



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:09 PM UTC

PDB ID : 5C6P / pdb_00005c6p
Title : protein C
Authors : Lu, M.
Deposited on : 2015-06-23
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

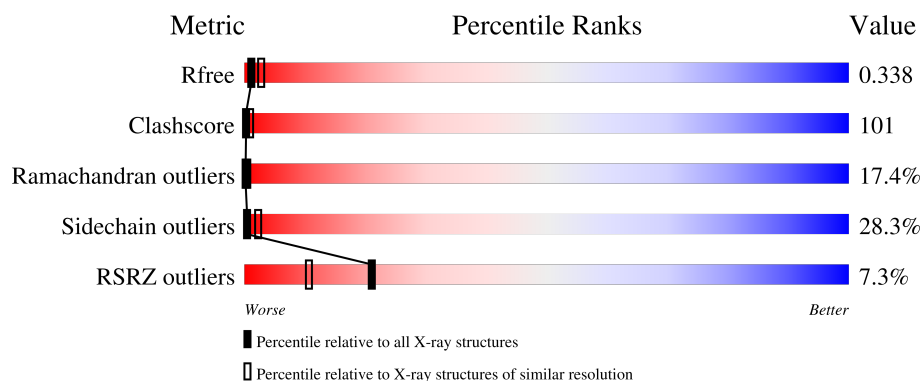
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	459	
2	B	99	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4248 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 C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	0	0	0
			3508	2338	558	589	23			

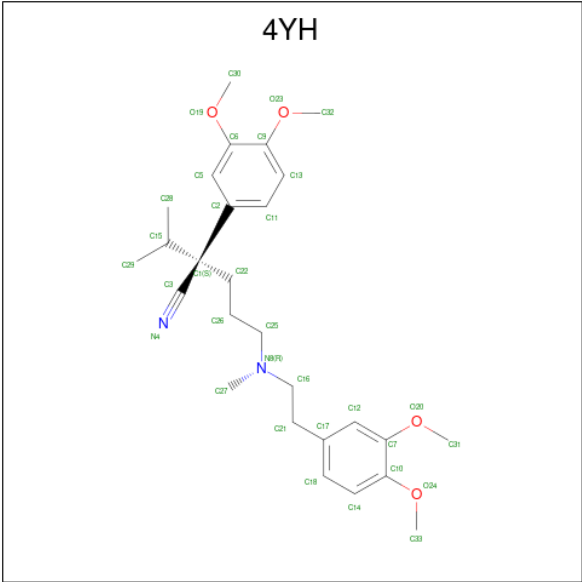
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	460	SER	-	expression tag	UNP Q5F9J8
A	461	SER	-	expression tag	UNP Q5F9J8
A	462	GLY	-	expression tag	UNP Q5F9J8
A	463	LEU	-	expression tag	UNP Q5F9J8

- Molecule 2 is a protein called protein D.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	91	Total	C	N	O	0	0	0
			707	457	110	140			

- Molecule 3 is (2S)-2-(3,4-dimethoxyphenyl)-5-{[2-(3,4-dimethoxyphenyl)ethyl](methyl)amino}-2-(propan-2-yl)pentanenitrile (CCD ID: 4YH) (formula: C₂₇H₃₈N₂O₄).

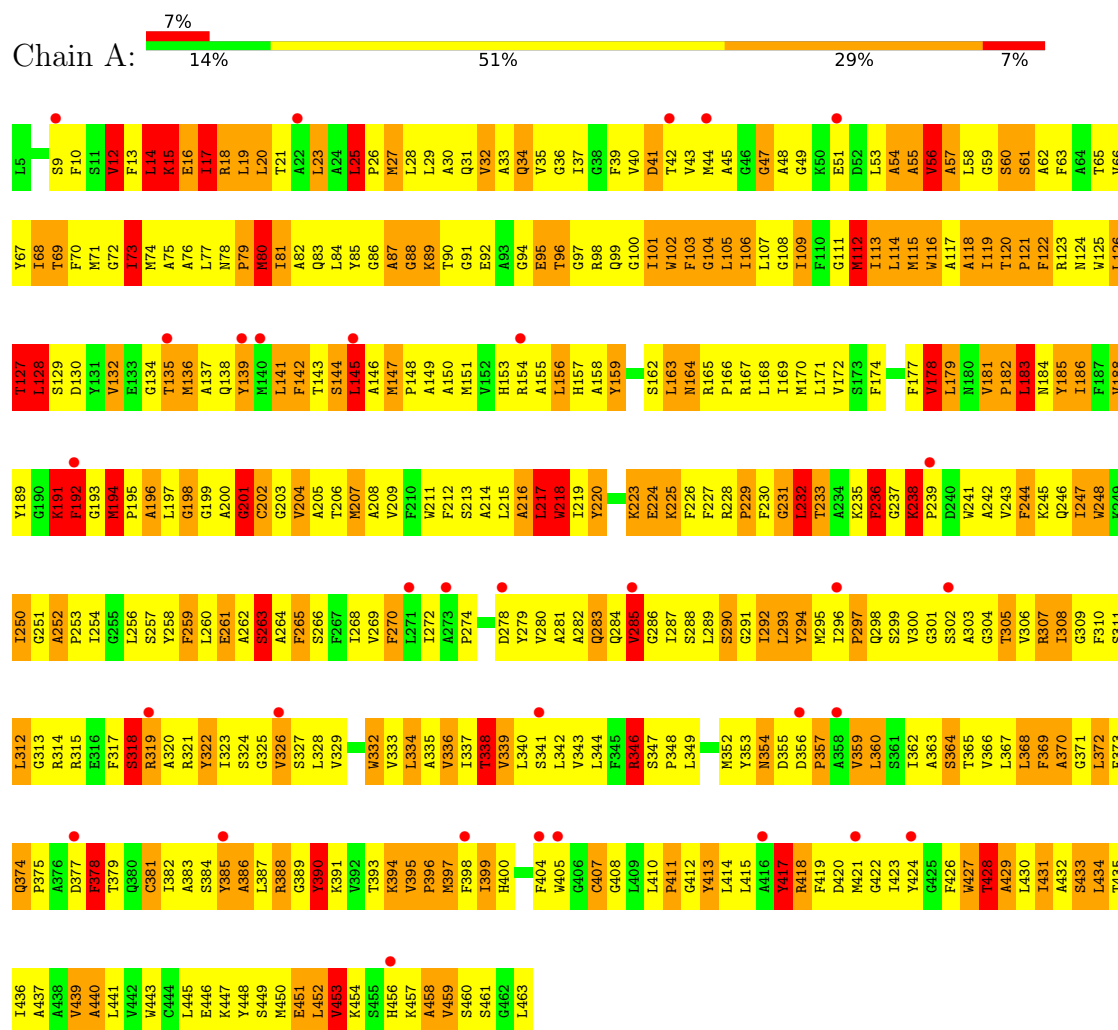


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			33	27	2	4		

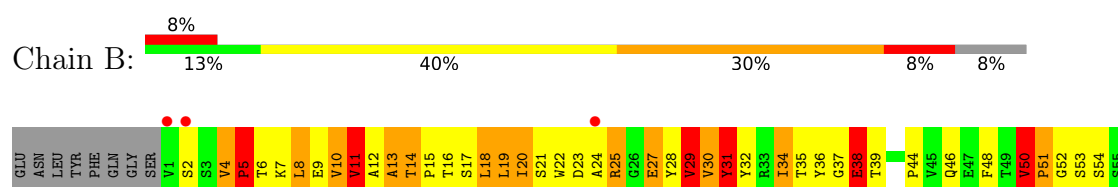
3 Residue-property plots

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 C



• Molecule 2: protein D





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	117.64Å 117.64Å 225.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.01	Depositor EDS
% Data completeness (in resolution range)	91.0 (20.00-3.00) 94.2 (20.00-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 3.04Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.280 , 0.290 0.345 , 0.338	Depositor DCC
R_{free} test set	1719 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	75.5	Xtriage
Anisotropy	0.661	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.15 , 90.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.159 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4248	wwPDB-VP
Average B, all atoms (Å ²)	161.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.79	2/3605 (0.1%)	1.32	36/4898 (0.7%)
2	B	0.91	0/729	1.57	22/1004 (2.2%)
All	All	0.81	2/4334 (0.0%)	1.36	58/5902 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	13
2	B	0	4
All	All	0	17

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	346	ARG	C-O	14.86	1.42	1.23
1	A	125	TRP	CA-C	5.44	1.57	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	339	VAL	N-CA-C	-14.27	99.55	113.53
1	A	346	ARG	O-C-N	-13.96	104.81	123.24
1	A	360	LEU	N-CA-C	11.96	125.70	111.82
1	A	56	VAL	N-CA-C	-10.59	101.60	111.45
1	A	142	PHE	N-CA-C	-10.09	97.51	112.04
1	A	294	TYR	N-CA-C	-9.44	103.86	114.62
2	B	50	VAL	CA-C-N	-8.63	109.06	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	50	VAL	C-N-CA	-8.63	109.06	119.84
1	A	122	PHE	N-CA-C	-7.88	104.62	112.97
1	A	130	ASP	N-CA-C	7.84	122.30	112.03
2	B	11	VAL	N-CA-C	-7.71	104.28	111.45
1	A	127	THR	N-CA-C	7.58	126.94	110.80
1	A	285	VAL	N-CA-C	-7.47	101.58	112.04
1	A	216	ALA	N-CA-C	-7.42	104.25	113.38
1	A	433	SER	N-CA-C	-7.39	103.31	111.36
1	A	215	LEU	N-CA-C	-7.26	102.68	112.26
1	A	145	LEU	CA-CB-CG	7.17	141.41	116.30
2	B	5	PRO	N-CA-C	-7.09	97.85	112.47
2	B	10	VAL	N-CA-C	-7.02	99.66	109.21
2	B	89	TYR	N-CA-C	6.97	119.79	108.63
2	B	90	ARG	N-CA-C	6.97	120.28	107.73
1	A	223	LYS	N-CA-C	6.92	118.52	110.97
1	A	198	GLY	N-CA-C	-6.69	97.33	113.18
1	A	451	GLU	N-CA-C	-6.50	105.27	113.72
1	A	141	LEU	N-CA-C	-6.39	103.15	111.71
2	B	69	THR	N-CA-C	6.26	119.07	107.99
2	B	70	ILE	CB-CA-C	6.25	118.86	110.42
1	A	179	LEU	N-CA-C	-6.18	103.69	111.11
1	A	16	GLU	N-CA-C	6.10	117.79	108.52
2	B	9	GLU	N-CA-C	6.03	119.86	107.37
1	A	178	VAL	N-CA-C	-5.97	105.52	112.98
2	B	8	LEU	CA-CB-CG	5.94	137.10	116.30
2	B	81	TRP	N-CA-C	5.86	118.37	107.99
1	A	388	ARG	N-CA-C	-5.84	104.83	111.07
2	B	29	VAL	N-CA-C	-5.83	97.22	109.34
1	A	453	VAL	N-CA-C	-5.79	97.31	109.34
1	A	32	VAL	N-CA-C	-5.61	106.98	111.81
1	A	231	GLY	N-CA-C	-5.60	101.71	111.62
2	B	86	SER	N-CA-C	5.52	117.46	109.07
1	A	101	ILE	N-CA-C	-5.51	104.20	111.09
1	A	53	LEU	N-CA-C	-5.35	106.60	113.02
2	B	5	PRO	CA-C-N	-5.34	111.33	121.54
2	B	5	PRO	C-N-CA	-5.34	111.33	121.54
1	A	55	ALA	N-CA-C	-5.30	98.36	108.17
1	A	346	ARG	N-CA-C	-5.30	98.39	107.61
1	A	114	LEU	N-CA-C	-5.29	105.20	110.97
1	A	125	TRP	N-CA-C	5.26	119.17	112.12
1	A	418	ARG	N-CA-C	5.20	117.78	110.14
2	B	73	TYR	N-CA-C	5.20	116.88	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	LYS	N-CA-C	-5.18	102.40	109.71
2	B	14	THR	CA-C-N	5.14	126.27	119.84
2	B	14	THR	C-N-CA	5.14	126.27	119.84
1	A	459	VAL	N-CA-C	5.10	118.21	111.17
2	B	8	LEU	CB-CA-C	-5.09	104.16	111.70
2	B	2	SER	N-CA-C	5.08	114.33	108.49
1	A	128	LEU	N-CA-C	5.08	118.29	110.42
1	A	370	ALA	N-CA-C	-5.04	106.23	112.38
2	B	31	TYR	N-CA-C	-5.01	100.14	110.80

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	LEU	Peptide
1	A	127	THR	Peptide
1	A	14	LEU	Peptide
1	A	201	GLY	Peptide
1	A	220	TYR	Peptide
1	A	25	LEU	Peptide
1	A	263	SER	Peptide
1	A	322	TYR	Peptide
1	A	338	THR	Peptide
1	A	346	ARG	Mainchain
1	A	359	VAL	Peptide
1	A	390	TYR	Peptide
1	A	54	ALA	Peptide
2	B	13	ALA	Peptide
2	B	4	VAL	Peptide
2	B	80	GLY	Peptide
2	B	89	TYR	Peptide

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	3508	0	3587	710	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	707	0	681	167	1
3	A	33	0	38	9	0
All	All	4248	0	4306	868	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 101.

