:360:LEU:HA	1:B:363:LEU:HB2	1.92	0.50
1:B:286:TRP:CZ2	1:B:327:ALA:CB	2.95	0.50
1:B:296:THR:O	1:B:297:LEU:C	2.54	0.50
1:A:324:GLN:H	1:A:339:GLU:HG2	1.76	0.50
1:A:519:TYR:HE1	1:A:523:THR:HG21	1.67	0.50
1:B:347:LEU:O	1:B:351:LYS:HG2	2.11	0.50
1:B:317:LEU:HD12	1:B:317:LEU:O	2.11	0.49
1:A:382:TYR:CZ	1:A:410:LEU:HD13	2.48	0.49
1:B:323:VAL:HG23	1:B:402:VAL:O	2.12	0.49
1:A:334:ILE:C	1:A:335:TYR:CD2	2.89	0.49
1:A:482:PRO:O	1:A:484:PRO:HD3	2.12	0.49
1:A:264:ARG:O	1:A:267:LEU:HD12	2.12	0.49
1:B:397:ASN:O	1:B:398:LEU:HB2	2.13	0.49
1:B:384:HIS:CD2	1:B:384:HIS:C	2.88	0.49
1:A:320:GLU:O	1:A:401:LYS:HE2	2.13	0.49
1:A:432:GLU:H	1:A:432:GLU:CD	2.19	0.49
1:A:490:SER:HB2	1:A:519:TYR:OH	2.13	0.49
1:B:366:MET:O	1:B:367:ALA:C	2.54	0.49
1:A:360:LEU:HB3	1:A:361:PRO:HD3	1.95	0.48
1:A:470:GLU:O	1:A:474:GLN:HG2	2.12	0.48
1:B:319:HIS:CD2	1:B:373:GLY:HA2	2.48	0.48
1:B:385:ARG:HG2	1:B:439:PHE:CD2	2.47	0.48
1:B:480:ARG:CG	1:B:480:ARG:NH1	2.76	0.48
1:A:450:ILE:HD13	1:A:499:TRP:CE2	2.48	0.48
1:A:473:ASP:HA	1:A:476:GLU:HB2	1.95	0.48
1:B:325:LEU:HA	1:B:338:MET:HB3	1.96	0.48
1:B:359:ARG:HH11	1:B:359:ARG:CG	2.27	0.48
1:B:440:THR:O	1:B:443:SER:OG	2.15	0.48
1:A:291:ARG:HD2	1:A:340:TYR:CD2	2.48	0.48
1:A:297:LEU:HD23	1:A:307:PHE:CG	2.49	0.48
1:A:359:ARG:O	1:A:363:LEU:HG	2.14	0.48
1:A:431:PRO:HG2	1:A:501:LYS:HE2	1.95	0.48
1:A:440:THR:OG1	1:A:442:LYS:CB	2.60	0.48
1:A:441:ILE:O	1:A:444:ASP:HB2	2.14	0.48
1:A:451:LEU:O	1:A:454:GLU:HG2	2.12	0.48
1:B:476:GLU:OE1	1:B:476:GLU:HA	2.10	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ALA:HB1	1:A:439:PHE:CE1	2.49	0.48
1:A:462:PRO:HB3	1:A:481:MET:CE	2.41	0.48
1:B:485:PRO:O	1:B:486:GLU:HB2	2.14	0.48
1:A:282:TRP:N	1:A:282:TRP:CD1	2.82	0.48
1:B:312:GLN:O	1:B:316:LYS:HB2	2.13	0.48
1:B:451:LEU:HA	1:B:454:GLU:HB2	1.96	0.48
1:B:457:THR:O	1:B:458:LYS:HB2	2.14	0.48
1:A:360:LEU:HG	1:A:364:VAL:HG23	1.95	0.47
1:B:271:VAL:HG21	1:B:283:MET:CE	2.44	0.47
1:B:346:LEU:O	1:B:349:PHE:HB3	2.13	0.47
1:A:310:GLU:HG3	1:A:405:PHE:CB	2.43	0.47
1:A:264:ARG:CZ	1:A:264:ARG:CB	2.92	0.47
1:A:297:LEU:CD2	1:A:307:PHE:CD1	2.97	0.47
1:B:516:LEU:HA	1:B:519:TYR:HB2	1.96	0.47
1:A:344:GLY:HA2	2:A:601:G97:C4	2.45	0.47
1:B:399:VAL:HG12	1:B:400:CYS:N	2.29	0.47
1:A:364:VAL:O	1:A:367:ALA:HB3	2.15	0.47
1:A:474:GLN:O	1:A:479:TYR:HB3	2.14	0.47
1:B:314:MET:O	1:B:317:LEU:HG	2.14	0.47
1:B:359:ARG:O	1:B:363:LEU:CG	2.59	0.47
1:B:479:TYR:C	1:B:479:TYR:CD2	2.93	0.47
1:A:396:GLU:O	1:A:397:ASN:CB	2.62	0.47
1:A:442:LYS:O	1:A:445:VAL:HB	2.14	0.47
1:A:524:GLU:N	1:A:525:PRO:CD	2.76	0.47
1:B:441:ILE:HG23	1:B:442:LYS:N	2.30	0.47
1:A:297:LEU:CD2	1:A:307:PHE:CD2	2.97	0.47
1:B:489[B]:GLU:HA	1:B:492:HIS:HB3	1.96	0.47
1:A:273:LEU:O	2:A:601:G97:HAI	2.14	0.47
1:B:258:ASP:OD1	1:B:260:TRP:N	2.39	0.47
1:B:426:ILE:HD11	1:B:468:ASN:O	2.15	0.46
1:B:484:PRO:O	1:B:487:CYS:HB3	2.15	0.46
1:B:296:THR:HG22	1:B:335:TYR:HA	1.97	0.46
1:B:424:PHE:CB	1:B:425:PRO:CA	2.89	0.46
1:A:313:VAL:HG13	1:A:382:TYR:CE2	2.50	0.46
1:A:387:LEU:O	1:A:388:ARG:HG3	2.14	0.46
1:A:297:LEU:HD23	1:A:307:PHE:CD2	2.50	0.46
