



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:24 AM UTC

PDB ID : 4PRG / pdb_00004prg
Title : 0072 PARTIAL AGONIST PPAR GAMMA COCRYSTAL
Authors : Milburn, M.V.
Deposited on : 1999-05-07
Resolution : 2.90 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

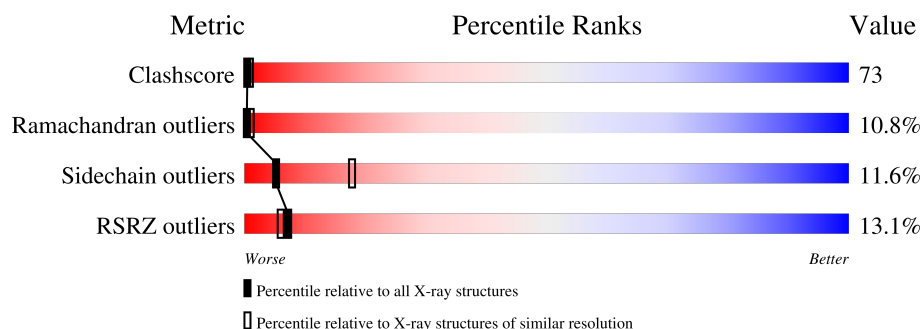
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	270	13% 16% 61% 19% .
1	B	270	16% 17% 61% 20% .
1	C	270	10% 14% 62% 21% .
1	D	270	14% 20% 59% 19% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	072	A	1	-	X	-	-
2	072	D	4	-	X	-	-

2 Entry composition [i](#)

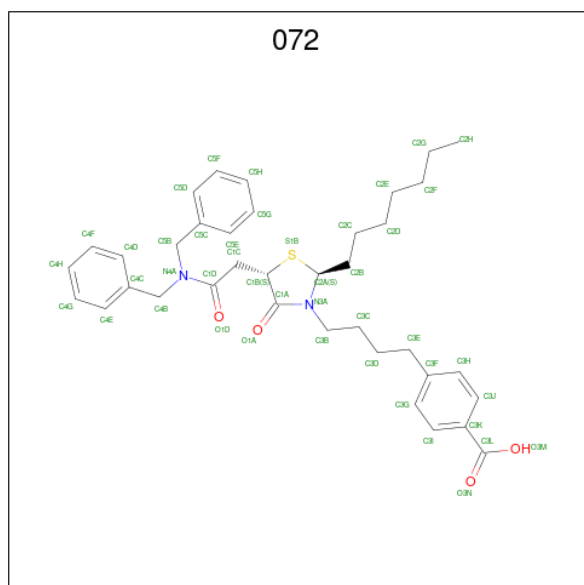
There are 2 unique types of molecules in this entry. The entry contains 8840 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR GAMMA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2166	1397	354	405	10			
1	B	270	Total	C	N	O	S	0	0	0
			2166	1397	354	405	10			
1	C	270	Total	C	N	O	S	0	0	0
			2166	1397	354	405	10			
1	D	270	Total	C	N	O	S	0	0	0
			2166	1397	354	405	10			

- Molecule 2 is (+/-)(2S,5S)-3-(4-(4-CARBOXYPHENYL)BUTYL)-2-HEPTYL-4-OXO-5-T HIAZOLIDINE (CCD ID: 072) (formula: C₃₇H₄₆N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			44	37	2	4	1		

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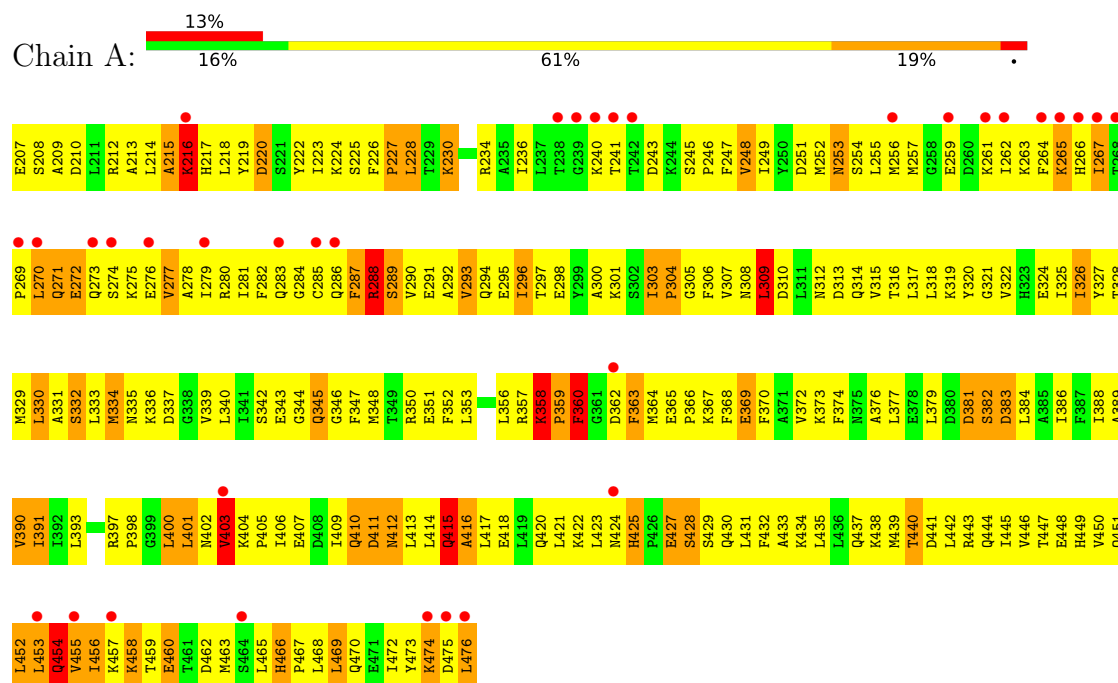
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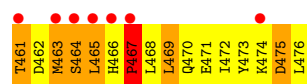
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			44	37	2	4	1		
2	C	1	Total	C	N	O	S	0	0
			44	37	2	4	1		
2	D	1	Total	C	N	O	S	0	0
			44	37	2	4	1		

3 Residue-property plots

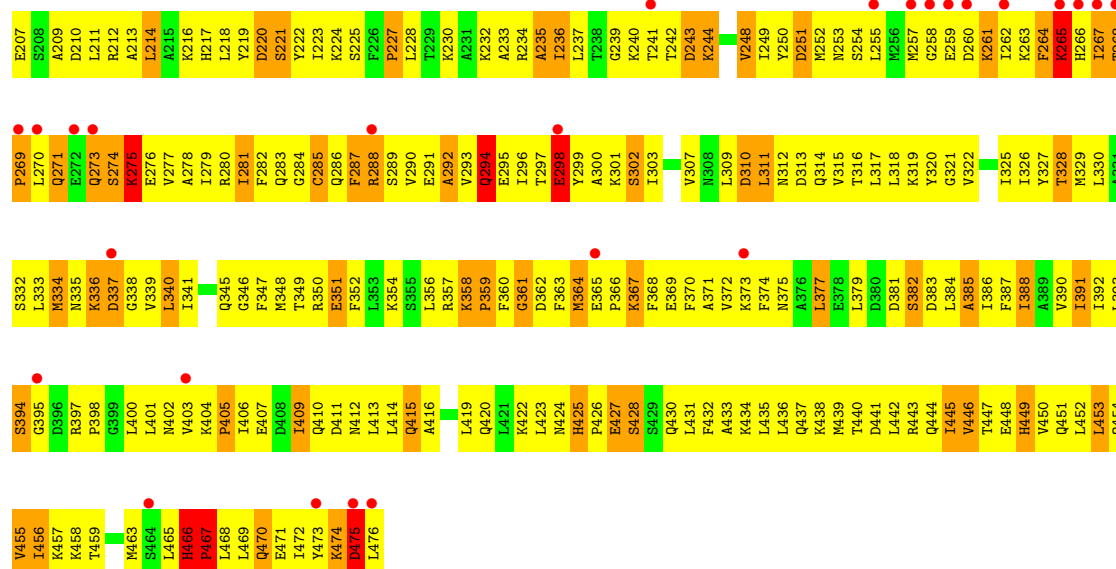
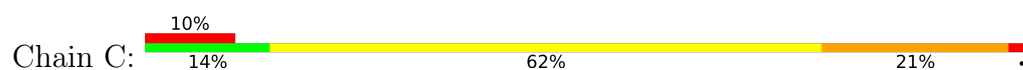
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: PROTEIN (PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR GAMMA)

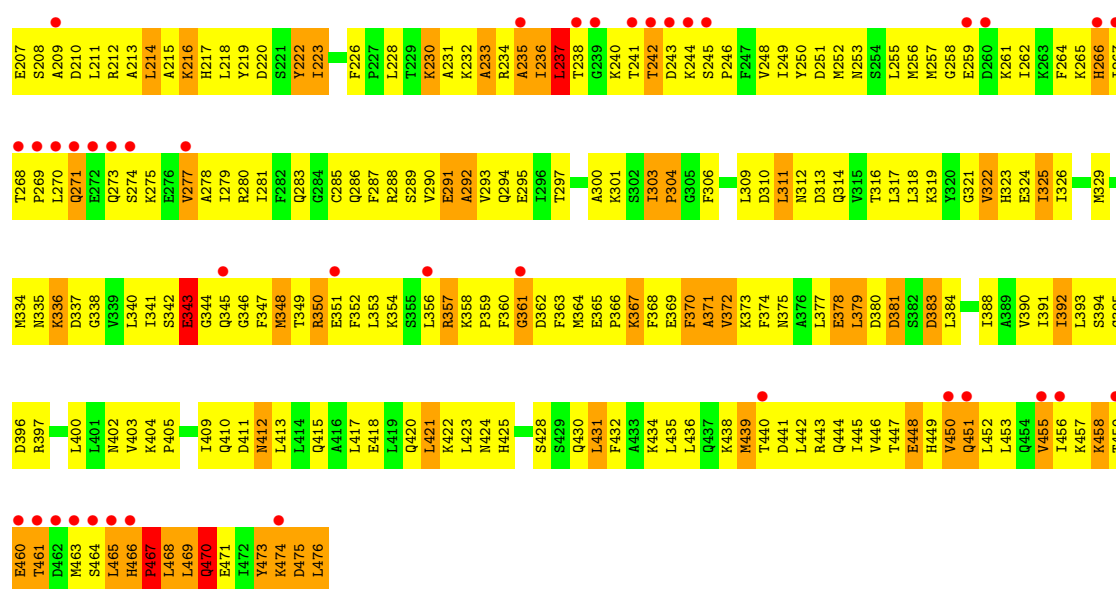




● Molecule 1: PROTEIN (PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR GAMMA)



● Molecule 1: PROTEIN (PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR GAMMA)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	92.72Å 61.54Å 118.81Å 90.00° 102.57° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90 10.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	78.6 (10.00-2.90) 85.1 (10.00-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.59Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.240 , 0.283 0.273 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.527	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 120.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8840	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 83.80 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9712e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 072

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.56	0/2203	1.13	22/2967 (0.7%)
1	B	0.56	0/2203	1.11	22/2967 (0.7%)
1	C	0.57	0/2203	1.10	21/2967 (0.7%)
1	D	0.59	0/2203	1.11	19/2967 (0.6%)
All	All	0.57	0/8812	1.11	84/11868 (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	D	0	1

There are no bond length outliers.

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	ASP	N-CA-C	-9.24	101.18	111.07
1	C	453	LEU	N-CA-C	-9.03	102.39	113.50
1	A	462	ASP	N-CA-C	-8.22	103.03	113.23
1	D	431	LEU	N-CA-C	-7.72	101.98	111.40
1	D	470	GLN	N-CA-C	-7.57	103.93	113.01
1	A	415	GLN	N-CA-C	-7.45	101.63	111.24
1	A	288	ARG	N-CA-C	-7.38	103.24	111.28
1	D	465	LEU	N-CA-C	-7.21	101.42	111.81
1	C	298	GLU	N-CA-C	-7.18	103.14	110.97
1	A	403	VAL	N-CA-C	7.16	118.47	111.67
1	A	230	LYS	N-CA-C	-7.10	103.54	111.28
1	C	248	VAL	N-CA-C	7.05	118.79	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	404	LYS	CA-C-N	7.04	126.86	119.05
1	B	404	LYS	C-N-CA	7.04	126.86	119.05
1	B	337	ASP	N-CA-C	6.98	121.03	112.23
1	B	262	ILE	N-CA-C	6.88	118.25	108.42
1	C	425	HIS	CA-C-N	6.79	127.34	119.47
1	C	425	HIS	C-N-CA	6.79	127.34	119.47
1	C	449	HIS	N-CA-C	-6.79	103.81	111.14
1	A	236	ILE	N-CA-C	-6.70	106.60	113.10
1	D	448	GLU	N-CA-C	-6.67	103.93	111.07
1	C	377	LEU	N-CA-C	-6.66	105.12	113.18
1	A	277	VAL	N-CA-C	6.66	116.79	110.53
1	B	214	LEU	N-CA-C	-6.64	103.96	111.07
1	D	291	GLU	N-CA-C	-6.55	104.06	111.07
1	C	334	MET	N-CA-C	6.55	120.08	109.40
1	B	414	LEU	N-CA-C	-6.54	104.24	111.36
1	B	285	CYS	N-CA-C	-6.53	103.86	110.97
1	D	222	TYR	N-CA-C	-6.48	104.29	111.36
1	C	292	ALA	N-CA-C	-6.45	104.29	111.71
1	B	400	LEU	N-CA-C	-6.44	100.89	110.23
1	A	363	PHE	N-CA-C	6.41	118.81	111.11
1	B	451	GLN	N-CA-C	-6.39	105.37	113.43
1	A	454	GLN	N-CA-C	-6.38	104.25	111.07
1	B	461	THR	N-CA-C	-6.30	105.61	113.55
1	A	356	LEU	N-CA-C	6.30	118.00	110.19
1	A	273	GLN	N-CA-C	6.20	118.83	111.33
1	B	367	LYS	N-CA-C	-6.15	104.13	111.69
1	C	281	ILE	CB-CA-C	-6.14	106.49	111.71
1	C	235	ALA	N-CA-C	-6.11	101.58	111.04
1	C	287	PHE	N-CA-C	-5.99	104.33	111.69
1	A	466	HIS	CA-C-N	5.96	127.29	119.84
1	A	466	HIS	C-N-CA	5.96	127.29	119.84
1	A	334	MET	N-CA-C	5.92	118.40	109.41
1	C	382	SER	N-CA-C	-5.88	104.78	111.07
1	A	328	THR	N-CA-C	-5.77	104.68	110.97
1	D	230	LYS	N-CA-C	-5.75	104.38	111.40
1	C	388	ILE	N-CA-C	-5.72	104.28	112.35
1	D	383	ASP	N-CA-C	-5.66	104.75	111.03
1	B	469	LEU	N-CA-C	-5.63	105.14	112.23
1	B	289	SER	N-CA-C	-5.60	105.09	111.14
1	B	452	LEU	N-CA-C	-5.58	106.45	113.20
1	A	303	ILE	CA-C-N	5.56	126.79	119.84
1	A	303	ILE	C-N-CA	5.56	126.79	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	326	ILE	N-CA-C	5.51	115.65	110.30
1	C	240	LYS	N-CA-C	-5.47	106.68	113.19
1	D	367	LYS	N-CA-C	-5.46	105.33	111.28
1	B	454	GLN	N-CA-C	-5.46	104.73	111.33
1	A	411	ASP	N-CA-C	-5.44	104.99	111.03
1	C	214	LEU	N-CA-C	-5.43	104.40	111.02
1	D	209	ALA	N-CA-C	-5.43	105.26	111.07
1	D	303	ILE	CA-C-N	5.41	126.60	119.84
1	D	303	ILE	C-N-CA	5.41	126.60	119.84
1	B	230	LYS	N-CA-C	-5.39	105.49	111.36
1	B	465	LEU	N-CA-C	-5.36	106.33	112.92
1	A	248	VAL	N-CA-C	5.33	116.97	108.87
1	D	251	ASP	N-CA-C	5.32	117.06	109.14
1	D	271	GLN	N-CA-C	-5.30	106.58	112.57
1	B	358	LYS	N-CA-C	5.29	120.75	113.77
1	B	441	ASP	N-CA-C	-5.26	105.46	111.14
1	B	387	PHE	N-CA-C	-5.23	105.58	111.28
1	C	466	HIS	CA-C-N	5.20	126.34	119.84
1	C	466	HIS	C-N-CA	5.20	126.34	119.84
1	D	233	ALA	N-CA-C	-5.18	106.65	112.87
1	B	445	ILE	CB-CA-C	-5.15	105.38	111.97
1	C	340	LEU	N-CA-C	-5.14	103.70	110.43
1	D	412	ASN	N-CA-C	-5.13	105.58	111.07
1	C	337	ASP	N-CA-C	5.12	119.39	113.20
1	D	235	ALA	N-CA-C	-5.12	105.88	111.82
1	A	425	HIS	CA-C-N	5.10	124.71	119.05
1	A	425	HIS	C-N-CA	5.10	124.71	119.05
1	D	343	GLU	N-CA-C	-5.09	105.72	112.24
1	C	415	GLN	N-CA-C	-5.07	105.21	111.40
1	D	350	ARG	N-CA-C	-5.07	106.61	112.89

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	473	TYR	Sidechain

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	2166	0	2232	334	0
1	B	2166	0	2232	329	0
1	C	2166	0	2232	353	0
1	D	2166	0	2232	324	1
2	A	44	0	45	6	0
2	B	44	0	45	4	0
2	C	44	0	45	5	0
2	D	44	0	45	1	0
All	All	8840	0	9108	1316	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 73.

