



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:51 PM UTC

PDB ID : 3CKR / pdb_00003ckr
Title : Crystal structure of BACE-1 in complex with inhibitor
Authors : Min, K.
Deposited on : 2008-03-16
Resolution : 2.70 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

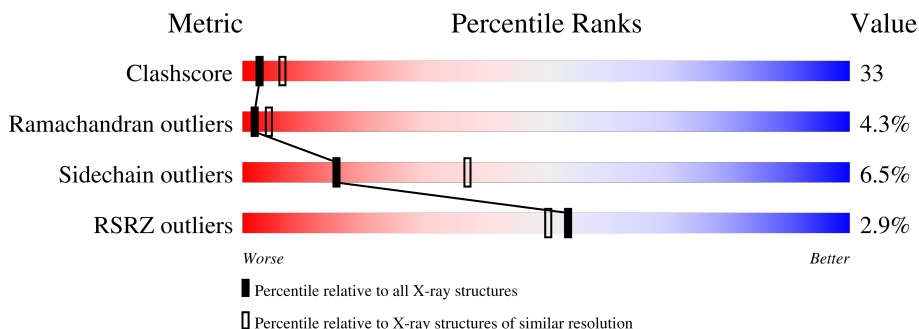
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	412	
1	B	412	
1	C	412	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9135 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.

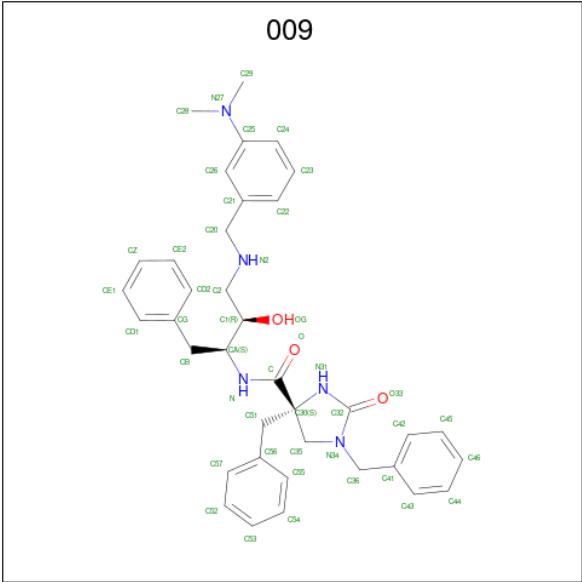
- Molecule 1 is a protein called Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	0	0
			2974	1904	496	560	14			
1	B	377	Total	C	N	O	S	0	0	0
			2968	1901	493	560	14			
1	C	377	Total	C	N	O	S	0	0	0
			2967	1900	494	559	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LYS	ARG	engineered mutation	UNP P56817
A	-5	LYS	ARG	engineered mutation	UNP P56817
B	-6	LYS	ARG	engineered mutation	UNP P56817
B	-5	LYS	ARG	engineered mutation	UNP P56817
C	-6	LYS	ARG	engineered mutation	UNP P56817
C	-5	LYS	ARG	engineered mutation	UNP P56817

- Molecule 2 is (4S)-1,4-dibenzyl-N-[(1S,2R)-1-benzyl-3-{[3-(dimethylamino)benzyl]amino}-2-hydroxypropyl]-2-oxoimidazolidine-4-carboxamide (CCD ID: 009) (formula: C₃₇H₄₃N₅O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			45	37	5	3		
2	B	1	Total	C	N	O	0	0
			45	37	5	3		
2	C	1	Total	C	N	O	0	0
			45	37	5	3		

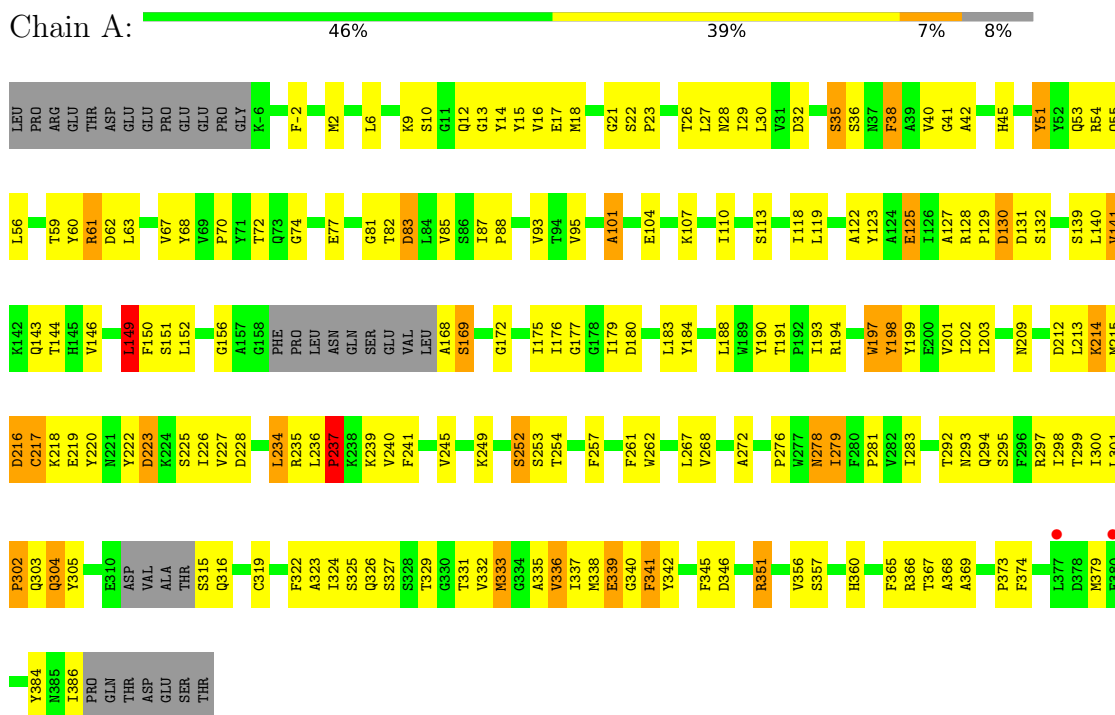
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total	O	0	0
			38	38		
3	B	35	Total	O	0	0
			35	35		
3	C	18	Total	O	0	0
			18	18		

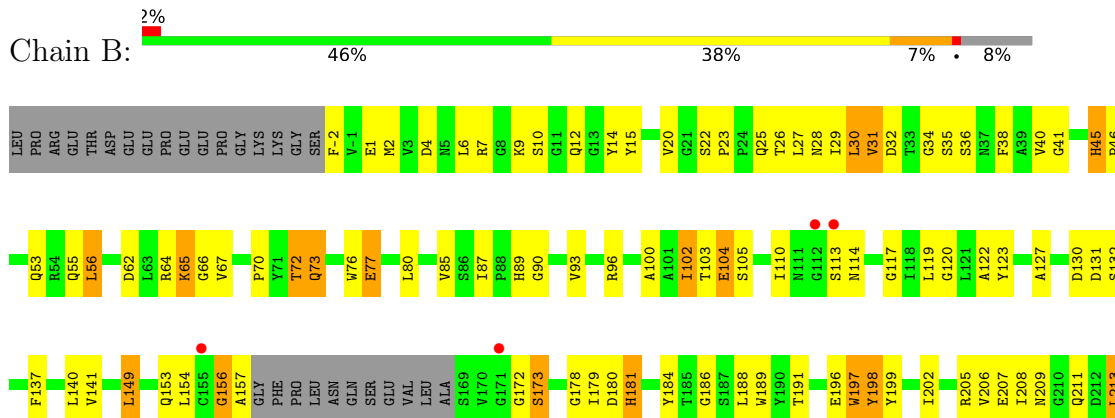
3 Residue-property plots

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: Beta-secretase 1



- Molecule 1: Beta-secretase 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	224.46Å 108.13Å 61.13Å 90.00° 100.87° 90.00°	Depositor
Resolution (Å)	19.96 – 2.70 19.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	84.2 (19.96-2.70) 84.9 (19.96-2.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.71Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.251 , 0.257 0.267 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	43.5	Xtriage
Anisotropy	0.911	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.1	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	0.92	EDS
Total number of atoms	9135	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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:
009

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	0.55	0/3048	1.08	22/4138 (0.5%)
1	B	0.55	0/3043	1.11	22/4136 (0.5%)
1	C	0.50	0/3041	1.05	25/4129 (0.6%)
All	All	0.54	0/9132	1.08	69/12403 (0.6%)

There are no bond length outliers.