1:B:404:ASP:OD1	1:B:404:ASP:N	2.47	0.46
1:B:441:ILE:HG23	1:B:442:LYS:HD3	1.98	0.46
1:A:480:ARG:CA	1:A:480:ARG:HH11	2.28	0.46
1:A:293:ALA:HB3	1:A:338:MET:CE	2.45	0.46
1:B:482:PRO:O	1:B:484:PRO:CD	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:ILE:C	1:B:453:THR:OG1	2.58	0.46
1:A:279:GLY:CA	1:A:297:LEU:HA	2.37	0.46
1:A:473:ASP:O	1:A:477:ARG:HB2	2.16	0.46
1:A:488:PRO:C	1:A:490:SER:N	2.71	0.46
1:A:523:THR:HG22	1:A:524:GLU:HG2	1.97	0.46
1:B:359:ARG:H	1:B:362:GLN:HE21	1.63	0.46
1:B:441:ILE:HG13	1:B:509:PHE:HE2	1.80	0.46
1:B:290:THR:HG22	1:B:291:ARG:O	2.16	0.46
1:A:509:PHE:O	1:A:513:GLN:HB3	2.16	0.45
1:B:268:ARG:O	1:B:284:GLY:HA3	2.15	0.45
1:B:297:LEU:HD12	1:B:334:ILE:N	2.31	0.45
1:B:319:HIS:CD2	1:B:321:LYS:HB2	2.51	0.45
1:A:266:SER:OG	1:A:287:ASN:HA	2.16	0.45
1:A:297:LEU:CD2	1:A:307:PHE:CB	2.94	0.45
1:A:442:LYS:HD2	1:A:503:PRO:O	2.16	0.45
1:A:344:GLY:HA2	2:A:601:G97:C5	2.46	0.45
1:A:452:LEU:O	1:A:456:THR:OG1	2.31	0.45
1:B:445:VAL:HG22	1:B:509:PHE:CZ	2.52	0.45
1:B:480:ARG:HD3	1:B:499:TRP:HB3	1.97	0.45
1:B:491:LEU:CD1	1:B:494:LEU:HD23	2.47	0.45
1:A:311:ALA:HB1	1:A:325:LEU:HD21	1.99	0.45
1:A:271:VAL:CG1	1:A:272:LYS:N	2.80	0.45
1:A:296:THR:OG1	1:A:297:LEU:N	2.48	0.45
1:B:433:ALA:HB1	1:B:439:PHE:CZ	2.51	0.45
1:B:290:THR:HG22	1:B:291:ARG:N	2.31	0.45
1:B:399:VAL:O	1:B:400:CYS:SG	2.70	0.45
1:A:271:VAL:O	1:A:282:TRP:HE3	1.99	0.45
1:B:360:LEU:O	1:B:364:VAL:N	2.50	0.45
1:B:378:GLU:HG3	1:B:441:ILE:CG1	2.46	0.45
1:B:350:LEU:HD21	1:B:455:LEU:HD23	1.98	0.44
1:B:297:LEU:CD1	1:B:334:ILE:O	2.63	0.44
1:A:440:THR:OG1	1:A:442:LYS:N	2.49	0.44
1:B:307:PHE:O	1:B:307:PHE:CD2	2.71	0.44
1:B:396:GLU:O	1:B:397:ASN:CB	2.63	0.44
1:A:297:LEU:HD22	1:A:307:PHE:HB2	1.99	0.44
1:B:389:ALA:HB2	1:B:454:GLU:OE2	2.17	0.44
1:A:297:LEU:CD2	1:A:307:PHE:HB2	2.48	0.44
1:A:264:ARG:HH11	1:A:264:ARG:HG3	1.82	0.44
1:A:501:LYS:HA	1:A:501:LYS:HD3	1.55	0.44
1:B:429:THR:HG22	1:B:434:ALA:HB2	1.98	0.44
1:B:466:MET:HE2	1:B:471:VAL:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:PHE:C	1:B:440:THR:HG1	2.27	0.43
1:B:483:CYS:HA	1:B:484:PRO:HD2	1.85	0.43
1:A:296:THR:HB	1:A:335:TYR:CD2	2.51	0.43
1:A:334:ILE:O	1:A:335:TYR:HD2	1.90	0.43
1:A:375:ALA:HA	1:A:509:PHE:HB2	1.99	0.43
1:A:460:ARG:HD2	1:A:460:ARG:HA	1.63	0.43
1:B:527:TYR:HE2	1:B:529:PRO:HG3	1.82	0.43
1:A:369:GLN:O	1:A:372:SER:HB3	2.19	0.43
1:B:262:ILE:HD12	1:B:267:LEU:CD2	2.48	0.43
1:B:375:ALA:HA	1:B:509:PHE:HB2	2.00	0.43
1:A:286:TRP:CD1	1:A:287:ASN:N	2.87	0.43
1:A:362:GLN:N	1:A:362:GLN:OE1	2.50	0.43
1:A:499:TRP:O	1:A:500:ARG:C	2.61	0.43
1:B:379:ARG:HH11	1:B:379:ARG:CG	2.24	0.43
1:A:325:LEU:HD12	1:A:326:TYR:N	2.28	0.43
1:A:508:THR:OG1	1:A:509:PHE:N	2.51	0.43
1:B:294:ILE:HG23	1:B:336:ILE:O	2.18	0.43
1:B:312:GLN:O	1:B:313:VAL:C	2.62	0.43
1:B:360:LEU:O	1:B:364:VAL:HG23	2.17	0.43
1:A:286:TRP:CG	1:A:287:ASN:HB2	2.53	0.43
1:B:388:ARG:HG2	1:B:428:TRP:CD1	2.54	0.43
1:B:264:ARG:HH12	1:B:335:TYR:HD2	1.66	0.43
1:B:399:VAL:C	1:B:400:CYS:SG	3.01	0.43
1:B:457:THR:O	1:B:458:LYS:CB	2.67	0.43