All (1316) 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:400:LEU:HD12	1:A:403:VAL:HG22	1.27	1.10
1:D:290:VAL:HG21	1:D:473:TYR:HD1	1.17	1.08
1:D:452:LEU:O	1:D:456:ILE:HG12	1.54	1.07
1:C:320:TYR:HB2	1:C:397:ARG:HH11	1.22	1.02
1:D:259:GLU:HA	1:D:262:ILE:HG22	1.35	1.02
1:A:357:ARG:HG2	1:A:359:PRO:HD2	1.36	1.02
1:B:311:LEU:HD12	1:B:311:LEU:H	1.24	1.01
1:C:212:ARG:HH11	1:C:423:LEU:HD13	1.26	0.99
1:B:419:LEU:HA	1:B:422:LYS:HD2	1.41	0.99
1:A:212:ARG:O	1:A:216:LYS:HD3	1.60	0.99
1:A:288:ARG:NH1	1:A:289:SER:HA	1.77	0.99
1:C:276:GLU:O	1:C:280:ARG:HB2	1.64	0.98
1:C:358:LYS:HE2	1:C:358:LYS:H	1.29	0.97
1:A:288:ARG:C	1:A:288:ARG:HD2	1.91	0.95
1:D:259:GLU:HB3	1:D:269:PRO:HD3	1.49	0.94
1:D:233:ALA:O	1:D:237:LEU:HB2	1.68	0.94
1:C:271:GLN:O	1:C:276:GLU:HA	1.69	0.93
1:B:462:ASP:HB3	1:D:423:LEU:HB3	1.51	0.93
1:B:279:ILE:HD12	1:B:279:ILE:H	1.34	0.92
1:C:291:GLU:HA	1:C:294:GLN:HG2	1.49	0.92
1:C:357:ARG:HG2	1:C:359:PRO:HD2	1.48	0.92
1:C:212:ARG:NH1	1:C:423:LEU:HD13	1.84	0.92
1:D:256:MET:HE1	1:D:280:ARG:NH2	1.83	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:VAL:HG21	1:D:473:TYR:CD1	2.04	0.91
1:D:358:LYS:H	1:D:358:LYS:HD2	1.35	0.91
1:D:460:GLU:HG2	1:D:463:MET:SD	2.11	0.91
1:C:286:GLN:HA	1:C:289:SER:OG	1.71	0.90
1:D:270:LEU:HB3	1:D:274:SER:HB3	1.51	0.90
1:D:402:ASN:O	1:D:405:PRO:HD2	1.73	0.89
1:C:370:PHE:HA	1:C:373:LYS:HE3	1.54	0.89
1:A:454:GLN:HG2	1:A:475:ASP:OD2	1.73	0.89
1:A:448:GLU:O	1:A:451:GLN:HG2	1.73	0.88
1:C:212:ARG:O	1:C:216:LYS:HD3	1.73	0.88
1:D:447:THR:O	1:D:450:VAL:HG22	1.73	0.88
1:C:348:MET:HE2	1:C:352:PHE:HE2	1.38	0.87
1:D:288:ARG:NH2	1:D:342:SER:HA	1.89	0.87
1:C:334:MET:HE1	1:C:364:MET:HE1	1.53	0.87
1:C:442:LEU:O	1:C:446:VAL:HG23	1.72	0.87
1:A:271:GLN:O	1:A:276:GLU:HA	1.75	0.87
1:B:466:HIS:CB	1:B:470:GLN:HB2	2.05	0.87
1:C:440:THR:HG23	1:C:441:ASP:H	1.39	0.87
1:D:476:LEU:H	1:D:476:LEU:HD23	1.39	0.87
1:C:268:THR:H	1:C:269:PRO:HD2	1.38	0.86
1:C:334:MET:HE2	1:C:339:VAL:HB	1.59	0.85
1:A:270:LEU:HD22	1:A:271:GLN:H	1.41	0.85
1:A:469:LEU:HD12	1:A:472:ILE:HD11	1.58	0.85
1:B:212:ARG:HA	1:B:212:ARG:NH1	1.91	0.84
1:B:234:ARG:HH12	1:B:237:LEU:HD13	1.42	0.84
1:B:312:ASN:N	1:B:312:ASN:HD22	1.73	0.84
1:C:437:GLN:O	1:C:440:THR:HG22	1.77	0.84
1:A:374:PHE:HA	1:A:438:LYS:HZ3	1.40	0.84
1:B:321:GLY:O	1:B:325:ILE:HG12	1.77	0.83
1:C:294:GLN:HE21	1:C:294:GLN:HA	1.41	0.83
1:A:256:MET:HA	1:A:259:GLU:HG3	1.60	0.83
1:C:212:ARG:HH21	1:C:216:LYS:HE3	1.44	0.83
1:D:325:ILE:HG22	1:D:329:MET:HE2	1.61	0.82
1:D:259:GLU:OE2	1:D:264:PHE:HB3	1.79	0.82
1:D:252:MET:O	1:D:255:LEU:HB3	1.78	0.82
1:C:290:VAL:O	1:C:293:VAL:HB	1.80	0.82
1:D:343:GLU:HB3	1:D:345:GLN:HG2	1.61	0.81
1:B:381:ASP:HA	1:B:384:LEU:HD13	1.63	0.80
1:D:288:ARG:HH21	1:D:342:SER:HA	1.45	0.80
1:D:208:SER:HA	1:D:211:LEU:HD12	1.62	0.80
1:D:311:LEU:HD12	1:D:311:LEU:H	1.44	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:MET:HE1	1:D:280:ARG:HH22	1.44	0.79
1:C:287:PHE:O	1:C:290:VAL:HG12	1.82	0.79
1:B:340:LEU:O	1:B:341:ILE:HD12	1.82	0.79
1:D:264:PHE:CZ	1:D:266:HIS:HB3	2.18	0.79
1:B:439:MET:HA	1:B:442:LEU:HD12	1.64	0.79
1:C:419:LEU:HG	1:C:423:LEU:HD11	1.64	0.79
1:A:425:HIS:HB3	1:A:428:SER:HB2	1.63	0.79
1:C:449:HIS:NE2	1:C:453:LEU:HD12	1.98	0.79
1:C:232:LYS:O	1:C:236:ILE:HD12	1.83	0.78
1:D:357:ARG:HG2	1:D:358:LYS:N	1.97	0.78
1:A:359:PRO:HG2	1:A:360:PHE:HD1	1.48	0.78
1:B:325:ILE:HD12	1:B:388:ILE:HG23	1.65	0.78
1:C:370:PHE:HD1	1:C:373:LYS:HZ1	1.31	0.78
1:B:380:ASP:O	1:B:384:LEU:HD12	1.83	0.78
1:B:476:LEU:HD22	1:B:476:LEU:H	1.49	0.78
1:A:226:PHE:CD1	1:A:329:MET:HE1	2.18	0.77
1:C:341:ILE:HD13	1:C:348:MET:HB2	1.66	0.77
1:A:350:ARG:NH2	1:A:368:PHE:HB2	2.00	0.77
1:A:465:LEU:HD21	1:A:473:TYR:HD2	1.50	0.77
1:B:411:ASP:O	1:B:415:GLN:HG3	1.85	0.77
1:A:427:GLU:CD	1:A:427:GLU:H	1.92	0.77
1:A:249:ILE:HD12	1:A:255:LEU:HA	1.67	0.77
1:A:220:ASP:O	1:A:223:ILE:HB	1.85	0.77
1:C:207:GLU:HG2	1:C:209:ALA:H	1.50	0.77
1:B:288:ARG:HH12	1:B:343:GLU:H	1.30	0.77
1:A:290:VAL:O	1:A:294:GLN:HG2	1.84	0.76
1:A:460:GLU:O	1:A:463:MET:HB3	1.84	0.76
1:B:258:GLY:HA2	1:B:261:LYS:HD2	1.65	0.76
1:D:289:SER:O	1:D:292:ALA:HB3	1.85	0.76
1:B:212:ARG:HA	1:B:212:ARG:HH11	1.49	0.76
1:C:320:TYR:OH	1:C:398:PRO:HB2	1.86	0.76
1:D:430:GLN:O	1:D:434:LYS:HG3	1.86	0.76
1:A:430:GLN:HG2	1:B:414:LEU:HD12	1.67	0.76
1:A:212:ARG:HE	1:A:216:LYS:HE3	1.51	0.76
1:B:355:SER:O	1:B:356:LEU:HD23	1.86	0.76
1:A:252:MET:HB3	1:A:256:MET:CE	2.15	0.76
1:A:336:LYS:HZ2	1:A:350:ARG:HH12	1.34	0.76
1:A:439:MET:HA	1:A:442:LEU:HD13	1.68	0.75
1:D:358:LYS:HD2	1:D:358:LYS:N	1.99	0.75
1:B:312:ASN:HD22	1:B:312:ASN:H	1.32	0.75
1:D:259:GLU:HA	1:D:262:ILE:CG2	2.12	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LYS:O	1:A:234:ARG:HG2	1.86	0.75
1:B:264:PHE:CZ	1:B:266:HIS:HB3	2.22	0.75
1:C:265:LYS:HA	1:C:265:LYS:NZ	2.02	0.75
1:D:357:ARG:HG2	1:D:358:LYS:H	1.51	0.74
1:A:403:VAL:C	1:A:405:PRO:HD2	2.12	0.74
1:A:265:LYS:HB3	1:A:265:LYS:NZ	2.03	0.74
1:C:455:VAL:HG12	1:C:459:THR:HG21	1.70	0.74
1:A:277:VAL:HG22	1:A:281:ILE:HG13	1.68	0.74
1:B:343:GLU:HG2	1:B:345:GLN:HE21	1.52	0.74
1:C:370:PHE:HD1	1:C:373:LYS:NZ	1.86	0.74
1:D:465:LEU:O	1:D:466:HIS:HD2	1.71	0.74
1:C:320:TYR:HB2	1:C:397:ARG:NH1	1.99	0.74
1:D:264:PHE:HE2	1:D:267:ILE:H	1.36	0.74
1:B:343:GLU:HB3	1:B:345:GLN:HG2	1.70	0.73
1:B:463:MET:C	1:B:465:LEU:H	1.96	0.73
1:C:288:ARG:NH1	1:C:326:ILE:HD13	2.04	0.73
1:A:465:LEU:HD21	1:A:473:TYR:CD2	2.23	0.73
1:A:309:LEU:HD21	1:A:409:ILE:CD1	2.19	0.73
1:A:441:ASP:O	1:A:445:ILE:HG13	1.88	0.73
1:D:364:MET:HA	1:D:367:LYS:HG2	1.68	0.73
1:B:466:HIS:HB3	1:B:470:GLN:HB2	1.71	0.73
1:D:440:THR:O	1:D:444:GLN:HG2	1.89	0.73
1:A:379:LEU:HD21	1:A:435:LEU:HD22	1.69	0.73
1:A:466:HIS:CE1	1:A:468:LEU:HG	2.24	0.73
1:B:421:LEU:HD12	1:B:432:PHE:HA	1.71	0.73
1:A:320:TYR:CB	1:A:397:ARG:HH11	2.02	0.72
1:A:212:ARG:HB3	1:A:216:LYS:NZ	2.04	0.72
1:D:411:ASP:O	1:D:415:GLN:HG3	1.89	0.72
1:A:449:HIS:O	1:A:452:LEU:HB2	1.90	0.72
1:C:318:LEU:O	1:C:322:VAL:HB	1.90	0.72
1:A:257:MET:O	1:A:261:LYS:HG2	1.90	0.72
1:B:441:ASP:O	1:B:445:ILE:HG12	1.89	0.72
1:C:366:PRO:HA	1:C:369:GLU:CD	2.15	0.72
1:C:425:HIS:HB3	1:C:428:SER:OG	1.89	0.72
1:A:292:ALA:O	1:A:296:ILE:HG13	1.90	0.71
1:B:343:GLU:CG	1:B:345:GLN:HE21	2.03	0.71
1:A:456:ILE:O	1:A:460:GLU:HB2	1.91	0.71
1:C:358:LYS:H	1:C:358:LYS:CE	2.03	0.71
1:D:269:PRO:HA	1:D:280:ARG:NH2	2.05	0.71
1:D:466:HIS:H	1:D:467:PRO:HD2	1.55	0.71
1:A:247:PHE:CE2	1:A:261:LYS:HG3	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:405:PRO:O	1:C:409:ILE:HG13	1.89	0.71
1:D:232:LYS:C	1:D:234:ARG:H	1.98	0.71
1:B:260:ASP:OD1	1:B:269:PRO:HG3	1.91	0.71
1:D:234:ARG:CZ	1:D:237:LEU:HD13	2.20	0.71
1:D:311:LEU:HD12	1:D:311:LEU:N	2.04	0.71
1:A:400:LEU:CD1	1:A:403:VAL:HG22	2.12	0.71
1:C:393:LEU:CD1	1:C:409:ILE:HB	2.22	0.70
1:A:324:GLU:HG2	1:A:446:VAL:HG21	1.74	0.70
1:D:365:GLU:O	1:D:369:GLU:HG3	1.90	0.70
1:C:274:SER:O	1:C:275:LYS:HB2	1.90	0.70
1:A:350:ARG:HH21	1:A:368:PHE:HB2	1.56	0.70
1:A:437:GLN:O	1:A:440:THR:HG22	1.90	0.70
1:B:430:GLN:HE21	1:B:433:ALA:CB	2.03	0.70
1:C:251:ASP:OD1	1:C:253:ASN:HB3	1.91	0.70
1:C:334:MET:HE1	1:C:364:MET:CE	2.22	0.70
1:B:460:GLU:HG2	1:B:463:MET:SD	2.32	0.70
1:B:249:ILE:HD12	1:B:348:MET:HE2	1.74	0.70
1:C:291:GLU:HA	1:C:294:GLN:CG	2.21	0.70
1:C:440:THR:HG23	1:C:441:ASP:N	2.07	0.70
1:D:292:ALA:HA	1:D:295:GLU:OE1	1.92	0.70
1:D:476:LEU:H	1:D:476:LEU:CD2	2.05	0.70
1:A:348:MET:SD	1:A:353:LEU:HD21	2.31	0.69
1:D:358:LYS:H	1:D:358:LYS:CD	2.05	0.69
1:B:341:ILE:HD13	1:B:348:MET:HB2	1.73	0.69
1:B:369:GLU:O	1:B:372:VAL:HB	1.91	0.69
1:B:461:THR:HB	1:D:423:LEU:HD21	1.73	0.69
1:C:293:VAL:HG11	1:C:468:LEU:HD13	1.74	0.69
1:C:403:VAL:HG12	1:C:407:GLU:HG3	1.75	0.69
1:D:371:ALA:HB1	1:D:375:ASN:HD21	1.56	0.69
1:B:460:GLU:OE2	1:B:463:MET:HB2	1.93	0.69
1:C:419:LEU:HG	1:C:423:LEU:CD1	2.22	0.69
1:C:455:VAL:O	1:C:459:THR:HG23	1.91	0.69
1:B:417:LEU:O	1:B:420:GLN:HB3	1.92	0.69
1:A:214:LEU:HD23	1:A:416:ALA:HB2	1.75	0.69
1:D:232:LYS:HD2	1:D:235:ALA:HB3	1.74	0.69
1:A:330:LEU:O	1:A:333:LEU:HB2	1.93	0.69
1:B:475:ASP:OD1	1:B:476:LEU:HD22	1.93	0.69
1:A:288:ARG:C	1:A:288:ARG:CD	2.63	0.69
1:A:288:ARG:O	1:A:291:GLU:HB2	1.93	0.69
1:B:462:ASP:H	1:D:423:LEU:HD22	1.57	0.69
1:D:468:LEU:HD12	1:D:468:LEU:H	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:THR:N	1:C:269:PRO:HD2	2.07	0.69
1:D:271:GLN:HE21	1:D:271:GLN:HA	1.58	0.68
1:C:288:ARG:C	1:C:288:ARG:HD2	2.18	0.68
1:D:364:MET:HA	1:D:367:LYS:CG	2.22	0.68
1:B:286:GLN:O	1:B:290:VAL:HG23	1.92	0.68
1:B:317:LEU:HD22	1:B:393:LEU:HA	1.74	0.68
1:B:357:ARG:HB3	1:B:360:PHE:HD2	1.58	0.68
1:B:466:HIS:HB2	1:B:470:GLN:HB2	1.75	0.68
1:C:474:LYS:HB2	1:C:474:LYS:NZ	2.06	0.68
1:D:445:ILE:HA	1:D:448:GLU:HG3	1.76	0.68
1:A:340:LEU:HB3	1:A:344:GLY:HA2	1.76	0.68
1:A:286:GLN:HA	1:A:289:SER:OG	1.94	0.68
1:B:282:PHE:C	1:B:284:GLY:H	2.01	0.68
1:B:466:HIS:N	1:B:467:PRO:CD	2.57	0.68
1:D:410:GLN:HA	1:D:413:LEU:HD12	1.75	0.68
1:A:309:LEU:HD21	1:A:409:ILE:HD11	1.74	0.68
1:D:301:LYS:HD2	1:D:301:LYS:N	2.09	0.68
1:A:310:ASP:OD2	1:A:312:ASN:HB2	1.94	0.67
1:B:466:HIS:N	1:B:467:PRO:HD2	2.09	0.67
1:A:270:LEU:HD13	1:A:271:GLN:N	2.09	0.67
1:A:438:LYS:O	1:A:442:LEU:HD12	1.95	0.67
1:D:417:LEU:O	1:D:420:GLN:HB3	1.94	0.67
1:A:305:GLY:HA2	1:A:308:ASN:HD22	1.58	0.67
1:D:455:VAL:O	1:D:458:LYS:HG2	1.95	0.67
1:A:334:MET:HB3	1:A:339:VAL:HB	1.76	0.67
1:B:424:ASN:ND2	1:B:425:HIS:NE2	2.43	0.67
1:B:475:ASP:CG	1:B:476:LEU:HD22	2.19	0.67
1:C:433:ALA:O	1:C:437:GLN:HG2	1.95	0.67
1:D:311:LEU:H	1:D:311:LEU:CD1	2.07	0.67
1:B:247:PHE:CE2	1:B:258:GLY:HA3	2.30	0.67
1:B:404:LYS:HB3	1:B:405:PRO:HD3	1.77	0.67
1:C:348:MET:HE2	1:C:352:PHE:CE2	2.26	0.67
1:A:359:PRO:HG2	1:A:360:PHE:CD1	2.29	0.67
1:B:230:LYS:HA	1:B:332:SER:HB3	1.76	0.67
1:B:430:GLN:HE21	1:B:433:ALA:HB3	1.59	0.67
1:D:259:GLU:C	1:D:261:LYS:H	2.02	0.67
1:C:283:GLN:HG2	1:C:463:MET:HE1	1.77	0.67
1:C:330:LEU:HD12	1:C:333:LEU:HD12	1.77	0.67
1:B:457:LYS:HG3	1:B:458:LYS:N	2.09	0.66
1:A:252:MET:HE3	1:A:256:MET:HE2	1.77	0.66
1:D:270:LEU:HD13	1:D:274:SER:OG	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:GLN:HA	1:D:271:GLN:NE2	2.10	0.66
1:D:256:MET:SD	1:D:269:PRO:HB2	2.35	0.66
1:C:400:LEU:HD22	1:C:406:ILE:CD1	2.25	0.66
1:C:465:LEU:HB3	1:C:470:GLN:NE2	2.11	0.66
1:A:212:ARG:NE	1:A:216:LYS:HE3	2.10	0.66
1:C:339:VAL:HG22	1:C:340:LEU:O	1.95	0.66
1:C:358:LYS:HE2	1:C:358:LYS:N	2.08	0.66
1:A:411:ASP:O	1:A:415:GLN:HG3	1.96	0.65
1:B:252:MET:HE1	1:B:355:SER:O	1.96	0.65
1:C:419:LEU:O	1:C:423:LEU:HD12	1.95	0.65
1:A:219:TYR:CE1	1:A:382:SER:HA	2.30	0.65
1:A:370:PHE:HA	1:A:373:LYS:HE3	1.78	0.65
1:A:427:GLU:O	1:A:429:SER:N	2.28	0.65
1:D:466:HIS:H	1:D:467:PRO:CD	2.08	0.65
1:A:225:SER:O	1:A:295:GLU:HB3	1.96	0.65
1:D:212:ARG:HA	1:D:212:ARG:NH1	2.12	0.65
1:D:340:LEU:C	1:D:341:ILE:HD12	2.21	0.65
1:C:359:PRO:HG2	1:C:360:PHE:H	1.61	0.65
1:D:214:LEU:O	1:D:218:LEU:HG	1.97	0.65
1:D:357:ARG:HB3	1:D:360:PHE:HD2	1.62	0.65
1:C:330:LEU:HG	1:C:334:MET:HE3	1.78	0.64
1:A:293:VAL:HG22	1:A:322:VAL:HG21	1.78	0.64
1:A:453:LEU:HD13	1:A:473:TYR:CE1	2.32	0.64
1:C:230:LYS:O	1:C:234:ARG:HG2	1.97	0.64
1:B:472:ILE:C	1:B:473:TYR:HD1	2.05	0.64
1:A:366:PRO:HG2	1:A:367:LYS:HE3	1.79	0.64
1:B:348:MET:HG2	1:B:353:LEU:HD21	1.80	0.64
1:D:301:LYS:HD2	1:D:301:LYS:H	1.62	0.64
1:C:309:LEU:HD21	1:C:409:ILE:HD11	1.78	0.64
1:A:329:MET:O	1:A:331:ALA:N	2.30	0.64
1:C:214:LEU:HD21	1:C:413:LEU:HD23	1.78	0.64
1:C:268:THR:H	1:C:269:PRO:CD	2.09	0.64
1:C:307:VAL:HA	1:C:314:GLN:OE1	1.97	0.64
1:C:404:LYS:N	1:C:405:PRO:HD2	2.13	0.64
1:D:208:SER:O	1:D:212:ARG:HG2	1.97	0.64
1:D:439:MET:O	1:D:443:ARG:HB2	1.96	0.64
1:A:320:TYR:HB3	1:A:397:ARG:HH11	1.61	0.64
1:B:451:GLN:C	1:B:451:GLN:NE2	2.56	0.64
1:A:369:GLU:O	1:A:373:LYS:HG2	1.98	0.64
1:D:453:LEU:HD23	1:D:475:ASP:OD2	1.97	0.63
1:A:295:GLU:O	1:A:298:GLU:HB3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:THR:OG1	1:A:318:LEU:HD13	1.98	0.63
1:A:319:LYS:HA	1:A:472:ILE:HG22	1.79	0.63
1:B:253:ASN:HB3	1:B:257:MET:SD	2.39	0.63
1:D:232:LYS:C	1:D:234:ARG:N	2.52	0.63
1:A:230:LYS:HG3	1:A:332:SER:HB3	1.78	0.63
1:A:469:LEU:HA	1:A:472:ILE:HG12	1.80	0.63
1:B:312:ASN:N	1:B:312:ASN:ND2	2.46	0.63
1:A:364:MET:SD	2:A:1:072:H4F	2.39	0.63
1:A:373:LYS:HG3	1:A:438:LYS:HE3	1.81	0.63
1:C:357:ARG:CG	1:C:359:PRO:HD2	2.25	0.63
1:B:357:ARG:HG2	1:B:359:PRO:CD	2.29	0.63
1:B:402:ASN:OD1	1:B:405:PRO:HD3	1.99	0.63
1:D:411:ASP:C	1:D:415:GLN:HE21	2.07	0.63
1:B:223:ILE:HG22	1:B:224:LYS:HD3	1.80	0.62
1:D:412:ASN:HA	1:D:415:GLN:NE2	2.14	0.62
1:C:250:TYR:O	1:C:251:ASP:HB3	1.98	0.62
1:A:357:ARG:CG	1:A:359:PRO:HD2	2.24	0.62
1:B:264:PHE:CG	1:B:265:LYS:N	2.68	0.62
1:B:353:LEU:O	1:B:356:LEU:HG	2.00	0.62
1:B:357:ARG:HB3	1:B:360:PHE:CD2	2.34	0.62
1:D:334:MET:HE2	1:D:368:PHE:CE1	2.33	0.62
1:A:428:SER:HB3	1:A:431:LEU:HB2	1.81	0.62
1:C:364:MET:HB3	1:C:368:PHE:HE1	1.64	0.62
1:A:288:ARG:HD2	1:A:288:ARG:O	1.99	0.62
1:D:466:HIS:N	1:D:467:PRO:HD2	2.14	0.62
1:C:454:GLN:O	1:C:457:LYS:N	2.28	0.62
1:C:440:THR:HB	1:D:440:THR:HG22	1.82	0.62
1:B:256:MET:HE1	1:B:280:ARG:HH22	1.65	0.62
1:B:421:LEU:HD11	1:B:435:LEU:HD23	1.81	0.62
1:C:466:HIS:CG	1:C:467:PRO:HD2	2.35	0.62
1:A:276:GLU:OE2	1:A:279:ILE:HG12	1.99	0.61
1:B:348:MET:HG2	1:B:353:LEU:CG	2.29	0.61
1:C:294:GLN:HE21	1:C:294:GLN:CA	2.05	0.61
1:D:232:LYS:HD2	1:D:235:ALA:CB	2.29	0.61
1:A:324:GLU:OE2	1:A:443:ARG:HD3	2.00	0.61
1:A:336:LYS:NZ	1:A:350:ARG:HH12	1.98	0.61
1:B:381:ASP:HA	1:B:384:LEU:CD1	2.30	0.61
1:C:311:LEU:HD23	1:C:312:ASN:N	2.15	0.61
1:A:363:PHE:HE1	2:A:1:072:H4H	1.65	0.61
1:B:462:ASP:CA	1:D:423:LEU:HD13	2.30	0.61
1:C:403:VAL:C	1:C:405:PRO:HD2	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:VAL:HG13	1:A:278:ALA:N	2.13	0.61
1:A:288:ARG:CZ	1:A:289:SER:HA	2.30	0.61
1:C:393:LEU:HD11	1:C:409:ILE:HB	1.81	0.61
1:A:267:ILE:HD13	1:A:274:SER:O	2.01	0.61
1:C:453:LEU:HD13	1:C:473:TYR:CE1	2.35	0.61
1:A:282:PHE:C	1:A:284:GLY:H	2.08	0.61
1:A:466:HIS:ND1	1:A:467:PRO:HD2	2.15	0.61
1:A:251:ASP:OD1	1:A:253:ASN:N	2.34	0.61
1:B:458:LYS:O	1:B:458:LYS:HE3	1.99	0.61
1:C:265:LYS:HA	1:C:265:LYS:HZ3	1.64	0.61
1:C:277:VAL:HG13	1:C:278:ALA:N	2.15	0.61
1:D:356:LEU:O	1:D:361:GLY:HA3	2.00	0.61
1:A:364:MET:HA	1:A:367:LYS:HG2	1.83	0.61
1:D:318:LEU:O	1:D:322:VAL:HG23	2.01	0.61
1:D:470:GLN:HE22	1:D:471:GLU:CD	2.09	0.61
1:A:276:GLU:OE2	1:A:278:ALA:HB3	2.01	0.61
1:B:325:ILE:O	1:B:329:MET:HG3	2.01	0.61
1:A:320:TYR:HB2	1:A:397:ARG:HH11	1.66	0.60
1:A:433:ALA:O	1:A:437:GLN:HG2	2.01	0.60
1:C:296:ILE:O	1:C:300:ALA:N	2.19	0.60
1:C:349:THR:HG22	1:C:350:ARG:H	1.65	0.60
1:C:249:ILE:HG21	1:C:255:LEU:HD13	1.82	0.60
1:C:264:PHE:C	1:C:266:HIS:H	2.09	0.60
1:D:325:ILE:O	1:D:329:MET:HG3	2.00	0.60
1:D:417:LEU:HD21	1:D:435:LEU:CD2	2.31	0.60
1:A:288:ARG:HH11	1:A:289:SER:HA	1.65	0.60
1:A:218:LEU:HD11	1:A:413:LEU:HD22	1.82	0.60
1:A:458:LYS:HE3	1:C:210:ASP:OD1	2.00	0.60
1:B:234:ARG:HH22	1:B:237:LEU:CD1	2.14	0.60
1:C:212:ARG:HD3	1:C:423:LEU:CD1	2.32	0.60
1:D:249:ILE:O	1:D:349:THR:HG23	2.01	0.60
1:D:341:ILE:HD13	1:D:348:MET:H	1.67	0.60
1:D:371:ALA:O	1:D:372:VAL:C	2.45	0.60
1:B:404:LYS:N	1:B:405:PRO:HD2	2.17	0.60
1:C:249:ILE:HD12	1:C:255:LEU:HA	1.82	0.60
1:D:325:ILE:HG23	1:D:388:ILE:HG23	1.82	0.60
1:D:358:LYS:HB2	1:D:359:PRO:HD3	1.84	0.60
1:D:450:VAL:CG2	1:D:451:GLN:N	2.64	0.60
1:A:330:LEU:HD11	1:A:334:MET:HE3	1.83	0.60
1:C:248:VAL:HG22	1:C:347:PHE:HB3	1.83	0.60
1:A:404:LYS:N	1:A:405:PRO:HD2	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:GLN:HA	1:B:271:GLN:HE21	1.67	0.60
1:A:265:LYS:HB3	1:A:265:LYS:HZ3	1.66	0.60
1:A:474:LYS:HB2	1:A:474:LYS:HZ2	1.67	0.60
1:B:341:ILE:HG12	1:B:348:MET:HE3	1.84	0.60
1:D:232:LYS:O	1:D:236:ILE:HG12	2.02	0.60
1:C:349:THR:HG22	1:C:350:ARG:N	2.17	0.59
1:D:457:LYS:C	1:D:459:THR:H	2.10	0.59
1:B:384:LEU:O	1:B:388:ILE:HG13	2.01	0.59
1:C:454:GLN:O	1:C:455:VAL:C	2.45	0.59
1:D:314:GLN:O	1:D:318:LEU:HD13	2.01	0.59
1:A:274:SER:O	1:A:275:LYS:HB3	2.02	0.59
1:A:360:PHE:HD1	1:A:360:PHE:H	1.50	0.59
1:A:433:ALA:O	1:A:437:GLN:CG	2.50	0.59
1:A:374:PHE:HA	1:A:438:LYS:NZ	2.16	0.59
1:D:344:GLY:C	1:D:346:GLY:H	2.11	0.59
1:D:356:LEU:HB2	1:D:361:GLY:HA2	1.84	0.59
1:C:242:THR:O	1:C:243:ASP:C	2.45	0.59
1:D:241:THR:O	1:D:242:THR:C	2.44	0.59
1:A:252:MET:HB3	1:A:256:MET:HE3	1.85	0.59
1:B:214:LEU:HD23	1:B:416:ALA:HB2	1.83	0.59
1:B:343:GLU:O	1:B:345:GLN:NE2	2.35	0.59
1:A:234:ARG:NH1	1:A:332:SER:HA	2.17	0.59
1:A:289:SER:O	1:A:290:VAL:C	2.46	0.59
1:C:288:ARG:O	1:C:292:ALA:N	2.36	0.59
1:B:327:TYR:CE1	1:B:367:LYS:HD2	2.38	0.59
1:D:213:ALA:O	1:D:214:LEU:C	2.45	0.59
1:D:420:GLN:O	1:D:424:ASN:N	2.35	0.59
1:B:288:ARG:HH12	1:B:343:GLU:N	2.00	0.58
1:D:421:LEU:N	1:D:421:LEU:HD23	2.17	0.58
1:B:268:THR:HB	1:B:269:PRO:HD2	1.85	0.58
1:C:250:TYR:CE1	1:C:254:SER:HB3	2.38	0.58
1:D:277:VAL:O	1:D:278:ALA:C	2.44	0.58
1:A:218:LEU:HD11	1:A:413:LEU:CD2	2.33	0.58
1:A:451:GLN:O	1:A:455:VAL:HG23	2.03	0.58
1:B:348:MET:HG2	1:B:353:LEU:CD2	2.33	0.58
1:D:417:LEU:HD21	1:D:435:LEU:HD21	1.85	0.58
1:A:214:LEU:HD21	1:A:413:LEU:HD23	1.85	0.58
1:C:336:LYS:HE2	1:C:372:VAL:HG11	1.85	0.58
1:D:341:ILE:HG12	1:D:348:MET:HE3	1.83	0.58
1:A:271:GLN:HB3	1:A:280:ARG:NH2	2.18	0.58
1:B:288:ARG:NH1	1:B:343:GLU:H	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:HIS:O	1:B:470:GLN:N	2.30	0.58
1:D:380:ASP:O	1:D:384:LEU:HD12	2.02	0.58
1:A:288:ARG:HD2	1:A:289:SER:N	2.18	0.58
1:A:401:LEU:C	1:A:402:ASN:HD22	2.12	0.58
1:D:379:LEU:HD12	1:D:425:HIS:HE2	1.68	0.58
1:C:259:GLU:HG2	1:C:264:PHE:CD2	2.39	0.57
1:D:338:GLY:HA3	1:D:347:PHE:CZ	2.38	0.57
1:D:343:GLU:C	1:D:345:GLN:H	2.13	0.57
1:D:279:ILE:O	1:D:283:GLN:HG3	2.04	0.57
1:B:461:THR:HG22	1:D:212:ARG:HD3	1.86	0.57
1:B:234:ARG:HH21	1:B:332:SER:C	2.13	0.57
1:C:397:ARG:H	1:C:400:LEU:HD12	1.69	0.57
1:B:322:VAL:HG13	1:B:323:HIS:N	2.19	0.57
1:B:348:MET:HG2	1:B:353:LEU:HG	1.85	0.57
1:D:370:PHE:HA	1:D:373:LYS:CE	2.34	0.57
1:A:365:GLU:N	1:A:366:PRO:HD2	2.19	0.57
1:B:306:PHE:O	1:B:308:ASN:N	2.37	0.57
1:B:343:GLU:HG2	1:B:345:GLN:NE2	2.20	0.57
1:B:445:ILE:HA	1:B:448:GLU:OE1	2.05	0.57
1:C:360:PHE:O	1:C:362:ASP:N	2.38	0.57
1:D:288:ARG:HH22	1:D:343:GLU:H	1.53	0.57
1:C:403:VAL:O	1:C:404:LYS:C	2.47	0.57
1:C:320:TYR:CB	1:C:397:ARG:HH11	2.07	0.57
1:C:430:GLN:HG3	1:C:433:ALA:HB3	1.87	0.57
1:D:259:GLU:CA	1:D:262:ILE:HG22	2.24	0.57
1:C:288:ARG:C	1:C:288:ARG:CD	2.78	0.57
1:A:220:ASP:HB2	1:A:224:LYS:HE3	1.86	0.56
1:A:207:GLU:HB3	1:A:210:ASP:HB2	1.86	0.56
1:D:216:LYS:O	1:D:220:ASP:CG	2.49	0.56
1:A:465:LEU:HD23	1:A:470:GLN:HA	1.88	0.56
1:C:252:MET:SD	1:C:255:LEU:HD23	2.45	0.56
1:C:368:PHE:O	1:C:372:VAL:HG23	2.05	0.56
1:C:444:GLN:O	1:C:448:GLU:HG3	2.06	0.56
1:D:286:GLN:O	1:D:290:VAL:HG23	2.05	0.56
1:B:333:LEU:HB3	1:B:340:LEU:HB2	1.85	0.56
1:B:436:LEU:C	1:B:438:LYS:H	2.12	0.56
1:C:288:ARG:HH12	1:C:326:ILE:HD13	1.70	0.56
1:D:222:TYR:O	1:D:226:PHE:HD2	1.88	0.56
1:D:432:PHE:O	1:D:435:LEU:HB3	2.06	0.56
1:C:371:ALA:O	1:C:375:ASN:ND2	2.39	0.56