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	198	TYR	N-CA-C	-10.07	95.45	109.95
1	A	213	LEU	N-CA-C	-7.94	102.22	112.23
1	B	199	TYR	N-CA-C	-7.88	98.60	109.71
1	A	198	TYR	N-CA-C	-7.79	98.40	110.17
1	B	87	ILE	CA-C-N	7.65	129.40	119.84
1	B	87	ILE	C-N-CA	7.65	129.40	119.84
1	B	38	PHE	N-CA-C	-7.52	97.00	108.96
1	C	198	TYR	N-CA-C	-7.48	97.98	109.65
1	C	-1	VAL	N-CA-C	7.01	120.85	111.17
1	B	45	HIS	CA-C-N	6.92	127.50	119.47
1	B	45	HIS	C-N-CA	6.92	127.50	119.47
1	B	233	ASN	N-CA-C	6.64	119.10	110.53
1	C	216	ASP	N-CA-C	-6.57	100.10	109.96
1	C	38	PHE	N-CA-C	-6.48	99.96	110.20
1	C	246	LYS	N-CA-C	-6.46	102.91	111.24
1	B	311	ASP	N-CA-C	6.41	124.45	110.80
1	B	342	TYR	N-CA-C	-6.21	97.00	107.99
1	C	13	GLY	N-CA-C	6.04	122.28	112.61
1	A	197	TRP	N-CA-C	-6.00	102.39	111.34
1	A	51	TYR	N-CA-C	5.98	116.99	108.74
1	B	275	THR	CA-C-N	5.97	127.30	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	275	THR	C-N-CA	5.97	127.30	119.84
1	A	38	PHE	N-CA-C	-5.97	99.01	108.73
1	C	233	ASN	N-CA-C	5.92	118.52	110.35
1	A	351	ARG	N-CA-C	5.86	116.29	108.38
1	B	31	VAL	N-CA-C	5.86	115.04	106.55
1	B	173	SER	N-CA-C	5.83	118.26	109.23
1	C	124	ALA	N-CA-C	5.82	117.31	110.97
1	A	341	PHE	N-CA-C	5.78	118.20	109.41
1	B	278	ASN	N-CA-C	5.74	119.54	112.54
1	C	365	PHE	N-CA-C	5.68	120.34	113.41
1	A	279	ILE	N-CA-C	-5.66	106.80	113.42
1	A	227	VAL	N-CA-C	-5.62	99.78	107.99
1	A	302	PRO	N-CA-C	-5.60	105.74	113.53
1	B	202	ILE	N-CA-C	5.60	115.93	107.75
1	A	214	LYS	N-CA-C	5.59	117.46	110.91
1	A	87	ILE	CA-C-N	5.55	126.78	119.84
1	A	87	ILE	C-N-CA	5.55	126.78	119.84
1	A	13	GLY	N-CA-C	5.55	121.03	112.81
1	B	102	ILE	N-CA-C	5.54	116.75	109.21
1	A	365	PHE	N-CA-C	5.53	120.16	113.41
1	C	90	GLY	N-CA-C	-5.53	101.06	112.34
1	C	275	THR	CA-C-N	5.53	126.75	119.84
1	C	275	THR	C-N-CA	5.53	126.75	119.84
1	C	228	ASP	N-CA-C	5.52	119.24	107.70
1	C	360	HIS	N-CA-C	5.47	117.80	110.35
1	A	40	VAL	N-CA-C	5.42	117.59	108.81
1	B	246	LYS	N-CA-C	-5.41	105.07	110.97
1	C	331	THR	N-CA-C	5.40	117.53	108.73
1	C	15	TYR	N-CA-C	5.38	117.17	108.41
1	B	369	ALA	N-CA-C	5.37	117.01	108.79
1	A	141	VAL	N-CA-C	5.30	115.96	110.82
1	A	184	TYR	N-CA-C	5.29	117.46	109.41
1	A	45	HIS	CA-C-N	5.29	126.45	119.84
1	A	45	HIS	C-N-CA	5.29	126.45	119.84
1	C	223	ASP	N-CA-C	-5.26	99.60	110.80
1	B	343	VAL	N-CA-C	5.26	115.34	107.51
1	C	328	SER	N-CA-C	-5.26	106.77	114.39
1	C	191	THR	N-CA-C	-5.20	102.97	110.40
1	B	341	PHE	N-CA-C	5.20	116.88	109.14
1	C	87	ILE	CA-C-N	5.18	126.32	119.84
1	C	87	ILE	C-N-CA	5.18	126.32	119.84
1	C	191	THR	CA-C-N	-5.18	115.23	120.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	191	THR	C-N-CA	-5.18	115.23	120.31
1	A	101	ALA	N-CA-C	-5.18	100.64	108.67
1	C	278	ASN	N-CA-C	5.17	118.36	111.75
1	A	216	ASP	N-CA-C	-5.12	102.06	109.59
1	C	51	TYR	N-CA-C	5.06	116.22	108.42
1	B	31	VAL	CB-CA-C	-5.02	106.95	112.68

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2974	0	2889	165	1
1	B	2968	0	2884	172	0
1	C	2967	0	2886	261	1
2	A	45	0	43	4	0
2	B	45	0	43	2	0
2	C	45	0	43	1	0
3	A	38	0	0	4	0
3	B	35	0	0	1	0
3	C	18	0	0	2	0
All	All	9135	0	8788	586	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 33.