1:A:446:TRP:CZ3	1:A:499:TRP:O	2.71	0.43
1:A:480:ARG:HH11	1:A:480:ARG:HA	1.84	0.43
1:B:275:GLN:CG	1:B:276:GLY:H	2.30	0.43
1:B:281:VAL:HG22	1:B:295:LYS:HG3	2.00	0.43
1:B:466:MET:HE2	1:B:471:VAL:HG22	1.99	0.43
1:A:386:ASP:CG	1:A:391:ASN:HD21	2.26	0.43
1:B:371:ALA:O	1:B:375:ALA:N	2.51	0.43
1:B:262:ILE:HD11	1:B:267:LEU:HD22	1.97	0.42
1:B:349:PHE:CE1	1:B:394:VAL:HG11	2.54	0.42
1:B:389:ALA:N	1:B:454:GLU:OE2	2.48	0.42
1:A:264:ARG:HH11	1:A:264:ARG:CG	2.31	0.42
1:A:495:MET:O	1:A:498:CYS:CB	2.54	0.42
1:B:433:ALA:HB1	1:B:439:PHE:CE2	2.53	0.42
1:B:378:GLU:HG3	1:B:441:ILE:CD1	2.49	0.42
1:B:327:ALA:HB3	1:B:337:VAL:HG11	2.01	0.42
1:B:388:ARG:O	1:B:392:ILE:HG12	2.19	0.42
1:A:368:ALA:O	1:A:369:GLN:C	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:GLU:OE1	1:A:432:GLU:N	2.37	0.42
1:A:360:LEU:O	1:A:364:VAL:HG23	2.19	0.42
1:A:472:LEU:O	1:A:476:GLU:HG2	2.20	0.42
1:A:528:GLN:CG	1:A:529:PRO:HD2	2.50	0.42
1:B:312:GLN:O	1:B:316:LYS:N	2.42	0.42
1:B:505:GLU:OE2	1:B:505:GLU:CA	2.67	0.42
1:A:431:PRO:O	1:A:432:GLU:C	2.61	0.42
1:B:379:ARG:HG3	1:B:379:ARG:NH1	2.28	0.42
1:B:262:ILE:H	1:B:262:ILE:HG13	1.75	0.42
1:A:265:GLU:CG	1:A:266:SER:N	2.82	0.41
1:A:519:TYR:CE1	1:A:523:THR:HG22	2.52	0.41
1:B:297:LEU:HD13	1:B:297:LEU:N	2.35	0.41
1:B:283:MET:CG	1:B:284:GLY:N	2.83	0.41
1:B:297:LEU:HD11	1:B:333:PRO:HB3	2.01	0.41
1:A:286:TRP:HB2	1:A:292:VAL:HG21	2.02	0.41
1:A:402:VAL:HG12	1:A:403:ALA:N	2.35	0.41
1:A:479:TYR:O	1:A:479:TYR:HD2	2.03	0.41
1:A:283:MET:HG3	1:A:340:TYR:CD1	2.52	0.41
1:A:286:TRP:CG	1:A:287:ASN:N	2.88	0.41
1:B:495:MET:O	1:B:498:CYS:N	2.53	0.41
1:A:426:ILE:HA	1:A:429:THR:OG1	2.20	0.41
1:A:523:THR:C	1:A:525:PRO:HD3	2.46	0.41
1:B:331:GLU:O	1:B:333:PRO:C	2.57	0.41
1:B:452:LEU:HB3	1:B:495:MET:HE2	2.01	0.41
1:A:273:LEU:N	1:A:281:VAL:O	2.42	0.41
1:A:328:VAL:HG23	1:A:335:TYR:O	2.19	0.41
1:A:509:PHE:O	1:A:513:GLN:CB	2.69	0.41
1:A:312:GLN:O	1:A:316:LYS:NZ	2.31	0.41
1:A:360:LEU:HG	1:A:364:VAL:CG2	2.50	0.41
1:A:388:ARG:HG2	1:A:428:TRP:CG	2.56	0.41
1:A:277:CYS:CB	1:A:278:PHE:CE2	3.04	0.41
1:A:325:LEU:HA	1:A:338:MET:HB3	2.02	0.41
1:A:453:THR:O	1:A:456:THR:OG1	2.39	0.41
1:B:286:TRP:O	1:B:287:ASN:HB2	2.20	0.41
1:B:308:LEU:HA	1:B:309:GLN:C	2.45	0.41
1:B:341:MET:HE3	1:B:341:MET:HA	2.03	0.41
1:A:286:TRP:CD1	1:A:287:ASN:HB2	2.56	0.40
1:B:365:ASP:O	1:B:368:ALA:HB3	2.21	0.40
1:A:481:MET:HB3	1:A:482:PRO:HD2	2.02	0.40
1:A:322:LEU:O	1:A:323:VAL:C	2.64	0.40
1:A:376:TYR:O	1:A:379:ARG:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ALA:H	1:B:337:VAL:CB	2.30	0.40
1:B:440:THR:CG2	1:B:441:ILE:N	2.84	0.40
1:B:466:MET:HE3	1:B:474:GLN:HG3	2.03	0.40
1:B:319:HIS:HB3	1:B:322:LEU:HB2	2.04	0.40
1:A:450:ILE:HD13	1:A:499:TRP:HZ2	1.79	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:ASN:OD1	1:B:438:ARG:CG[1_655]	2.15	0.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	255/286 (89%)	236 (92%)	18 (7%)	1 (0%)	30	65
1	B	249/286 (87%)	226 (91%)	23 (9%)	0	100	100
All	All	504/572 (88%)	462 (92%)	41 (8%)	1 (0%)	43	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	PHE