1:C:379:LEU:HD11	1:C:435:LEU:HD22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:THR:CG2	1:C:441:ASP:H	2.14	0.56
1:D:255:LEU:HD22	1:D:352:PHE:HZ	1.70	0.56
1:D:340:LEU:HB3	1:D:344:GLY:HA2	1.87	0.56
1:D:450:VAL:HG23	1:D:451:GLN:N	2.21	0.56
1:D:418:GLU:O	1:D:422:LYS:HG3	2.06	0.56
1:C:220:ASP:O	1:C:224:LYS:N	2.36	0.56
1:C:230:LYS:HG3	1:C:332:SER:HB2	1.87	0.56
1:C:271:GLN:HE22	1:C:277:VAL:N	2.04	0.56
1:C:366:PRO:HA	1:C:369:GLU:OE2	2.06	0.56
1:C:270:LEU:HD22	1:C:271:GLN:H	1.71	0.56
1:D:370:PHE:O	1:D:371:ALA:C	2.49	0.56
1:A:305:GLY:O	1:A:308:ASN:HB2	2.05	0.56
1:A:458:LYS:NZ	1:A:458:LYS:HB2	2.20	0.56
1:B:402:ASN:OD1	1:B:405:PRO:CD	2.54	0.56
1:B:468:LEU:O	1:B:472:ILE:HG13	2.06	0.56
1:A:430:GLN:O	1:A:434:LYS:HG2	2.07	0.55
1:B:214:LEU:HD21	1:B:413:LEU:HD23	1.87	0.55
1:B:325:ILE:HD12	1:B:388:ILE:CG2	2.36	0.55
1:B:433:ALA:O	1:B:437:GLN:HG2	2.07	0.55
1:C:291:GLU:CA	1:C:294:GLN:HG2	2.32	0.55
1:C:387:PHE:O	1:C:391:ILE:HG13	2.06	0.55
1:D:334:MET:HE2	1:D:368:PHE:CD1	2.41	0.55
1:D:340:LEU:O	1:D:341:ILE:HD12	2.07	0.55
1:D:397:ARG:O	1:D:400:LEU:HD12	2.05	0.55
1:A:277:VAL:HG23	1:A:280:ARG:HH21	1.71	0.55
1:A:334:MET:HB3	1:A:339:VAL:CB	2.35	0.55
1:A:400:LEU:HD11	1:A:406:ILE:HD12	1.87	0.55
1:C:368:PHE:O	1:C:369:GLU:C	2.49	0.55
1:D:278:ALA:HB1	1:D:360:PHE:CD2	2.42	0.55
1:D:384:LEU:O	1:D:388:ILE:HG13	2.07	0.55
1:C:410:GLN:HG2	1:C:414:LEU:HG	1.89	0.55
1:A:320:TYR:CE2	1:A:398:PRO:HD2	2.42	0.55
1:D:325:ILE:HD13	1:D:325:ILE:N	2.22	0.55
1:D:412:ASN:C	1:D:412:ASN:HD22	2.12	0.55
1:D:461:THR:C	1:D:463:MET:H	2.14	0.55
1:A:300:ALA:HA	1:A:303:ILE:CD1	2.37	0.55
1:C:220:ASP:O	1:C:221:SER:C	2.50	0.55
1:C:239:GLY:C	1:C:241:THR:H	2.12	0.55
1:D:249:ILE:HD12	1:D:348:MET:HE2	1.88	0.55
1:D:457:LYS:HD2	1:D:461:THR:HG21	1.87	0.55
1:A:410:GLN:O	1:A:414:LEU:HG	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:LYS:O	1:B:236:ILE:HG13	2.07	0.55
1:B:252:MET:O	1:B:255:LEU:HB3	2.06	0.55
1:D:338:GLY:O	1:D:368:PHE:HE1	1.89	0.55
1:D:357:ARG:CG	1:D:358:LYS:H	2.16	0.55
1:D:368:PHE:O	1:D:369:GLU:C	2.50	0.55
1:A:412:ASN:HA	1:A:415:GLN:OE1	2.06	0.55
1:C:225:SER:O	1:C:295:GLU:HG2	2.07	0.55
1:C:230:LYS:HG3	1:C:332:SER:CB	2.36	0.55
1:B:357:ARG:HG2	1:B:359:PRO:HD2	1.88	0.55
1:C:249:ILE:HG23	1:C:255:LEU:HA	1.88	0.55
1:D:222:TYR:HE2	1:D:388:ILE:HD11	1.72	0.55
1:A:457:LYS:HD2	1:A:460:GLU:O	2.07	0.55
1:B:287:PHE:C	1:B:287:PHE:HD1	2.15	0.55
1:B:311:LEU:HD12	1:B:311:LEU:N	2.08	0.55
1:B:357:ARG:HG2	1:B:359:PRO:HD3	1.88	0.54
1:D:240:LYS:HG2	1:D:242:THR:H	1.71	0.54
1:D:383:ASP:OD2	1:D:425:HIS:NE2	2.39	0.54
1:B:330:LEU:C	1:B:330:LEU:HD23	2.32	0.54
1:B:336:LYS:O	1:B:350:ARG:HD2	2.07	0.54
1:D:237:LEU:HD11	1:D:334:MET:O	2.06	0.54
1:A:457:LYS:C	1:A:459:THR:H	2.14	0.54
1:A:470:GLN:HA	1:A:470:GLN:NE2	2.22	0.54
1:B:326:ILE:HG23	2:B:2:072:H5E	1.88	0.54
1:D:222:TYR:HD1	1:D:223:ILE:HD13	1.72	0.54
1:A:390:VAL:O	1:A:391:ILE:C	2.50	0.54
1:A:350:ARG:HG3	1:A:368:PHE:CZ	2.43	0.54
1:A:421:LEU:CD1	1:A:432:PHE:HA	2.38	0.54
1:B:276:GLU:O	1:B:277:VAL:C	2.50	0.54
1:B:474:LYS:O	1:B:475:ASP:HB3	2.07	0.54
1:C:290:VAL:HG13	1:C:291:GLU:N	2.23	0.54
1:C:393:LEU:HD11	1:C:409:ILE:HD12	1.90	0.54
1:D:316:THR:O	1:D:317:LEU:C	2.51	0.54
1:D:343:GLU:C	1:D:345:GLN:N	2.64	0.54
1:A:383:ASP:N	1:A:383:ASP:OD1	2.41	0.54
1:B:292:ALA:HA	1:B:295:GLU:HG3	1.88	0.54
1:A:370:PHE:HA	1:A:373:LYS:CE	2.37	0.54
1:B:287:PHE:C	1:B:287:PHE:CD1	2.86	0.54
1:B:348:MET:SD	1:B:353:LEU:HD21	2.48	0.54
1:C:251:ASP:OD1	1:C:251:ASP:C	2.50	0.54
1:D:271:GLN:HE21	1:D:271:GLN:CA	2.21	0.54
1:B:241:THR:O	1:B:243:ASP:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:PHE:C	1:B:284:GLY:N	2.61	0.54
1:B:330:LEU:HD23	1:B:330:LEU:O	2.08	0.54
1:C:212:ARG:HD3	1:C:423:LEU:HD11	1.90	0.54
1:C:335:ASN:O	1:C:336:LYS:C	2.51	0.54
1:D:322:VAL:O	1:D:326:ILE:HG13	2.08	0.54
1:D:364:MET:O	1:D:367:LYS:N	2.41	0.53
1:A:334:MET:HE2	1:A:339:VAL:HB	1.89	0.53
1:C:264:PHE:O	1:C:266:HIS:N	2.40	0.53
1:D:358:LYS:HB2	1:D:359:PRO:CD	2.37	0.53
1:B:418:GLU:O	1:B:422:LYS:HG3	2.08	0.53
1:B:444:GLN:O	1:B:448:GLU:HG3	2.07	0.53
1:B:453:LEU:O	1:B:456:ILE:N	2.42	0.53
1:A:331:ALA:C	1:A:333:LEU:H	2.16	0.53
1:A:400:LEU:HD12	1:A:403:VAL:CG2	2.18	0.53
1:B:325:ILE:CD1	1:B:388:ILE:HG23	2.37	0.53
1:C:281:ILE:O	1:C:284:GLY:N	2.41	0.53
1:D:465:LEU:C	1:D:466:HIS:HD2	2.17	0.53
1:A:379:LEU:HD11	1:A:435:LEU:HD13	1.88	0.53
1:A:474:LYS:HE3	1:A:474:LYS:HA	1.90	0.53
1:B:271:GLN:HE22	1:B:276:GLU:HA	1.73	0.53
1:B:436:LEU:O	1:B:438:LYS:N	2.33	0.53
1:C:293:VAL:O	1:C:297:THR:OG1	2.21	0.53
1:B:234:ARG:NH1	1:B:237:LEU:HD13	2.17	0.53
1:B:404:LYS:HB3	1:B:405:PRO:CD	2.38	0.53
1:C:251:ASP:OD1	1:C:253:ASN:N	2.41	0.53
1:C:445:ILE:O	1:C:446:VAL:C	2.50	0.53
1:D:268:THR:O	1:D:270:LEU:N	2.42	0.53
1:B:341:ILE:CD1	1:B:348:MET:HB2	2.39	0.53
1:D:451:GLN:O	1:D:455:VAL:HB	2.09	0.53
1:A:457:LYS:HE2	1:A:463:MET:O	2.08	0.53
1:B:463:MET:C	1:B:465:LEU:N	2.63	0.53
1:C:290:VAL:HG23	1:C:468:LEU:HD12	1.90	0.53
1:A:252:MET:C	1:A:256:MET:HE3	2.34	0.53
1:A:266:HIS:O	1:A:267:ILE:C	2.51	0.53
1:B:234:ARG:HH22	1:B:237:LEU:HD12	1.74	0.53
1:B:371:ALA:O	1:B:375:ASN:HB2	2.08	0.53
1:C:227:PRO:HD2	1:C:295:GLU:CD	2.34	0.53
1:D:360:PHE:C	1:D:362:ASP:H	2.16	0.53
1:A:293:VAL:HG22	1:A:322:VAL:CG2	2.39	0.53
1:C:370:PHE:HA	1:C:373:LYS:HG2	1.91	0.53
1:C:381:ASP:HA	1:C:384:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:LEU:O	1:C:388:ILE:HG12	2.08	0.53
1:C:448:GLU:HA	1:C:451:GLN:HG2	1.91	0.53
1:D:217:HIS:O	1:D:220:ASP:HB2	2.09	0.53
1:A:335:ASN:OD1	1:A:347:PHE:HZ	1.91	0.52
1:D:321:GLY:O	1:D:322:VAL:C	2.52	0.52
1:A:288:ARG:HG3	2:A:1:072:C1D	2.39	0.52
1:A:342:SER:O	1:A:343:GLU:HB2	2.08	0.52
1:B:424:ASN:OD1	1:B:424:ASN:O	2.26	0.52
1:C:440:THR:CB	1:D:440:THR:HG22	2.38	0.52
1:D:351:GLU:O	1:D:354:LYS:N	2.40	0.52
1:A:216:LYS:HD3	1:A:216:LYS:H	1.74	0.52
1:A:291:GLU:O	1:A:295:GLU:HG3	2.09	0.52
1:A:358:LYS:HA	1:A:358:LYS:HE3	1.91	0.52
1:B:393:LEU:O	1:B:410:GLN:HG3	2.10	0.52
1:C:227:PRO:O	1:C:228:LEU:C	2.52	0.52
1:C:424:ASN:C	1:C:426:PRO:HD3	2.34	0.52
1:D:259:GLU:C	1:D:261:LYS:N	2.62	0.52
1:B:270:LEU:HB2	1:B:274:SER:OG	2.10	0.52
1:B:279:ILE:HG22	1:B:283:GLN:OE1	2.09	0.52
1:B:457:LYS:CG	1:B:458:LYS:N	2.73	0.52
1:C:288:ARG:CZ	1:C:289:SER:OG	2.57	0.52
1:A:212:ARG:HB3	1:A:216:LYS:HZ1	1.75	0.52
1:B:271:GLN:O	1:B:271:GLN:HG3	2.08	0.52
1:B:410:GLN:O	1:B:413:LEU:HB2	2.10	0.52
1:C:410:GLN:O	1:C:413:LEU:N	2.43	0.52
1:A:270:LEU:CD2	1:A:271:GLN:H	2.15	0.52
1:C:363:PHE:O	1:C:367:LYS:HE3	2.09	0.52
1:D:451:GLN:HE22	1:D:455:VAL:HG21	1.74	0.52
1:B:351:GLU:O	1:B:352:PHE:C	2.53	0.52
1:C:251:ASP:OD1	1:C:253:ASN:CB	2.57	0.52
1:C:251:ASP:HA	1:C:352:PHE:CD1	2.45	0.52
1:C:258:GLY:HA3	1:C:264:PHE:CZ	2.44	0.52
1:C:334:MET:HB3	1:C:339:VAL:HB	1.91	0.52
1:C:393:LEU:HD12	1:C:409:ILE:HB	1.92	0.52
1:C:397:ARG:HB2	1:C:400:LEU:HG	1.92	0.52
1:D:232:LYS:O	1:D:234:ARG:N	2.42	0.52
1:D:258:GLY:O	1:D:262:ILE:N	2.43	0.52
1:B:463:MET:O	1:B:465:LEU:N	2.40	0.52
1:C:288:ARG:HD2	1:C:289:SER:N	2.24	0.52
1:D:311:LEU:C	1:D:313:ASP:H	2.16	0.52
1:D:365:GLU:N	1:D:366:PRO:HD2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:GLU:O	1:A:279:ILE:HB	2.10	0.52
1:C:268:THR:N	1:C:269:PRO:CD	2.71	0.52
1:C:450:VAL:HG11	1:C:475:ASP:HA	1.91	0.52
1:D:222:TYR:CE1	1:D:381:ASP:HB3	2.45	0.52
1:D:392:ILE:HG22	1:D:393:LEU:HD22	1.91	0.52
1:B:209:ALA:O	1:B:212:ARG:HB2	2.09	0.52
1:B:234:ARG:O	1:B:235:ALA:C	2.52	0.52
1:C:212:ARG:NH1	1:C:420:GLN:HA	2.24	0.52
1:D:268:THR:HB	1:D:269:PRO:HD2	1.92	0.52
1:B:237:LEU:O	1:B:239:GLY:N	2.43	0.51
1:D:349:THR:O	1:D:353:LEU:HD12	2.09	0.51
1:B:462:ASP:HA	1:D:423:LEU:HD13	1.90	0.51
1:C:220:ASP:HA	1:C:223:ILE:HB	1.93	0.51
1:C:394:SER:CB	1:C:397:ARG:HE	2.23	0.51
1:D:273:GLN:OE1	1:D:273:GLN:HA	2.10	0.51
1:D:394:SER:HB3	1:D:397:ARG:NE	2.25	0.51
1:A:276:GLU:OE2	1:A:279:ILE:N	2.43	0.51
1:B:317:LEU:CD2	1:B:393:LEU:HA	2.39	0.51
1:D:402:ASN:O	1:D:402:ASN:CG	2.54	0.51
1:B:384:LEU:HD12	1:B:384:LEU:H	1.75	0.51
1:D:379:LEU:HD12	1:D:383:ASP:OD2	2.11	0.51
1:D:434:LYS:O	1:D:438:LYS:HD3	2.10	0.51
1:A:249:ILE:HB	1:A:348:MET:HA	1.93	0.51
1:A:290:VAL:CG1	1:A:291:GLU:N	2.74	0.51
1:A:331:ALA:O	1:A:333:LEU:N	2.44	0.51
1:C:350:ARG:HB3	1:C:351:GLU:OE1	2.11	0.51
1:C:364:MET:O	1:C:367:LYS:HB2	2.10	0.51
1:D:270:LEU:HB3	1:D:274:SER:CB	2.34	0.51
1:A:313:ASP:OD1	1:A:401:LEU:HB2	2.10	0.51
1:A:331:ALA:C	1:A:333:LEU:N	2.68	0.51
1:B:421:LEU:HD12	1:B:432:PHE:CA	2.39	0.51
1:A:230:LYS:HG3	1:A:332:SER:CB	2.41	0.51
1:A:282:PHE:C	1:A:284:GLY:N	2.69	0.51
1:B:333:LEU:O	1:B:339:VAL:HA	2.11	0.51
1:D:435:LEU:O	1:D:438:LYS:HB2	2.11	0.51
1:D:459:THR:HG22	1:D:460:GLU:N	2.26	0.51
1:A:467:PRO:HA	1:A:470:GLN:HB3	1.91	0.51
1:C:370:PHE:O	1:C:373:LYS:HG2	2.11	0.51
1:A:325:ILE:O	1:A:329:MET:HG3	2.11	0.51
1:B:208:SER:O	1:B:211:LEU:N	2.44	0.51
1:C:363:PHE:HZ	1:C:449:HIS:HD2	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:HIS:CD2	1:C:467:PRO:HD2	2.45	0.51
1:D:457:LYS:O	1:D:459:THR:N	2.43	0.51
1:C:266:HIS:HB2	2:C:3:072:H3I	1.93	0.51
1:C:370:PHE:HA	1:C:373:LYS:CE	2.33	0.51
1:B:253:ASN:C	1:B:255:LEU:N	2.67	0.50
1:B:338:GLY:HA3	1:B:347:PHE:CZ	2.45	0.50
1:C:365:GLU:N	1:C:366:PRO:HD2	2.26	0.50
1:D:323:HIS:O	1:D:326:ILE:HB	2.11	0.50
1:D:324:GLU:OE2	1:D:443:ARG:HD2	2.11	0.50
1:C:271:GLN:HE22	1:C:277:VAL:H	1.58	0.50
1:B:291:GLU:O	1:B:293:VAL:N	2.45	0.50
1:B:322:VAL:CG1	1:B:323:HIS:N	2.74	0.50
1:C:299:TYR:O	1:C:302:SER:HB3	2.11	0.50
1:A:251:ASP:OD1	1:A:252:MET:N	2.44	0.50
1:B:324:GLU:OE1	1:B:397:ARG:NH2	2.44	0.50
1:C:311:LEU:O	1:C:314:GLN:HB2	2.11	0.50
1:C:357:ARG:HG2	1:C:358:LYS:N	2.24	0.50
1:A:277:VAL:O	1:A:278:ALA:C	2.54	0.50
1:B:430:GLN:HE21	1:B:433:ALA:HB2	1.77	0.50
1:C:363:PHE:O	1:C:364:MET:HG2	2.11	0.50
1:A:350:ARG:HG3	1:A:368:PHE:CE1	2.46	0.50
1:A:421:LEU:HD12	1:A:432:PHE:HA	1.94	0.50
1:B:457:LYS:C	1:B:457:LYS:HD2	2.37	0.50
1:D:384:LEU:HD12	1:D:384:LEU:H	1.76	0.50
1:D:461:THR:C	1:D:463:MET:N	2.68	0.50
1:A:364:MET:C	1:A:366:PRO:HD2	2.36	0.50
1:B:266:HIS:CG	1:B:267:ILE:N	2.79	0.50
1:B:289:SER:O	1:B:293:VAL:HG23	2.11	0.50
1:C:474:LYS:HB2	1:C:474:LYS:HZ2	1.74	0.50
1:A:219:TYR:CD1	1:A:382:SER:HA	2.47	0.50
1:C:221:SER:O	1:C:222:TYR:C	2.55	0.50
1:C:405:PRO:O	1:C:406:ILE:C	2.53	0.50
1:C:414:LEU:HB3	1:D:430:GLN:HG3	1.92	0.50
1:D:240:LYS:C	1:D:242:THR:H	2.18	0.50
1:B:312:ASN:H	1:B:312:ASN:ND2	2.06	0.50
1:C:386:ILE:O	1:C:390:VAL:HG23	2.12	0.50
1:D:377:LEU:HB2	1:D:379:LEU:HD22	1.94	0.50
1:B:266:HIS:CD2	1:B:267:ILE:HG22	2.47	0.49
1:C:443:ARG:O	1:C:446:VAL:HB	2.12	0.49
1:D:278:ALA:O	1:D:279:ILE:C	2.54	0.49
1:A:305:GLY:HA2	1:A:308:ASN:ND2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:HIS:N	1:C:426:PRO:HD3	2.27	0.49
1:D:277:VAL:O	1:D:280:ARG:N	2.46	0.49
1:A:362:ASP:O	1:A:366:PRO:CD	2.60	0.49
1:B:447:THR:O	1:B:450:VAL:HG22	2.11	0.49
1:C:239:GLY:C	1:C:241:THR:N	2.70	0.49
1:C:293:VAL:CG1	1:C:468:LEU:HD13	2.41	0.49
1:C:410:GLN:O	1:C:411:ASP:C	2.55	0.49
1:B:236:ILE:O	1:B:237:LEU:O	2.31	0.49
1:B:279:ILE:H	1:B:279:ILE:CD1	2.08	0.49
1:C:220:ASP:O	1:C:221:SER:O	2.31	0.49
1:C:401:LEU:HB2	1:C:402:ASN:OD1	2.12	0.49
1:A:262:ILE:HG22	1:A:263:LYS:H	1.78	0.49
1:A:357:ARG:O	1:A:358:LYS:C	2.56	0.49
1:A:453:LEU:HD13	1:A:473:TYR:CZ	2.47	0.49
1:B:374:PHE:O	1:B:377:LEU:HG	2.13	0.49
1:B:430:GLN:HA	1:B:430:GLN:NE2	2.28	0.49
1:D:277:VAL:O	1:D:280:ARG:HB2	2.13	0.49
1:A:222:TYR:HE2	1:A:381:ASP:OD1	1.95	0.49
1:A:245:SER:HB3	1:A:246:PRO:HD2	1.94	0.49
1:A:438:LYS:O	1:A:441:ASP:HB2	2.12	0.49
1:A:468:LEU:O	1:A:472:ILE:HG12	2.12	0.49
1:B:220:ASP:O	1:B:224:LYS:HG2	2.12	0.49
1:C:360:PHE:O	1:C:361:GLY:C	2.54	0.49
1:D:438:LYS:C	1:D:440:THR:N	2.71	0.49
1:A:276:GLU:OE1	1:A:278:ALA:N	2.45	0.49
1:A:289:SER:O	1:A:292:ALA:N	2.43	0.49
1:B:333:LEU:HD22	1:B:340:LEU:HD12	1.93	0.49
1:B:476:LEU:HD22	1:B:476:LEU:N	2.24	0.49
1:A:415:GLN:O	1:A:416:ALA:C	2.54	0.49
1:A:470:GLN:HA	1:A:470:GLN:HE21	1.78	0.49
1:A:306:PHE:C	1:A:308:ASN:H	2.21	0.49
1:B:448:GLU:O	1:B:452:LEU:HD13	2.13	0.49
1:C:360:PHE:O	1:C:363:PHE:N	2.34	0.49
1:C:405:PRO:HG2	1:C:406:ILE:H	1.77	0.49
1:D:275:LYS:HB3	1:D:280:ARG:HD2	1.94	0.49
1:D:466:HIS:N	1:D:467:PRO:CD	2.71	0.49
1:A:275:LYS:HG3	1:A:279:ILE:HG21	1.95	0.49
1:A:293:VAL:HG13	1:A:322:VAL:HG21	1.94	0.49
1:B:323:HIS:O	1:B:326:ILE:N	2.46	0.49
1:B:419:LEU:O	1:B:422:LYS:HB2	2.13	0.49
1:C:311:LEU:O	1:C:312:ASN:C	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:LEU:O	1:C:456:ILE:HD12	2.13	0.49
1:D:281:ILE:HG12	2:D:4:072:H3H	1.95	0.49
1:D:316:THR:O	1:D:319:LYS:N	2.45	0.49
1:D:460:GLU:C	1:D:460:GLU:CD	2.81	0.49
1:D:465:LEU:C	1:D:466:HIS:CD2	2.91	0.49
1:C:453:LEU:HD23	1:C:453:LEU:O	2.12	0.48
1:B:221:SER:O	1:B:224:LYS:N	2.46	0.48
1:B:287:PHE:O	1:B:290:VAL:HB	2.13	0.48
1:B:429:SER:O	1:B:434:LYS:NZ	2.43	0.48
1:B:460:GLU:HG2	1:B:463:MET:CG	2.43	0.48
1:D:255:LEU:HD21	1:D:277:VAL:CG1	2.43	0.48
1:D:362:ASP:OD1	1:D:362:ASP:N	2.44	0.48
1:A:411:ASP:O	1:A:412:ASN:C	2.56	0.48
1:B:246:PRO:HB2	1:B:346:GLY:CA	2.43	0.48
1:B:249:ILE:HD13	1:B:255:LEU:HD13	1.94	0.48
1:B:348:MET:CG	1:B:353:LEU:HD21	2.44	0.48
1:C:390:VAL:HG13	1:C:410:GLN:HG3	1.95	0.48
1:D:374:PHE:O	1:D:377:LEU:HG	2.13	0.48
1:D:460:GLU:CD	1:D:460:GLU:O	2.56	0.48
1:A:251:ASP:OD1	1:A:251:ASP:C	2.57	0.48
1:A:264:PHE:O	1:A:266:HIS:N	2.44	0.48
1:A:440:THR:HG23	1:A:441:ASP:N	2.28	0.48
1:B:340:LEU:HB3	1:B:344:GLY:HA2	1.95	0.48
1:C:440:THR:HA	1:D:440:THR:HG22	1.94	0.48
1:D:418:GLU:HG3	1:D:422:LYS:HE3	1.96	0.48
1:A:210:ASP:O	1:A:213:ALA:HB3	2.14	0.48
1:A:440:THR:HG23	1:A:441:ASP:H	1.79	0.48
1:A:474:LYS:HZ2	1:A:474:LYS:CB	2.26	0.48
1:B:228:LEU:CD2	1:B:233:ALA:HB2	2.43	0.48
1:B:453:LEU:O	1:B:454:GLN:C	2.57	0.48
1:C:271:GLN:O	1:C:275:LYS:O	2.32	0.48
1:C:294:GLN:CA	1:C:294:GLN:NE2	2.74	0.48
1:C:299:TYR:O	1:C:300:ALA:C	2.55	0.48
1:C:404:LYS:N	1:C:405:PRO:CD	2.76	0.48
1:D:267:ILE:HD11	1:D:270:LEU:HD12	1.95	0.48
1:D:291:GLU:O	1:D:292:ALA:C	2.55	0.48
1:D:364:MET:O	1:D:365:GLU:C	2.56	0.48
1:D:371:ALA:O	1:D:374:PHE:N	2.46	0.48
1:C:257:MET:O	1:C:260:ASP:HB3	2.13	0.48
1:C:319:LYS:NZ	1:C:471:GLU:O	2.47	0.48
1:C:444:GLN:N	1:C:444:GLN:NE2	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:ASP:C	1:B:464:SER:H	2.22	0.48
1:D:335:ASN:C	1:D:337:ASP:N	2.72	0.48
1:D:335:ASN:O	1:D:337:ASP:N	2.47	0.48
1:D:438:LYS:C	1:D:440:THR:H	2.21	0.48
1:A:403:VAL:C	1:A:405:PRO:CD	2.86	0.48
1:A:442:LEU:HD12	1:A:442:LEU:H	1.78	0.48
1:B:222:TYR:O	1:B:226:PHE:HD1	1.96	0.48
1:C:207:GLU:HG2	1:C:209:ALA:HB3	1.94	0.48
1:D:292:ALA:O	1:D:293:VAL:C	2.57	0.48
1:A:320:TYR:CZ	1:A:398:PRO:HD2	2.48	0.48
1:A:364:MET:HG3	2:A:1:072:H2D1	1.95	0.48
1:C:456:ILE:HA	1:C:459:THR:OG1	2.14	0.48
1:D:432:PHE:CZ	1:D:436:LEU:HD11	2.48	0.48
1:D:464:SER:C	1:D:466:HIS:H	2.21	0.48
1:A:270:LEU:HD13	1:A:272:GLU:N	2.29	0.47
1:A:365:GLU:O	1:A:369:GLU:OE2	2.32	0.47
1:B:291:GLU:C	1:B:293:VAL:N	2.69	0.47
1:B:449:HIS:CE1	1:B:453:LEU:HD22	2.49	0.47
1:C:363:PHE:CZ	1:C:449:HIS:HD2	2.31	0.47
1:C:403:VAL:C	1:C:405:PRO:CD	2.87	0.47
1:D:248:VAL:HG12	1:D:249:ILE:N	2.29	0.47
1:D:452:LEU:O	1:D:456:ILE:N	2.47	0.47
1:B:323:HIS:O	1:B:324:GLU:C	2.57	0.47
1:B:430:GLN:O	1:B:431:LEU:C	2.57	0.47
1:C:236:ILE:HD12	1:C:236:ILE:H	1.79	0.47
1:C:274:SER:O	1:C:275:LYS:CB	2.60	0.47
1:C:330:LEU:O	1:C:333:LEU:HB2	2.14	0.47
1:C:384:LEU:O	1:C:385:ALA:C	2.57	0.47
1:D:219:TYR:O	1:D:220:ASP:C	2.56	0.47
1:A:271:GLN:O	1:A:276:GLU:CA	2.57	0.47
1:A:319:LYS:HG3	1:A:472:ILE:HA	1.96	0.47
1:A:444:GLN:O	1:A:448:GLU:HG3	2.13	0.47
1:C:258:GLY:O	1:C:262:ILE:HB	2.14	0.47
1:C:440:THR:HG23	1:C:441:ASP:OD1	2.13	0.47
1:A:377:LEU:HB3	1:A:431:LEU:HD11	1.95	0.47
1:B:277:VAL:HA	1:B:280:ARG:HH11	1.78	0.47
1:B:306:PHE:C	1:B:308:ASN:N	2.72	0.47
1:C:232:LYS:O	1:C:236:ILE:CD1	2.60	0.47
1:C:391:ILE:O	1:C:392:ILE:C	2.57	0.47
1:D:265:LYS:O	1:D:266:HIS:CB	2.62	0.47
1:D:442:LEU:O	1:D:446:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:ARG:HH21	2:B:2:072:H1C2	1.79	0.47
1:B:328:THR:O	1:B:331:ALA:HB3	2.14	0.47
1:B:339:VAL:N	1:B:347:PHE:CE1	2.83	0.47
1:B:446:VAL:O	1:B:450:VAL:HG13	2.15	0.47
1:C:244:LYS:HB2	1:C:244:LYS:NZ	2.30	0.47
1:C:277:VAL:CG1	1:C:278:ALA:N	2.78	0.47
1:C:293:VAL:O	1:C:294:GLN:C	2.58	0.47
1:C:444:GLN:NE2	1:C:444:GLN:H	2.12	0.47
1:D:250:TYR:HA	1:D:349:THR:HG21	1.96	0.47
1:A:214:LEU:O	1:A:215:ALA:C	2.58	0.47
1:A:316:THR:O	1:A:320:TYR:HD1	1.98	0.47
1:A:457:LYS:C	1:A:459:THR:N	2.73	0.47
1:A:475:ASP:O	1:A:476:LEU:HB2	2.14	0.47
1:B:207:GLU:O	1:B:211:LEU:HG	2.15	0.47
1:B:218:LEU:HD12	1:B:386:ILE:HG12	1.97	0.47
1:B:218:LEU:CD1	1:B:386:ILE:HG12	2.45	0.47
1:B:338:GLY:O	1:B:368:PHE:HE1	1.98	0.47
1:B:367:LYS:O	1:B:370:PHE:HB3	2.14	0.47
1:B:465:LEU:C	1:B:467:PRO:HD2	2.39	0.47
1:B:473:TYR:N	1:B:473:TYR:CD1	2.82	0.47
1:C:258:GLY:C	1:C:260:ASP:H	2.23	0.47
1:C:282:PHE:O	1:C:285:CYS:HB3	2.15	0.47
1:C:409:ILE:O	1:C:412:ASN:HB3	2.15	0.47
1:C:465:LEU:O	1:C:466:HIS:O	2.33	0.47
1:D:469:LEU:HD22	1:D:473:TYR:HE2	1.79	0.47
1:B:237:LEU:C	1:B:239:GLY:N	2.73	0.47
1:C:281:ILE:HG12	2:C:3:072:C3H	2.45	0.47
1:D:285:CYS:O	1:D:286:GLN:C	2.57	0.47
1:A:374:PHE:HB2	1:A:438:LYS:HE2	1.95	0.47
1:C:465:LEU:HB3	1:C:470:GLN:HE22	1.80	0.47
1:A:449:HIS:CE1	1:A:453:LEU:HD12	2.50	0.46
1:A:469:LEU:HA	1:A:472:ILE:CG1	2.45	0.46
1:B:436:LEU:C	1:B:438:LYS:N	2.73	0.46
1:B:472:ILE:O	1:B:472:ILE:HG22	2.14	0.46
1:D:259:GLU:HG2	1:D:262:ILE:CG2	2.46	0.46
1:A:320:TYR:N	1:A:320:TYR:CD1	2.83	0.46
1:B:317:LEU:HD21	1:B:406:ILE:CG2	2.45	0.46
1:B:393:LEU:HD22	1:B:393:LEU:N	2.29	0.46
1:B:418:GLU:HG3	1:B:432:PHE:CD2	2.50	0.46
1:C:374:PHE:O	1:C:375:ASN:C	2.55	0.46
1:C:430:GLN:C	1:C:432:PHE:N	2.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:PHE:CD1	1:D:287:PHE:C	2.94	0.46
1:A:220:ASP:O	1:A:224:LYS:HG3	2.16	0.46
1:A:262:ILE:HG22	1:A:263:LYS:N	2.30	0.46
1:A:277:VAL:CG1	1:A:278:ALA:N	2.77	0.46
1:B:409:ILE:O	1:B:412:ASN:N	2.49	0.46
1:B:456:ILE:HA	1:B:459:THR:HB	1.96	0.46
1:C:225:SER:O	1:C:227:PRO:HD3	2.15	0.46
1:C:235:ALA:O	1:C:236:ILE:C	2.58	0.46
1:C:470:GLN:HE21	1:C:470:GLN:HB2	1.48	0.46
1:A:228:LEU:HD11	1:A:343:GLU:O	2.16	0.46
1:B:234:ARG:NH2	1:B:332:SER:O	2.43	0.46
1:B:357:ARG:HD2	1:B:360:PHE:HE2	1.79	0.46
1:B:439:MET:O	1:B:443:ARG:HB2	2.14	0.46
1:B:476:LEU:H	1:B:476:LEU:CD2	2.21	0.46
1:D:364:MET:CA	1:D:367:LYS:HG2	2.42	0.46
1:A:442:LEU:O	1:A:446:VAL:HG23	2.15	0.46
1:B:246:PRO:HB2	1:B:346:GLY:HA2	1.98	0.46
1:B:305:GLY:O	1:B:308:ASN:HB2	2.15	0.46
1:B:352:PHE:O	1:B:355:SER:N	2.37	0.46
1:B:441:ASP:O	1:B:444:GLN:HB2	2.15	0.46
1:D:240:LYS:C	1:D:242:THR:N	2.73	0.46
1:D:353:LEU:O	1:D:361:GLY:HA2	2.16	0.46
1:A:287:PHE:O	1:A:290:VAL:HG12	2.15	0.46
1:B:233:ALA:O	1:B:234:ARG:C	2.59	0.46
1:C:315:VAL:O	1:C:316:THR:C	2.59	0.46
1:C:315:VAL:O	1:C:318:LEU:HB2	2.16	0.46
1:C:437:GLN:O	1:C:439:MET:N	2.49	0.46
1:D:391:ILE:O	1:D:392:ILE:C	2.56	0.46
1:A:434:LYS:O	1:A:437:GLN:HB2	2.15	0.46
1:B:322:VAL:O	1:B:325:ILE:HB	2.16	0.46
1:B:460:GLU:CG	1:B:463:MET:SD	3.03	0.46
1:A:291:GLU:O	1:A:294:GLN:HB2	2.16	0.46
1:B:324:GLU:HB2	1:B:391:ILE:HG21	1.98	0.46
1:B:466:HIS:C	1:B:470:GLN:HB2	2.41	0.46
1:D:335:ASN:C	1:D:337:ASP:H	2.24	0.46