All (868) 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:458:ALA:HB3	2:B:8:LEU:O	1.31	1.26
2:B:27:GLU:HB3	2:B:52:GLY:O	1.39	1.23
1:A:158:ALA:CB	1:A:217:LEU:HD11	1.67	1.23
1:A:292:ILE:HG13	1:A:293:LEU:H	1.11	1.13
1:A:146:ALA:HB3	1:A:147:MET:HE2	1.15	1.13
1:A:151:MET:SD	1:A:214:ALA:CB	2.39	1.10
1:A:77:LEU:HA	1:A:80:MET:HG3	1.31	1.10
2:B:67:ASP:HA	2:B:90:ARG:HG2	1.10	1.09
2:B:63:SER:HB3	2:B:64:PRO:HD2	1.28	1.09
1:A:112:MET:HB2	1:A:149:ALA:HB3	1.21	1.09
2:B:10:VAL:HG13	2:B:19:LEU:O	1.52	1.08
1:A:254:ILE:HB	1:A:394:LYS:HE2	1.33	1.08
1:A:146:ALA:CB	1:A:147:MET:HE2	1.83	1.08
1:A:321:ARG:HD3	1:A:449:SER:HA	1.35	1.08
1:A:445:LEU:O	1:A:449:SER:HB2	1.52	1.08
1:A:259:PHE:HA	1:A:262:ALA:HB3	1.32	1.07
1:A:334:LEU:HA	1:A:337:ILE:HG12	1.36	1.07
1:A:158:ALA:HB2	1:A:217:LEU:CD1	1.84	1.06
1:A:329:VAL:HA	1:A:332:TRP:HB2	1.11	1.06
1:A:189:TYR:O	1:A:197:LEU:HD12	1.57	1.05
1:A:151:MET:SD	1:A:214:ALA:HB1	1.98	1.04
1:A:349:LEU:CD1	1:A:360:LEU:HA	1.89	1.02
2:B:20:ILE:HG12	2:B:58:THR:HA	1.36	1.02
1:A:250:ILE:O	1:A:394:LYS:HD2	1.60	1.01
1:A:339:VAL:HG23	1:A:370:ALA:O	1.61	1.01
1:A:396:PRO:HA	1:A:399:ILE:HG13	1.38	1.01
1:A:439:VAL:HG23	1:A:440:ALA:H	1.24	1.00
1:A:97:GLY:HA3	1:A:227:PHE:HE2	1.27	0.99
2:B:35:THR:O	2:B:70:ILE:HG13	1.62	0.99
1:A:192:PHE:HB3	1:A:196:ALA:HA	1.42	0.98
1:A:305:THR:OG1	1:A:389:GLY:HA2	1.64	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:ASP:HA	2:B:90:ARG:CG	1.93	0.97
1:A:82:ALA:HB1	1:A:310:PHE:HB2	1.46	0.97
1:A:248:TRP:CZ3	1:A:252:ALA:HB2	2.01	0.96
1:A:78:ASN:HA	1:A:163:LEU:HD11	1.47	0.96
1:A:184:ASN:O	1:A:188:VAL:HG23	1.67	0.95
1:A:458:ALA:CB	2:B:8:LEU:O	2.15	0.94
1:A:97:GLY:HA3	1:A:227:PHE:CE2	2.02	0.94
2:B:20:ILE:CG1	2:B:58:THR:HA	1.97	0.94
1:A:31:GLN:HE22	1:A:300:VAL:HB	1.29	0.93
2:B:17:SER:HA	2:B:61:GLY:HA3	1.49	0.93
1:A:95:GLU:O	1:A:99:GLN:HG2	1.68	0.93
2:B:8:LEU:HD22	2:B:87:ILE:HG12	1.48	0.92
1:A:349:LEU:HD13	1:A:360:LEU:HA	1.50	0.92
2:B:4:VAL:C	2:B:5:PRO:O	2.04	0.92
2:B:67:ASP:CA	2:B:90:ARG:HG2	2.00	0.92
1:A:218:TRP:HA	1:A:218:TRP:CE3	2.02	0.92
1:A:318:SER:C	1:A:320:ALA:H	1.72	0.92
1:A:159:TYR:HB3	1:A:170:MET:SD	2.09	0.91
1:A:284:GLN:O	1:A:288:SER:HB3	1.69	0.91
1:A:340:LEU:O	1:A:344:LEU:HB2	1.69	0.91
1:A:426:PHE:HA	1:A:428:THR:HG22	1.52	0.91
1:A:147:MET:N	1:A:148:PRO:HD2	1.86	0.91
1:A:159:TYR:CB	1:A:170:MET:SD	2.59	0.91
2:B:30:VAL:CG1	2:B:51:PRO:O	2.19	0.91
1:A:329:VAL:HA	1:A:332:TRP:CB	1.99	0.91
1:A:158:ALA:HB2	1:A:217:LEU:HD11	0.94	0.90
1:A:184:ASN:ND2	1:A:205:ALA:HB1	1.84	0.90
1:A:292:ILE:HG13	1:A:293:LEU:N	1.78	0.90
2:B:36:TYR:HA	2:B:70:ILE:HD11	1.52	0.90
1:A:120:THR:HB	1:A:121:PRO:CD	2.01	0.90
1:A:359:VAL:HG12	1:A:360:LEU:H	1.36	0.89
1:A:287:ILE:HA	1:A:290:SER:HB3	1.53	0.89
1:A:424:TYR:HA	1:A:427:TRP:CD1	2.08	0.89
2:B:68:TYR:H	2:B:90:ARG:HB3	1.37	0.89
2:B:38:GLU:HA	2:B:68:TYR:HA	1.53	0.89
1:A:395:VAL:HG13	1:A:396:PRO:HD3	1.54	0.87
1:A:426:PHE:C	1:A:428:THR:H	1.83	0.86
2:B:31:TYR:HD1	2:B:75:ARG:HH12	1.23	0.85
1:A:251:GLY:O	1:A:254:ILE:HG22	1.77	0.85
1:A:148:PRO:HD3	1:A:207:MET:HB2	1.57	0.85
1:A:458:ALA:HB1	2:B:8:LEU:HB3	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:LEU:HD22	2:B:20:ILE:H	1.40	0.85
1:A:146:ALA:HB3	1:A:147:MET:CE	2.03	0.85
1:A:322:TYR:HE1	1:A:449:SER:HG	0.87	0.85
1:A:70:PHE:HB3	1:A:153:HIS:CE1	2.12	0.85
1:A:283:GLN:O	1:A:287:ILE:HG12	1.77	0.85
1:A:82:ALA:HB1	1:A:310:PHE:CB	2.07	0.84
1:A:89:LYS:CD	1:A:89:LYS:H	1.90	0.84
1:A:410:LEU:HD12	1:A:413:TYR:HD1	1.39	0.84
1:A:120:THR:HB	1:A:121:PRO:HD3	1.60	0.84
2:B:19:LEU:HA	2:B:58:THR:HG22	1.58	0.84
1:A:40:VAL:HG23	1:A:178:VAL:HG22	1.60	0.84
2:B:4:VAL:HG23	2:B:5:PRO:O	1.76	0.84
2:B:20:ILE:HD11	2:B:59:ILE:HG12	1.59	0.84
1:A:384:SER:HA	1:A:387:LEU:HB2	1.59	0.83
1:A:216:ALA:HA	1:A:219:ILE:HD11	1.58	0.83
1:A:300:VAL:O	1:A:304:GLY:N	2.11	0.83
1:A:387:LEU:HD12	1:A:393:THR:HG21	1.61	0.83
1:A:397:MET:HA	1:A:400:HIS:HB3	1.58	0.83
1:A:254:ILE:HB	1:A:394:LYS:CE	2.07	0.83
1:A:414:LEU:HD23	1:A:428:THR:HG21	1.60	0.83
2:B:74:ALA:HB1	2:B:82:TYR:HB2	1.60	0.83
1:A:112:MET:CB	1:A:149:ALA:HB3	2.06	0.83
2:B:63:SER:HB3	2:B:64:PRO:CD	2.09	0.82
2:B:30:VAL:HG13	2:B:51:PRO:O	1.78	0.82
1:A:334:LEU:HD12	1:A:337:ILE:HD11	1.61	0.82
1:A:334:LEU:HA	1:A:337:ILE:CG1	2.10	0.81
1:A:77:LEU:HA	1:A:80:MET:CG	2.10	0.81
1:A:218:TRP:HA	1:A:218:TRP:HE3	1.44	0.81
2:B:11:VAL:H	2:B:19:LEU:HD12	1.45	0.81
1:A:321:ARG:HH12	1:A:391:LYS:HD2	1.45	0.81
1:A:184:ASN:HD22	1:A:205:ALA:HB1	1.42	0.81
1:A:15:LYS:HZ3	1:A:15:LYS:HB2	1.43	0.81
1:A:31:GLN:HE22	1:A:300:VAL:CB	1.94	0.81
1:A:151:MET:SD	1:A:214:ALA:HB2	2.19	0.81
1:A:15:LYS:HB2	1:A:15:LYS:NZ	1.95	0.80
1:A:40:VAL:CG2	1:A:178:VAL:HG22	2.11	0.80
2:B:74:ALA:CB	2:B:82:TYR:HB2	2.12	0.80
1:A:148:PRO:O	1:A:151:MET:N	2.15	0.80
1:A:264:ALA:O	1:A:268:ILE:HG12	1.81	0.80
1:A:386:ALA:HA	1:A:389:GLY:HA3	1.62	0.80
1:A:216:ALA:HA	1:A:219:ILE:CD1	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:GLU:HA	1:A:264:ALA:HB3	1.64	0.80
1:A:461:SER:HA	2:B:8:LEU:HG	1.64	0.80
2:B:28:TYR:H	2:B:30:VAL:HB	1.47	0.80
2:B:75:ARG:CB	2:B:75:ARG:HH11	1.95	0.79
1:A:76:ALA:HB1	1:A:250:ILE:HD12	1.65	0.79
1:A:339:VAL:HA	1:A:342:LEU:HD12	1.64	0.79
2:B:5:PRO:HD2	2:B:83:SER:O	1.83	0.79
1:A:55:ALA:HB1	1:A:58:LEU:HD21	1.62	0.79
1:A:318:SER:HA	1:A:321:ARG:H	1.47	0.79
2:B:75:ARG:HD2	2:B:79:TRP:O	1.83	0.79
1:A:308:ILE:HD11	1:A:386:ALA:HA	1.65	0.79
1:A:113:ILE:HA	1:A:116:TRP:HB3	1.64	0.78
2:B:10:VAL:CG1	2:B:19:LEU:O	2.32	0.78
1:A:78:ASN:HA	1:A:163:LEU:HD21	1.65	0.78
1:A:70:PHE:HB3	1:A:153:HIS:HE1	1.46	0.78
1:A:32:VAL:O	1:A:35:VAL:HG12	1.84	0.78
1:A:394:LYS:HA	1:A:397:MET:HG2	1.66	0.78
1:A:146:ALA:C	1:A:148:PRO:HD2	2.09	0.78
1:A:439:VAL:HG23	1:A:440:ALA:N	1.99	0.77
1:A:73:ILE:HD12	1:A:73:ILE:H	1.49	0.77
1:A:14:LEU:O	1:A:322:TYR:CE2	2.38	0.77
1:A:81:ILE:HB	1:A:163:LEU:HD12	1.66	0.77
1:A:99:GLN:O	1:A:244:PHE:HE1	1.67	0.77
2:B:35:THR:HG23	2:B:73:TYR:HE1	1.50	0.77
1:A:74:MET:C	1:A:76:ALA:H	1.91	0.77
1:A:374:GLN:O	1:A:378:PHE:HD1	1.68	0.77
1:A:137:ALA:HB3	1:A:138:GLN:HE21	1.49	0.77
2:B:29:VAL:O	2:B:76:SER:HA	1.84	0.77
2:B:13:ALA:HA	2:B:18:LEU:HA	1.68	0.76
1:A:339:VAL:HA	1:A:342:LEU:CD1	2.15	0.76
2:B:66:VAL:O	2:B:90:ARG:HB2	1.85	0.76
1:A:177:PHE:HE1	1:A:213:SER:HB2	1.51	0.76
1:A:356:ASP:CG	1:A:357:PRO:HD3	2.09	0.76
1:A:322:TYR:HE1	1:A:449:SER:OG	1.66	0.76
1:A:387:LEU:HB3	1:A:393:THR:HB	1.66	0.76
1:A:329:VAL:CA	1:A:332:TRP:HB2	2.05	0.75
2:B:27:GLU:CB	2:B:52:GLY:O	2.28	0.75
1:A:410:LEU:C	1:A:412:GLY:H	1.95	0.75
1:A:78:ASN:CA	1:A:163:LEU:HD11	2.15	0.75
1:A:147:MET:N	1:A:148:PRO:CD	2.50	0.75
1:A:318:SER:C	1:A:320:ALA:N	2.43	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:ARG:HD2	2:B:79:TRP:C	2.10	0.75
1:A:159:TYR:HB2	1:A:170:MET:SD	2.27	0.74
2:B:74:ALA:O	2:B:81:TRP:HE3	1.69	0.74
1:A:30:ALA:O	1:A:34:GLN:HB2	1.87	0.74
2:B:34:ILE:HD12	2:B:48:PHE:HB2	1.68	0.74
1:A:192:PHE:HB3	1:A:196:ALA:CA	2.17	0.74
1:A:418:ARG:HG2	1:A:422:GLY:HA3	1.67	0.74
1:A:174:PHE:HA	1:A:177:PHE:HB2	1.70	0.74
1:A:31:GLN:NE2	1:A:300:VAL:HB	2.02	0.74
1:A:369:PHE:HB3	1:A:372:LEU:HD12	1.70	0.74
1:A:198:GLY:O	1:A:201:GLY:N	2.19	0.74
2:B:74:ALA:O	2:B:81:TRP:CE3	2.41	0.73
1:A:408:GLY:HA2	1:A:411:PRO:HB2	1.70	0.73
1:A:248:TRP:HZ3	1:A:252:ALA:HB2	1.54	0.73
1:A:369:PHE:HA	1:A:372:LEU:HB2	1.71	0.73
1:A:384:SER:O	1:A:387:LEU:N	2.18	0.73
2:B:76:SER:HB3	2:B:82:TYR:CE2	2.24	0.73
1:A:458:ALA:HB1	2:B:8:LEU:HD13	1.71	0.73
2:B:18:LEU:HB2	2:B:59:ILE:HD11	1.69	0.73
2:B:90:ARG:O	2:B:91:THR:HB	1.87	0.73
1:A:248:TRP:CE3	1:A:252:ALA:HB2	2.24	0.73
1:A:252:ALA:HB3	1:A:253:PRO:HD3	1.71	0.73
1:A:372:LEU:HD11	1:A:424:TYR:HB2	1.70	0.72
1:A:89:LYS:CG	1:A:92:GLU:HB3	2.18	0.72
2:B:32:TYR:HB2	2:B:50:VAL:HG23	1.72	0.72
1:A:383:ALA:O	1:A:387:LEU:HD23	1.90	0.72
1:A:373:PHE:HB2	1:A:434:LEU:HD13	1.70	0.72
2:B:90:ARG:O	2:B:90:ARG:HD2	1.90	0.72
1:A:181:VAL:O	1:A:185:TYR:HB3	1.90	0.72
1:A:429:ALA:O	1:A:433:SER:HB2	1.90	0.71
1:A:183:LEU:O	1:A:186:ILE:HG13	1.89	0.71
1:A:284:GLN:O	1:A:288:SER:CB	2.38	0.71
1:A:321:ARG:CD	1:A:449:SER:HA	2.18	0.71
1:A:343:VAL:HG13	1:A:367:LEU:O	1.91	0.71
2:B:78:TYR:C	2:B:80:GLY:H	1.96	0.71
1:A:177:PHE:CE1	1:A:213:SER:HB2	2.26	0.71
1:A:461:SER:HB2	2:B:6:THR:O	1.91	0.71
1:A:200:ALA:C	1:A:202:CYS:H	1.98	0.71
1:A:369:PHE:CD2	1:A:424:TYR:HB3	2.25	0.71
1:A:216:ALA:HA	1:A:219:ILE:CG1	2.21	0.71
1:A:457:LYS:HB3	2:B:10:VAL:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:TYR:CB	1:A:362:ILE:HG23	2.22	0.70
1:A:89:LYS:H	1:A:89:LYS:HD3	1.56	0.70
1:A:458:ALA:CB	2:B:8:LEU:HB3	2.22	0.70
2:B:78:TYR:O	2:B:80:GLY:N	2.18	0.70
1:A:189:TYR:HB2	1:A:199:GLY:O	1.91	0.70
1:A:397:MET:HB3	1:A:400:HIS:ND1	2.06	0.70
2:B:63:SER:CB	2:B:64:PRO:HD2	2.17	0.70
1:A:148:PRO:CD	1:A:207:MET:HB2	2.21	0.70
1:A:78:ASN:HA	1:A:163:LEU:CD1	2.21	0.70
1:A:305:THR:HA	1:A:308:ILE:HD11	1.72	0.70
1:A:76:ALA:HB1	1:A:250:ILE:CD1	2.22	0.69
1:A:410:LEU:HD12	1:A:413:TYR:CD1	2.24	0.69
2:B:4:VAL:HG23	2:B:6:THR:HA	1.73	0.69
1:A:120:THR:O	1:A:122:PHE:N	2.22	0.69
1:A:450:MET:HA	1:A:450:MET:HE2	1.74	0.69
2:B:36:TYR:HE2	2:B:59:ILE:HG22	1.56	0.69
1:A:123:ARG:HE	1:A:128:LEU:HB2	1.57	0.69
1:A:373:PHE:HB2	1:A:434:LEU:CD1	2.22	0.69
1:A:72:GLY:C	1:A:254:ILE:HG23	2.17	0.68