All (586) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:GLN:HB3	1:B:55:GLN:HE22	1.21	1.02
1:C:41:GLY:HA2	1:C:102:ILE:HB	1.42	1.01
1:B:73:GLN:HA	1:B:73:GLN:HE21	1.24	1.01
1:C:55:GLN:H	1:C:55:GLN:HE21	1.09	0.97
1:C:267:LEU:HD13	1:C:319:CYS:HB3	1.44	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:TRP:CD1	1:B:198:TYR:H	1.84	0.96
1:B:53:GLN:HB3	1:B:55:GLN:NE2	1.81	0.95
1:C:55:GLN:HG2	1:C:56:LEU:HD12	1.51	0.92
1:C:68:TYR:HB2	1:C:77:GLU:HG2	1.49	0.92
1:B:9:LYS:HD3	1:B:12:GLN:OE1	1.72	0.89
1:B:279:ILE:HG22	1:C:211:GLN:HE21	1.36	0.88
1:B:55:GLN:HG2	1:B:56:LEU:HD23	1.54	0.88
1:B:309:VAL:C	1:B:311:ASP:H	1.79	0.87
1:B:340:GLY:HA2	1:B:360:HIS:HB2	1.58	0.86
1:B:357:SER:HB3	1:B:360:HIS:HB3	1.58	0.85
1:C:45:HIS:HD2	1:C:46:PRO:HD2	1.42	0.84
1:A:267:LEU:HD13	1:A:319:CYS:HB3	1.60	0.84
1:A:215:MET:HE1	1:A:240:VAL:HG22	1.60	0.84
1:B:29:ILE:HD12	1:B:117:GLY:HA3	1.61	0.83
1:C:113:SER:HG	1:C:115:TRP:CD1	1.98	0.82
1:A:245:VAL:O	1:A:249:LYS:HB2	1.80	0.81
1:A:180:ASP:HB3	1:A:183:LEU:HG	1.62	0.80
1:B:73:GLN:HA	1:B:73:GLN:NE2	1.97	0.80
1:A:70:PRO:HD2	1:A:128:ARG:NH1	1.95	0.80
1:C:241:PHE:HE1	1:C:324:ILE:O	1.63	0.80
1:B:271:GLN:CD	1:B:271:GLN:H	1.90	0.80
1:A:95:VAL:HG11	1:A:140:LEU:HA	1.64	0.79
1:C:67:VAL:HG23	1:C:129:PRO:HG3	1.62	0.79
1:A:304:GLN:O	1:A:336:VAL:HG12	1.83	0.79
1:A:18:MET:SD	1:A:29:ILE:HG13	2.23	0.79
1:A:53:GLN:HB3	1:A:55:GLN:HE22	1.48	0.78
1:C:32:ASP:OD1	1:C:230:GLY:HA3	1.83	0.78
1:C:322:PHE:CZ	1:C:324:ILE:HB	2.18	0.78
1:B:279:ILE:HG22	1:C:211:GLN:NE2	1.99	0.77
1:C:301:LEU:HD11	1:C:367:THR:HA	1.65	0.77
1:B:113:SER:O	1:B:114:ASN:HB2	1.84	0.76
1:A:261:PHE:CD1	1:A:268:VAL:HG23	2.21	0.76
1:C:65:LYS:HE3	1:C:80:LEU:HD12	1.68	0.76
1:C:77:GLU:HB2	1:C:104:GLU:HB2	1.68	0.76
1:A:35:SER:O	1:A:122:ALA:HB3	1.86	0.76
1:A:168:ALA:O	1:A:169:SER:HB2	1.86	0.76
1:C:55:GLN:H	1:C:55:GLN:NE2	1.81	0.75
1:B:285:LEU:HD12	1:B:298:ILE:HD11	1.68	0.75
1:A:93:VAL:HB	1:A:144:THR:HG21	1.67	0.74
1:C:193:ILE:HD12	1:C:350:LYS:HA	1.68	0.74
1:C:195:ARG:O	1:C:197:TRP:HD1	1.70	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:VAL:HG23	1:A:129:PRO:HG3	1.70	0.73
1:C:245:VAL:O	1:C:249:LYS:HB2	1.89	0.73
1:B:188:LEU:HD23	1:B:355:ALA:HB2	1.71	0.72
1:C:203:ILE:HD13	1:C:285:LEU:HD22	1.71	0.71
1:A:235:ARG:HB2	1:A:332:VAL:HB	1.72	0.71
1:A:322:PHE:CE2	1:A:324:ILE:HB	2.24	0.71
1:C:149:LEU:HD23	1:C:149:LEU:C	2.15	0.71
1:C:335:ALA:O	1:C:339:GLU:HG3	1.90	0.70
1:C:69:VAL:HG22	1:C:128:ARG:HB2	1.73	0.70
1:C:68:TYR:CB	1:C:77:GLU:HG2	2.21	0.70
1:C:37:ASN:HD21	1:C:128:ARG:H	1.38	0.70
1:B:238:LYS:O	1:B:242:GLU:HG3	1.91	0.69
1:C:70:PRO:HA	1:C:75:LYS:HB3	1.74	0.69
1:C:229:SER:HB3	1:C:338:MET:HE1	1.74	0.69
1:C:29:ILE:HD12	1:C:117:GLY:HA3	1.73	0.69
1:B:301:LEU:HB3	1:B:302:PRO:HD2	1.73	0.69
1:A:197:TRP:CD1	1:A:198:TYR:H	2.11	0.69
1:C:-4:GLY:O	1:C:180:ASP:HA	1.92	0.69
1:B:31:VAL:HG12	1:B:31:VAL:O	1.92	0.68
1:B:211:GLN:HE22	1:C:254:THR:HG21	1.55	0.68
1:B:236:LEU:HD13	1:B:240:VAL:HG12	1.74	0.68
1:C:341:PHE:HB3	1:C:355:ALA:O	1.93	0.68
1:A:82:THR:O	1:A:83:ASP:HB2	1.93	0.68
1:C:267:LEU:HD22	1:C:309:VAL:HG21	1.75	0.68
1:B:4:ASP:H	1:B:173:SER:HB3	1.58	0.68
1:C:38:PHE:HD2	1:C:39:ALA:N	1.92	0.68
1:C:55:GLN:HE21	1:C:55:GLN:N	1.87	0.68
1:C:61:ARG:HB2	1:C:82:THR:OG1	1.93	0.68
1:C:301:LEU:H	1:C:304:GLN:NE2	1.91	0.68
1:A:53:GLN:HB3	1:A:55:GLN:NE2	2.09	0.68
1:B:53:GLN:CB	1:B:55:GLN:HE22	2.03	0.68
1:A:12:GLN:HE22	1:A:113:SER:HA	1.58	0.68
1:A:70:PRO:HD2	1:A:128:ARG:HH12	1.58	0.68
1:A:152:LEU:HD12	1:A:345:PHE:CE2	2.29	0.67
1:A:217:CYS:HA	1:A:220:TYR:CD1	2.28	0.67
1:A:384:TYR:OH	1:A:386:ILE:HD13	1.94	0.67
1:A:149:LEU:HD23	1:A:149:LEU:C	2.20	0.67
1:B:179:ILE:HD11	1:B:344:VAL:HG11	1.76	0.67
1:C:68:TYR:HB2	1:C:77:GLU:CG	2.24	0.67