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	222/245 (91%)	166 (75%)	56 (25%)	0	3
1	B	211/245 (86%)	157 (74%)	54 (26%)	0	3
All	All	433/490 (88%)	323 (75%)	110 (25%)	0	3

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	261	GLU
1	A	262	ILE
1	A	264	ARG
1	A	267	LEU
1	A	269	LEU
1	A	273	LEU
1	A	278	PHE
1	A	283	MET
1	A	285	THR
1	A	296	THR
1	A	297	LEU
1	A	303	SER
1	A	305	GLU
1	A	309	GLN
1	A	314	MET
1	A	322	LEU
1	A	325	LEU
1	A	328	VAL
1	A	330	SER
1	A	332	GLU
1	A	338	MET
1	A	341	MET
1	A	342	SER
1	A	362	GLN
1	A	366	MET
1	A	378	GLU
1	A	380	MET
1	A	385	ARG
1	A	393	LEU
1	A	398	LEU
1	A	404	ASP
1	A	407	LEU
1	A	410	LEU

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Mol	Chain	Res	Type
1	A	426	ILE
1	A	429	THR
1	A	442	LYS
1	A	451	LEU
1	A	454	GLU
1	A	456	THR
1	A	457	THR
1	A	466	MET
1	A	469	ARG
1	A	472	LEU
1	A	475	VAL
1	A	477	ARG
1	A	479	TYR
1	A	480	ARG
1	A	497	GLN
1	A	501	LYS
1	A	510	GLU
1	A	521	THR
1	A	522	SER
1	A	526[A]	GLN
1	A	526[B]	GLN
1	A	527	TYR
1	A	531	GLU
1	B	260	TRP
1	B	262	ILE
1	B	265	GLU
1	B	266	SER
1	B	267	LEU
1	B	282	TRP
1	B	289	THR
1	B	291	ARG
1	B	294	ILE
1	B	295	LYS
1	B	297	LEU
1	B	305	GLU
1	B	314	MET
1	B	316	LYS
1	B	318	ARG
1	B	322	LEU
1	B	328	VAL
1	B	332	GLU
1	B	334	ILE