1:A:141:LEU:O	1:A:145:LEU:HD23	1.93	0.68
1:A:339:VAL:HG21	1:A:375:PRO:HD3	1.73	0.68
1:A:101:ILE:HG12	1:A:154:ARG:HG2	1.75	0.68
1:A:186:ILE:HA	1:A:189:TYR:HD2	1.56	0.68
2:B:5:PRO:HD3	2:B:74:ALA:HB2	1.74	0.68
2:B:22:TRP:O	2:B:56:THR:HG23	1.93	0.68
1:A:339:VAL:HA	1:A:342:LEU:CG	2.24	0.68
1:A:15:LYS:NZ	1:A:446:GLU:CD	2.52	0.68
1:A:308:ILE:CD1	1:A:386:ALA:HA	2.23	0.68
1:A:74:MET:CE	1:A:107:LEU:HD12	2.24	0.68
1:A:137:ALA:HB3	1:A:138:GLN:NE2	2.08	0.68
1:A:306:VAL:O	1:A:308:ILE:N	2.27	0.67
2:B:76:SER:HB3	2:B:82:TYR:CZ	2.29	0.67
1:A:192:PHE:HB2	1:A:194:MET:C	2.19	0.67
2:B:28:TYR:N	2:B:30:VAL:HB	2.08	0.67
1:A:365:THR:HB	1:A:423:ILE:HG21	1.75	0.67
1:A:186:ILE:HA	1:A:189:TYR:CD2	2.28	0.67
1:A:411:PRO:HG2	1:A:429:ALA:HB3	1.77	0.66
2:B:19:LEU:HD11	2:B:21:SER:OG	1.95	0.66
1:A:411:PRO:HB3	1:A:428:THR:HG23	1.77	0.66
2:B:5:PRO:CD	2:B:83:SER:O	2.43	0.66
2:B:31:TYR:C	2:B:32:TYR:CD2	2.74	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ILE:O	1:A:76:ALA:HB3	1.95	0.66
1:A:112:MET:O	1:A:116:TRP:HB2	1.95	0.66
1:A:69:THR:HG23	1:A:70:PHE:H	1.61	0.66
1:A:135:THR:HA	1:A:138:GLN:HG2	1.78	0.66
1:A:266:SER:O	1:A:270:PHE:HB2	1.95	0.66
1:A:15:LYS:HZ2	1:A:446:GLU:CD	2.04	0.66
1:A:42:THR:HA	1:A:45:ALA:HB3	1.78	0.66
2:B:28:TYR:H	2:B:30:VAL:CB	2.08	0.66
1:A:238:LYS:HB2	1:A:239:PRO:HD2	1.78	0.65
1:A:404:PHE:HA	1:A:433:SER:OG	1.96	0.65
2:B:7:LYS:H	2:B:23:ASP:HB3	1.61	0.65
1:A:99:GLN:O	1:A:244:PHE:CE1	2.47	0.65
1:A:202:CYS:O	1:A:206:THR:N	2.25	0.65
1:A:283:GLN:O	1:A:283:GLN:HG2	1.96	0.65
1:A:40:VAL:HG22	1:A:181:VAL:HG21	1.78	0.65
2:B:36:TYR:HB3	2:B:46:GLN:HB2	1.78	0.65
1:A:77:LEU:O	1:A:163:LEU:HD11	1.96	0.65
1:A:371:GLY:O	1:A:375:PRO:HD2	1.96	0.65
1:A:141:LEU:O	1:A:145:LEU:CD2	2.45	0.65
1:A:426:PHE:C	1:A:428:THR:N	2.53	0.65
1:A:66:VAL:HA	1:A:69:THR:HG22	1.79	0.64
1:A:366:VAL:HA	1:A:369:PHE:CZ	2.31	0.64
1:A:428:THR:C	1:A:430:LEU:H	2.05	0.64
1:A:439:VAL:O	1:A:441:LEU:N	2.29	0.64
1:A:279:TYR:HB3	1:A:362:ILE:HG23	1.78	0.64
1:A:386:ALA:CA	1:A:389:GLY:HA3	2.27	0.64
1:A:247:ILE:HA	1:A:250:ILE:HD11	1.80	0.64
1:A:247:ILE:O	1:A:247:ILE:HG22	1.98	0.64
1:A:374:GLN:O	1:A:378:PHE:CD1	2.50	0.64
2:B:35:THR:OG1	2:B:71:THR:N	2.29	0.64
1:A:216:ALA:HA	1:A:219:ILE:HG12	1.79	0.64
1:A:95:GLU:O	1:A:99:GLN:CG	2.44	0.64
1:A:377:ASP:O	1:A:378:PHE:C	2.40	0.64
2:B:28:TYR:C	2:B:30:VAL:HB	2.22	0.64
2:B:11:VAL:N	2:B:19:LEU:HD12	2.13	0.63
1:A:372:LEU:HD13	1:A:431:ILE:HG21	1.79	0.63
1:A:89:LYS:HB2	1:A:92:GLU:CB	2.28	0.63
1:A:224:GLU:HG2	1:A:225:LYS:N	2.13	0.63
2:B:8:LEU:HD22	2:B:87:ILE:CG1	2.27	0.63
1:A:73:ILE:H	1:A:73:ILE:CD1	2.11	0.63
1:A:338:THR:HG23	1:A:341:SER:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:TYR:HD1	2:B:75:ARG:NH1	1.96	0.62
1:A:135:THR:O	1:A:139:TYR:N	2.32	0.62
1:A:268:ILE:HB	1:A:287:ILE:CD1	2.29	0.62
1:A:298:GLN:HG2	1:A:382:ILE:HG22	1.82	0.62
1:A:102:TRP:CD1	1:A:233:THR:HG1	2.18	0.62
1:A:76:ALA:CB	1:A:250:ILE:HD12	2.30	0.62
1:A:377:ASP:HB2	1:A:434:LEU:HG	1.82	0.62
1:A:33:ALA:O	1:A:36:GLY:N	2.25	0.62
1:A:320:ALA:O	1:A:323:ILE:HG12	1.99	0.62
1:A:148:PRO:HA	1:A:211:TRP:HE1	1.64	0.62
1:A:398:PHE:HD2	1:A:399:ILE:HG12	1.64	0.62
1:A:426:PHE:CA	1:A:428:THR:HG22	2.27	0.62
1:A:439:VAL:CG2	1:A:440:ALA:H	1.99	0.62
1:A:76:ALA:O	1:A:79:PRO:HD2	2.00	0.62
1:A:431:ILE:HA	1:A:434:LEU:HB3	1.81	0.62
1:A:120:THR:CB	1:A:121:PRO:CD	2.75	0.62
1:A:445:LEU:O	1:A:449:SER:CB	2.40	0.62
1:A:36:GLY:HA2	1:A:39:PHE:CE2	2.35	0.61
1:A:66:VAL:HG21	1:A:115:MET:HG3	1.80	0.61
1:A:40:VAL:O	1:A:43:VAL:HG12	2.00	0.61
1:A:139:TYR:HA	1:A:142:PHE:CD1	2.36	0.61
1:A:323:ILE:C	1:A:325:GLY:H	2.08	0.61
1:A:334:LEU:HD12	1:A:337:ILE:CD1	2.30	0.61
1:A:158:ALA:HA	1:A:217:LEU:HD21	1.81	0.61
1:A:400:HIS:HB2	1:A:441:LEU:HD11	1.83	0.61
1:A:272:ILE:HB	1:A:281:ALA:HA	1.82	0.61
1:A:138:GLN:OE1	1:A:200:ALA:HB3	2.01	0.61
1:A:362:ILE:HG22	1:A:363:ALA:O	2.01	0.61
2:B:34:ILE:CD1	2:B:48:PHE:HB2	2.31	0.61
1:A:61:SER:HB2	3:A:601:4YH:H37	1.83	0.61
1:A:115:MET:CE	1:A:146:ALA:HB2	2.31	0.61
1:A:336:VAL:HA	1:A:339:VAL:HG12	1.83	0.61
2:B:31:TYR:C	2:B:32:TYR:HD2	2.09	0.60
1:A:146:ALA:CB	1:A:147:MET:CE	2.70	0.60
1:A:238:LYS:CB	1:A:239:PRO:CD	2.80	0.60
2:B:4:VAL:HG11	2:B:85:ILE:HD13	1.84	0.60
2:B:90:ARG:HD2	2:B:90:ARG:C	2.26	0.60
1:A:13:PHE:O	1:A:15:LYS:N	2.34	0.60
1:A:61:SER:C	1:A:63:PHE:H	2.09	0.60
1:A:82:ALA:CB	1:A:310:PHE:HB2	2.27	0.60
1:A:61:SER:O	1:A:63:PHE:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ASN:HA	1:A:163:LEU:CD2	2.32	0.60
1:A:339:VAL:HA	1:A:342:LEU:HG	1.82	0.60
1:A:328:LEU:HD23	1:A:329:VAL:HG22	1.83	0.60
1:A:74:MET:C	1:A:76:ALA:N	2.57	0.60
1:A:202:CYS:O	1:A:205:ALA:N	2.34	0.60
2:B:75:ARG:HH11	2:B:75:ARG:CG	2.14	0.60
1:A:132:VAL:HA	1:A:136:MET:HE3	1.84	0.60
1:A:162:SER:O	1:A:163:LEU:C	2.44	0.60
1:A:181:VAL:HA	1:A:184:ASN:OD1	2.01	0.60
1:A:295:MET:O	1:A:299:SER:HB3	2.02	0.60
1:A:44:MET:HE2	1:A:181:VAL:CG1	2.31	0.59
1:A:48:ALA:HB1	1:A:54:ALA:HB1	1.84	0.59
1:A:320:ALA:HA	1:A:323:ILE:HG12	1.83	0.59
2:B:75:ARG:HH11	2:B:75:ARG:HB2	1.65	0.59
1:A:383:ALA:C	1:A:387:LEU:HD23	2.27	0.59
1:A:384:SER:O	1:A:386:ALA:N	2.25	0.59
1:A:155:ALA:HB2	1:A:214:ALA:HA	1.84	0.59
1:A:313:GLY:C	1:A:315:ARG:H	2.10	0.59
2:B:20:ILE:HG13	2:B:58:THR:HA	1.85	0.59
1:A:86:GLY:HA3	1:A:313:GLY:C	2.28	0.59
1:A:306:VAL:C	1:A:308:ILE:H	2.11	0.59
1:A:359:VAL:HG12	1:A:360:LEU:N	2.14	0.59
1:A:322:TYR:CE1	1:A:449:SER:OG	2.48	0.59
1:A:377:ASP:C	1:A:379:THR:N	2.59	0.59
1:A:225:LYS:HD2	1:A:226:PHE:H	1.68	0.59
1:A:332:TRP:CD1	1:A:379:THR:HG1	2.21	0.59
1:A:158:ALA:CB	1:A:217:LEU:CD1	2.60	0.58
1:A:301:GLY:O	1:A:385:TYR:O	2.21	0.58
1:A:79:PRO:O	1:A:80:MET:C	2.46	0.58
1:A:113:ILE:HA	1:A:116:TRP:CB	2.32	0.58
2:B:63:SER:HB2	2:B:68:TYR:OH	2.04	0.58
1:A:74:MET:HE2	1:A:107:LEU:HD12	1.85	0.58
1:A:98:ARG:HG3	1:A:233:THR:HG22	1.84	0.58
2:B:71:THR:HG23	2:B:86:SER:HB2	1.83	0.58
1:A:305:THR:O	1:A:389:GLY:O	2.20	0.58
1:A:236:PHE:N	1:A:241:TRP:HB2	2.18	0.58
1:A:315:ARG:HG3	1:A:317:PHE:CE1	2.39	0.58
2:B:34:ILE:CD1	2:B:48:PHE:CB	2.82	0.58
1:A:56:VAL:O	1:A:58:LEU:N	2.36	0.58
1:A:231:GLY:O	1:A:232:LEU:C	2.47	0.58
1:A:84:LEU:O	1:A:87:ALA:HB3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:PRO:HG3	1:A:207:MET:HB2	1.84	0.58
2:B:27:GLU:CB	2:B:30:VAL:HG11	2.33	0.58
1:A:97:GLY:O	1:A:157:HIS:CE1	2.57	0.58
2:B:7:LYS:HG2	2:B:8:LEU:N	2.19	0.58
1:A:200:ALA:O	1:A:202:CYS:N	2.37	0.58
2:B:5:PRO:HG2	2:B:72:VAL:HG13	1.84	0.58
2:B:21:SER:HA	2:B:56:THR:HA	1.85	0.58
1:A:145:LEU:HD13	1:A:203:GLY:CA	2.33	0.57
1:A:306:VAL:C	1:A:308:ILE:N	2.61	0.57
1:A:410:LEU:O	1:A:414:LEU:HB2	2.04	0.57
1:A:73:ILE:HA	1:A:251:GLY:CA	2.34	0.57
1:A:356:ASP:OD2	3:A:601:4YH:H26	2.04	0.57
1:A:369:PHE:HD2	1:A:424:TYR:HB3	1.69	0.57
2:B:4:VAL:HB	2:B:85:ILE:HB	1.86	0.57
1:A:132:VAL:HG13	1:A:136:MET:HG2	1.87	0.57
1:A:235:LYS:HB2	1:A:241:TRP:HB3	1.85	0.57
1:A:235:LYS:O	1:A:236:PHE:HB2	2.04	0.57
1:A:56:VAL:HG13	1:A:57:ALA:H	1.69	0.57
1:A:253:PRO:HB3	1:A:398:PHE:HB2	1.86	0.57
1:A:328:LEU:HD23	1:A:329:VAL:CG2	2.34	0.57
1:A:148:PRO:CG	1:A:207:MET:HB2	2.34	0.57
1:A:333:VAL:HG12	1:A:334:LEU:HD13	1.87	0.57
1:A:349:LEU:HA	1:A:355:ASP:OD2	2.04	0.57
2:B:36:TYR:HD1	2:B:46:GLN:CD	2.13	0.57
1:A:40:VAL:O	1:A:41:ASP:C	2.48	0.57
1:A:71:MET:HG2	1:A:156:LEU:CD2	2.35	0.57
1:A:248:TRP:HZ3	1:A:252:ALA:CB	2.17	0.57
1:A:305:THR:HG1	1:A:389:GLY:HA2	1.68	0.57
1:A:395:VAL:CG1	1:A:396:PRO:HD3	2.32	0.57
1:A:33:ALA:HB2	1:A:171:LEU:HA	1.87	0.56
2:B:34:ILE:HG22	2:B:71:THR:O	2.04	0.56
1:A:329:VAL:HG13	1:A:332:TRP:HB3	1.87	0.56
1:A:445:LEU:O	1:A:445:LEU:HG	2.05	0.56
1:A:205:ALA:O	1:A:208:ALA:HB3	2.05	0.56
1:A:447:LYS:HD2	1:A:448:TYR:CE1	2.40	0.56
1:A:89:LYS:HG3	1:A:92:GLU:HB3	1.85	0.56
2:B:19:LEU:HD13	2:B:20:ILE:N	2.20	0.56
1:A:14:LEU:O	1:A:322:TYR:HE2	1.87	0.56
1:A:136:MET:O	1:A:139:TYR:CD2	2.59	0.56
1:A:384:SER:O	1:A:388:ARG:HG3	2.04	0.56
1:A:386:ALA:O	1:A:390:TYR:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:LEU:C	1:A:412:GLY:N	2.62	0.56
1:A:263:SER:C	1:A:265:PHE:H	2.13	0.56
2:B:4:VAL:HG12	2:B:84:PRO:O	2.05	0.56
1:A:44:MET:HE2	1:A:181:VAL:HB	1.87	0.56
1:A:411:PRO:CG	1:A:429:ALA:HB3	2.36	0.56
1:A:163:LEU:O	1:A:164:ASN:C	2.49	0.55
1:A:200:ALA:C	1:A:202:CYS:N	2.64	0.55
1:A:231:GLY:O	1:A:233:THR:N	2.40	0.55
1:A:335:ALA:HA	1:A:378:PHE:CG	2.41	0.55
1:A:384:SER:C	1:A:386:ALA:H	2.10	0.55
1:A:145:LEU:HB2	1:A:203:GLY:HA3	1.88	0.55
1:A:301:GLY:C	1:A:303:ALA:H	2.12	0.55
1:A:87:ALA:HB1	1:A:89:LYS:NZ	2.20	0.55
1:A:211:TRP:H	1:A:211:TRP:CD1	2.23	0.55
1:A:238:LYS:HB2	1:A:239:PRO:CD	2.35	0.55
2:B:68:TYR:N	2:B:90:ARG:HB3	2.16	0.55
1:A:83:GLN:HA	1:A:309:GLY:O	2.07	0.55
1:A:398:PHE:CD2	1:A:399:ILE:HG12	2.42	0.55
1:A:411:PRO:C	1:A:426:PHE:HB2	2.31	0.55
1:A:51:GLU:O	1:A:54:ALA:HB3	2.07	0.55
1:A:134:GLY:O	1:A:136:MET:N	2.40	0.55
1:A:138:GLN:OE1	1:A:200:ALA:CB	2.55	0.55
1:A:189:TYR:O	1:A:189:TYR:CD1	2.60	0.55
2:B:36:TYR:CA	2:B:70:ILE:HD11	2.29	0.55
1:A:288:SER:O	1:A:292:ILE:HG23	2.07	0.55
1:A:47:GLY:HA3	1:A:185:TYR:OH	2.06	0.55
1:A:56:VAL:HG13	1:A:57:ALA:N	2.22	0.55
1:A:305:THR:OG1	1:A:389:GLY:CA	2.48	0.55
1:A:339:VAL:CG2	1:A:375:PRO:HD3	2.36	0.55
2:B:75:ARG:CD	2:B:79:TRP:O	2.53	0.55
1:A:73:ILE:O	1:A:76:ALA:CB	2.54	0.54
1:A:71:MET:HG2	1:A:156:LEU:HD22	1.88	0.54