1:D:391:ILE:O	1:D:394:SER:HB2	2.16	0.46
1:D:445:ILE:CA	1:D:448:GLU:HG3	2.45	0.46
1:A:222:TYR:CD1	1:A:226:PHE:CD2	3.04	0.46
1:A:277:VAL:HG22	1:A:281:ILE:CG1	2.44	0.46
1:A:336:LYS:HE2	1:A:372:VAL:HG21	1.98	0.46
1:A:450:VAL:C	1:A:452:LEU:N	2.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:HIS:CG	1:A:467:PRO:HD2	2.50	0.46
1:B:338:GLY:O	1:B:368:PHE:CE1	2.69	0.46
1:B:471:GLU:O	1:B:474:LYS:HG3	2.15	0.46
1:C:262:ILE:HG22	1:C:263:LYS:N	2.31	0.46
1:C:288:ARG:NE	2:C:3:072:O1D	2.47	0.46
1:C:316:THR:O	1:C:319:LYS:HB3	2.15	0.46
1:C:370:PHE:CZ	1:C:442:LEU:HD21	2.50	0.46
1:C:455:VAL:HG12	1:C:459:THR:CG2	2.44	0.46
1:D:381:ASP:HA	1:D:384:LEU:HD13	1.98	0.46
1:D:403:VAL:O	1:D:404:LYS:C	2.58	0.46
1:D:471:GLU:C	1:D:473:TYR:N	2.72	0.46
1:C:319:LYS:O	1:C:322:VAL:HG12	2.16	0.46
1:C:434:LYS:HA	1:C:437:GLN:HG2	1.97	0.46
1:D:243:ASP:OD2	1:D:244:LYS:HE2	2.16	0.46
1:D:262:ILE:HD11	1:D:342:SER:HB3	1.97	0.46
1:D:476:LEU:CD2	1:D:476:LEU:N	2.78	0.46
1:A:360:PHE:O	1:A:363:PHE:HB2	2.16	0.45
1:A:458:LYS:CE	1:C:210:ASP:OD1	2.63	0.45
1:B:352:PHE:O	1:B:355:SER:OG	2.31	0.45
1:C:383:ASP:OD2	1:C:425:HIS:HE1	1.99	0.45
1:C:444:GLN:O	1:C:447:THR:OG1	2.32	0.45
1:C:450:VAL:CG1	1:C:475:ASP:HA	2.46	0.45
1:D:421:LEU:HD12	1:D:432:PHE:HA	1.99	0.45
1:A:389:ALA:HB1	1:A:413:LEU:HD13	1.97	0.45
1:C:214:LEU:HD23	1:C:416:ALA:HB2	1.98	0.45
1:C:252:MET:HA	1:C:255:LEU:HB3	1.98	0.45
1:C:364:MET:HB3	1:C:368:PHE:CE1	2.48	0.45
1:D:364:MET:O	1:D:367:LYS:HG2	2.16	0.45
1:A:406:ILE:HA	1:A:409:ILE:HD12	1.97	0.45
1:B:237:LEU:HD22	1:B:238:THR:H	1.82	0.45
1:D:264:PHE:CE2	1:D:266:HIS:HB3	2.50	0.45
1:D:265:LYS:O	1:D:265:LYS:HG3	2.17	0.45
1:D:371:ALA:C	1:D:375:ASN:ND2	2.74	0.45
1:D:469:LEU:C	1:D:471:GLU:H	2.24	0.45
1:A:384:LEU:O	1:A:388:ILE:HG12	2.16	0.45
1:A:386:ILE:O	1:A:389:ALA:HB3	2.16	0.45
1:A:469:LEU:HG	1:A:473:TYR:CE2	2.50	0.45
1:A:473:TYR:C	1:A:474:LYS:HZ1	2.22	0.45
1:B:317:LEU:HD21	1:B:406:ILE:HG21	1.98	0.45
1:B:334:MET:HG2	1:B:339:VAL:HG23	1.98	0.45
1:B:339:VAL:HG13	1:B:341:ILE:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:PRO:HD2	1:C:295:GLU:OE1	2.17	0.45
1:C:425:HIS:HB3	1:C:428:SER:CB	2.46	0.45
1:C:264:PHE:C	1:C:266:HIS:N	2.74	0.45
1:C:364:MET:O	1:C:368:PHE:HD1	1.98	0.45
1:C:465:LEU:O	1:C:466:HIS:C	2.59	0.45
1:D:234:ARG:NH2	1:D:334:MET:O	2.49	0.45
1:A:271:GLN:HB3	1:A:280:ARG:HH22	1.81	0.45
1:B:425:HIS:N	1:B:426:PRO:CD	2.79	0.45
1:C:377:LEU:CB	1:C:379:LEU:HG	2.47	0.45
1:A:298:GLU:O	1:A:301:LYS:HB2	2.15	0.45
1:B:281:ILE:HG12	2:B:2:072:H3H	1.99	0.45
1:B:341:ILE:HG13	2:B:2:072:C1A	2.45	0.45
1:B:380:ASP:C	1:B:384:LEU:HD12	2.41	0.45
1:B:448:GLU:O	1:B:449:HIS:C	2.58	0.45
1:D:465:LEU:O	1:D:466:HIS:CD2	2.60	0.45
1:A:248:VAL:HG22	1:A:347:PHE:HB3	1.99	0.45
1:A:397:ARG:O	1:A:400:LEU:HB2	2.16	0.45
1:B:311:LEU:H	1:B:311:LEU:CD1	2.01	0.45
1:D:325:ILE:CG2	1:D:388:ILE:HG23	2.47	0.45
1:D:356:LEU:O	1:D:357:ARG:O	2.35	0.45
1:D:456:ILE:O	1:D:457:LYS:C	2.60	0.45
1:D:470:GLN:O	1:D:470:GLN:HG2	2.15	0.45
1:A:319:LYS:O	1:A:322:VAL:HG12	2.17	0.45
1:A:358:LYS:HB2	1:A:359:PRO:CD	2.47	0.45
1:A:474:LYS:HA	1:A:474:LYS:CE	2.46	0.45
1:B:472:ILE:HG22	1:B:473:TYR:CD1	2.52	0.45
1:C:379:LEU:CD1	1:C:435:LEU:HD22	2.47	0.45
1:A:320:TYR:HB2	1:A:397:ARG:HD2	1.98	0.44
1:B:275:LYS:HB3	1:B:280:ARG:HG3	1.99	0.44
1:B:341:ILE:HG12	1:B:348:MET:CE	2.45	0.44
1:C:270:LEU:HD13	1:C:271:GLN:N	2.31	0.44
1:D:452:LEU:HD12	1:D:452:LEU:H	1.81	0.44
1:A:207:GLU:HG2	1:A:210:ASP:OD2	2.18	0.44
1:A:283:GLN:HG3	1:A:463:MET:HE1	1.97	0.44
1:A:340:LEU:HA	1:A:346:GLY:O	2.17	0.44
1:A:368:PHE:O	1:A:369:GLU:C	2.60	0.44
1:A:390:VAL:O	1:A:393:LEU:N	2.51	0.44
1:A:400:LEU:HD11	1:A:406:ILE:CD1	2.46	0.44
1:B:228:LEU:HD22	1:B:233:ALA:HB2	1.99	0.44
1:C:212:ARG:HD3	1:C:423:LEU:HD13	1.97	0.44
1:C:213:ALA:O	1:C:214:LEU:C	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:VAL:HA	1:C:280:ARG:HB3	1.99	0.44
1:C:381:ASP:O	1:C:382:SER:C	2.59	0.44
1:C:384:LEU:O	1:C:387:PHE:N	2.50	0.44
1:C:434:LYS:HA	1:C:437:GLN:CG	2.48	0.44
1:D:288:ARG:HH21	1:D:342:SER:CA	2.23	0.44
1:D:380:ASP:C	1:D:384:LEU:CD1	2.91	0.44
1:A:216:LYS:H	1:A:216:LYS:CD	2.29	0.44
1:B:430:GLN:HG3	1:B:433:ALA:HB3	1.99	0.44
1:C:330:LEU:HA	1:C:333:LEU:HG	1.98	0.44
1:C:374:PHE:O	1:C:377:LEU:HG	2.17	0.44
1:C:469:LEU:HD12	1:C:469:LEU:H	1.82	0.44
1:A:315:VAL:O	1:A:316:THR:C	2.60	0.44
1:A:451:GLN:HA	1:A:454:GLN:HB2	1.99	0.44
1:A:466:HIS:ND1	1:A:468:LEU:HG	2.32	0.44
1:B:409:ILE:O	1:B:410:GLN:C	2.60	0.44
1:C:317:LEU:HD23	1:C:317:LEU:N	2.31	0.44
1:C:325:ILE:O	1:C:328:THR:HB	2.17	0.44
1:C:411:ASP:O	1:C:415:GLN:HG3	2.17	0.44
1:D:289:SER:O	1:D:293:VAL:HG23	2.18	0.44
1:D:344:GLY:C	1:D:346:GLY:N	2.75	0.44
1:D:446:VAL:O	1:D:449:HIS:HB3	2.17	0.44
1:A:255:LEU:HD22	1:A:352:PHE:HZ	1.82	0.44
1:A:432:PHE:HE2	1:B:433:ALA:HB2	1.82	0.44
1:A:450:VAL:O	1:A:452:LEU:N	2.51	0.44
1:A:466:HIS:HA	1:A:467:PRO:HD3	1.83	0.44
1:A:475:ASP:O	1:A:476:LEU:CB	2.66	0.44
1:B:237:LEU:HD22	1:B:238:THR:HG23	1.99	0.44
1:B:352:PHE:O	1:B:353:LEU:C	2.60	0.44
1:B:380:ASP:C	1:B:380:ASP:OD1	2.60	0.44
1:B:457:LYS:C	1:B:457:LYS:CD	2.90	0.44
1:C:290:VAL:HG23	1:C:466:HIS:CE1	2.52	0.44
1:D:207:GLU:HB3	1:D:210:ASP:OD1	2.18	0.44
1:D:377:LEU:O	1:D:378:GLU:C	2.61	0.44
1:D:469:LEU:C	1:D:471:GLU:N	2.75	0.44
1:A:267:ILE:HB	1:A:280:ARG:HH11	1.82	0.44
1:A:449:HIS:ND1	1:A:449:HIS:C	2.75	0.44
1:B:253:ASN:O	1:B:255:LEU:N	2.51	0.44
1:B:430:GLN:O	1:B:434:LYS:N	2.49	0.44
1:B:451:GLN:NE2	1:B:451:GLN:O	2.49	0.44
1:B:462:ASP:HB3	1:D:423:LEU:HD13	1.99	0.44
1:D:243:ASP:OD2	1:D:244:LYS:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:GLY:O	1:D:323:HIS:N	2.51	0.44
1:D:348:MET:HE3	1:D:348:MET:HB2	1.77	0.44
1:D:421:LEU:HB3	1:D:431:LEU:HD23	1.99	0.44
1:A:214:LEU:O	1:A:215:ALA:O	2.35	0.44
1:B:405:PRO:HA	1:B:408:ASP:HB2	1.98	0.44
1:D:453:LEU:C	1:D:455:VAL:H	2.25	0.44
1:D:470:GLN:C	1:D:470:GLN:NE2	2.76	0.44
1:A:414:LEU:O	1:A:418:GLU:HB2	2.18	0.44
1:A:430:GLN:NE2	1:B:414:LEU:HB3	2.33	0.44
1:B:241:THR:HG22	1:B:243:ASP:OD2	2.18	0.44
1:B:271:GLN:HA	1:B:271:GLN:NE2	2.33	0.44
1:B:313:ASP:OD1	1:B:400:LEU:HA	2.18	0.44
1:D:234:ARG:HD3	1:D:234:ARG:HA	1.61	0.44
1:D:292:ALA:O	1:D:295:GLU:N	2.50	0.44
1:D:457:LYS:C	1:D:459:THR:N	2.76	0.44
1:D:466:HIS:O	1:D:467:PRO:C	2.61	0.44
1:A:383:ASP:OD2	1:A:424:ASN:ND2	2.50	0.44
1:A:415:GLN:O	1:A:418:GLU:HB3	2.18	0.44
1:A:458:LYS:HE3	1:C:210:ASP:CG	2.42	0.44
1:B:460:GLU:O	1:B:460:GLU:CD	2.60	0.44
1:B:462:ASP:HA	1:D:212:ARG:NE	2.33	0.44
1:D:303:ILE:HG21	1:D:393:LEU:HD21	2.00	0.44
1:A:226:PHE:HA	1:A:227:PRO:HD3	1.80	0.43
1:B:275:LYS:N	1:B:275:LYS:HD2	2.33	0.43
1:B:297:THR:O	1:B:301:LYS:HD3	2.18	0.43
1:C:297:THR:O	1:C:301:LYS:HD3	2.18	0.43
1:D:232:LYS:HD2	1:D:232:LYS:HA	1.83	0.43
1:D:232:LYS:HE2	1:D:244:LYS:HE3	2.00	0.43
1:D:349:THR:OG1	1:D:352:PHE:CB	2.66	0.43
1:D:364:MET:HA	1:D:367:LYS:HG3	1.97	0.43
1:A:403:VAL:O	1:A:404:LYS:C	2.59	0.43
1:B:431:LEU:HD12	1:B:431:LEU:HA	1.90	0.43
1:C:394:SER:OG	1:C:397:ARG:HG3	2.19	0.43
1:C:447:THR:HA	1:C:450:VAL:HB	1.99	0.43
1:D:348:MET:SD	1:D:353:LEU:HD21	2.58	0.43
1:D:394:SER:O	1:D:396:ASP:N	2.50	0.43
1:A:234:ARG:HH11	1:A:332:SER:C	2.25	0.43
1:B:214:LEU:O	1:B:218:LEU:HG	2.18	0.43
1:B:243:ASP:OD1	1:B:244:LYS:N	2.51	0.43
1:B:248:VAL:HG12	1:B:249:ILE:N	2.33	0.43
1:B:255:LEU:O	1:B:256:MET:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ILE:HG23	1:B:388:ILE:HG23	2.00	0.43
1:C:219:TYR:O	1:C:222:TYR:HB3	2.17	0.43
1:C:338:GLY:HA2	1:C:368:PHE:HE2	1.82	0.43
1:B:223:ILE:HD13	1:B:223:ILE:HA	1.85	0.43
1:C:212:ARG:NH2	1:C:216:LYS:HE3	2.24	0.43
1:D:303:ILE:HG23	1:D:304:PRO:HD2	2.00	0.43
1:D:476:LEU:HD23	1:D:476:LEU:N	2.19	0.43
1:A:254:SER:O	1:A:255:LEU:C	2.61	0.43
1:A:393:LEU:N	1:A:393:LEU:HD22	2.33	0.43
1:A:404:LYS:N	1:A:405:PRO:CD	2.81	0.43
1:D:360:PHE:O	1:D:362:ASP:N	2.50	0.43
1:D:370:PHE:CE1	1:D:441:ASP:HB2	2.53	0.43
1:A:358:LYS:HB2	1:A:359:PRO:HD3	2.00	0.43
1:A:364:MET:O	1:A:365:GLU:C	2.62	0.43
1:A:365:GLU:N	1:A:366:PRO:CD	2.80	0.43
1:B:207:GLU:HB3	1:B:210:ASP:HB2	2.00	0.43
1:C:299:TYR:O	1:C:302:SER:N	2.51	0.43
1:D:245:SER:HA	1:D:246:PRO:HD3	1.75	0.43
1:A:379:LEU:HD21	1:A:435:LEU:CD2	2.44	0.43
1:C:290:VAL:CG1	1:C:291:GLU:N	2.81	0.43
1:C:325:ILE:HG23	1:C:388:ILE:HG23	2.01	0.43
1:C:326:ILE:HG22	1:C:327:TYR:N	2.33	0.43
1:A:314:GLN:HA	1:A:317:LEU:HD12	2.00	0.43
1:A:342:SER:O	1:A:345:GLN:HB2	2.18	0.43
1:B:463:MET:O	1:B:466:HIS:CD2	2.72	0.43
1:B:472:ILE:HG22	1:B:473:TYR:CE1	2.54	0.43
1:C:288:ARG:NH1	1:C:289:SER:HA	2.34	0.43
1:C:320:TYR:CE2	1:C:398:PRO:HD2	2.54	0.43
1:C:466:HIS:CE1	1:C:468:LEU:H	2.35	0.43
1:D:380:ASP:O	1:D:383:ASP:HB2	2.18	0.43
1:A:293:VAL:HG13	1:A:322:VAL:CG2	2.49	0.43
1:A:373:LYS:O	1:A:376:ALA:HB3	2.18	0.43
1:B:404:LYS:N	1:B:405:PRO:CD	2.82	0.43
1:B:431:LEU:O	1:B:432:PHE:C	2.60	0.43
1:D:222:TYR:HE2	1:D:388:ILE:CD1	2.31	0.43
1:D:230:LYS:O	1:D:231:ALA:C	2.61	0.43
1:D:256:MET:SD	1:D:271:GLN:HB2	2.59	0.43
1:D:297:THR:HG23	1:D:318:LEU:CD2	2.48	0.43
1:D:380:ASP:O	1:D:383:ASP:N	2.50	0.43
1:A:270:LEU:CD1	1:A:272:GLU:N	2.82	0.43
1:A:360:PHE:CD1	1:A:360:PHE:N	2.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:SER:OG	1:A:383:ASP:OD1	2.36	0.43
1:B:264:PHE:CE2	1:B:266:HIS:HB3	2.53	0.43
1:B:275:LYS:C	1:B:280:ARG:HD2	2.44	0.43
1:B:279:ILE:O	1:B:283:GLN:HG3	2.19	0.43
1:B:407:GLU:O	1:B:411:ASP:CG	2.61	0.43
1:C:311:LEU:O	1:C:314:GLN:N	2.52	0.43
1:C:313:ASP:O	1:C:314:GLN:C	2.61	0.43
1:C:407:GLU:O	1:C:411:ASP:OD2	2.37	0.43
1:A:281:ILE:HG22	2:A:1:072:H2F1	2.01	0.42
1:B:213:ALA:O	1:B:214:LEU:C	2.60	0.42
1:B:317:LEU:HD22	1:B:393:LEU:HD13	2.01	0.42
1:B:462:ASP:OD1	1:B:463:MET:N	2.52	0.42
1:C:232:LYS:O	1:C:235:ALA:HB3	2.19	0.42
1:C:310:ASP:O	1:C:311:LEU:C	2.60	0.42
1:C:367:LYS:H	1:C:367:LYS:HD3	1.83	0.42
1:C:427:GLU:CD	1:C:427:GLU:H	2.26	0.42
1:D:348:MET:HG2	1:D:353:LEU:CG	2.49	0.42
1:D:349:THR:OG1	1:D:352:PHE:HB3	2.19	0.42
1:A:271:GLN:HE21	1:A:271:GLN:C	2.28	0.42
1:A:297:THR:O	1:A:300:ALA:HB3	2.18	0.42
1:B:306:PHE:C	1:B:308:ASN:H	2.26	0.42
1:C:249:ILE:HG21	1:C:255:LEU:CD1	2.47	0.42
1:C:258:GLY:HA3	1:C:264:PHE:CE2	2.54	0.42
1:D:370:PHE:HA	1:D:373:LYS:HE2	2.01	0.42
1:D:418:GLU:CG	1:D:422:LYS:HE3	2.49	0.42
1:A:351:GLU:O	1:A:352:PHE:C	2.62	0.42
1:B:405:PRO:HG2	1:B:406:ILE:H	1.84	0.42
1:C:207:GLU:O	1:C:211:LEU:HG	2.19	0.42
1:C:288:ARG:HD2	1:C:292:ALA:HB2	2.00	0.42
1:C:466:HIS:HE1	1:C:468:LEU:HG	1.84	0.42
1:D:243:ASP:CG	1:D:244:LYS:H	2.27	0.42
1:D:417:LEU:HD21	1:D:435:LEU:HD23	2.00	0.42
1:A:327:TYR:OH	1:A:449:HIS:CD2	2.72	0.42
1:C:370:PHE:CD1	1:C:373:LYS:NZ	2.76	0.42
1:C:387:PHE:HZ	1:C:439:MET:HG3	1.84	0.42
1:C:449:HIS:CD2	1:C:453:LEU:HD12	2.53	0.42
1:D:294:GLN:O	1:D:295:GLU:C	2.62	0.42
1:D:470:GLN:C	1:D:470:GLN:HE21	2.27	0.42
1:A:359:PRO:O	1:A:362:ASP:OD1	2.36	0.42
1:A:389:ALA:O	1:A:390:VAL:C	2.63	0.42
1:A:417:LEU:O	1:A:420:GLN:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:GLU:CD	1:B:397:ARG:HH22	2.26	0.42
1:B:334:MET:HE2	1:B:368:PHE:CE1	2.55	0.42
1:B:472:ILE:C	1:B:473:TYR:CD1	2.92	0.42
1:C:214:LEU:HD23	1:C:416:ALA:CB	2.49	0.42
1:C:218:LEU:HD11	1:C:413:LEU:CD2	2.50	0.42
1:C:261:LYS:HE3	1:C:261:LYS:HB3	1.92	0.42
1:C:294:GLN:HB2	1:C:295:GLU:H	1.72	0.42
1:D:336:LYS:O	1:D:350:ARG:CD	2.67	0.42
1:A:444:GLN:O	1:A:447:THR:HB	2.18	0.42
1:B:330:LEU:HD23	1:B:334:MET:HG3	2.01	0.42
1:C:259:GLU:HG2	1:C:264:PHE:HD2	1.83	0.42
1:C:267:ILE:HD12	1:C:275:LYS:HB3	2.01	0.42
1:A:252:MET:HB3	1:A:256:MET:HE1	1.96	0.42
1:A:270:LEU:HD22	1:A:271:GLN:N	2.21	0.42
1:A:325:ILE:HG13	1:A:391:ILE:HG21	2.00	0.42
1:A:438:LYS:HA	1:A:441:ASP:OD2	2.19	0.42
1:B:291:GLU:O	1:B:292:ALA:C	2.61	0.42
1:B:334:MET:HG2	1:B:339:VAL:CG2	2.50	0.42
1:B:410:GLN:HE21	1:B:410:GLN:HB3	1.49	0.42
1:B:475:ASP:OD2	1:B:476:LEU:HD13	2.20	0.42
1:C:233:ALA:C	1:C:235:ALA:N	2.77	0.42
1:C:303:ILE:HG21	1:C:413:LEU:HD11	2.02	0.42
1:C:319:LYS:HD2	1:C:472:ILE:HA	2.00	0.42
1:C:330:LEU:CG	1:C:334:MET:HE3	2.45	0.42
1:C:367:LYS:O	1:C:368:PHE:C	2.62	0.42
1:C:386:ILE:HD12	1:C:420:GLN:HG2	2.00	0.42
1:D:297:THR:HG23	1:D:318:LEU:HD21	2.01	0.42
1:D:357:ARG:HB3	1:D:360:PHE:CD2	2.48	0.42
1:B:333:LEU:CD2	1:B:340:LEU:HD12	2.49	0.42
1:C:207:GLU:C	1:C:209:ALA:N	2.77	0.42
1:C:351:GLU:HA	1:C:354:LYS:HB3	2.01	0.42
1:D:232:LYS:O	1:D:235:ALA:N	2.53	0.42
1:D:285:CYS:O	1:D:288:ARG:N	2.52	0.42
1:D:453:LEU:C	1:D:455:VAL:N	2.76	0.42
1:A:212:ARG:NH1	1:A:423:LEU:HD12	2.34	0.42
1:C:211:LEU:C	1:C:213:ALA:H	2.28	0.42
1:C:237:LEU:CD2	1:C:340:LEU:HD21	2.50	0.42
1:C:377:LEU:CD1	1:C:435:LEU:HD13	2.50	0.42
1:C:436:LEU:HA	1:C:439:MET:SD	2.59	0.42
1:A:212:ARG:HB3	1:A:216:LYS:HZ2	1.83	0.42
1:A:252:MET:O	1:A:256:MET:HE3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:ARG:O	1:A:446:VAL:N	2.53	0.42
1:C:325:ILE:HG23	1:C:388:ILE:HD12	2.01	0.42
1:C:390:VAL:CG1	1:C:410:GLN:OE1	2.68	0.42
1:D:213:ALA:C	1:D:215:ALA:N	2.75	0.42
1:D:289:SER:HB3	1:D:326:ILE:HD13	2.01	0.42
1:D:336:LYS:O	1:D:350:ARG:HD2	2.20	0.42
1:D:467:PRO:C	1:D:469:LEU:H	2.27	0.42
1:A:226:PHE:CE1	1:A:329:MET:HE1	2.55	0.41
1:A:330:LEU:HA	1:A:333:LEU:HD23	2.02	0.41
1:A:363:PHE:O	1:A:367:LYS:HE3	2.20	0.41
1:A:393:LEU:HG	1:A:409:ILE:CG2	2.50	0.41
1:A:430:GLN:CG	1:B:414:LEU:HD12	2.45	0.41
1:B:271:GLN:HE21	1:B:271:GLN:CA	2.28	0.41
1:C:318:LEU:O	1:C:319:LYS:C	2.63	0.41
1:C:422:LYS:O	1:C:423:LEU:C	2.62	0.41
1:D:216:LYS:HE3	1:D:220:ASP:OD1	2.19	0.41
1:D:457:LYS:HD2	1:D:461:THR:CG2	2.50	0.41
1:D:464:SER:O	1:D:467:PRO:HD2	2.19	0.41
1:A:213:ALA:O	1:A:214:LEU:C	2.63	0.41
1:A:295:GLU:O	1:A:296:ILE:C	2.63	0.41
1:A:322:VAL:O	1:A:326:ILE:HD12	2.20	0.41
1:B:277:VAL:N	1:B:280:ARG:HH11	2.18	0.41
1:B:340:LEU:C	1:B:341:ILE:HD12	2.45	0.41
1:C:384:LEU:O	1:C:386:ILE:N	2.53	0.41
1:C:397:ARG:HA	1:C:398:PRO:HD3	1.80	0.41
1:D:237:LEU:CD2	1:D:238:THR:H	2.33	0.41
1:D:243:ASP:OD1	1:D:243:ASP:N	2.53	0.41
1:D:409:ILE:O	1:D:410:GLN:C	2.61	0.41
1:A:208:SER:OG	1:A:209:ALA:N	2.52	0.41
1:A:247:PHE:CD1	1:A:247:PHE:C	2.98	0.41
1:B:326:ILE:HG22	1:B:327:TYR:N	2.35	0.41
1:B:453:LEU:C	1:B:455:VAL:N	2.77	0.41
1:B:457:LYS:HG3	1:B:458:LYS:H	1.82	0.41
1:B:467:PRO:O	1:B:471:GLU:N	2.53	0.41
1:C:379:LEU:CD2	1:C:431:LEU:HD21	2.50	0.41
1:C:430:GLN:O	1:C:432:PHE:N	2.53	0.41
1:C:437:GLN:C	1:C:439:MET:N	2.77	0.41
1:D:288:ARG:NH2	1:D:342:SER:CA	2.73	0.41
1:A:215:ALA:O	1:A:217:HIS:N	2.54	0.41
1:A:263:LYS:O	1:A:264:PHE:HD1	2.03	0.41
1:A:285:CYS:SG	2:A:1:072:H2A	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:LYS:NZ	1:A:438:LYS:HE3	2.35	0.41
1:B:249:ILE:HD13	1:B:255:LEU:CD1	2.51	0.41
1:B:278:ALA:HB3	1:B:279:ILE:HD12	2.03	0.41
1:C:383:ASP:OD2	1:C:425:HIS:CE1	2.74	0.41
1:D:222:TYR:CE2	1:D:388:ILE:CD1	3.03	0.41
1:D:288:ARG:NH2	1:D:343:GLU:H	2.17	0.41
1:D:366:PRO:HA	1:D:369:GLU:CD	2.46	0.41
1:D:451:GLN:NE2	1:D:455:VAL:HG21	2.34	0.41
1:B:235:ALA:O	1:B:239:GLY:O	2.39	0.41
1:B:277:VAL:HG12	1:B:278:ALA:N	2.35	0.41
1:B:292:ALA:O	1:B:296:ILE:HG13	2.20	0.41
1:C:279:ILE:O	1:C:283:GLN:HG3	2.20	0.41
1:C:321:GLY:N	1:C:397:ARG:NH1	2.68	0.41
1:C:455:VAL:C	1:C:459:THR:HG23	2.46	0.41
1:D:348:MET:HG2	1:D:353:LEU:HD21	2.01	0.41
1:D:390:VAL:HG22	1:D:413:LEU:HB3	2.03	0.41
1:A:220:ASP:HB2	1:A:224:LYS:CE	2.51	0.41
1:A:270:LEU:HD13	1:A:271:GLN:H	1.85	0.41
1:A:320:TYR:O	1:A:322:VAL:N	2.53	0.41
1:B:240:LYS:HG2	1:B:241:THR:N	2.34	0.41
1:B:365:GLU:O	1:B:369:GLU:HG3	2.21	0.41
1:B:475:ASP:CG	1:B:476:LEU:N	2.79	0.41
1:B:475:ASP:O	1:B:476:LEU:O	2.39	0.41
1:C:255:LEU:HD22	1:C:352:PHE:HZ	1.84	0.41
1:C:348:MET:HE1	2:C:3:072:H3H	2.03	0.41
1:C:414:LEU:HB2	1:D:430:GLN:HG2	2.02	0.41
1:C:430:GLN:O	1:C:431:LEU:C	2.60	0.41
1:D:300:ALA:HB1	1:D:306:PHE:CE1	2.56	0.41
1:C:364:MET:O	1:C:365:GLU:C	2.64	0.41
1:C:400:LEU:HB3	1:C:403:VAL:HG22	2.02	0.41
1:C:437:GLN:OE1	1:D:439:MET:HE1	2.21	0.41
1:D:277:VAL:CG1	1:D:281:ILE:HD11	2.51	0.41
1:D:363:PHE:HB2	1:D:452:LEU:HD21	2.03	0.41
1:A:256:MET:CA	1:A:259:GLU:HG3	2.41	0.41
1:A:288:ARG:CZ	1:A:289:SER:CA	2.98	0.41
1:A:330:LEU:CA	1:A:333:LEU:HD23	2.51	0.41
1:A:430:GLN:NE2	1:B:414:LEU:CB	2.83	0.41
1:B:462:ASP:HB3	1:D:423:LEU:CB	2.35	0.41
1:C:273:GLN:C	1:C:275:LYS:H	2.27	0.41
1:C:293:VAL:CB	1:C:468:LEU:HD13	2.50	0.41
1:C:419:LEU:C	1:C:423:LEU:HD12	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:473:TYR:O	1:D:474:LYS:C	2.64	0.41
1:A:421:LEU:HD12	1:A:432:PHE:CA	2.51	0.41
1:A:421:LEU:O	1:A:422:LYS:C	2.64	0.41
1:A:425:HIS:HB3	1:A:428:SER:CB	2.42	0.41
1:B:241:THR:O	1:B:243:ASP:CG	2.63	0.41
1:B:299:TYR:O	1:B:302:SER:N	2.54	0.41
1:B:475:ASP:OD1	1:B:476:LEU:CD2	2.65	0.41
1:C:207:GLU:C	1:C:209:ALA:H	2.29	0.41
1:C:237:LEU:HD21	1:C:340:LEU:HG	2.02	0.41
1:C:295:GLU:O	1:C:298:GLU:HB3	2.21	0.41
1:C:325:ILE:HG22	1:C:329:MET:HG3	2.03	0.41
1:C:397:ARG:H	1:C:400:LEU:CD1	2.33	0.41
1:C:466:HIS:C	1:C:466:HIS:ND1	2.79	0.41
1:C:474:LYS:HE3	1:C:474:LYS:HA	2.03	0.41
1:D:207:GLU:O	1:D:210:ASP:HB2	2.21	0.41
1:D:241:THR:O	1:D:241:THR:HG22	2.21	0.41
1:D:310:ASP:OD2	1:D:312:ASN:ND2	2.50	0.41
1:A:207:GLU:O	1:A:210:ASP:N	2.54	0.41
1:A:259:GLU:HA	1:A:264:PHE:CD2	2.55	0.41
1:A:443:ARG:O	1:A:444:GLN:C	2.64	0.41
1:B:323:HIS:CE1	1:B:476:LEU:HD12	2.56	0.41
1:B:331:ALA:C	1:B:333:LEU:H	2.29	0.41
1:B:337:ASP:OD1	1:B:337:ASP:N	2.53	0.41
1:B:350:ARG:HG3	1:B:368:PHE:CD2	2.56	0.41
1:C:377:LEU:HB3	1:C:379:LEU:HG	2.02	0.41
1:C:455:VAL:O	1:C:457:LYS:N	2.54	0.41
1:D:232:LYS:O	1:D:233:ALA:C	2.64	0.41
1:A:271:GLN:NE2	1:A:272:GLU:N	2.69	0.40
1:B:338:GLY:O	1:B:339:VAL:HB	2.21	0.40
1:B:454:GLN:O	1:B:457:LYS:HB3	2.21	0.40
1:C:359:PRO:HG2	1:C:360:PHE:CD2	2.56	0.40
1:C:360:PHE:HA	1:C:363:PHE:HB2	2.02	0.40
1:A:276:GLU:CD	1:A:279:ILE:H	2.28	0.40
1:B:212:ARG:CZ	1:B:212:ARG:HB3	2.51	0.40
1:B:243:ASP:CG	1:B:244:LYS:H	2.29	0.40
1:B:360:PHE:O	1:B:361:GLY:C	2.62	0.40
1:C:221:SER:O	1:C:224:LYS:N	2.54	0.40
1:C:288:ARG:HD2	1:C:289:SER:HA	2.02	0.40
1:C:363:PHE:C	1:C:367:LYS:HE3	2.46	0.40
1:D:348:MET:HG2	1:D:353:LEU:HG	2.03	0.40
1:A:287:PHE:CD2	1:A:288:ARG:N	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:LYS:O	1:A:442:LEU:CD1	2.66	0.40
1:A:473:TYR:C	1:A:474:LYS:NZ	2.79	0.40
1:B:234:ARG:NH1	1:B:237:LEU:HB3	2.37	0.40
1:B:349:THR:OG1	1:B:352:PHE:HB3	2.20	0.40
1:B:380:ASP:OD1	1:B:382:SER:N	2.50	0.40
1:B:405:PRO:HG2	1:B:406:ILE:N	2.37	0.40
1:B:431:LEU:O	1:B:434:LYS:N	2.53	0.40
1:B:448:GLU:C	1:B:452:LEU:HD13	2.47	0.40
1:C:333:LEU:HD11	2:C:3:072:H5B2	2.04	0.40
1:C:432:PHE:O	1:C:433:ALA:C	2.65	0.40
1:D:321:GLY:O	1:D:324:GLU:N	2.52	0.40
1:D:469:LEU:O	1:D:473:TYR:HD2	2.05	0.40
1:A:340:LEU:HD23	1:A:347:PHE:HD1	1.85	0.40
1:B:335:ASN:HD21	1:B:337:ASP:HB2	1.86	0.40
1:C:276:GLU:OE2	1:C:279:ILE:HG12	2.21	0.40
1:C:428:SER:CB	1:C:431:LEU:HD22	2.52	0.40
1:C:440:THR:CA	1:D:440:THR:HG22	2.51	0.40
1:B:411:ASP:C	1:B:413:LEU:N	2.77	0.40
1:B:420:GLN:O	1:B:421:LEU:C	2.63	0.40
1:B:421:LEU:CD1	1:B:432:PHE:HA	2.45	0.40
1:B:460:GLU:OE2	1:B:466:HIS:CE1	2.74	0.40
1:C:249:ILE:HG23	1:C:255:LEU:CA	2.51	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:D:245:SER:OG	1:D:245:SER:OG[2_756]	1.79	0.41