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Mol	Chain	Res	Type
1	B	337	VAL
1	B	338	MET
1	B	339	GLU
1	B	341	MET
1	B	342	SER
1	B	348	ASP
1	B	351	LYS
1	B	356	LYS
1	B	359	ARG
1	B	360	LEU
1	B	379	ARG
1	B	380	MET
1	B	384	HIS
1	B	385	ARG
1	B	387	LEU
1	B	402	VAL
1	B	404	ASP
1	B	407	LEU
1	B	442	LYS
1	B	450	ILE
1	B	453	THR
1	B	456	THR
1	B	457	THR
1	B	466	MET
1	B	472	LEU
1	B	473	ASP
1	B	480	ARG
1	B	490	SER
1	B	501[A]	LYS
1	B	501[B]	LYS
1	B	505	GLU
1	B	516	LEU
1	B	521	THR
1	B	528	GLN
1	B	533	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	319	HIS
1	A	384	HIS
1	B	309	GLN

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Mol	Chain	Res	Type
1	B	319	HIS
1	B	362	GLN
1	B	384	HIS
1	B	391	ASN
1	B	526	GLN
1	B	528	GLN

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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	G97	A	601	-	29,30,30	1.78	8 (27%)	38,41,41	2.54	12 (31%)
2	G97	B	601	-	29,30,30	1.84	8 (27%)	38,41,41	2.24	12 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	G97	A	601	-	-	4/14/14/14	0/4/4/4
2	G97	B	601	-	-	0/14/14/14	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	G97	C6-C5	4.58	1.50	1.44
2	B	601	G97	CAM-C4	-4.40	1.35	1.41
2	B	601	G97	C4-N3	-3.98	1.31	1.37
2	A	601	G97	C5-C4	3.86	1.48	1.42
2	B	601	G97	C6-C5	3.64	1.49	1.44
2	B	601	G97	C6-N1	3.62	1.37	1.33
2	A	601	G97	CAM-C4	-3.25	1.36	1.41
2	A	601	G97	CAU-NAQ	-3.20	1.35	1.41
2	B	601	G97	C5-C4	2.96	1.47	1.42
2	A	601	G97	NAS-NAN	2.53	1.41	1.36
2	A	601	G97	CAL-CAK	2.51	1.42	1.36
2	A	601	G97	C4-N3	-2.42	1.33	1.37
2	B	601	G97	CAU-NAQ	-2.41	1.36	1.41
2	B	601	G97	CAL-CAK	2.32	1.41	1.36
2	A	601	G97	C6-N1	2.10	1.35	1.33
2	B	601	G97	NAS-NAN	2.09	1.40	1.36

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	G97	C2-N3-C4	7.84	121.92	116.56
2	A	601	G97	C5-C6-NAR	6.64	126.41	119.78
2	A	601	G97	C2-N3-C4	6.61	121.08	116.56
2	A	601	G97	C6-N1-C2	6.11	125.32	117.20
2	A	601	G97	CAG-CAJ-CAV	4.90	107.96	103.85
2	B	601	G97	CAW-C2-N1	4.25	124.43	117.40
2	A	601	G97	N3-C2-N1	-4.24	120.85	126.49
2	A	601	G97	C5-C6-N1	-3.87	116.26	122.07
2	A	601	G97	CAM-CAU-NAQ	-3.82	110.64	123.10
2	B	601	G97	C6-N1-C2	3.68	122.09	117.20
2	B	601	G97	N3-C2-N1	-3.52	121.80	126.49
2	B	601	G97	CAG-CAJ-CAV	3.50	106.78	103.85
2	B	601	G97	CAM-CAU-NAQ	-3.28	112.39	123.10
2	B	601	G97	C5-C6-N1	-3.23	117.23	122.07
2	A	601	G97	CAL-C5-C6	3.06	128.57	124.16
2	B	601	G97	CAJ-CAV-NAR	2.74	133.83	125.86
2	A	601	G97	CAW-C2-N1	2.65	121.78	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	G97	CAK-CAU-NAQ	2.60	129.15	120.41
2	A	601	G97	CAJ-CAV-NAR	2.35	132.67	125.86
2	B	601	G97	C5-C6-NAR	2.24	122.01	119.78
2	B	601	G97	CAI-CAW-C2	-2.18	117.20	120.78
2	A	601	G97	C6-C5-C4	-2.08	114.62	115.86
2	B	601	G97	CAK-CAU-NAQ	2.05	127.29	120.41
2	B	601	G97	CAM-C4-C5	2.00	121.81	119.58

There are no chirality outliers.