1:C:69:VAL:O	1:C:75:LYS:HB2	1.95	0.67
1:B:234:LEU:HB2	1:B:336:VAL:CG2	2.24	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:VAL:HG13	1:B:366:ARG:NH1	2.10	0.67
1:A:146:VAL:HG11	1:A:176:ILE:HG22	1.76	0.66
1:A:107:LYS:HE2	1:A:107:LYS:H	1.60	0.66
1:C:136:PHE:HD2	1:C:136:PHE:C	2.04	0.66
1:C:242:GLU:O	1:C:245:VAL:HG23	1.95	0.66
1:A:367:THR:HG23	1:A:368:ALA:O	1.95	0.66
1:C:123:TYR:CD2	1:C:196:GLU:HB3	2.31	0.66
1:C:235:ARG:HE	1:C:332:VAL:HG21	1.59	0.66
1:A:278:ASN:HA	1:A:366:ARG:HH12	1.60	0.66
1:B:4:ASP:N	1:B:173:SER:HB3	2.11	0.66
1:B:40:VAL:HG12	1:B:117:GLY:HA3	1.79	0.65
1:A:22:SER:HB2	1:A:59:THR:HG23	1.79	0.65
1:A:183:LEU:HD12	1:A:342:TYR:CE1	2.31	0.65
1:B:76:TRP:HB2	1:B:102:ILE:HG23	1.77	0.65
1:C:70:PRO:HD2	1:C:128:ARG:NH1	2.11	0.65
1:C:386:ILE:HD13	1:C:386:ILE:C	2.21	0.65
1:C:55:GLN:C	1:C:57:SER:H	2.05	0.65
1:A:302:PRO:HG2	1:A:303:GLN:OE1	1.97	0.65
1:C:69:VAL:HG22	1:C:128:ARG:CB	2.27	0.65
1:C:301:LEU:HB3	1:C:302:PRO:HD2	1.76	0.65
1:C:233:ASN:HA	1:C:336:VAL:CG1	2.27	0.65
1:C:193:ILE:HG13	1:C:350:LYS:C	2.23	0.64
1:C:113:SER:OG	1:C:115:TRP:NE1	2.31	0.64
1:A:12:GLN:NE2	1:A:113:SER:HA	2.12	0.64
1:A:15:TYR:HB2	1:A:29:ILE:O	1.98	0.64
1:C:267:LEU:CD1	1:C:319:CYS:HB3	2.24	0.63
1:A:36:SER:HB2	1:A:127:ALA:HB2	1.80	0.63
1:A:219:GLU:HG3	1:A:239:LYS:HD3	1.79	0.63
1:A:305:TYR:HA	1:A:336:VAL:CG1	2.29	0.63
1:A:22:SER:HA	1:A:23:PRO:C	2.24	0.62
1:A:55:GLN:O	1:A:56:LEU:HD23	2.00	0.62
1:B:29:ILE:HG23	1:B:117:GLY:C	2.24	0.62
1:B:29:ILE:HD12	1:B:117:GLY:CA	2.28	0.62
1:C:251:ALA:HB2	3:C:504:HOH:O	1.99	0.62
1:B:2:MET:HG2	1:B:90:GLY:HA2	1.82	0.62
1:B:184:TYR:CE2	1:B:188:LEU:HG	2.35	0.62
1:B:279:ILE:CG2	1:C:211:GLN:HE21	2.12	0.62
1:B:309:VAL:O	1:B:311:ASP:N	2.32	0.62
1:B:316:GLN:NE2	1:B:316:GLN:HA	2.15	0.61
1:C:136:PHE:C	1:C:136:PHE:CD2	2.75	0.61
1:A:305:TYR:HA	1:A:336:VAL:HG12	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:ASP:OD2	1:C:183:LEU:HG	2.00	0.61
1:B:211:GLN:HA	1:C:278:ASN:OD1	2.00	0.61
1:C:8:GLY:HA2	1:C:15:TYR:CE2	2.35	0.61
1:C:341:PHE:HA	1:C:357:SER:HB2	1.83	0.60
1:A:346:ASP:OD1	1:A:346:ASP:C	2.45	0.60
1:C:2:MET:HG2	1:C:89:HIS:O	2.00	0.60
1:C:15:TYR:OH	1:C:114:ASN:ND2	2.29	0.60
1:A:72:THR:HB	2:A:501:009:H51	1.83	0.60
1:B:278:ASN:H	1:B:278:ASN:ND2	2.00	0.60
1:A:316:GLN:CD	1:A:316:GLN:H	2.10	0.60
1:A:357:SER:HB3	1:A:360:HIS:HB3	1.84	0.60
1:A:107:LYS:HE2	1:A:107:LYS:N	2.17	0.59
1:C:83:ASP:O	1:C:96:ARG:HG3	2.01	0.59
1:C:154:LEU:HD11	1:C:338:MET:HE2	1.83	0.59
1:A:17:GLU:OE2	1:A:88:PRO:HG2	2.01	0.59
1:A:63:LEU:HD21	1:C:-3:SER:HB2	1.85	0.59
1:A:179:ILE:HG23	1:A:342:TYR:HE2	1.67	0.59
1:C:71:TYR:O	1:C:72:THR:C	2.45	0.59
1:A:315:SER:HB2	1:A:316:GLN:NE2	2.17	0.59
1:B:55:GLN:HE21	1:B:56:LEU:CD2	2.15	0.59
1:B:376:THR:HG22	1:B:379:MET:HG2	1.83	0.59
1:A:303:GLN:OE1	1:A:303:GLN:N	2.34	0.59
1:C:42:ALA:HB3	1:C:101:ALA:HB1	1.84	0.59
1:C:180:ASP:HB3	1:C:183:LEU:CD1	2.33	0.59
1:C:193:ILE:N	1:C:350:LYS:O	2.31	0.59
1:C:225:SER:OG	1:C:331:THR:HB	2.03	0.59
1:C:267:LEU:C	1:C:267:LEU:HD12	2.28	0.59
1:C:276:PRO:O	1:C:279:ILE:HG12	2.02	0.59
1:C:37:ASN:ND2	1:C:128:ARG:H	2.01	0.58
1:A:143:GLN:HG3	1:C:1:GLU:OE1	2.04	0.58
1:B:4:ASP:CG	1:B:7:ARG:HH12	2.12	0.58
1:C:25:GLN:HE22	1:C:53:GLN:H	1.50	0.58
1:A:197:TRP:CG	1:A:198:TYR:H	2.20	0.58
1:B:271:GLN:CD	1:B:271:GLN:N	2.57	0.58
1:C:124:ALA:O	1:C:126:ILE:N	2.36	0.58
1:C:283:ILE:N	1:C:283:ILE:HD12	2.18	0.58
1:C:294:GLN:O	1:C:379:MET:HE1	2.04	0.58
1:B:65:LYS:HD3	1:B:66:GLY:H	1.69	0.58
1:B:245:VAL:O	1:B:249:LYS:HG3	2.03	0.58
1:C:45:HIS:O	1:C:47:PHE:N	2.37	0.58
1:B:211:GLN:NE2	1:C:254:THR:HG21	2.19	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:PHE:HE1	1:B:324:ILE:O	1.87	0.58
1:C:55:GLN:HG2	1:C:56:LEU:N	2.18	0.58