1:A:86:GLY:HA3	1:A:314:ARG:N	2.22	0.54
2:B:13:ALA:HB1	2:B:17:SER:O	2.08	0.54
1:A:77:LEU:CA	1:A:80:MET:HG3	2.21	0.54
1:A:105:LEU:C	1:A:109:ILE:HD12	2.32	0.54
1:A:366:VAL:C	1:A:368:LEU:H	2.16	0.54
1:A:368:LEU:O	1:A:372:LEU:HG	2.08	0.54
1:A:387:LEU:HD22	1:A:445:LEU:HD13	1.88	0.54
1:A:461:SER:CB	2:B:7:LYS:HA	2.37	0.54
1:A:36:GLY:HA2	1:A:39:PHE:CD2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:SER:C	1:A:265:PHE:N	2.66	0.54
1:A:69:THR:HG23	1:A:70:PHE:HD1	1.72	0.54
1:A:268:ILE:HD12	1:A:269:VAL:HG23	1.88	0.54
1:A:317:PHE:C	1:A:319:ARG:H	2.16	0.54
1:A:439:VAL:O	1:A:443:TRP:HB3	2.08	0.54
2:B:7:LYS:HB3	2:B:23:ASP:HB2	1.90	0.54
2:B:59:ILE:HD12	2:B:61:GLY:CA	2.37	0.54
1:A:106:ILE:CD1	1:A:244:PHE:HZ	2.21	0.54
1:A:119:ILE:HG22	1:A:120:THR:N	2.22	0.54
1:A:207:MET:HE3	1:A:208:ALA:HA	1.90	0.54
1:A:217:LEU:O	1:A:218:TRP:C	2.50	0.54
1:A:301:GLY:O	1:A:305:THR:HB	2.07	0.53
1:A:336:VAL:O	1:A:339:VAL:HG12	2.09	0.53
2:B:7:LYS:H	2:B:23:ASP:CB	2.21	0.53
2:B:34:ILE:HA	2:B:71:THR:O	2.08	0.53
1:A:57:ALA:O	1:A:61:SER:N	2.37	0.53
1:A:104:GLY:O	1:A:153:HIS:HB2	2.08	0.53
1:A:127:THR:HG23	1:A:128:LEU:HD22	1.89	0.53
1:A:69:THR:HG23	1:A:70:PHE:N	2.22	0.53
1:A:76:ALA:HB2	1:A:251:GLY:HA2	1.89	0.53
1:A:145:LEU:HD13	1:A:203:GLY:HA2	1.88	0.53
1:A:186:ILE:HG22	1:A:189:TYR:HE2	1.72	0.53
1:A:349:LEU:HD13	1:A:360:LEU:CA	2.32	0.53
1:A:397:MET:O	1:A:400:HIS:CG	2.61	0.53
1:A:94:GLY:HA2	1:A:227:PHE:CZ	2.44	0.53
1:A:224:GLU:CG	1:A:225:LYS:N	2.72	0.53
2:B:37:GLY:O	2:B:70:ILE:CD1	2.56	0.53
2:B:38:GLU:HB2	2:B:67:ASP:O	2.08	0.53
1:A:28:LEU:O	1:A:32:VAL:HG23	2.09	0.53
1:A:17:ILE:HG22	1:A:18:ARG:N	2.23	0.53
1:A:263:SER:HB3	1:A:405:TRP:CD1	2.44	0.53
1:A:296:ILE:HB	1:A:297:PRO:HD3	1.89	0.53
1:A:408:GLY:HA3	1:A:430:LEU:HD11	1.90	0.53
1:A:431:ILE:HD12	1:A:431:ILE:O	2.08	0.53
1:A:224:GLU:CG	1:A:225:LYS:H	2.22	0.53
1:A:411:PRO:HA	1:A:428:THR:CG2	2.38	0.53
1:A:143:THR:O	1:A:146:ALA:HB3	2.09	0.53
1:A:185:TYR:O	1:A:189:TYR:HB3	2.09	0.52
1:A:252:ALA:HB3	1:A:253:PRO:CD	2.39	0.52
2:B:28:TYR:O	2:B:30:VAL:HB	2.09	0.52
1:A:108:GLY:O	1:A:112:MET:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:VAL:O	1:A:440:ALA:C	2.52	0.52
2:B:14:THR:O	2:B:16:THR:N	2.42	0.52
2:B:36:TYR:HE2	2:B:59:ILE:CG2	2.21	0.52
1:A:327:SER:O	1:A:328:LEU:C	2.52	0.52
1:A:163:LEU:HD22	1:A:306:VAL:HG22	1.92	0.52
2:B:19:LEU:CD1	2:B:21:SER:H	2.23	0.52
1:A:144:SER:C	1:A:146:ALA:H	2.16	0.52
2:B:27:GLU:HB2	2:B:30:VAL:CG1	2.40	0.52
1:A:158:ALA:CA	1:A:217:LEU:HD11	2.37	0.52
2:B:27:GLU:HB2	2:B:30:VAL:HG11	1.90	0.52
1:A:339:VAL:CA	1:A:342:LEU:HG	2.39	0.52
1:A:15:LYS:HA	1:A:322:TYR:CD2	2.45	0.51
1:A:89:LYS:HB2	1:A:92:GLU:HB3	1.92	0.51
1:A:135:THR:O	1:A:135:THR:CG2	2.58	0.51
1:A:254:ILE:HD11	1:A:385:TYR:HE1	1.75	0.51
1:A:346:ARG:O	1:A:347:SER:HB3	2.10	0.51
1:A:284:GLN:HE21	3:A:601:4YH:C13	2.23	0.51
1:A:217:LEU:O	1:A:220:TYR:N	2.32	0.51
2:B:67:ASP:HA	2:B:90:ARG:CB	2.39	0.51
1:A:15:LYS:NZ	1:A:446:GLU:OE2	2.44	0.51
1:A:203:GLY:O	1:A:207:MET:HB3	2.11	0.51
1:A:295:MET:HE3	1:A:296:ILE:HG13	1.92	0.51
1:A:74:MET:O	1:A:76:ALA:N	2.44	0.51
1:A:92:GLU:HA	1:A:95:GLU:HG2	1.93	0.51
1:A:118:ALA:O	1:A:119:ILE:C	2.53	0.51
1:A:461:SER:CA	2:B:8:LEU:HG	2.37	0.51
2:B:71:THR:HG22	2:B:72:VAL:N	2.25	0.51
1:A:44:MET:HG3	1:A:206:THR:CG2	2.41	0.51
1:A:103:PHE:O	1:A:106:ILE:HB	2.11	0.51
1:A:135:THR:O	1:A:135:THR:HG22	2.10	0.51
1:A:40:VAL:O	1:A:43:VAL:N	2.43	0.51
1:A:98:ARG:CG	1:A:233:THR:HG22	2.40	0.51
1:A:108:GLY:C	1:A:150:ALA:HA	2.35	0.51
1:A:127:THR:HG23	1:A:128:LEU:N	2.26	0.51
1:A:284:GLN:NE2	3:A:601:4YH:C13	2.74	0.51
1:A:40:VAL:HG22	1:A:178:VAL:HG22	1.92	0.51
1:A:159:TYR:CD1	1:A:159:TYR:C	2.88	0.51
1:A:337:ILE:HA	1:A:340:LEU:HD12	1.93	0.51
1:A:136:MET:N	1:A:136:MET:HE2	2.26	0.51
1:A:189:TYR:CD1	1:A:189:TYR:C	2.82	0.51
1:A:214:ALA:O	1:A:217:LEU:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ILE:C	1:A:325:GLY:N	2.69	0.51
1:A:414:LEU:CD2	1:A:428:THR:HG21	2.37	0.51
2:B:17:SER:HA	2:B:61:GLY:CA	2.33	0.51
1:A:27:MET:HE2	1:A:27:MET:N	2.25	0.50
1:A:74:MET:HE3	1:A:107:LEU:HD12	1.90	0.50
1:A:138:GLN:C	1:A:141:LEU:H	2.19	0.50
2:B:36:TYR:CD1	2:B:46:GLN:HB2	2.46	0.50
2:B:36:TYR:CB	2:B:46:GLN:HB2	2.40	0.50
1:A:70:PHE:O	1:A:73:ILE:HB	2.12	0.50
1:A:415:LEU:HB2	1:A:426:PHE:HD2	1.76	0.50
1:A:440:ALA:O	1:A:443:TRP:HE3	1.94	0.50
2:B:7:LYS:HG2	2:B:8:LEU:H	1.74	0.50
2:B:24:ALA:O	2:B:53:SER:OG	2.27	0.50
1:A:18:ARG:NE	1:A:20:LEU:HD12	2.26	0.50
1:A:25:LEU:H	1:A:26:PRO:CD	2.25	0.50
1:A:74:MET:HE1	1:A:104:GLY:N	2.26	0.50
1:A:89:LYS:HB2	1:A:92:GLU:HB2	1.92	0.50
1:A:238:LYS:CB	1:A:239:PRO:HD2	2.39	0.50
1:A:253:PRO:O	1:A:257:SER:HB2	2.11	0.50
2:B:19:LEU:HD22	2:B:20:ILE:N	2.18	0.50
2:B:34:ILE:HD12	2:B:48:PHE:CB	2.40	0.50
2:B:69:THR:OG1	2:B:88:ASN:CB	2.59	0.50
1:A:12:VAL:HG23	1:A:13:PHE:H	1.76	0.50
1:A:65:THR:O	1:A:69:THR:HG22	2.12	0.50
1:A:308:ILE:HB	1:A:390:TYR:CD1	2.47	0.50
1:A:411:PRO:CB	1:A:428:THR:HG23	2.39	0.50
2:B:19:LEU:HD13	2:B:19:LEU:C	2.36	0.50
2:B:34:ILE:HG23	2:B:72:VAL:HG23	1.92	0.50
1:A:9:SER:HB2	1:A:443:TRP:HD1	1.75	0.50
1:A:279:TYR:HB2	1:A:362:ILE:HG23	1.92	0.50
1:A:339:VAL:CG2	1:A:370:ALA:O	2.47	0.50
1:A:397:MET:HA	1:A:400:HIS:CB	2.35	0.50
1:A:415:LEU:HD12	1:A:423:ILE:O	2.11	0.50
1:A:57:ALA:O	1:A:61:SER:HB2	2.11	0.50
1:A:137:ALA:CB	1:A:138:GLN:NE2	2.75	0.50
1:A:415:LEU:HB2	1:A:426:PHE:CD2	2.47	0.50
1:A:458:ALA:HB1	2:B:8:LEU:CD1	2.40	0.50
2:B:76:SER:O	2:B:78:TYR:O	2.30	0.50
1:A:19:LEU:O	1:A:21:THR:N	2.44	0.50
1:A:400:HIS:HD2	1:A:404:PHE:CD1	2.30	0.50
1:A:169:ILE:HD11	1:A:223:LYS:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:TYR:O	1:A:297:PRO:HB2	2.11	0.50
1:A:308:ILE:CD1	1:A:386:ALA:CB	2.90	0.50
1:A:23:LEU:HD23	1:A:25:LEU:HB2	1.93	0.50
1:A:47:GLY:C	1:A:49:GLY:H	2.20	0.50
1:A:79:PRO:O	1:A:81:ILE:N	2.45	0.50
1:A:439:VAL:CG2	1:A:440:ALA:N	2.68	0.50
1:A:100:GLY:O	1:A:104:GLY:N	2.21	0.49
1:A:335:ALA:HA	1:A:378:PHE:CD2	2.46	0.49
3:A:601:4YH:H27	3:A:601:4YH:H17	1.94	0.49
1:A:151:MET:HG2	1:A:211:TRP:CG	2.47	0.49
1:A:307:ARG:O	1:A:311:SER:OG	2.17	0.49
1:A:342:LEU:HB3	1:A:370:ALA:HB1	1.94	0.49
1:A:29:LEU:HA	1:A:32:VAL:HB	1.94	0.49
1:A:66:VAL:HA	1:A:69:THR:CG2	2.43	0.49
1:A:141:LEU:CD2	1:A:203:GLY:HA3	2.42	0.49
1:A:143:THR:O	1:A:146:ALA:N	2.44	0.49
1:A:159:TYR:C	1:A:159:TYR:HD1	2.21	0.49
1:A:321:ARG:HG2	1:A:449:SER:OG	2.13	0.49
1:A:397:MET:O	1:A:398:PHE:C	2.54	0.49
1:A:18:ARG:HE	1:A:20:LEU:HD12	1.77	0.49
1:A:31:GLN:HG3	1:A:296:ILE:HA	1.95	0.49
1:A:113:ILE:CA	1:A:116:TRP:HB3	2.41	0.49
1:A:430:LEU:HA	1:A:433:SER:HB3	1.94	0.49
1:A:61:SER:C	1:A:63:PHE:N	2.71	0.49
1:A:73:ILE:HD12	1:A:73:ILE:N	2.24	0.49
1:A:461:SER:HB3	2:B:7:LYS:HA	1.93	0.49
1:A:73:ILE:HA	1:A:251:GLY:C	2.38	0.49
1:A:104:GLY:O	1:A:153:HIS:CB	2.60	0.49
1:A:366:VAL:HA	1:A:369:PHE:CE1	2.47	0.49
2:B:18:LEU:HB2	2:B:59:ILE:CD1	2.39	0.49
2:B:28:TYR:H	2:B:30:VAL:CG2	2.25	0.49
1:A:115:MET:O	1:A:116:TRP:C	2.55	0.49
1:A:141:LEU:O	1:A:141:LEU:HD23	2.13	0.49
1:A:448:TYR:HA	1:A:451:GLU:HG2	1.95	0.49
2:B:4:VAL:CG2	2:B:5:PRO:O	2.53	0.49
1:A:397:MET:O	1:A:400:HIS:ND1	2.46	0.48
2:B:4:VAL:CB	2:B:85:ILE:HB	2.43	0.48
1:A:121:PRO:C	1:A:123:ARG:H	2.19	0.48
1:A:259:PHE:CA	1:A:262:ALA:HB3	2.23	0.48
1:A:292:ILE:CG1	1:A:293:LEU:N	2.62	0.48
1:A:353:TYR:O	1:A:354:ASN:CG	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:GLU:H	2:B:27:GLU:CD	2.21	0.48
2:B:34:ILE:HD11	2:B:48:PHE:HB3	1.94	0.48
1:A:72:GLY:HA2	1:A:258:TYR:CE1	2.48	0.48
1:A:308:ILE:CD1	1:A:386:ALA:HB1	2.43	0.48
1:A:310:PHE:C	1:A:312:LEU:H	2.21	0.48
1:A:381:CYS:C	1:A:383:ALA:N	2.70	0.48
1:A:415:LEU:HG	1:A:422:GLY:O	2.12	0.48
1:A:44:MET:HE3	1:A:206:THR:CG2	2.44	0.48
1:A:148:PRO:O	1:A:150:ALA:N	2.47	0.48
1:A:342:LEU:HD13	1:A:374:GLN:HG3	1.95	0.48
1:A:89:LYS:H	1:A:89:LYS:HD2	1.75	0.48
1:A:372:LEU:HD22	1:A:431:ILE:HG12	1.96	0.48
1:A:186:ILE:O	1:A:189:TYR:CD2	2.67	0.48
1:A:281:ALA:O	1:A:284:GLN:HG2	2.14	0.48
1:A:283:GLN:O	1:A:283:GLN:CG	2.62	0.48
1:A:294:TYR:C	1:A:294:TYR:CD2	2.91	0.48
1:A:387:LEU:C	1:A:393:THR:HB	2.38	0.48
1:A:55:ALA:CB	1:A:58:LEU:HD11	2.44	0.48
1:A:186:ILE:CA	1:A:189:TYR:HD2	2.27	0.48
1:A:318:SER:OG	1:A:321:ARG:HB3	2.14	0.48
1:A:394:LYS:HA	1:A:397:MET:CG	2.40	0.48
1:A:112:MET:HG3	1:A:146:ALA:O	2.12	0.47
1:A:216:ALA:CA	1:A:219:ILE:HG12	2.43	0.47
1:A:407:CYS:O	1:A:411:PRO:HG2	2.13	0.47
2:B:28:TYR:CA	2:B:30:VAL:HB	2.43	0.47
1:A:135:THR:CG2	1:A:142:PHE:HE1	2.27	0.47
1:A:357:PRO:HG3	3:A:601:4YH:H20	1.96	0.47
1:A:369:PHE:CE2	1:A:424:TYR:HB3	2.48	0.47
1:A:17:ILE:HG22	1:A:18:ARG:H	1.78	0.47
1:A:209:VAL:HA	1:A:212:PHE:HB3	1.96	0.47
1:A:301:GLY:C	1:A:303:ALA:N	2.69	0.47
1:A:325:GLY:O	1:A:328:LEU:HB3	2.14	0.47
1:A:356:ASP:CG	1:A:357:PRO:CD	2.86	0.47
1:A:78:ASN:CA	1:A:163:LEU:HD21	2.39	0.47
1:A:105:LEU:O	1:A:107:LEU:N	2.48	0.47
1:A:284:GLN:NE2	3:A:601:4YH:H8	2.30	0.47
1:A:391:LYS:C	1:A:393:THR:H	2.23	0.47
1:A:105:LEU:O	1:A:106:ILE:C	2.57	0.47
1:A:111:GLY:C	1:A:113:ILE:N	2.71	0.47
1:A:115:MET:HE1	1:A:146:ALA:HB2	1.96	0.47
1:A:135:THR:HA	1:A:138:GLN:CG	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:MET:H	1:A:195:PRO:HD3	1.79	0.47
1:A:428:THR:C	1:A:430:LEU:N	2.72	0.47
1:A:396:PRO:HA	1:A:399:ILE:CG1	2.28	0.47
1:A:437:ALA:C	1:A:439:VAL:N	2.73	0.47
2:B:7:LYS:CG	2:B:8:LEU:H	2.27	0.47