All (4) torsion outliers are listed below:

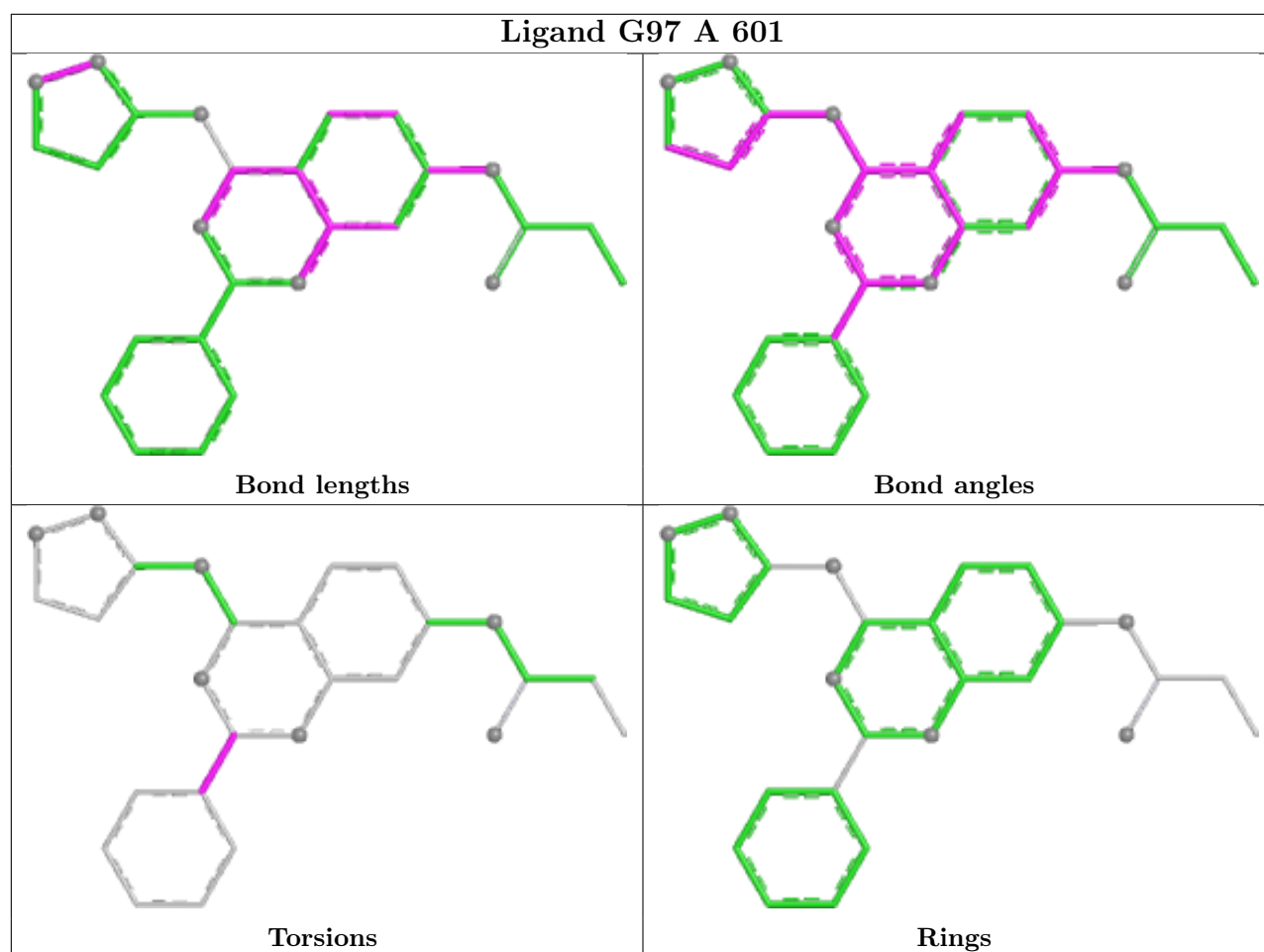
Mol	Chain	Res	Type	Atoms
2	A	601	G97	N1-C2-CAW-CAH
2	A	601	G97	N1-C2-CAW-CAI
2	A	601	G97	N3-C2-CAW-CAH
2	A	601	G97	N3-C2-CAW-CAI