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	268/270 (99%)	195 (73%)	46 (17%)	27 (10%)	0	1
1	B	268/270 (99%)	182 (68%)	56 (21%)	30 (11%)	0	1
1	C	268/270 (99%)	164 (61%)	68 (25%)	36 (13%)	0	0
1	D	268/270 (99%)	175 (65%)	70 (26%)	23 (9%)	0	1
All	All	1072/1080 (99%)	716 (67%)	240 (22%)	116 (11%)	0	1

All (116) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	ALA
1	A	240	LYS
1	A	267	ILE
1	A	269	PRO
1	A	272	GLU
1	A	309	LEU
1	A	330	LEU
1	A	359	PRO
1	A	428	SER
1	A	456	ILE
1	B	231	ALA
1	B	237	LEU
1	B	240	LYS
1	B	277	VAL
1	B	467	PRO
1	C	227	PRO
1	C	243	ASP
1	C	269	PRO
1	C	273	GLN
1	C	294	GLN
1	C	356	LEU
1	C	394	SER
1	C	428	SER
1	C	455	VAL
1	C	475	ASP
1	D	242	THR
1	D	266	HIS
1	D	277	VAL
1	D	322	VAL
1	D	357	ARG
1	D	370	PHE
1	D	371	ALA
1	D	372	VAL