1:A:56:VAL:C	1:A:58:LEU:N	2.71	0.47
1:A:89:LYS:CB	1:A:92:GLU:HB3	2.45	0.47
1:A:394:LYS:HA	1:A:397:MET:HB2	1.97	0.47
2:B:22:TRP:CH2	2:B:87:ILE:HB	2.50	0.47
2:B:77:TYR:CE2	2:B:82:TYR:OH	2.68	0.47
1:A:120:THR:C	1:A:122:PHE:H	2.16	0.46
1:A:317:PHE:HB3	1:A:452:LEU:HG	1.96	0.46
1:A:451:GLU:C	1:A:453:VAL:H	2.23	0.46
3:A:601:4YH:H17	3:A:601:4YH:C16	2.44	0.46
2:B:11:VAL:HB	2:B:19:LEU:HD12	1.98	0.46
1:A:15:LYS:HZ1	1:A:446:GLU:CD	2.23	0.46
1:A:98:ARG:HB3	1:A:229:PRO:HD2	1.96	0.46
1:A:397:MET:CB	1:A:400:HIS:ND1	2.76	0.46
1:A:225:LYS:HD2	1:A:226:PHE:N	2.29	0.46
1:A:308:ILE:CD1	1:A:386:ALA:CA	2.93	0.46
2:B:11:VAL:H	2:B:19:LEU:CD1	2.23	0.46
2:B:35:THR:HG23	2:B:71:THR:HB	1.97	0.46
2:B:38:GLU:CB	2:B:67:ASP:O	2.64	0.46
2:B:35:THR:HG23	2:B:73:TYR:CE1	2.40	0.46
1:A:56:VAL:C	1:A:58:LEU:H	2.23	0.46
1:A:111:GLY:O	1:A:114:LEU:N	2.45	0.46
1:A:136:MET:HE2	1:A:136:MET:H	1.80	0.46
2:B:22:TRP:HH2	2:B:87:ILE:HB	1.81	0.46
1:A:193:GLY:N	1:A:194:MET:HA	2.29	0.46
2:B:36:TYR:HB2	2:B:46:GLN:O	2.15	0.46
2:B:65:GLY:HA2	2:B:91:THR:OG1	2.15	0.46
1:A:124:ASN:N	1:A:127:THR:OG1	2.28	0.46
2:B:19:LEU:O	2:B:20:ILE:HD13	2.15	0.46
1:A:317:PHE:O	1:A:319:ARG:N	2.49	0.46
2:B:4:VAL:CA	2:B:5:PRO:O	2.64	0.46
1:A:94:GLY:HA2	1:A:227:PHE:CE2	2.50	0.46
1:A:429:ALA:HA	1:A:432:ALA:HB3	1.98	0.46
2:B:31:TYR:O	2:B:32:TYR:CD2	2.69	0.46
2:B:75:ARG:NH1	2:B:75:ARG:CG	2.74	0.46
1:A:51:GLU:HB3	1:A:54:ALA:HB2	1.97	0.45
1:A:69:THR:O	1:A:72:GLY:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LYS:HB3	1:A:225:LYS:HE3	1.63	0.45
1:A:396:PRO:O	1:A:400:HIS:N	2.49	0.45
2:B:78:TYR:C	2:B:80:GLY:N	2.67	0.45
1:A:90:THR:HG1	1:A:225:LYS:HZ1	1.62	0.45
1:A:246:GLN:C	1:A:248:TRP:H	2.23	0.45
1:A:31:GLN:HE22	1:A:300:VAL:CA	2.29	0.45
1:A:88:GLY:H	1:A:89:LYS:HD3	1.81	0.45
1:A:112:MET:O	1:A:116:TRP:CB	2.64	0.45
1:A:141:LEU:HD21	1:A:203:GLY:CA	2.46	0.45
1:A:356:ASP:CB	1:A:357:PRO:HD3	2.45	0.45
1:A:439:VAL:C	1:A:443:TRP:HB3	2.42	0.45
2:B:69:THR:HA	2:B:88:ASN:HA	1.97	0.45
1:A:14:LEU:HA	1:A:16:GLU:HG3	1.98	0.45
1:A:349:LEU:HD12	1:A:360:LEU:HD23	1.99	0.45
1:A:74:MET:HG3	1:A:153:HIS:ND1	2.31	0.45
1:A:95:GLU:O	1:A:98:ARG:HG2	2.16	0.45
1:A:115:MET:O	1:A:117:ALA:N	2.50	0.45
1:A:186:ILE:CG2	1:A:191:LYS:HD2	2.47	0.45
1:A:298:GLN:HA	1:A:382:ILE:HG21	1.98	0.45
1:A:340:LEU:C	1:A:342:LEU:H	2.24	0.45
1:A:27:MET:HB3	1:A:300:VAL:CG2	2.47	0.45
1:A:55:ALA:HB3	1:A:58:LEU:HD11	1.98	0.45
1:A:181:VAL:N	1:A:182:PRO:HD2	2.31	0.45
1:A:184:ASN:HD21	1:A:205:ALA:HB1	1.77	0.45
1:A:285:VAL:O	1:A:289:LEU:HB2	2.16	0.45
1:A:251:GLY:O	1:A:254:ILE:CG2	2.59	0.45
1:A:310:PHE:C	1:A:312:LEU:N	2.75	0.45
1:A:457:LYS:O	1:A:458:ALA:HB2	2.16	0.45
1:A:95:GLU:C	1:A:98:ARG:HG2	2.41	0.45
1:A:118:ALA:O	1:A:121:PRO:HD2	2.17	0.45
1:A:141:LEU:CD2	1:A:200:ALA:O	2.65	0.45
1:A:321:ARG:HA	1:A:390:TYR:HE1	1.81	0.45
1:A:397:MET:C	1:A:400:HIS:H	2.24	0.45
1:A:120:THR:C	1:A:122:PHE:N	2.74	0.45
1:A:201:GLY:HA2	1:A:204:VAL:HB	1.98	0.45
1:A:315:ARG:HG3	1:A:317:PHE:HE1	1.80	0.45
1:A:459:VAL:HG23	1:A:460:SER:OG	2.16	0.45
1:A:63:PHE:HD1	1:A:115:MET:SD	2.39	0.44
1:A:72:GLY:HA2	1:A:258:TYR:HE1	1.83	0.44
1:A:81:ILE:O	1:A:81:ILE:CG2	2.64	0.44
1:A:377:ASP:O	1:A:379:THR:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:GLY:O	1:A:157:HIS:NE2	2.51	0.44
1:A:151:MET:O	1:A:151:MET:HG3	2.17	0.44
1:A:279:TYR:HB3	1:A:362:ILE:HG12	1.99	0.44
1:A:373:PHE:HA	1:A:434:LEU:HD21	2.00	0.44
1:A:98:ARG:HD3	1:A:229:PRO:HB2	2.00	0.44
1:A:168:LEU:HA	1:A:171:LEU:HD12	2.00	0.44
1:A:40:VAL:O	1:A:42:THR:N	2.51	0.44
1:A:59:GLY:C	1:A:61:SER:N	2.72	0.44
1:A:141:LEU:HD23	1:A:145:LEU:HB2	2.00	0.44
1:A:338:THR:C	1:A:342:LEU:HG	2.42	0.44
1:A:373:PHE:HB2	1:A:434:LEU:HD11	1.97	0.44
1:A:138:GLN:O	1:A:141:LEU:C	2.61	0.44
1:A:313:GLY:C	1:A:315:ARG:N	2.76	0.44
2:B:30:VAL:HG11	2:B:51:PRO:O	2.15	0.44
2:B:59:ILE:HD12	2:B:61:GLY:N	2.33	0.44
1:A:105:LEU:O	1:A:108:GLY:N	2.51	0.44
1:A:151:MET:O	1:A:151:MET:CG	2.65	0.44
1:A:248:TRP:CZ3	1:A:252:ALA:CB	2.86	0.44
1:A:272:ILE:HA	1:A:280:VAL:HG12	2.00	0.44
2:B:34:ILE:CD1	2:B:48:PHE:HB3	2.48	0.44
1:A:44:MET:HE2	1:A:181:VAL:CB	2.48	0.44
1:A:77:LEU:O	1:A:163:LEU:CD1	2.64	0.44
1:A:111:GLY:O	1:A:113:ILE:N	2.50	0.43
1:A:264:ALA:C	1:A:268:ILE:HG12	2.41	0.43
1:A:414:LEU:HD12	1:A:414:LEU:HA	1.72	0.43
1:A:78:ASN:N	1:A:79:PRO:HD2	2.34	0.43
1:A:120:THR:CB	1:A:121:PRO:HD2	2.49	0.43
2:B:25:ARG:O	2:B:25:ARG:NH1	2.49	0.43
1:A:112:MET:O	1:A:116:TRP:N	2.42	0.43
1:A:285:VAL:HG11	1:A:348:PRO:HB2	1.99	0.43
1:A:136:MET:O	1:A:139:TYR:HD2	1.99	0.43
1:A:268:ILE:HB	1:A:287:ILE:HD12	2.00	0.43
1:A:457:LYS:O	1:A:458:ALA:CB	2.66	0.43
2:B:18:LEU:N	2:B:59:ILE:HD11	2.33	0.43
2:B:7:LYS:CG	2:B:8:LEU:N	2.82	0.43
1:A:143:THR:O	1:A:144:SER:C	2.60	0.43
1:A:384:SER:C	1:A:386:ALA:N	2.71	0.43
1:A:115:MET:HE2	1:A:119:ILE:HD11	2.01	0.43
1:A:78:ASN:N	1:A:79:PRO:CD	2.82	0.43
1:A:82:ALA:O	1:A:85:TYR:N	2.42	0.43
1:A:15:LYS:NZ	1:A:15:LYS:CB	2.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:SER:O	2:B:62:LEU:HD22	2.19	0.42
1:A:77:LEU:HD12	1:A:77:LEU:N	2.34	0.42
1:A:217:LEU:O	1:A:219:ILE:N	2.52	0.42
1:A:224:GLU:CD	1:A:225:LYS:H	2.27	0.42
1:A:91:GLY:O	1:A:95:GLU:N	2.45	0.42
1:A:364:SER:C	1:A:366:VAL:H	2.27	0.42
1:A:58:LEU:H	1:A:58:LEU:HG	1.58	0.42
1:A:156:LEU:C	1:A:158:ALA:N	2.76	0.42
1:A:169:ILE:HD13	1:A:220:TYR:HB3	2.02	0.42
1:A:235:LYS:HB2	1:A:241:TRP:CB	2.48	0.42
1:A:242:ALA:HA	1:A:245:LYS:HB3	2.00	0.42
1:A:397:MET:CA	1:A:400:HIS:ND1	2.81	0.42
1:A:426:PHE:HD2	1:A:426:PHE:H	1.67	0.42
1:A:428:THR:OG1	1:A:429:ALA:N	2.53	0.42
2:B:22:TRP:N	2:B:22:TRP:CD1	2.87	0.42
2:B:51:PRO:HD2	2:B:54:SER:OG	2.20	0.42
1:A:98:ARG:CG	1:A:99:GLN:N	2.83	0.42
1:A:242:ALA:C	1:A:244:PHE:N	2.75	0.42
3:A:601:4YH:H31	3:A:601:4YH:H38	1.74	0.42
1:A:132:VAL:O	1:A:136:MET:HB2	2.19	0.42
1:A:282:ALA:C	1:A:284:GLN:H	2.26	0.42
1:A:308:ILE:HG13	1:A:309:GLY:H	1.85	0.42
1:A:430:LEU:HA	1:A:433:SER:CB	2.50	0.42
1:A:68:ILE:HA	1:A:68:ILE:HD13	1.75	0.42
1:A:79:PRO:HG2	1:A:80:MET:H	1.85	0.42
1:A:151:MET:HG2	1:A:211:TRP:HA	2.00	0.42
1:A:304:GLY:O	1:A:306:VAL:N	2.53	0.42
1:A:447:LYS:HD2	1:A:448:TYR:CD1	2.55	0.42
1:A:141:LEU:HD21	1:A:200:ALA:O	2.19	0.42
1:A:241:TRP:O	1:A:244:PHE:HB3	2.19	0.42
1:A:347:SER:N	1:A:348:PRO:CD	2.83	0.42
1:A:304:GLY:O	1:A:307:ARG:N	2.53	0.42
2:B:35:THR:N	2:B:71:THR:O	2.52	0.42
2:B:64:PRO:HB2	2:B:65:GLY:H	1.61	0.42
1:A:40:VAL:HG22	1:A:181:VAL:CG2	2.46	0.41
1:A:96:THR:HG23	1:A:243:VAL:HB	2.01	0.41
1:A:418:ARG:HG3	1:A:419:PHE:H	1.85	0.41
2:B:69:THR:OG1	2:B:88:ASN:HB3	2.20	0.41
1:A:29:LEU:HB3	1:A:171:LEU:HD11	2.02	0.41
1:A:410:LEU:HG	1:A:414:LEU:HD13	2.01	0.41
2:B:7:LYS:CB	2:B:23:ASP:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLU:HA	1:A:98:ARG:CD	2.50	0.41
1:A:172:VAL:C	1:A:174:PHE:H	2.29	0.41
1:A:412:GLY:HA2	1:A:426:PHE:HD1	1.85	0.41
1:A:456:HIS:CD2	1:A:459:VAL:HA	2.55	0.41
2:B:19:LEU:HD13	2:B:21:SER:H	1.84	0.41
1:A:98:ARG:HG3	1:A:99:GLN:N	2.36	0.41
1:A:139:TYR:O	1:A:142:PHE:HB2	2.20	0.41
1:A:397:MET:C	1:A:399:ILE:N	2.76	0.41
2:B:31:TYR:CD1	2:B:75:ARG:NH1	2.78	0.41
2:B:75:ARG:HG3	2:B:76:SER:N	2.34	0.41
1:A:105:LEU:HA	1:A:105:LEU:HD23	1.60	0.41
2:B:32:TYR:CD2	2:B:32:TYR:N	2.87	0.41
1:A:15:LYS:NZ	1:A:446:GLU:OE1	2.54	0.41
1:A:391:LYS:HZ3	1:A:448:TYR:HD2	1.69	0.41
1:A:27:MET:HE2	1:A:27:MET:H	1.85	0.41
1:A:106:ILE:HG22	1:A:107:LEU:N	2.36	0.41
1:A:128:LEU:CD2	1:A:128:LEU:H	2.34	0.41
1:A:211:TRP:CD1	1:A:211:TRP:N	2.88	0.41
1:A:318:SER:HA	1:A:321:ARG:N	2.26	0.41
1:A:103:PHE:CE1	1:A:107:LEU:HD11	2.56	0.41
1:A:322:TYR:CZ	1:A:446:GLU:OE2	2.74	0.41
1:A:366:VAL:C	1:A:368:LEU:N	2.74	0.41
1:A:428:THR:O	1:A:430:LEU:N	2.47	0.41
1:A:19:LEU:HB2	1:A:326:VAL:HG21	2.03	0.41
1:A:29:LEU:HD23	1:A:32:VAL:HG21	2.03	0.41
1:A:247:ILE:O	1:A:247:ILE:CG2	2.69	0.41
1:A:251:GLY:O	1:A:252:ALA:C	2.64	0.41
1:A:254:ILE:N	1:A:394:LYS:HD3	2.36	0.41
1:A:295:MET:O	1:A:296:ILE:C	2.64	0.41
1:A:339:VAL:CG2	1:A:371:GLY:HA2	2.51	0.41
1:A:379:THR:O	1:A:382:ILE:HG12	2.21	0.41
1:A:433:SER:O	1:A:436:ILE:HG13	2.21	0.41
1:A:25:LEU:H	1:A:26:PRO:HD2	1.85	0.41
2:B:7:LYS:HE2	2:B:23:ASP:N	2.36	0.41
1:A:44:MET:HE3	1:A:206:THR:HG23	2.02	0.40
1:A:103:PHE:CE2	1:A:107:LEU:HD21	2.56	0.40
1:A:168:LEU:O	1:A:172:VAL:HG23	2.21	0.40
1:A:182:PRO:O	1:A:183:LEU:C	2.63	0.40
1:A:297:PRO:HB3	1:A:378:PHE:CE2	2.56	0.40
1:A:337:ILE:HG13	1:A:338:THR:N	2.36	0.40
1:A:411:PRO:O	1:A:426:PHE:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:THR:HG23	1:A:138:GLN:HB2	2.02	0.40
1:A:182:PRO:O	1:A:185:TYR:HD2	2.03	0.40
1:A:387:LEU:CD2	1:A:445:LEU:HD13	2.51	0.40
1:A:44:MET:HE2	1:A:181:VAL:HG12	2.03	0.40
1:A:291:GLY:O	1:A:294:TYR:HB3	2.21	0.40
1:A:397:MET:N	1:A:397:MET:SD	2.94	0.40
1:A:418:ARG:CG	1:A:422:GLY:HA3	2.44	0.40
1:A:27:MET:SD	1:A:303:ALA:O	2.79	0.40
1:A:57:ALA:O	1:A:61:SER:CB	2.69	0.40
1:A:72:GLY:O	1:A:73:ILE:C	2.65	0.40
1:A:122:PHE:O	1:A:123:ARG:HG3	2.21	0.40
1:A:254:ILE:HB	1:A:394:LYS:CD	2.51	0.40
1:A:365:THR:C	1:A:368:LEU:HG	2.47	0.40
1:A:427:TRP:HB3	1:A:431:ILE:HG23	2.03	0.40
1:A:65:THR:HG22	1:A:66:VAL:HG13	2.03	0.40
1:A:369:PHE:C	1:A:371:GLY:N	2.74	0.40
1:A:414:LEU:HD12	1:A:417:TYR:HB3	2.02	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:A:196:ALA:N	2:B:31:TYR:OH[5_545]	2.13	0.07