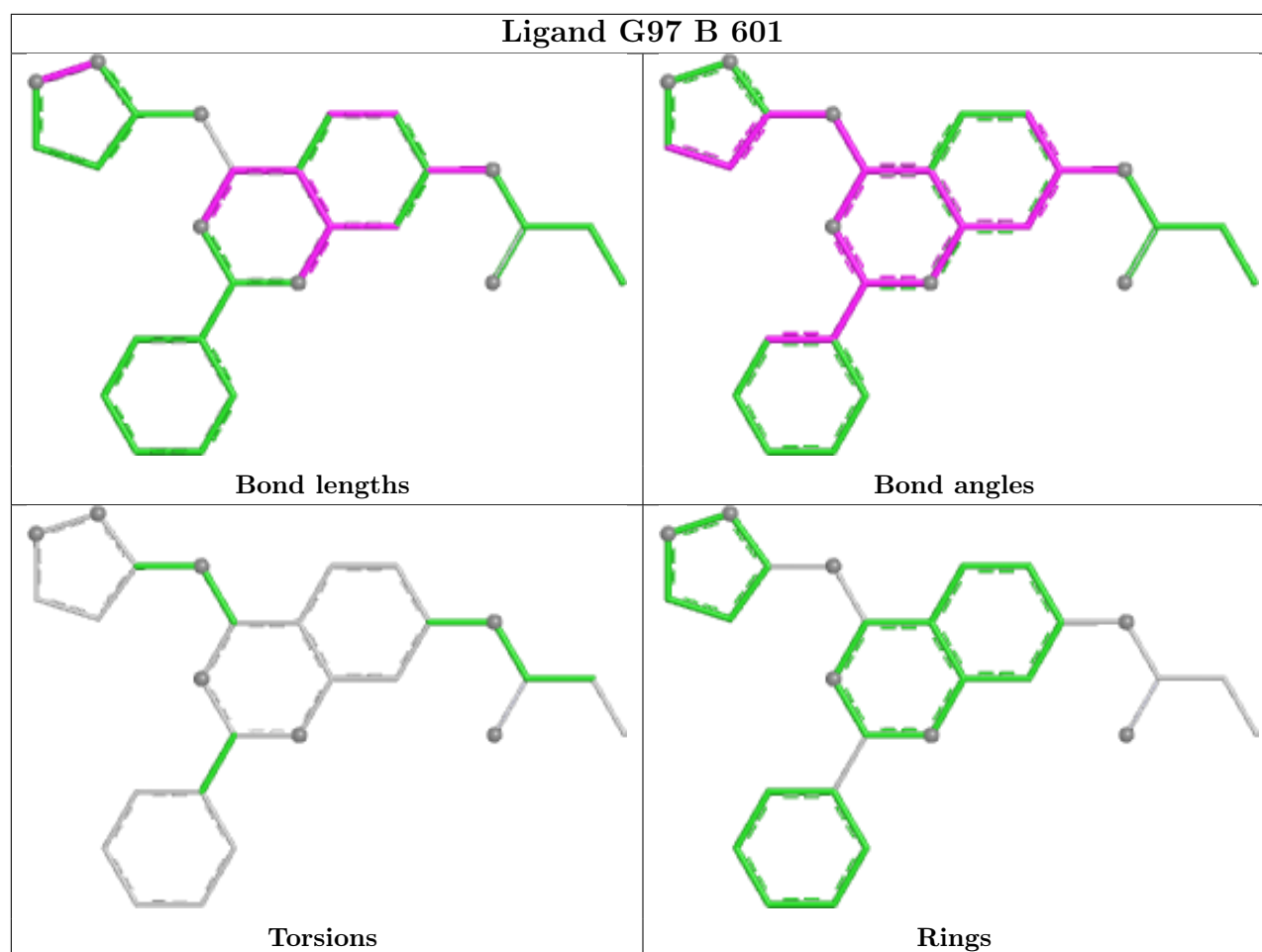
There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	G97	8	0
2	B	601	G97	2	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	260/286 (90%)	1.27	49 (18%) 3 2	13, 30, 63, 76	1 (0%)
1	B	253/286 (88%)	1.37	54 (21%) 2 1	10, 32, 62, 76	2 (0%)
All	All	513/572 (89%)	1.32	103 (20%) 3 2	10, 31, 62, 76	3 (0%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	311	ALA	6.7
1	A	276	GLY	5.9
1	A	405	PHE	5.1
1	B	309	GLN	5.0
1	B	307	PHE	4.9
1	A	267	LEU	4.8
1	B	404	ASP	4.8
1	B	313	VAL	4.6
1	B	277	CYS	4.2
1	A	278	PHE	4.1
1	A	486	GLU	3.9
1	B	472	LEU	3.7
1	B	278	PHE	3.6
1	A	277	CYS	3.6
1	B	348	ASP	3.5
1	A	289	THR	3.5
1	A	333	PRO	3.5
1	A	493	ASP	3.4
1	B	403	ALA	3.3
1	B	262	ILE	3.3
1	B	501[A]	LYS	3.3
1	A	265	GLU	3.3
1	B	471	VAL	3.2
1	A	389	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	266	SER	3.2
1	A	406	GLY	3.2
1	A	280	GLU	3.1
1	B	306	ALA	3.1
1	A	269	LEU	3.0
1	A	505	GLU	3.0
1	B	280	GLU	3.0
1	B	405	PHE	3.0
1	A	354	MET	3.0
1	B	276	GLY	2.9
1	A	404	ASP	2.9
1	A	270	GLU	2.9
1	B	532	ASN	2.9
1	A	282	TRP	2.9
1	A	473	ASP	2.8
1	A	288	GLY	2.8
1	A	408	ALA	2.8
1	B	440	THR	2.8
1	B	457	THR	2.8
1	B	308	LEU	2.8
1	A	271	VAL	2.8
1	B	493	ASP	2.7
1	B	456	THR	2.7
1	B	279	GLY	2.6
1	B	469	ARG	2.6
1	B	395	GLY	2.5
1	B	316	LYS	2.5
1	B	407	LEU	2.5
1	A	292	VAL	2.5
1	B	263	PRO	2.5
1	B	345	CYS	2.4
1	A	279	GLY	2.4
1	B	260	TRP	2.4
1	B	502	ASP	2.4
1	B	505	GLU	2.4
1	A	284	GLY	2.4
1	B	531	GLU	2.4
1	A	263	PRO	2.4
1	A	391	ASN	2.3
1	B	354	MET	2.3
1	A	306	ALA	2.3
1	B	286	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	287	ASN	2.3
1	A	532	ASN	2.3
1	B	424	PHE	2.3
1	B	312	GLN	2.3
1	A	426	ILE	2.2
1	A	425	PRO	2.2
1	A	494	LEU	2.2
1	A	285	THR	2.2
1	B	317	LEU	2.2
1	A	307	PHE	2.2
1	B	328	VAL	2.2
1	B	468	ASN	2.2
1	B	258	ASP	2.2
1	B	275	GLN	2.1
1	B	314	MET	2.1
1	A	454	GLU	2.1
1	B	332	GLU	2.1
1	B	391	ASN	2.1
1	B	523	THR	2.1
1	A	465	GLY	2.1
1	B	353	GLU	2.1
1	A	308	LEU	2.1
1	A	332	GLU	2.1
1	A	443	SER	2.1
1	B	282	TRP	2.1
1	B	436	TYR	2.1
1	B	470	GLU	2.1
1	A	281	VAL	2.0
1	B	381	ASN	2.0
1	B	499	TRP	2.0
1	A	502	ASP	2.0
1	A	304	PRO	2.0
1	A	272	LYS	2.0
1	B	454	GLU	2.0
1	A	424	PHE	2.0
1	A	501	LYS	2.0
1	A	409	ARG	2.0