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Mol	Chain	Res	Type
1	D	428	SER
1	D	467	PRO
1	A	216	LYS
1	A	265	LYS
1	A	270	LEU
1	A	391	ILE
1	A	455	VAL
1	B	227	PRO
1	B	238	THR
1	B	242	THR
1	B	266	HIS
1	B	275	LYS
1	B	278	ALA
1	B	307	VAL
1	B	475	ASP
1	C	221	SER
1	C	265	LYS
1	C	275	LYS
1	C	345	GLN
1	C	359	PRO
1	C	361	GLY
1	C	446	VAL
1	C	466	HIS
1	D	336	LYS
1	D	378	GLU
1	D	395	GLY
1	D	458	LYS
1	D	460	GLU
1	B	208	SER
1	B	265	LYS
1	B	292	ALA
1	B	306	PHE
1	B	464	SER
1	C	274	SER
1	C	311	LEU
1	C	336	LYS
1	C	358	LYS
1	C	385	ALA
1	C	438	LYS
1	C	467	PRO
1	D	361	GLY
1	D	466	HIS

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Mol	Chain	Res	Type
1	D	468	LEU
1	A	307	VAL
1	A	321	GLY
1	A	332	SER
1	A	382	SER
1	A	416	ALA
1	B	272	GLU
1	B	342	SER
1	B	422	LYS
1	B	459	THR
1	C	346	GLY
1	D	304	PRO
1	D	392	ILE
1	D	474	LYS
1	A	227	PRO
1	A	289	SER
1	A	360	PHE
1	B	274	SER
1	B	339	VAL
1	B	352	PHE
1	B	463	MET
1	C	251	ASP
1	C	264	PHE
1	C	364	MET
1	C	391	ILE
1	C	395	GLY
1	C	456	ILE
1	B	252	MET
1	B	437	GLN
1	C	267	ILE
1	C	268	THR
1	D	237	LEU
1	D	292	ALA
1	A	304	PRO
1	A	358	LYS
1	A	390	VAL
1	C	236	ILE
1	A	296	ILE
1	B	361	GLY
1	C	405	PRO
1	B	372	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	243/243 (100%)	207 (85%)	36 (15%)	3	10
1	B	243/243 (100%)	218 (90%)	25 (10%)	7	23
1	C	243/243 (100%)	217 (89%)	26 (11%)	6	22
1	D	243/243 (100%)	217 (89%)	26 (11%)	6	22
All	All	972/972 (100%)	859 (88%)	113 (12%)	5	18

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	LYS
1	A	220	ASP
1	A	228	LEU
1	A	241	THR
1	A	253	ASN
1	A	271	GLN
1	A	287	PHE
1	A	288	ARG
1	A	293	VAL
1	A	304	PRO
1	A	309	LEU
1	A	326	ILE
1	A	337	ASP
1	A	345	GLN
1	A	358	LYS
1	A	360	PHE
1	A	369	GLU
1	A	381	ASP
1	A	383	ASP
1	A	400	LEU
1	A	401	LEU
1	A	403	VAL
1	A	407	GLU
1	A	410	GLN

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Mol	Chain	Res	Type
1	A	412	ASN
1	A	415	GLN
1	A	427	GLU
1	A	440	THR
1	A	452	LEU
1	A	453	LEU
1	A	454	GLN
1	A	458	LYS
1	A	460	GLU
1	A	469	LEU
1	A	474	LYS
1	A	476	LEU
1	B	223	ILE
1	B	237	LEU
1	B	266	HIS
1	B	279	ILE
1	B	287	PHE
1	B	311	LEU
1	B	312	ASN
1	B	315	VAL
1	B	316	THR
1	B	341	ILE
1	B	343	GLU
1	B	348	MET
1	B	351	GLU
1	B	379	LEU
1	B	380	ASP
1	B	393	LEU
1	B	410	GLN
1	B	430	GLN
1	B	440	THR
1	B	443	ARG
1	B	444	GLN
1	B	457	LYS
1	B	458	LYS
1	B	467	PRO
1	B	469	LEU
1	C	217	HIS
1	C	220	ASP
1	C	244	LYS
1	C	261	LYS
1	C	265	LYS

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Mol	Chain	Res	Type
1	C	271	GLN
1	C	275	LYS
1	C	285	CYS
1	C	288	ARG
1	C	294	GLN
1	C	298	GLU
1	C	302	SER
1	C	310	ASP
1	C	328	THR
1	C	337	ASP
1	C	351	GLU
1	C	367	LYS
1	C	409	ILE
1	C	427	GLU
1	C	445	ILE
1	C	458	LYS
1	C	467	PRO
1	C	470	GLN
1	C	474	LYS
1	C	475	ASP
1	C	476	LEU
1	D	214	LEU
1	D	216	LYS
1	D	223	ILE
1	D	228	LEU
1	D	236	ILE
1	D	237	LEU
1	D	253	ASN
1	D	257	MET
1	D	309	LEU
1	D	311	LEU
1	D	325	ILE
1	D	343	GLU
1	D	348	MET
1	D	379	LEU
1	D	381	ASP
1	D	421	LEU
1	D	439	MET
1	D	450	VAL
1	D	451	GLN
1	D	455	VAL
1	D	461	THR

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Mol	Chain	Res	Type
1	D	467	PRO
1	D	469	LEU
1	D	470	GLN
1	D	475	ASP
1	D	476	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	GLN
1	A	283	GLN
1	A	308	ASN
1	A	314	GLN
1	A	345	GLN
1	A	402	ASN
1	A	410	GLN
1	A	412	ASN
1	A	424	ASN
1	A	430	GLN
1	A	437	GLN
1	A	449	HIS
1	A	451	GLN
1	A	470	GLN
1	B	217	HIS
1	B	253	ASN
1	B	266	HIS
1	B	271	GLN
1	B	308	ASN
1	B	312	ASN
1	B	345	GLN
1	B	410	GLN
1	B	412	ASN
1	B	420	GLN
1	B	424	ASN
1	B	430	GLN
1	B	437	GLN
1	B	444	GLN
1	B	449	HIS
1	B	451	GLN
1	B	454	GLN
1	B	466	HIS
1	B	470	GLN

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Mol	Chain	Res	Type
1	C	253	ASN
1	C	271	GLN
1	C	283	GLN
1	C	294	GLN
1	C	345	GLN
1	C	375	ASN
1	C	425	HIS
1	C	444	GLN
1	C	449	HIS
1	C	451	GLN
1	C	466	HIS
1	C	470	GLN
1	D	253	ASN
1	D	271	GLN
1	D	294	GLN
1	D	308	ASN
1	D	375	ASN
1	D	410	GLN
1	D	412	ASN
1	D	415	GLN
1	D	420	GLN
1	D	444	GLN
1	D	451	GLN
1	D	470	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	072	C	3	-	47,47,47	4.07	32 (68%)	53,61,61	2.86	14 (26%)
2	072	A	1	-	47,47,47	4.31	36 (76%)	53,61,61	3.16	15 (28%)
2	072	D	4	-	47,47,47	4.50	37 (78%)	53,61,61	2.56	17 (32%)
2	072	B	2	-	47,47,47	4.51	35 (74%)	53,61,61	2.55	13 (24%)

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	072	C	3	-	-	13/34/50/50	0/4/4/4
2	072	A	1	-	-	14/34/50/50	0/4/4/4
2	072	D	4	-	-	11/34/50/50	0/4/4/4
2	072	B	2	-	-	9/34/50/50	0/4/4/4