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	457/459 (100%)	258 (56%)	117 (26%)	82 (18%)	0	0
2	B	89/99 (90%)	55 (62%)	21 (24%)	13 (15%)	0	0
All	All	546/558 (98%)	313 (57%)	138 (25%)	95 (17%)	0	0

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	PHE
1	A	20	LEU
1	A	80	MET
1	A	106	ILE
1	A	119	ILE
1	A	135	THR
1	A	145	LEU
1	A	163	LEU
1	A	164	ASN
1	A	191	LYS
1	A	229	PRO
1	A	232	LEU
1	A	238	LYS
1	A	247	ILE
1	A	263	SER
1	A	278	ASP
1	A	297	PRO
1	A	305	THR
1	A	357	PRO
1	A	372	LEU
1	A	386	ALA
1	A	417	TYR
1	A	440	ALA
1	A	458	ALA
2	B	5	PRO
2	B	12	ALA
2	B	15	PRO
2	B	51	PRO
2	B	64	PRO
2	B	79	TRP
1	A	12	VAL
1	A	14	LEU
1	A	17	ILE
1	A	57	ALA
1	A	61	SER
1	A	62	ALA
1	A	73	ILE
1	A	79	PRO
1	A	112	MET
1	A	116	TRP
1	A	121	PRO
1	A	192	PHE