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

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](#)

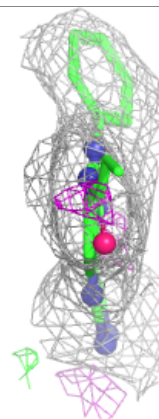
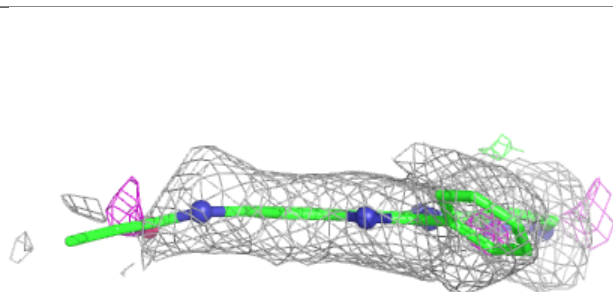
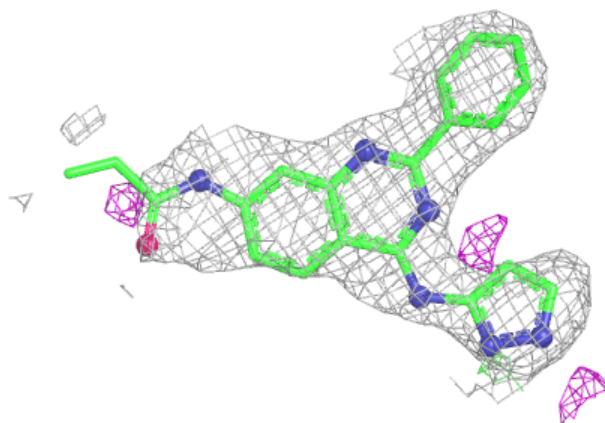
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	G97	A	601	27/27	0.80	0.19	29,33,42,43	0
2	G97	B	601	27/27	0.92	0.10	10,10,13,13	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.

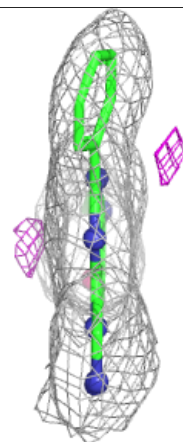
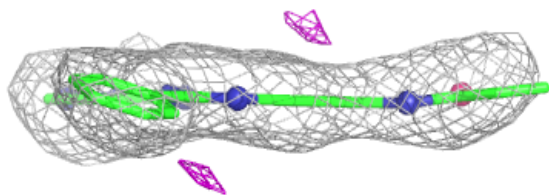
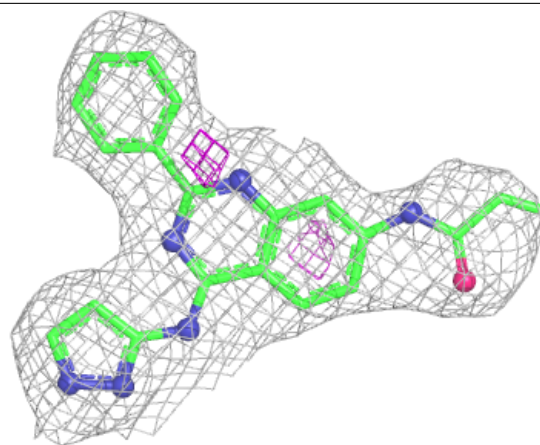
Electron density around G97 A 601:

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 G97 B 601:

$2mF_o-DF_c$ (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.