All (140) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	072	C2A-N3A	11.22	1.58	1.45
2	D	4	072	C1B-C1A	10.62	1.62	1.52
2	C	3	072	C4B-N4A	10.50	1.62	1.46
2	A	1	072	C4B-N4A	9.82	1.61	1.46
2	B	2	072	C1B-C1A	9.57	1.61	1.52
2	B	2	072	C3B-N3A	8.89	1.61	1.46
2	C	3	072	C2A-N3A	8.65	1.55	1.45
2	D	4	072	C3B-N3A	8.64	1.60	1.46
2	B	2	072	C1C-C1D	8.62	1.66	1.51
2	A	1	072	C2A-N3A	8.11	1.54	1.45
2	B	2	072	C5B-N4A	8.08	1.59	1.46
2	A	1	072	C3B-N3A	8.05	1.59	1.46
2	C	3	072	C4B-C4C	8.04	1.65	1.51
2	D	4	072	C4B-N4A	7.98	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	072	C5B-N4A	7.98	1.58	1.46
2	C	3	072	C5B-N4A	7.91	1.58	1.46
2	C	3	072	C3B-N3A	7.86	1.59	1.46
2	A	1	072	C5B-N4A	7.85	1.58	1.46
2	D	4	072	C2A-N3A	7.64	1.54	1.45
2	B	2	072	C4B-N4A	7.53	1.58	1.46
2	D	4	072	C1C-C1D	7.47	1.64	1.51
2	A	1	072	C1C-C1D	7.15	1.64	1.51
2	D	4	072	C4B-C4C	6.76	1.63	1.51
2	A	1	072	C1D-N4A	6.23	1.47	1.35
2	D	4	072	C3J-C3K	6.15	1.48	1.39
2	B	2	072	C1D-N4A	6.02	1.46	1.35
2	A	1	072	C4B-C4C	5.97	1.62	1.51
2	A	1	072	C5D-C5C	5.96	1.50	1.38
2	D	4	072	C5B-C5C	5.84	1.62	1.51
2	C	3	072	C1C-C1D	5.68	1.61	1.51
2	D	4	072	C1D-N4A	5.39	1.45	1.35
2	B	2	072	C3J-C3K	5.35	1.47	1.39
2	D	4	072	C3J-C3H	5.11	1.47	1.38
2	A	1	072	C4E-C4C	5.06	1.48	1.38
2	B	2	072	C4B-C4C	5.04	1.60	1.51
2	D	4	072	C3I-C3K	4.98	1.47	1.39
2	B	2	072	C5B-C5C	4.93	1.60	1.51
2	A	1	072	C3G-C3F	4.92	1.48	1.38
2	A	1	072	C5B-C5C	4.90	1.60	1.51
2	C	3	072	C1D-N4A	4.87	1.44	1.35
2	C	3	072	C3I-C3K	4.86	1.46	1.39
2	A	1	072	C3J-C3K	4.84	1.46	1.39
2	C	3	072	C4E-C4C	4.84	1.48	1.38
2	D	4	072	C3G-C3F	4.84	1.48	1.38
2	B	2	072	C3G-C3F	4.76	1.48	1.38
2	B	2	072	C3I-C3K	4.65	1.46	1.39
2	C	3	072	C3J-C3K	4.61	1.46	1.39
2	D	4	072	C1A-N3A	4.60	1.41	1.35
2	A	1	072	C2A-S1B	-4.55	1.76	1.83
2	B	2	072	C3I-C3G	4.49	1.46	1.38
2	B	2	072	C5E-C5C	4.48	1.47	1.38
2	B	2	072	C3H-C3F	4.48	1.47	1.38
2	B	2	072	C1A-N3A	4.48	1.41	1.35
2	D	4	072	C3I-C3G	4.47	1.46	1.38
2	A	1	072	C3I-C3K	4.47	1.46	1.39
2	D	4	072	C4G-C4E	4.46	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	072	C5H-C5G	4.43	1.48	1.38
2	A	1	072	C2B-C2A	4.42	1.62	1.52
2	A	1	072	C1A-N3A	4.40	1.41	1.35
2	D	4	072	C4E-C4C	4.36	1.47	1.38
2	A	1	072	C3I-C3G	4.34	1.45	1.38
2	D	4	072	C4D-C4C	4.30	1.47	1.38
2	C	3	072	C1A-N3A	4.29	1.40	1.35
2	B	2	072	C3J-C3H	4.27	1.45	1.38
2	C	3	072	C4G-C4E	4.25	1.46	1.38
2	B	2	072	C5D-C5C	4.20	1.47	1.38
2	A	1	072	C5F-C5D	4.17	1.46	1.38
2	C	3	072	C3G-C3F	4.14	1.47	1.38
2	C	3	072	C3H-C3F	4.11	1.47	1.38
2	A	1	072	C4D-C4C	4.10	1.47	1.38
2	A	1	072	C5E-C5C	4.10	1.47	1.38
2	B	2	072	C4D-C4C	4.09	1.47	1.38
2	B	2	072	C4G-C4E	4.07	1.45	1.38
2	C	3	072	C5B-C5C	4.03	1.58	1.51
2	D	4	072	C5F-C5D	4.02	1.45	1.38
2	D	4	072	C3H-C3F	3.99	1.46	1.38
2	D	4	072	C5E-C5C	3.93	1.46	1.38
2	D	4	072	C5D-C5C	3.92	1.46	1.38
2	A	1	072	C5G-C5E	3.91	1.45	1.38
2	C	3	072	C4D-C4C	3.89	1.46	1.38
2	C	3	072	C3E-C3F	3.89	1.62	1.51
2	A	1	072	C3H-C3F	3.85	1.46	1.38
2	D	4	072	C4F-C4D	3.83	1.45	1.38
2	C	3	072	C5E-C5C	3.81	1.46	1.38
2	B	2	072	C4E-C4C	3.81	1.46	1.38
2	A	1	072	C1B-C1A	3.75	1.55	1.52
2	D	4	072	C5H-C5F	3.73	1.46	1.38
2	A	1	072	C4G-C4E	3.69	1.45	1.38
2	C	3	072	C3I-C3G	3.68	1.44	1.38
2	D	4	072	C2B-C2A	3.67	1.60	1.52
2	D	4	072	C5G-C5E	3.64	1.45	1.38
2	A	1	072	C3E-C3F	3.61	1.61	1.51
2	C	3	072	C5G-C5E	3.59	1.45	1.38
2	C	3	072	C3J-C3H	3.53	1.44	1.38
2	B	2	072	C4F-C4D	3.51	1.44	1.38
2	C	3	072	C4F-C4D	3.49	1.44	1.38
2	B	2	072	C1B-S1B	3.41	1.89	1.80
2	B	2	072	C5F-C5D	3.35	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	072	C3E-C3F	3.30	1.61	1.51
2	B	2	072	C2B-C2A	3.30	1.59	1.52
2	C	3	072	C5D-C5C	3.19	1.45	1.38
2	D	4	072	C5H-C5G	3.18	1.45	1.38
2	D	4	072	C3E-C3F	3.14	1.60	1.51
2	C	3	072	C5H-C5F	3.05	1.45	1.38
2	B	2	072	C5H-C5F	2.98	1.44	1.38
2	D	4	072	C4H-C4G	2.90	1.44	1.38
2	D	4	072	O1A-C1A	2.84	1.27	1.22
2	D	4	072	C1C-C1B	2.80	1.61	1.52
2	A	1	072	C1B-S1B	-2.80	1.73	1.80
2	C	3	072	C4H-C4G	2.78	1.44	1.38
2	A	1	072	C4H-C4G	2.77	1.44	1.38
2	C	3	072	C5H-C5G	2.77	1.44	1.38
2	C	3	072	C2B-C2A	2.76	1.58	1.52
2	D	4	072	C4H-C4F	2.72	1.44	1.38
2	A	1	072	C4F-C4D	2.71	1.43	1.38
2	B	2	072	O1A-C1A	2.70	1.27	1.22
2	B	2	072	C1C-C1B	2.68	1.60	1.52
2	A	1	072	C5H-C5F	2.65	1.44	1.38
2	A	1	072	O1A-C1A	2.59	1.27	1.22
2	A	1	072	C3J-C3H	2.59	1.43	1.38
2	B	2	072	C5G-C5E	2.59	1.43	1.38
2	C	3	072	C4H-C4F	2.56	1.43	1.38
2	C	3	072	C5F-C5D	2.50	1.43	1.38
2	B	2	072	C2C-C2B	2.44	1.62	1.52
2	B	2	072	C5H-C5G	2.41	1.43	1.38
2	A	1	072	C3C-C3B	2.38	1.61	1.51
2	B	2	072	C3C-C3B	2.33	1.61	1.51
2	A	1	072	C4H-C4F	2.30	1.43	1.38
2	C	3	072	C2A-S1B	-2.30	1.79	1.83
2	C	3	072	C2C-C2B	2.29	1.61	1.52
2	D	4	072	C3C-C3B	2.26	1.60	1.51
2	B	2	072	C4H-C4F	2.25	1.43	1.38
2	D	4	072	C3D-C3E	2.21	1.62	1.52
2	B	2	072	C3D-C3E	2.19	1.62	1.52
2	D	4	072	C2E-C2D	2.11	1.62	1.51
2	D	4	072	C2F-C2E	2.10	1.62	1.51
2	C	3	072	C2F-C2E	2.06	1.62	1.51
2	A	1	072	C2D-C2C	2.05	1.62	1.51
2	D	4	072	C2D-C2C	2.04	1.61	1.51
2	A	1	072	C3D-C3E	2.00	1.61	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	072	C4C-C4B-N4A	12.80	133.27	113.15
2	A	1	072	C4C-C4B-N4A	11.83	131.75	113.15
2	A	1	072	C2A-S1B-C1B	10.02	101.34	94.12
2	D	4	072	C3C-C3B-N3A	8.98	126.86	113.25
2	B	2	072	C3C-C3B-N3A	8.65	126.37	113.25
2	A	1	072	C5C-C5B-N4A	7.85	125.49	113.15
2	B	2	072	C1C-C1D-N4A	7.08	131.41	118.37
2	B	2	072	O1D-C1D-C1C	-7.04	108.93	122.07
2	D	4	072	C1C-C1D-N4A	6.91	131.10	118.37
2	C	3	072	O1D-C1D-C1C	-6.13	110.61	122.07
2	C	3	072	C2A-S1B-C1B	6.13	98.54	94.12
2	A	1	072	C3C-C3B-N3A	6.10	122.50	113.25
2	C	3	072	C1C-C1D-N4A	5.99	129.41	118.37
2	A	1	072	O1D-C1D-C1C	-5.93	110.99	122.07
2	C	3	072	C5C-C5B-N4A	5.93	122.48	113.15
2	B	2	072	C1A-C1B-S1B	5.89	107.99	105.19
2	A	1	072	C1C-C1D-N4A	5.87	129.19	118.37
2	D	4	072	C1A-C1B-S1B	5.71	107.91	105.19
2	D	4	072	C4C-C4B-N4A	5.69	122.09	113.15
2	D	4	072	O1D-C1D-C1C	-5.67	111.49	122.07
2	B	2	072	C2A-S1B-C1B	-5.56	90.12	94.12
2	C	3	072	C1A-C1B-S1B	-5.07	102.78	105.19
2	A	1	072	C1C-C1B-S1B	-4.66	105.11	115.10
2	C	3	072	O1A-C1A-C1B	-4.21	115.34	124.52
2	C	3	072	C3C-C3B-N3A	4.17	119.57	113.25
2	B	2	072	C4C-C4B-N4A	4.02	119.47	113.15
2	D	4	072	C3D-C3E-C3F	4.02	128.67	113.67
2	A	1	072	C1A-C1B-S1B	-3.99	103.30	105.19
2	B	2	072	C2C-C2B-C2A	3.97	124.76	113.22
2	D	4	072	C5C-C5B-N4A	3.82	119.16	113.15
2	B	2	072	C3B-N3A-C1A	-3.69	117.81	122.36
2	A	1	072	O1A-C1A-C1B	-3.20	117.56	124.52
2	A	1	072	C3C-C3D-C3E	3.08	126.61	113.74
2	A	1	072	C2E-C2D-C2C	3.04	129.72	114.37
2	A	1	072	C3D-C3E-C3F	3.02	124.92	113.67
2	D	4	072	C1C-C1B-S1B	-2.96	108.76	115.10
2	D	4	072	C3C-C3D-C3E	2.94	126.03	113.74
2	C	3	072	C2D-C2C-C2B	2.88	124.49	113.62
2	C	3	072	O3M-C3L-C3K	2.80	122.03	114.84
2	A	1	072	C2C-C2B-C2A	2.80	121.36	113.22
2	D	4	072	C3D-C3C-C3B	2.76	125.72	113.17
2	B	2	072	C3D-C3E-C3F	2.69	123.70	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	072	C3D-C3C-C3B	2.67	125.29	113.17
2	D	4	072	O1D-C1D-N4A	-2.66	117.39	122.12
2	D	4	072	C2C-C2B-C2A	2.50	120.50	113.22
2	B	2	072	C2D-C2C-C2B	2.48	122.96	113.62
2	D	4	072	C2D-C2C-C2B	2.46	122.90	113.62
2	A	1	072	O3M-C3L-C3K	2.37	120.92	114.84
2	C	3	072	C2F-C2E-C2D	2.34	126.19	114.37
2	B	2	072	C3C-C3D-C3E	2.32	123.45	113.74
2	D	4	072	C2A-S1B-C1B	-2.31	92.46	94.12
2	A	1	072	C2D-C2C-C2B	2.21	121.94	113.62
2	C	3	072	C2C-C2B-C2A	2.18	119.55	113.22
2	D	4	072	O3M-C3L-C3K	2.15	120.35	114.84
2	C	3	072	O3M-C3L-O3N	-2.14	118.75	123.35
2	D	4	072	C3B-N3A-C1A	-2.12	119.74	122.36
2	D	4	072	C4D-C4C-C4E	-2.11	115.09	118.23
2	C	3	072	C2E-C2D-C2C	2.04	124.70	114.37
2	B	2	072	C2E-C2D-C2C	2.03	124.64	114.37

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	072	S1B-C2A-C2B-C2C
2	A	1	072	N3A-C2A-C2B-C2C
2	A	1	072	C4C-C4B-N4A-C1D
2	C	3	072	S1B-C1B-C1C-C1D
2	C	3	072	C1A-C1B-C1C-C1D
2	C	3	072	S1B-C2A-C2B-C2C
2	C	3	072	N3A-C2A-C2B-C2C
2	C	3	072	C4C-C4B-N4A-C1D
2	D	4	072	S1B-C2A-C2B-C2C
2	D	4	072	N3A-C2A-C2B-C2C
2	B	2	072	C3J-C3K-C3L-O3N
2	D	4	072	C3I-C3K-C3L-O3N
2	B	2	072	C3J-C3K-C3L-O3M
2	D	4	072	C3I-C3K-C3L-O3M
2	B	2	072	C3I-C3K-C3L-O3N
2	D	4	072	C3J-C3K-C3L-O3N
2	B	2	072	C3I-C3K-C3L-O3M
2	D	4	072	C3J-C3K-C3L-O3M
2	A	1	072	N3A-C3B-C3C-C3D
2	A	1	072	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
2	B	2	072	C3C-C3D-C3E-C3F
2	A	1	072	C3I-C3K-C3L-O3N
2	D	4	072	C3C-C3D-C3E-C3F
2	C	3	072	C4C-C4B-N4A-C5B
2	D	4	072	O1D-C1D-N4A-C4B
2	A	1	072	C3J-C3K-C3L-O3N
2	D	4	072	N3A-C3B-C3C-C3D
2	A	1	072	C1C-C1D-N4A-C4B
2	C	3	072	C1C-C1D-N4A-C4B
2	D	4	072	C1C-C1D-N4A-C4B
2	C	3	072	O1D-C1D-N4A-C4B
2	A	1	072	C3I-C3K-C3L-O3M
2	A	1	072	C3J-C3K-C3L-O3M
2	B	2	072	C2A-C2B-C2C-C2D
2	A	1	072	C4C-C4B-N4A-C5B
2	B	2	072	C2E-C2F-C2G-C2H
2	C	3	072	O1D-C1D-N4A-C5B
2	A	1	072	C2A-C2B-C2C-C2D
2	C	3	072	C2A-C2B-C2C-C2D
2	A	1	072	O1D-C1D-N4A-C4B
2	A	1	072	C1A-C1B-C1C-C1D
2	B	2	072	C1A-C1B-C1C-C1D
2	C	3	072	C2C-C2D-C2E-C2F
2	C	3	072	C1C-C1D-N4A-C5B
2	C	3	072	N3A-C3B-C3C-C3D
2	D	4	072	C2E-C2F-C2G-C2H
2	B	2	072	C2C-C2D-C2E-C2F

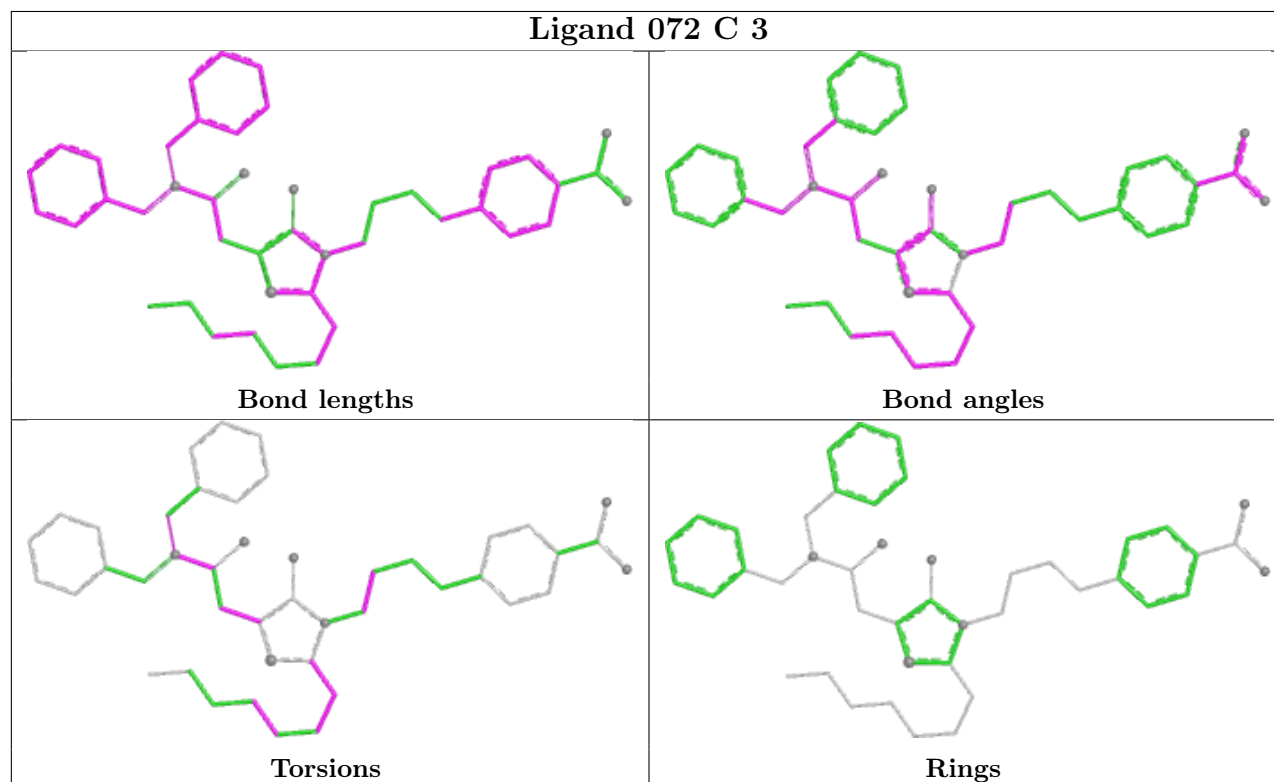
There are no ring outliers.

4 monomers are involved in 16 short contacts:

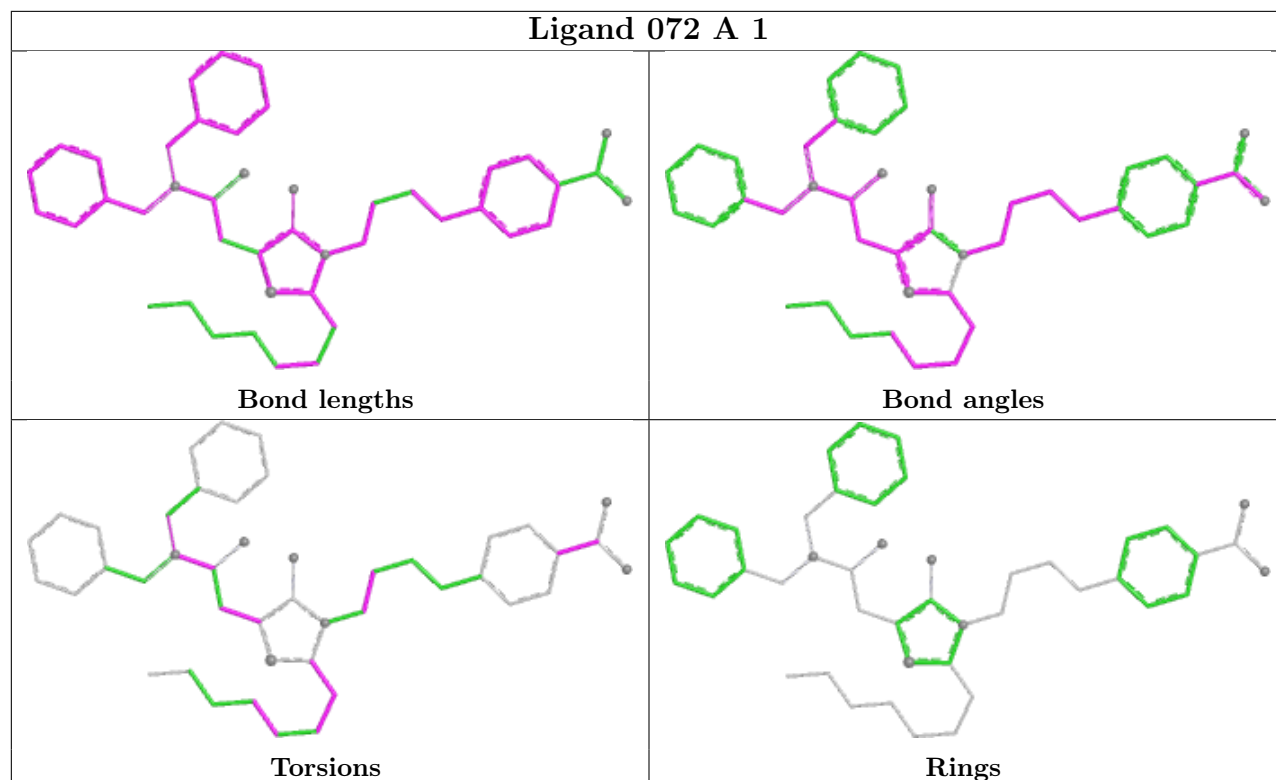
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	072	5	0
2	A	1	072	6	0
2	D	4	072	1	0
2	B	2	072	4	0

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.