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Mol	Chain	Res	Type
1	A	196	ALA
1	A	201	GLY
1	A	244	PHE
1	A	274	PRO
1	A	307	ARG
1	A	318	SER
1	A	319	ARG
1	A	324	SER
1	A	378	PHE
1	A	427	TRP
1	A	428	THR
1	A	47	GLY
1	A	69	THR
1	A	75	ALA
1	A	88	GLY
1	A	104	GLY
1	A	115	MET
1	A	118	ALA
1	A	165	ARG
1	A	182	PRO
1	A	217	LEU
1	A	236	PHE
1	A	270	PHE
1	A	352	MET
1	A	385	TYR
2	B	56	THR
1	A	41	ASP
1	A	105	LEU
1	A	166	PRO
1	A	260	LEU
1	A	354	ASN
2	B	44	PRO
1	A	25	LEU
1	A	183	LEU
1	A	218	TRP
1	A	230	PHE
1	A	237	GLY
1	A	411	PRO
1	A	429	ALA
2	B	38	GLU
1	A	60	SER
1	A	87	ALA

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Mol	Chain	Res	Type
1	A	194	MET
2	B	77	TYR
2	B	82	TYR
1	A	439	VAL
1	A	453	VAL
2	B	29	VAL
1	A	252	ALA
1	A	396	PRO
2	B	59	ILE
1	A	286	GLY
1	A	147	MET