1:C:204:VAL:HG11	1:C:379:MET:CG	2.33	0.58
1:B:26:THR:O	1:B:27:LEU:HG	2.04	0.57
1:C:232:THR:HG21	1:C:307:ARG:CZ	2.34	0.57
1:C:341:PHE:C	1:C:357:SER:HB2	2.29	0.57
1:C:301:LEU:H	1:C:304:GLN:HE21	1.50	0.57
1:B:110:ILE:HB	1:B:113:SER:HB3	1.85	0.57
1:A:215:MET:CE	1:A:240:VAL:HG22	2.32	0.57
1:B:311:ASP:O	1:B:312:VAL:HB	2.04	0.57
1:C:82:THR:O	1:C:83:ASP:HB2	2.05	0.57
1:C:204:VAL:HG11	1:C:379:MET:SD	2.45	0.57
1:C:241:PHE:CE1	1:C:325:SER:HA	2.40	0.57
1:A:60:TYR:CG	1:A:61:ARG:N	2.73	0.56
1:B:180:ASP:C	1:B:180:ASP:OD2	2.48	0.56
1:B:197:TRP:CD1	1:B:198:TYR:N	2.66	0.56
1:B:341:PHE:CA	1:B:357:SER:HB2	2.35	0.56
1:A:74:GLY:HA3	1:A:107:LYS:O	2.05	0.56
1:B:227:VAL:CG1	1:B:338:MET:HE3	2.35	0.56
1:C:78:GLY:HA3	1:C:101:ALA:O	2.05	0.56
1:C:302:PRO:O	1:C:306:LEU:HB2	2.06	0.56
1:B:186:GLY:HA3	3:B:513:HOH:O	2.06	0.56
1:C:71:TYR:O	1:C:73:GLN:N	2.39	0.56
1:C:48:LEU:HD22	1:C:116:GLU:HB3	1.86	0.56
1:C:135:PRO:HD2	1:C:138:ASP:OD2	2.06	0.56
1:A:297:ARG:HG2	1:A:374:PHE:CE1	2.40	0.56
1:B:309:VAL:O	1:B:309:VAL:HG23	2.06	0.56
1:A:241:PHE:O	1:A:245:VAL:HG23	2.06	0.56
1:C:188:LEU:HD23	1:C:355:ALA:HB2	1.88	0.56
1:A:2:MET:HE1	1:A:176:ILE:O	2.07	0.55
1:C:241:PHE:CE1	1:C:324:ILE:O	2.53	0.55
1:C:261:PHE:CD1	1:C:268:VAL:HG23	2.40	0.55
1:A:216:ASP:O	1:A:218:LYS:N	2.39	0.55
1:C:341:PHE:CA	1:C:357:SER:HB2	2.37	0.55
1:A:276:PRO:O	1:A:279:ILE:HG12	2.07	0.55
1:C:235:ARG:HB2	1:C:332:VAL:HG23	1.87	0.55
1:C:38:PHE:HD2	1:C:39:ALA:H	1.55	0.55
1:C:63:LEU:O	1:C:64:ARG:C	2.50	0.55
1:C:241:PHE:O	1:C:245:VAL:HG22	2.06	0.55
1:A:193:ILE:HG13	1:A:351:ARG:HA	1.89	0.55
1:B:205:ARG:NE	1:B:207:GLU:OE2	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:PRO:O	1:B:279:ILE:HG12	2.07	0.55
1:B:346:ASP:OD2	1:B:349:ARG:HB2	2.07	0.55
1:C:300:ILE:HD12	1:C:304:GLN:HB3	1.88	0.55
1:A:38:PHE:HE1	1:A:85:VAL:HG21	1.73	0.54
1:B:233:ASN:HA	1:B:336:VAL:HG13	1.87	0.54
1:C:232:THR:HG21	1:C:307:ARG:NH2	2.21	0.54
1:C:69:VAL:HG22	1:C:128:ARG:CG	2.37	0.54
1:C:136:PHE:HE2	1:C:140:LEU:HB2	1.72	0.54
1:C:300:ILE:HG21	1:C:337:ILE:HD13	1.89	0.54
1:A:225:SER:OG	1:A:331:THR:HB	2.08	0.54
1:C:37:ASN:HD21	1:C:128:ARG:N	2.04	0.54
1:C:70:PRO:CD	1:C:128:ARG:NH1	2.71	0.54
1:A:298:ILE:HB	1:A:341:PHE:CZ	2.43	0.53
1:C:69:VAL:HG22	1:C:128:ARG:HG3	1.90	0.53
1:A:29:ILE:HG21	1:A:119:LEU:HB2	1.88	0.53
1:C:267:LEU:HD22	1:C:309:VAL:CG2	2.39	0.53
1:B:181:HIS:HA	1:B:184:TYR:HE1	1.73	0.53
1:B:244:ALA:O	1:B:248:ILE:HG13	2.07	0.53
1:B:55:GLN:HG2	1:B:56:LEU:CD2	2.34	0.53
1:C:267:LEU:HB2	1:C:320:TYR:O	2.09	0.53
1:A:42:ALA:CB	1:A:101:ALA:HB1	2.39	0.53
1:C:257:PHE:HB3	1:C:258:PRO:HD2	1.90	0.53
1:B:197:TRP:CG	1:B:198:TYR:H	2.24	0.53
1:B:205:ARG:NH2	1:B:207:GLU:OE2	2.41	0.53
1:C:45:HIS:HD2	1:C:46:PRO:CD	2.20	0.53
1:C:99:ILE:HG22	1:C:100:ALA:N	2.24	0.53
1:B:207:GLU:O	1:B:208:ILE:HD13	2.08	0.52
1:B:270:TRP:CE3	1:B:275:THR:HG23	2.44	0.52
1:C:314:THR:HG21	1:C:316:GLN:HE21	1.74	0.52
1:C:222:TYR:O	1:C:223:ASP:CB	2.58	0.52
1:A:216:ASP:C	1:A:218:LYS:H	2.17	0.52
1:B:234:LEU:HB2	1:B:336:VAL:HG21	1.92	0.52
1:B:297:ARG:NH1	1:B:374:PHE:CZ	2.76	0.52
1:C:346:ASP:OD1	1:C:346:ASP:O	2.27	0.52
1:B:137:PHE:HD2	1:B:347:ARG:NH1	2.08	0.52
1:A:222:TYR:O	1:A:223:ASP:CB	2.57	0.52
1:C:76:TRP:O	1:C:77:GLU:HG3	2.10	0.52
1:C:149:LEU:HD23	1:C:150:PHE:N	2.25	0.52
1:C:252:SER:O	1:C:254:THR:N	2.42	0.52
1:B:6:LEU:HB2	1:B:172:GLY:O	2.09	0.52
1:B:309:VAL:C	1:B:311:ASP:N	2.52	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ASN:O	1:B:29:ILE:HD13	2.10	0.51
1:B:225:SER:OG	1:B:331:THR:HB	2.11	0.51
1:B:228:ASP:OD1	1:B:230:GLY:N	2.43	0.51
1:C:48:LEU:HD22	1:C:116:GLU:CB	2.40	0.51
1:A:257:PHE:HD1	1:A:262:TRP:CZ2	2.28	0.51
1:A:322:PHE:CZ	1:A:324:ILE:HB	2.45	0.51
1:B:346:ASP:OD1	1:B:346:ASP:C	2.54	0.51