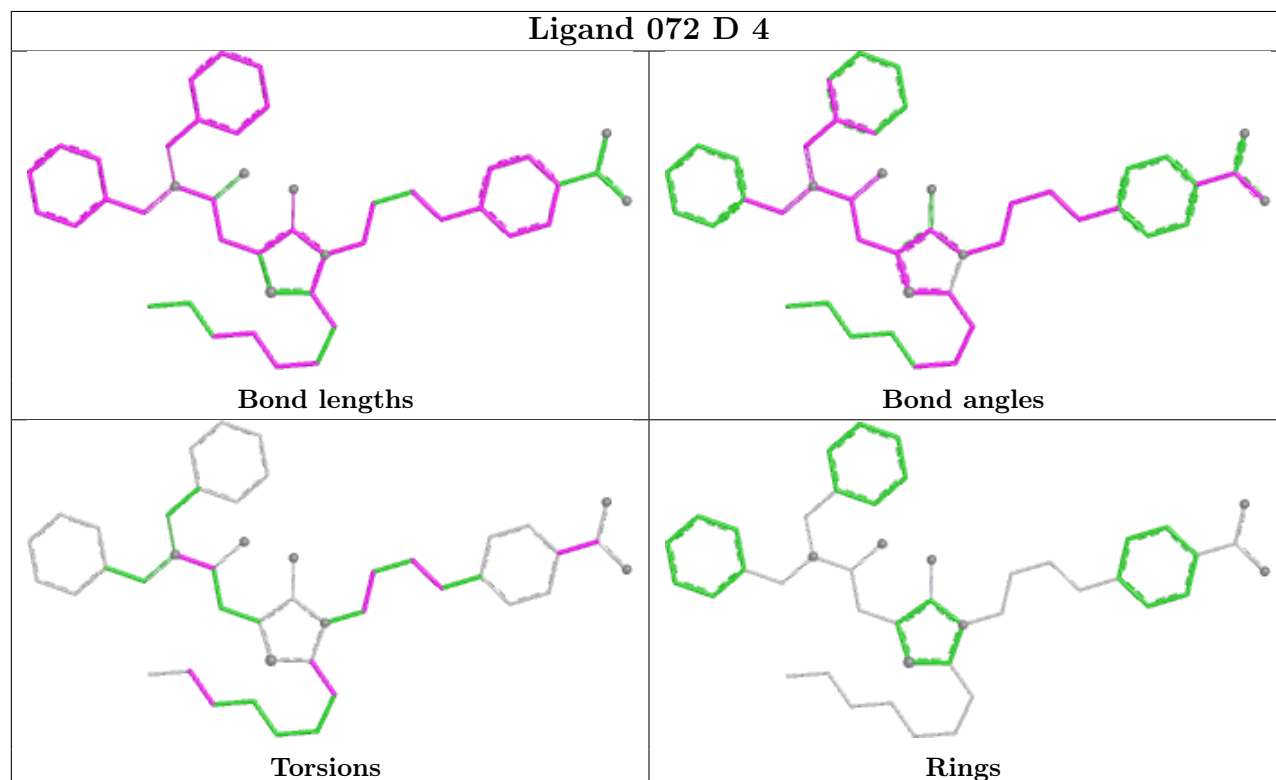
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

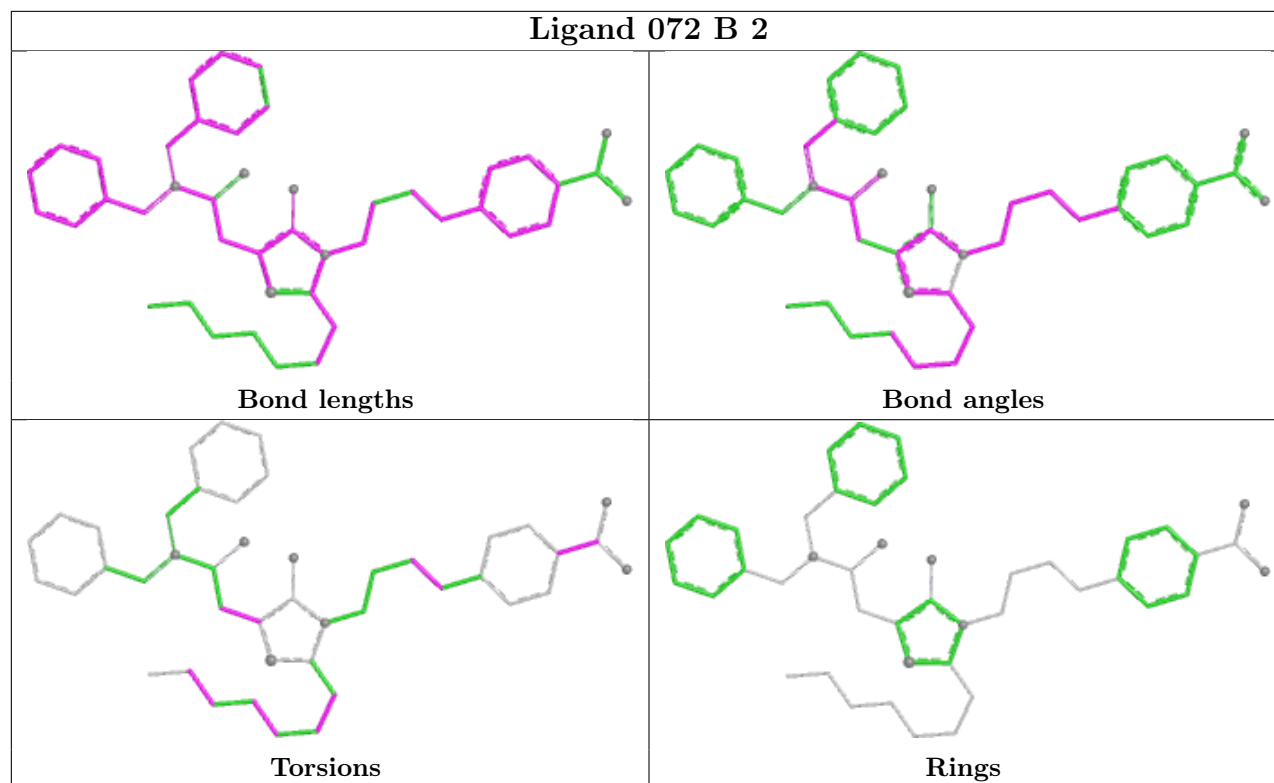


Ligand 072 A 1



Ligand 072 D 4





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	270/270 (100%)	0.74	34 (12%) 8 6	2, 15, 82, 111	0
1	B	270/270 (100%)	0.86	42 (15%) 5 4	2, 15, 75, 98	0
1	C	270/270 (100%)	0.72	26 (9%) 13 11	2, 13, 79, 103	0
1	D	270/270 (100%)	0.86	39 (14%) 6 5	2, 11, 75, 109	0
All	All	1080/1080 (100%)	0.80	141 (13%) 7 6	2, 14, 79, 111	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	464	SER	8.9
1	D	268	THR	8.2
1	A	270	LEU	6.9
1	B	270	LEU	6.5
1	A	274	SER	6.3
1	D	269	PRO	5.9
1	A	267	ILE	5.5
1	B	268	THR	5.3
1	B	274	SER	4.8
1	D	450	VAL	4.8
1	D	463	MET	4.7
1	C	272	GLU	4.6
1	D	243	ASP	4.5
1	C	268	THR	4.5
1	A	475	ASP	4.5
1	D	462	ASP	4.5
1	B	267	ILE	4.4
1	A	269	PRO	4.3
1	B	461	THR	4.3
1	C	241	THR	4.2
1	C	270	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	273	GLN	4.1
1	C	266	HIS	4.1
1	B	466	HIS	4.1
1	D	271	GLN	4.0
1	B	269	PRO	4.0
1	B	260	ASP	4.0
1	D	270	LEU	3.9
1	A	239	GLY	3.9
1	D	267	ILE	3.8
1	D	461	THR	3.8
1	A	264	PHE	3.8
1	A	262	ILE	3.8
1	B	271	GLN	3.7
1	A	268	THR	3.7
1	C	267	ILE	3.7
1	C	475	ASP	3.7
1	B	463	MET	3.6
1	A	241	THR	3.6
1	D	466	HIS	3.6
1	D	272	GLU	3.6
1	B	265	LYS	3.6
1	B	460	GLU	3.6
1	D	235	ALA	3.5
1	B	464	SER	3.5
1	D	239	GLY	3.5
1	B	455	VAL	3.4
1	D	266	HIS	3.3
1	D	351	GLU	3.3
1	D	274	SER	3.3
1	B	272	GLU	3.2
1	B	352	PHE	3.2
1	D	242	THR	3.2
1	D	459	THR	3.2
1	C	260	ASP	3.2
1	D	273	GLN	3.2
1	C	395	GLY	3.2
1	A	266	HIS	3.1
1	A	362	ASP	3.1
1	D	361	GLY	3.1
1	D	460	GLU	3.0
1	D	474	LYS	3.0
1	A	261	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	265	LYS	2.9
1	D	465	LEU	2.9
1	D	259	GLU	2.9
1	A	240	LYS	2.9
1	A	285	CYS	2.9
1	B	261	LYS	2.9
1	D	451	GLN	2.9
1	C	269	PRO	2.8
1	D	456	ILE	2.8
1	D	241	THR	2.8
1	B	351	GLU	2.8
1	B	458	LYS	2.8
1	A	242	THR	2.8
1	B	243	ASP	2.8
1	C	373	LYS	2.7
1	B	342	SER	2.7
1	D	245	SER	2.7
1	B	358	LYS	2.7
1	C	273	GLN	2.6
1	A	276	GLU	2.6
1	A	283	GLN	2.6
1	C	288	ARG	2.6
1	A	403	VAL	2.6
1	A	476	LEU	2.6
1	C	403	VAL	2.6
1	A	457	LYS	2.6
1	A	474	LYS	2.6
1	C	262	ILE	2.6
1	C	259	GLU	2.6
1	B	350	ARG	2.5
1	B	467	PRO	2.5
1	B	457	LYS	2.4
1	D	356	LEU	2.4
1	B	465	LEU	2.4
1	D	277	VAL	2.4
1	C	365	GLU	2.4
1	B	343	GLU	2.3
1	C	464	SER	2.3
1	D	209	ALA	2.3
1	C	258	GLY	2.3
1	A	453	LEU	2.2
1	B	266	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	241	THR	2.2
1	B	207	GLU	2.2
1	B	474	LYS	2.2
1	B	242	THR	2.2
1	C	257	MET	2.2
1	C	337	ASP	2.2
1	D	260	ASP	2.2
1	B	238	THR	2.2
1	D	440	THR	2.2
1	B	429	SER	2.2
1	B	453	LEU	2.2
1	B	454	GLN	2.2
1	D	455	VAL	2.2
1	C	473	TYR	2.2
1	B	239	GLY	2.1
1	B	249	ILE	2.1
1	B	253	ASN	2.1
1	A	216	LYS	2.1
1	C	265	LYS	2.1
1	A	279	ILE	2.1
1	C	298	GLU	2.1
1	D	244	LYS	2.1
1	C	255	LEU	2.1
1	A	259	GLU	2.1
1	B	279	ILE	2.1
1	B	369	GLU	2.1
1	A	424	ASN	2.1
1	D	238	THR	2.1
1	A	464	SER	2.0
1	C	476	LEU	2.0
1	A	238	THR	2.0
1	A	273	GLN	2.0
1	A	286	GLN	2.0
1	D	345	GLN	2.0
1	A	256	MET	2.0
1	A	455	VAL	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](#)

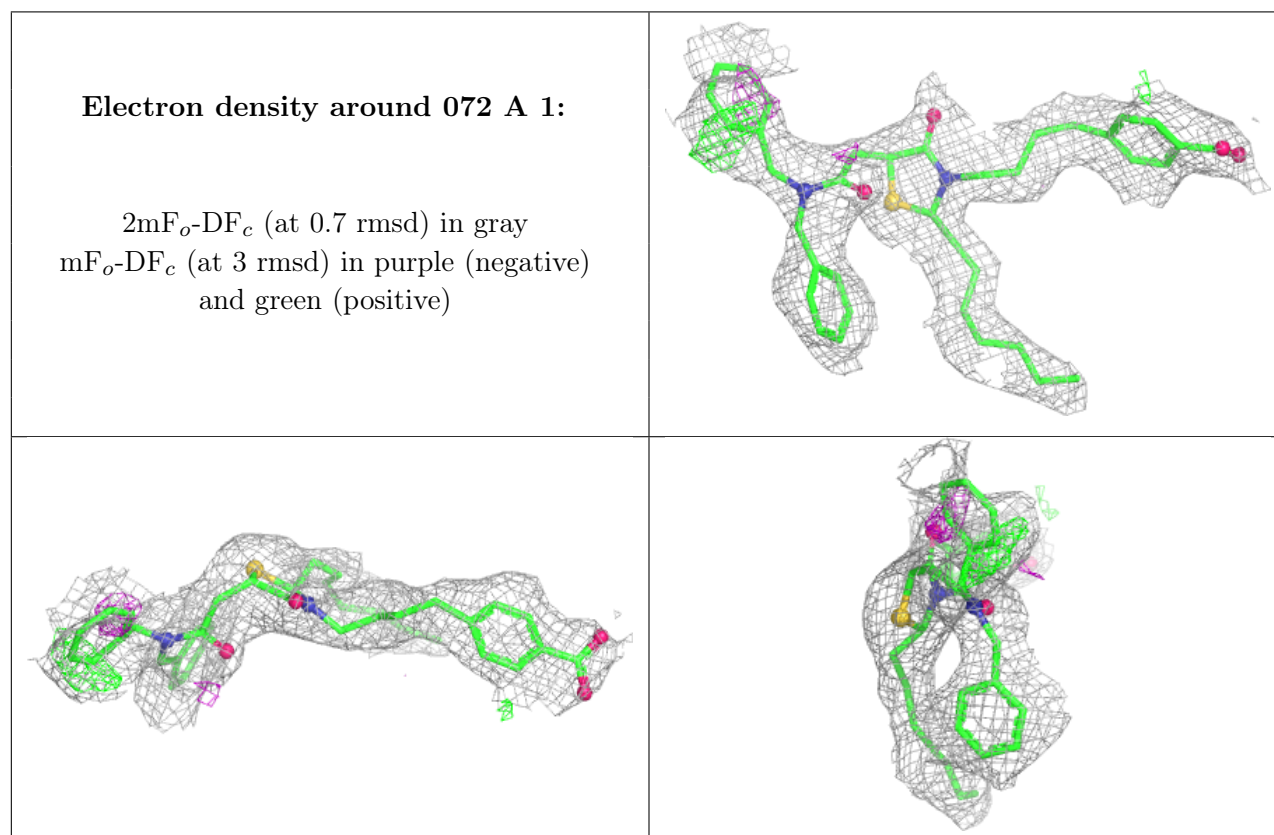
There are no oligosaccharides in this entry.

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.

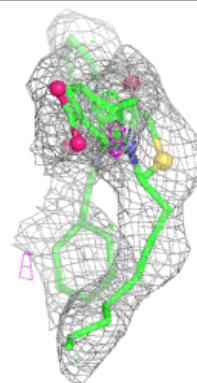
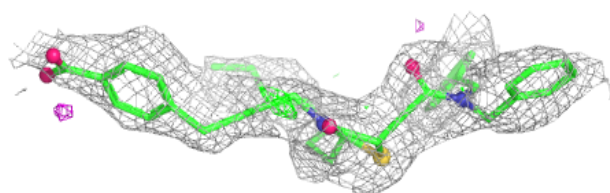
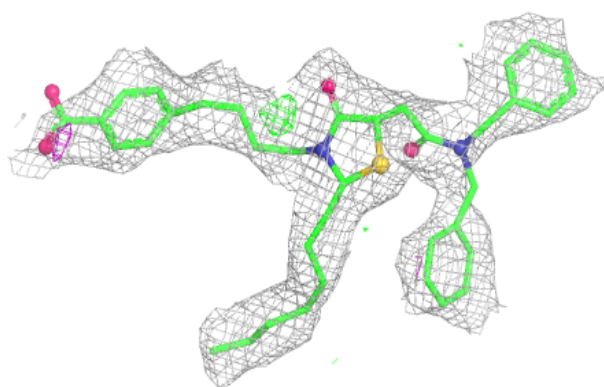
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	072	A	1	44/44	0.77	0.15	10,19,32,34	0
2	072	C	3	44/44	0.82	0.13	2,11,31,39	0
2	072	B	2	44/44	0.85	0.13	15,24,30,32	0
2	072	D	4	44/44	0.86	0.12	2,19,30,34	0

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.

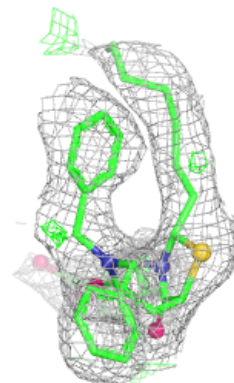
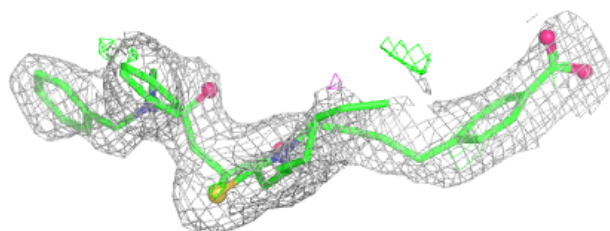
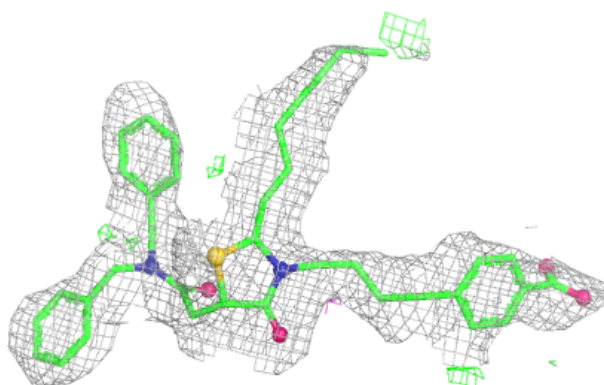


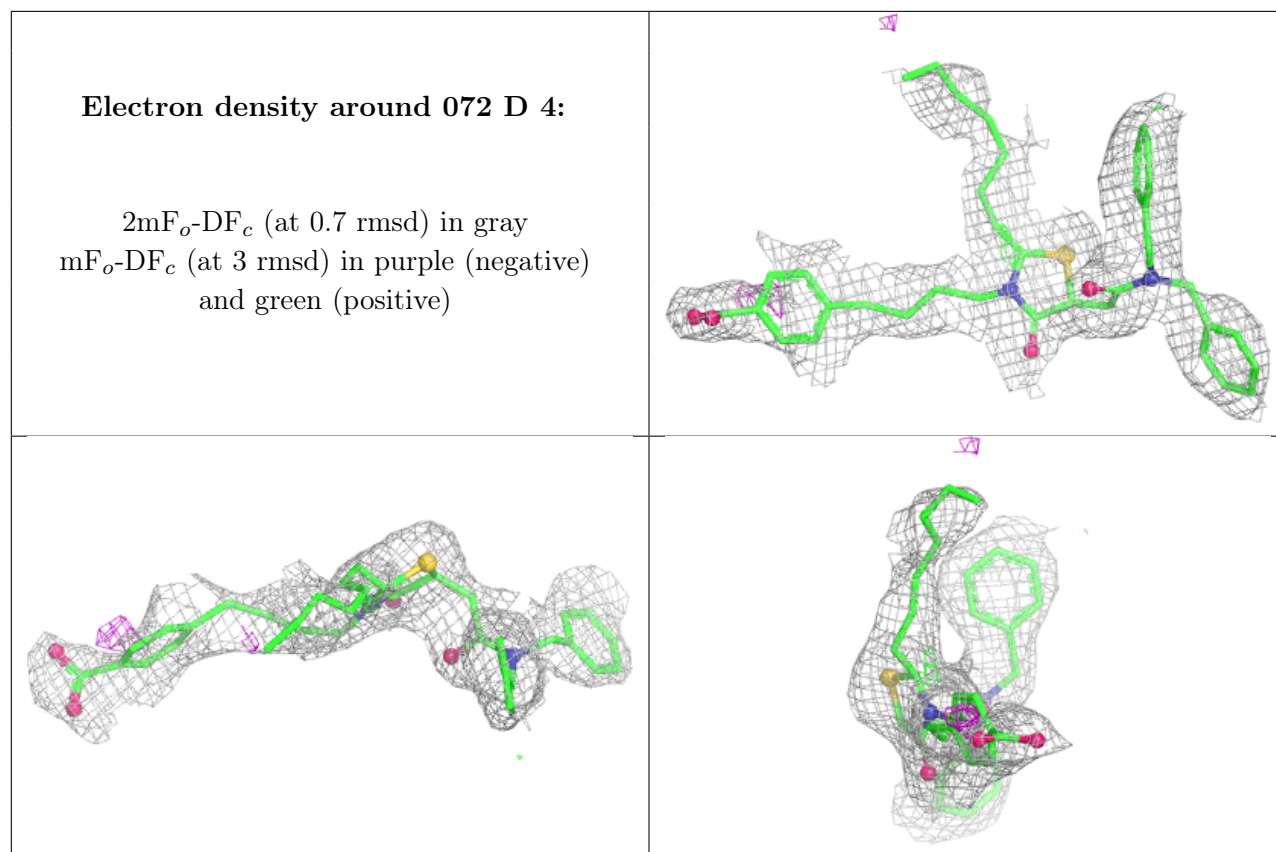
Electron density around 072 C 3:

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

**Electron density around 072 B 2:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.