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	353/353 (100%)	251 (71%)	102 (29%)	0	2
2	B	78/85 (92%)	58 (74%)	20 (26%)	0	3
All	All	431/438 (98%)	309 (72%)	122 (28%)	0	2

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	14	LEU
1	A	15	LYS
1	A	17	ILE
1	A	18	ARG
1	A	19	LEU
1	A	23	LEU
1	A	27	MET
1	A	34	GLN
1	A	37	ILE
1	A	56	VAL
1	A	60	SER

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Mol	Chain	Res	Type
1	A	67	TYR
1	A	68	ILE
1	A	73	ILE
1	A	80	MET
1	A	81	ILE
1	A	89	LYS
1	A	95	GLU
1	A	96	THR
1	A	102	TRP
1	A	103	PHE
1	A	109	ILE
1	A	112	MET
1	A	113	ILE
1	A	120	THR
1	A	126	LEU
1	A	128	LEU
1	A	129	SER
1	A	132	VAL
1	A	136	MET
1	A	139	TYR
1	A	144	SER
1	A	156	LEU
1	A	159	TYR
1	A	167	ARG
1	A	178	VAL
1	A	179	LEU
1	A	181	VAL
1	A	183	LEU
1	A	185	TYR
1	A	186	ILE
1	A	188	VAL
1	A	191	LYS
1	A	192	PHE
1	A	194	MET
1	A	202	CYS
1	A	204	VAL
1	A	207	MET
1	A	217	LEU
1	A	218	TRP
1	A	224	GLU
1	A	225	LYS
1	A	228	ARG

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Mol	Chain	Res	Type
1	A	232	LEU
1	A	233	THR
1	A	236	PHE
1	A	238	LYS
1	A	248	TRP
1	A	250	ILE
1	A	256	LEU
1	A	259	PHE
1	A	261	GLU
1	A	265	PHE
1	A	283	GLN
1	A	285	VAL
1	A	290	SER
1	A	292	ILE
1	A	293	LEU
1	A	302	SER
1	A	308	ILE
1	A	312	LEU
1	A	318	SER
1	A	326	VAL
1	A	332	TRP
1	A	334	LEU
1	A	336	VAL
1	A	338	THR
1	A	364	SER
1	A	368	LEU
1	A	369	PHE
1	A	374	GLN
1	A	378	PHE
1	A	381	CYS
1	A	390	TYR
1	A	394	LYS
1	A	395	VAL
1	A	397	MET
1	A	399	ILE
1	A	407	CYS
1	A	413	TYR
1	A	417	TYR
1	A	420	ASP
1	A	421	MET
1	A	428	THR
1	A	431	ILE

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Mol	Chain	Res	Type
1	A	434	LEU
1	A	435	THR
1	A	452	LEU
1	A	453	VAL
1	A	454	LYS
1	A	463	LEU
2	B	11	VAL
2	B	18	LEU
2	B	19	LEU
2	B	20	ILE
2	B	25	ARG
2	B	27	GLU
2	B	29	VAL
2	B	30	VAL
2	B	31	TYR
2	B	34	ILE
2	B	38	GLU
2	B	39	THR
2	B	50	VAL
2	B	62	LEU
2	B	70	ILE
2	B	75	ARG
2	B	85	ILE
2	B	87	ILE
2	B	90	ARG
2	B	91	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	184	ASN
1	A	284	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	4YH	A	601	-	33,34,34	1.72	3 (9%)	36,46,46	1.86	7 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	4YH	A	601	-	-	19/32/35/35	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	4YH	C1-C2	-6.84	1.40	1.53
3	A	601	4YH	C3-N4	4.17	1.20	1.14
3	A	601	4YH	C21-C17	-3.75	1.41	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	4YH	C1-C3-N4	-6.81	166.22	177.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	4YH	C31-O20-C7	-5.54	109.38	117.51
3	A	601	4YH	C30-O19-C6	-3.34	112.62	117.51
3	A	601	4YH	O20-C7-C10	2.35	118.58	115.40
3	A	601	4YH	O24-C10-C7	2.28	118.49	115.40
3	A	601	4YH	O20-C7-C12	-2.27	120.17	124.08
3	A	601	4YH	C32-O23-C9	-2.23	114.24	117.51

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	4YH	C3-C1-C2-C5
3	A	601	4YH	C3-C1-C2-C11
3	A	601	4YH	C2-C1-C15-C29
3	A	601	4YH	C2-C1-C15-C28
3	A	601	4YH	C3-C1-C15-C29
3	A	601	4YH	C3-C1-C15-C28
3	A	601	4YH	C22-C1-C15-C29
3	A	601	4YH	C22-C1-C15-C28
3	A	601	4YH	C2-C1-C22-C26
3	A	601	4YH	C6-C9-O23-C32
3	A	601	4YH	C7-C10-O24-C33
3	A	601	4YH	C9-C6-O19-C30
3	A	601	4YH	C13-C9-O23-C32
3	A	601	4YH	C5-C6-O19-C30
3	A	601	4YH	C14-C10-O24-C33
3	A	601	4YH	N8-C16-C21-C17
3	A	601	4YH	C21-C16-N8-C25
3	A	601	4YH	C15-C1-C22-C26
3	A	601	4YH	C10-C7-O20-C31

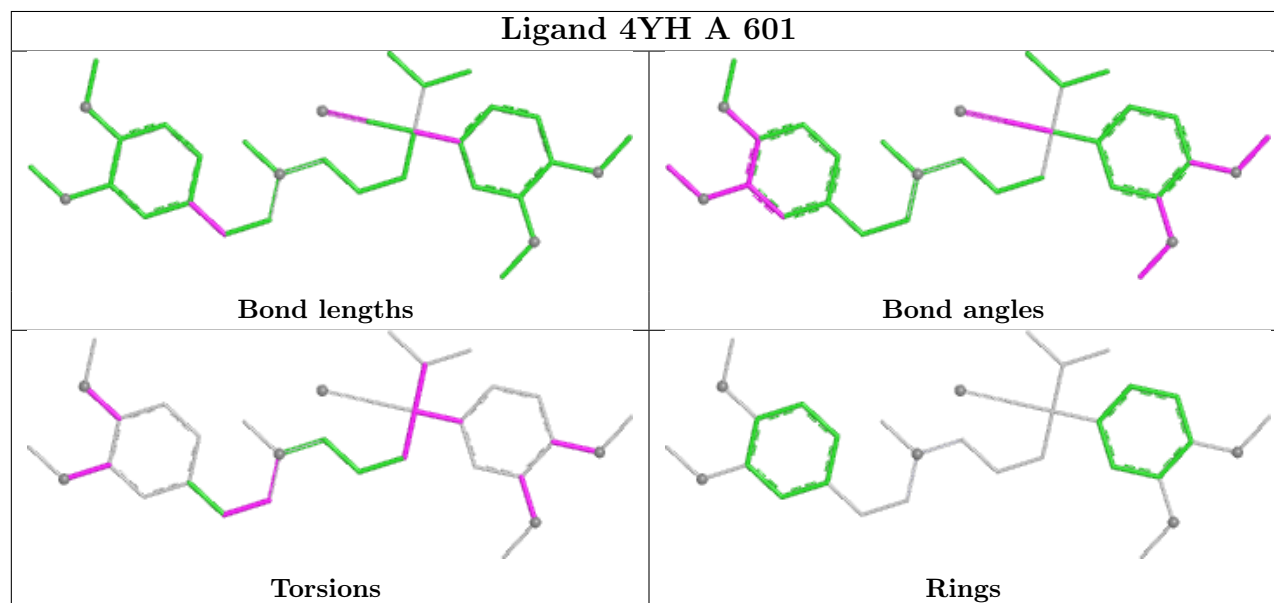
There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	4YH	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	459/459 (100%)	0.30	32 (6%)	22 12	51, 148, 322, 413	0
2	B	91/99 (91%)	0.46	8 (8%)	15 8	49, 116, 219, 349	0
All	All	550/558 (98%)	0.33	40 (7%)	21 11	49, 144, 309, 413	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2	SER	7.7
1	A	278	ASP	6.0
1	A	135	THR	5.4
1	A	9	SER	4.7
1	A	424	TYR	4.4
2	B	89	TYR	3.9
2	B	91	THR	3.9
1	A	139	TYR	3.6
1	A	456	HIS	3.5
2	B	1	VAL	3.5
1	A	273	ALA	3.5
1	A	302	SER	3.3
1	A	326	VAL	3.3
1	A	140	MET	3.3
1	A	271	LEU	3.0
2	B	90	ARG	2.9
1	A	405	TRP	2.8
1	A	239	PRO	2.7
1	A	319	ARG	2.7
1	A	358	ALA	2.7
1	A	404	PHE	2.7
1	A	154	ARG	2.7
1	A	385	TYR	2.6
1	A	356	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	377	ASP	2.6
1	A	192	PHE	2.5
1	A	285	VAL	2.5
2	B	77	TYR	2.4
1	A	421	MET	2.4
1	A	42	THR	2.3
1	A	44	MET	2.3
2	B	78	TYR	2.3
1	A	22	ALA	2.3
1	A	51	GLU	2.3
1	A	416	ALA	2.3
1	A	398	PHE	2.3
1	A	296	ILE	2.2
1	A	341	SER	2.2
2	B	24	ALA	2.1
1	A	145	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

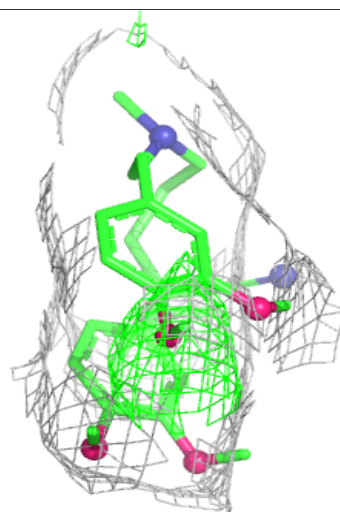
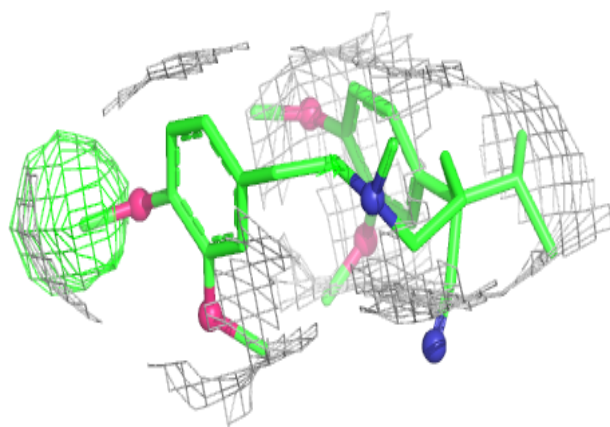
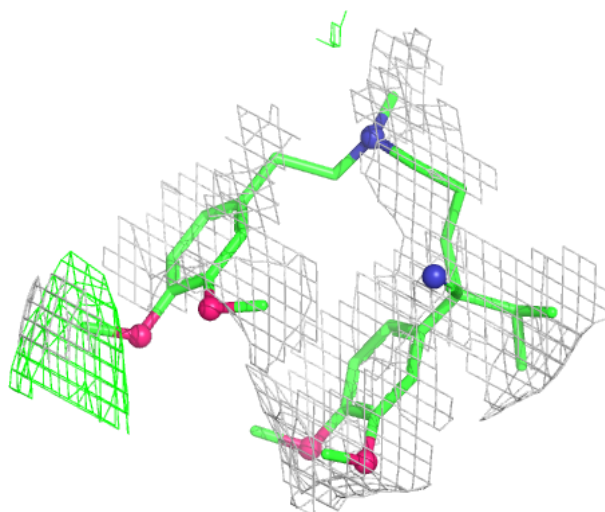
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	4YH	A	601	33/33	0.84	0.11	118,228,282,314	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 4YH A 601:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.