1:C:277:TRP:CH2	1:C:303:GLN:HG3	2.45	0.51
1:C:304:GLN:HB3	1:C:336:VAL:O	2.09	0.51
1:C:327:SER:OG	1:C:330:GLY:O	2.29	0.51
1:B:65:LYS:HD3	1:B:66:GLY:N	2.25	0.51
1:C:33:THR:HG23	1:C:229:SER:OG	2.09	0.51
1:B:197:TRP:CG	1:B:198:TYR:N	2.78	0.51
1:B:252:SER:O	1:B:254:THR:N	2.44	0.51
1:C:17:GLU:O	1:C:88:PRO:HD2	2.10	0.51
1:C:300:ILE:HG21	1:C:337:ILE:CD1	2.41	0.51
1:A:125:GLU:HB2	1:A:197:TRP:HA	1.92	0.51
1:C:55:GLN:O	1:C:57:SER:N	2.44	0.51
1:C:77:GLU:N	1:C:104:GLU:O	2.43	0.51
1:A:60:TYR:OH	1:A:62:ASP:HB2	2.11	0.51
1:A:146:VAL:HG13	1:A:177:GLY:HA3	1.93	0.51
1:C:35:SER:O	1:C:122:ALA:HB3	2.10	0.51
1:C:55:GLN:C	1:C:57:SER:N	2.68	0.51
1:A:36:SER:CB	1:A:127:ALA:HB2	2.40	0.51
1:B:153:GLN:HB2	1:B:342:TYR:HD1	1.76	0.51
1:C:55:GLN:CG	1:C:56:LEU:HD12	2.33	0.51
1:A:130:ASP:O	1:A:132:SER:N	2.44	0.50
1:C:66:GLY:HA2	1:C:79:GLU:HA	1.93	0.50
1:C:123:TYR:CE2	1:C:196:GLU:HB3	2.46	0.50
1:C:304:GLN:O	1:C:336:VAL:HB	2.10	0.50
1:A:72:THR:HB	2:A:501:009:C51	2.41	0.50
1:A:9:LYS:O	1:A:12:GLN:HB2	2.11	0.50
1:A:110:ILE:HB	1:A:113:SER:HB3	1.93	0.50
1:A:183:LEU:HA	3:A:525:HOH:O	2.12	0.50
1:B:55:GLN:HE21	1:B:56:LEU:HG	1.77	0.50
1:B:76:TRP:HA	1:B:104:GLU:O	2.12	0.50
1:C:369:ALA:HA	3:C:515:HOH:O	2.11	0.50
1:B:156:GLY:O	1:B:157:ALA:HB2	2.11	0.50
1:C:240:VAL:O	1:C:241:PHE:C	2.54	0.50
1:B:208:ILE:O	1:B:209:ASN:C	2.54	0.50
1:A:55:GLN:C	1:A:56:LEU:HD23	2.37	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:SER:OG	1:C:123:TYR:O	2.28	0.49
1:C:42:ALA:CB	1:C:101:ALA:HB1	2.41	0.49
1:C:296:PHE:CD1	1:C:296:PHE:C	2.89	0.49
1:A:295:SER:HB3	1:A:379:MET:SD	2.52	0.49
1:A:63:LEU:O	1:C:181:HIS:HD2	1.95	0.49
1:A:130:ASP:C	1:A:132:SER:H	2.20	0.49
1:B:267:LEU:CD2	1:B:321:LYS:HG3	2.42	0.49
1:C:69:VAL:CG2	1:C:128:ARG:HB2	2.41	0.49
1:C:189:TRP:O	1:C:353:GLY:HA2	2.12	0.49
1:C:237:PRO:O	1:C:238:LYS:C	2.55	0.49
1:A:245:VAL:HG12	1:A:249:LYS:HE3	1.93	0.49
1:A:301:LEU:HB3	1:A:302:PRO:HD2	1.94	0.49
1:A:294:GLN:O	1:A:379:MET:HE1	2.13	0.49
1:A:6:LEU:HB2	1:A:172:GLY:O	2.13	0.49
1:A:14:TYR:O	1:A:30:LEU:HD12	2.13	0.49
1:A:293:ASN:HA	1:A:379:MET:HE2	1.94	0.49
1:B:15:TYR:O	1:B:15:TYR:CD1	2.66	0.49
1:B:40:VAL:O	1:B:102:ILE:HG13	2.13	0.49
1:B:301:LEU:H	1:B:304:GLN:HE21	1.61	0.49
1:C:123:TYR:HE1	1:C:199:TYR:CE2	2.31	0.49
1:C:233:ASN:HB3	1:C:323:ALA:O	2.13	0.49
1:C:38:PHE:CD2	1:C:39:ALA:N	2.77	0.49
1:C:140:LEU:HD12	1:C:140:LEU:O	2.12	0.49
1:B:316:GLN:HA	1:B:316:GLN:HE21	1.76	0.49
1:C:320:TYR:N	1:C:320:TYR:CD1	2.81	0.49
1:C:234:LEU:HD23	1:C:337:ILE:HG13	1.95	0.49
1:A:194:ARG:HD2	1:A:202:ILE:HD11	1.95	0.48
1:B:235:ARG:CZ	2:B:502:009:H54	2.43	0.48
1:A:294:GLN:HG3	1:A:373:PRO:HB2	1.94	0.48
1:A:338:MET:C	1:A:340:GLY:H	2.21	0.48
1:B:340:GLY:HA2	1:B:360:HIS:CB	2.37	0.48
1:C:33:THR:O	1:C:199:TYR:HD1	1.96	0.48
1:C:300:ILE:HG13	1:C:304:GLN:HB2	1.95	0.48
1:A:123:TYR:HB2	1:A:197:TRP:O	2.13	0.48
1:A:252:SER:O	1:A:254:THR:N	2.47	0.48
1:C:32:ASP:C	1:C:34:GLY:H	2.18	0.48
1:C:70:PRO:HG2	1:C:128:ARG:HH22	1.78	0.48
1:B:1:GLU:OE2	1:B:89:HIS:HA	2.13	0.48
1:B:181:HIS:HA	1:B:184:TYR:CE1	2.48	0.48
1:B:279:ILE:HA	1:C:211:GLN:HE21	1.78	0.48
1:A:301:LEU:H	1:A:304:GLN:NE2	2.11	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:ILE:HD11	1:C:305:TYR:HB3	1.96	0.48
1:C:33:THR:HA	1:C:121:LEU:HB2	1.96	0.48
1:C:314:THR:HG22	1:C:315:SER:N	2.28	0.48
1:B:22:SER:HA	1:B:23:PRO:C	2.38	0.48
1:B:73:GLN:HE21	1:B:73:GLN:CA	2.00	0.48
1:A:190:TYR:CD2	1:A:351:ARG:HD2	2.48	0.48
1:A:234:LEU:HD11	1:A:236:LEU:HD21	1.96	0.48
1:C:149:LEU:C	1:C:149:LEU:CD2	2.85	0.48
1:B:20:VAL:HG12	1:B:85:VAL:HG13	1.96	0.47
1:B:310:GLU:C	1:B:311:ASP:OD1	2.57	0.47
1:C:28:ASN:C	1:C:29:ILE:HD13	2.39	0.47
1:C:229:SER:CB	1:C:338:MET:HE1	2.44	0.47
1:C:153:GLN:HB2	1:C:342:TYR:HD1	1.80	0.47
1:A:151:SER:OG	1:A:175:ILE:HB	2.14	0.47
1:A:283:ILE:O	1:A:299:THR:HA	2.13	0.47
1:B:311:ASP:O	1:B:312:VAL:CB	2.61	0.47
1:C:48:LEU:HD22	1:C:116:GLU:CG	2.45	0.47
1:B:375:VAL:HG12	1:B:375:VAL:O	2.13	0.47
1:A:197:TRP:CG	1:A:198:TYR:N	2.82	0.47
1:C:102:ILE:HD12	1:C:109:PHE:HZ	1.80	0.47
1:C:136:PHE:CE2	1:C:140:LEU:HB2	2.49	0.47
1:B:62:ASP:OD1	1:B:64:ARG:N	2.39	0.47
1:B:217:CYS:HA	1:B:220:TYR:CE1	2.49	0.47
1:C:83:ASP:O	1:C:96:ARG:HA	2.15	0.47
1:B:205:ARG:HB3	1:B:286:TYR:HB2	1.95	0.47
1:B:217:CYS:HA	1:B:220:TYR:CD1	2.49	0.47
1:B:335:ALA:O	1:B:339:GLU:HG3	2.15	0.47
1:A:302:PRO:CD	1:A:366:ARG:HH21	2.28	0.47
1:A:335:ALA:O	1:A:339:GLU:HG3	2.15	0.47
1:B:232:THR:O	1:B:336:VAL:HG13	2.15	0.47
1:B:341:PHE:C	1:B:357:SER:HB2	2.39	0.47
1:C:85:VAL:N	1:C:95:VAL:O	2.39	0.47
1:C:302:PRO:HA	1:C:305:TYR:CE2	2.50	0.47
1:A:326:GLN:HG2	1:A:327:SER:N	2.30	0.47
1:B:32:ASP:CG	1:B:34:GLY:H	2.23	0.47
1:C:235:ARG:HB2	1:C:332:VAL:CG2	2.44	0.47
1:C:133:LEU:O	1:C:135:PRO:HD3	2.15	0.46
1:C:205:ARG:HG2	1:C:206:VAL:N	2.29	0.46
1:A:386:ILE:O	1:A:386:ILE:HG23	2.16	0.46
1:B:32:ASP:O	1:B:120:GLY:HA2	2.15	0.46
1:B:72:THR:OG1	2:B:502:009:H51	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:PRO:HA	1:C:75:LYS:CB	2.43	0.46
1:B:137:PHE:O	1:B:141:VAL:HG23	2.15	0.46
1:B:376:THR:CG2	1:B:379:MET:HG2	2.45	0.46
1:A:32:ASP:OD2	1:A:35:SER:OG	2.34	0.46
1:A:209:ASN:OD1	1:A:281:PRO:HA	2.16	0.46
1:A:234:LEU:N	1:A:336:VAL:HG21	2.30	0.46
1:B:65:LYS:HB3	1:B:80:LEU:HD12	1.97	0.46
1:C:214:LYS:O	1:C:215:MET:HG3	2.15	0.46
1:C:235:ARG:HH12	1:C:329:THR:CG2	2.29	0.46
1:C:286:TYR:OH	1:C:297:ARG:NH1	2.48	0.46
1:A:21:GLY:HA2	1:A:83:ASP:OD1	2.14	0.46
1:A:70:PRO:CD	1:A:128:ARG:HH12	2.27	0.46
1:A:93:VAL:CB	1:A:144:THR:HG21	2.40	0.46
1:A:216:ASP:C	1:A:218:LYS:N	2.73	0.46
1:B:35:SER:O	1:B:122:ALA:HB3	2.14	0.46
1:B:153:GLN:HB2	1:B:342:TYR:CD1	2.50	0.46
1:C:267:LEU:HD12	1:C:267:LEU:O	2.14	0.46
1:B:341:PHE:N	1:B:357:SER:HB2	2.30	0.46
1:C:76:TRP:C	1:C:77:GLU:HG3	2.40	0.46
1:B:123:TYR:CZ	1:B:196:GLU:HG2	2.51	0.46
1:B:235:ARG:NH2	1:B:326:GLN:O	2.48	0.46
1:C:268:VAL:O	1:C:319:CYS:HA	2.15	0.46
1:C:310:GLU:C	1:C:310:GLU:CD	2.84	0.46
1:B:-2:PHE:HB3	1:B:2:MET:HE3	1.98	0.46
1:A:95:VAL:HB	1:A:143:GLN:OE1	2.16	0.46
1:A:326:GLN:HG2	1:A:327:SER:H	1.81	0.46
1:B:15:TYR:CE2	1:B:114:ASN:HB3	2.51	0.46
1:A:32:ASP:OD1	1:A:32:ASP:C	2.58	0.45
1:A:292:THR:HA	3:A:516:HOH:O	2.16	0.45
1:B:41:GLY:HA2	1:B:102:ILE:HB	1.98	0.45
1:B:297:ARG:HG2	1:B:374:PHE:CE1	2.51	0.45
1:C:54:ARG:HB3	1:C:60:TYR:CD2	2.51	0.45
1:A:217:CYS:HA	1:A:220:TYR:CE1	2.50	0.45
1:A:234:LEU:HB2	1:A:336:VAL:CG2	2.46	0.45
1:C:45:HIS:C	1:C:47:PHE:N	2.74	0.45
1:C:236:LEU:O	1:C:326:GLN:HA	2.16	0.45
1:C:277:TRP:CE3	1:C:302:PRO:HG2	2.51	0.45
1:A:32:ASP:OD2	2:A:501:009:HB	2.17	0.45
1:C:179:ILE:HG23	1:C:342:TYR:CE2	2.52	0.45
1:B:300:ILE:HG22	1:B:341:PHE:CE1	2.52	0.45
1:B:123:TYR:CE1	1:B:196:GLU:HG2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:TYR:CE2	1:C:154:LEU:HB3	2.52	0.45
1:C:31:VAL:HG13	1:C:121:LEU:HD11	1.98	0.45
1:C:62:ASP:OD1	1:C:63:LEU:N	2.50	0.45
1:C:225:SER:HA	1:C:331:THR:O	2.17	0.45
1:B:365:PHE:CE1	1:C:205:ARG:NH1	2.84	0.45
1:C:19:THR:HG22	1:C:26:THR:HA	1.98	0.45
1:C:318:ASP:N	1:C:318:ASP:OD2	2.49	0.45
1:C:37:ASN:HD21	1:C:128:ARG:HB2	1.82	0.45
1:C:98:ASN:C	1:C:99:ILE:HG13	2.41	0.45
1:C:237:PRO:HD3	1:C:331:THR:OG1	2.16	0.45
1:B:149:LEU:HB2	1:B:346:ASP:HA	1.98	0.45
1:B:206:VAL:HG11	1:B:213:LEU:HD22	1.99	0.45
1:B:307:ARG:HG2	1:B:307:ARG:HH11	1.81	0.45
1:C:70:PRO:HG2	1:C:128:ARG:NH2	2.32	0.45
1:C:15:TYR:O	1:C:15:TYR:CD1	2.70	0.45
1:C:19:THR:HA	1:C:25:GLN:O	2.16	0.45
1:A:305:TYR:HA	1:A:336:VAL:HG11	1.97	0.44
1:C:218:LYS:HG2	1:C:381:ASP:O	2.17	0.44
1:A:22:SER:CA	1:A:23:PRO:C	2.90	0.44
1:C:180:ASP:HB3	1:C:183:LEU:HG	1.99	0.44
1:C:337:ILE:HD13	1:C:337:ILE:HA	1.86	0.44
1:B:-2:PHE:CZ	1:B:178:GLY:HA3	2.51	0.44
1:B:227:VAL:HG12	1:B:338:MET:HE3	1.99	0.44
1:B:284:SER:HA	1:B:298:ILE:O	2.17	0.44
1:C:134:GLU:HG3	1:C:138:ASP:HB2	2.00	0.44
1:B:15:TYR:CD1	1:B:15:TYR:C	2.95	0.44
1:C:6:LEU:CD2	1:C:16:VAL:HB	2.47	0.44
1:C:253:SER:HA	1:C:256:LYS:HD3	1.99	0.44
1:A:35:SER:O	1:A:122:ALA:CB	2.63	0.44
1:B:73:GLN:NE2	1:B:73:GLN:CA	2.68	0.44
1:C:14:TYR:CD2	1:C:154:LEU:HD22	2.53	0.44
1:A:234:LEU:N	1:A:336:VAL:CG2	2.81	0.44
1:B:28:ASN:C	1:B:29:ILE:HD13	2.43	0.44
1:B:45:HIS:ND1	1:B:46:PRO:HD2	2.33	0.44
1:B:223:ASP:CA	1:B:384:TYR:HD2	2.31	0.44
1:C:135:PRO:O	1:C:136:PHE:C	2.60	0.44
1:C:277:TRP:CZ3	1:C:303:GLN:HG3	2.52	0.44
1:B:191:THR:HG23	1:B:191:THR:O	2.17	0.44
1:B:233:ASN:HA	1:B:336:VAL:CG1	2.48	0.44
1:C:-2:PHE:O	1:C:3:VAL:HG23	2.17	0.44
1:A:107:LYS:HE2	1:A:107:LYS:CA	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:TYR:O	1:A:223:ASP:HB2	2.16	0.44
1:A:32:ASP:OD2	1:A:118:ILE:HD11	2.17	0.44
1:A:110:ILE:CD1	2:A:501:009:H44	2.47	0.44
1:A:29:ILE:CG2	1:A:119:LEU:HB2	2.47	0.43
1:C:28:ASN:O	1:C:29:ILE:HD13	2.17	0.43
1:C:280:PHE:HB3	1:C:305:TYR:OH	2.18	0.43
1:A:316:GLN:H	1:A:316:GLN:NE2	2.16	0.43
1:B:223:ASP:HA	1:B:384:TYR:HD2	1.82	0.43
1:A:323:ALA:HB3	1:A:336:VAL:HG11	2.01	0.43
1:C:381:ASP:N	1:C:381:ASP:OD1	2.51	0.43
1:A:63:LEU:CD2	1:C:-3:SER:HB2	2.49	0.43
1:A:241:PHE:CE2	1:A:245:VAL:HG21	2.53	0.43
1:C:351:ARG:O	1:C:351:ARG:HG3	2.18	0.43
1:A:15:TYR:C	1:A:15:TYR:CD1	2.96	0.43
1:A:139:SER:O	1:A:140:LEU:C	2.61	0.43
1:B:20:VAL:O	1:B:25:GLN:HB2	2.18	0.43
1:B:267:LEU:HD23	1:B:321:LYS:HG3	2.00	0.43
1:A:123:TYR:CE1	1:A:199:TYR:CE2	3.07	0.43
1:B:30:LEU:HD22	1:B:31:VAL:N	2.34	0.43
1:C:41:GLY:HA3	1:C:48:LEU:HD11	2.01	0.43
1:A:18:MET:SD	1:A:29:ILE:CG1	3.00	0.43
1:C:34:GLY:HA3	1:C:228:ASP:OD1	2.19	0.43
1:C:124:ALA:C	1:C:126:ILE:H	2.26	0.43
1:C:204:VAL:O	1:C:205:ARG:HB2	2.19	0.43
1:C:386:ILE:C	1:C:386:ILE:CD1	2.90	0.43
1:A:63:LEU:H	1:A:81:GLY:HA2	1.83	0.43
1:A:300:ILE:HD11	1:A:305:TYR:HD2	1.84	0.43
1:C:288:MET:HE2	1:C:379:MET:HB3	2.00	0.43
1:B:307:ARG:HA	1:B:308:PRO:HD3	1.89	0.42
1:C:349:ARG:O	1:C:350:LYS:C	2.63	0.42
1:A:267:LEU:HD12	1:A:267:LEU:O	2.19	0.42
1:C:32:ASP:CB	1:C:118:ILE:HD11	2.50	0.42
1:C:67:VAL:CG2	1:C:129:PRO:HG3	2.41	0.42
1:C:235:ARG:HB2	1:C:332:VAL:HB	2.00	0.42
1:C:301:LEU:HD11	1:C:367:THR:CA	2.45	0.42
1:A:26:THR:O	1:A:27:LEU:HD23	2.19	0.42
1:A:168:ALA:O	1:A:169:SER:CB	2.62	0.42
1:C:238:LYS:HA	1:C:326:GLN:HB2	2.00	0.42
1:A:54:ARG:HD3	3:A:518:HOH:O	2.18	0.42
1:B:36:SER:HB2	1:B:127:ALA:HA	2.01	0.42
1:B:55:GLN:HE21	1:B:56:LEU:CG	2.33	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LEU:O	1:B:119:LEU:HG	2.19	0.42
1:B:267:LEU:HD21	1:B:321:LYS:HE3	2.01	0.42
1:C:146:VAL:HA	1:C:147:PRO:HD3	1.85	0.42
1:C:180:ASP:HB3	1:C:183:LEU:HD12	1.99	0.42
1:C:277:TRP:HE3	1:C:302:PRO:HG2	1.85	0.42
1:A:234:LEU:H	1:A:336:VAL:HG21	1.84	0.42
1:A:338:MET:C	1:A:340:GLY:N	2.78	0.42
1:B:205:ARG:HB3	1:B:286:TYR:CG	2.55	0.42
1:B:316:GLN:HE21	1:B:316:GLN:CA	2.30	0.42
1:C:45:HIS:CD2	1:C:46:PRO:HD2	2.34	0.42
1:A:28:ASN:HD22	1:A:28:ASN:HA	1.61	0.42
1:A:41:GLY:O	1:A:51:TYR:HB2	2.19	0.42
1:A:268:VAL:O	1:A:319:CYS:HA	2.19	0.42
1:C:59:THR:O	1:C:96:ARG:NH1	2.45	0.42
1:A:150:PHE:HE2	1:A:152:LEU:HD11	1.84	0.42
1:B:205:ARG:HB3	1:B:286:TYR:CB	2.50	0.42
1:C:233:ASN:ND2	1:C:323:ALA:HA	2.35	0.42
1:C:288:MET:HE2	1:C:379:MET:CB	2.50	0.42
1:B:9:LYS:O	1:B:10:SER:C	2.62	0.42
1:B:247:SER:O	1:B:248:ILE:C	2.60	0.42
1:C:235:ARG:HB2	1:C:332:VAL:CB	2.50	0.42
1:B:76:TRP:HB2	1:B:102:ILE:CG2	2.46	0.42
1:B:77:GLU:HB3	1:B:104:GLU:HB3	2.02	0.42
1:B:184:TYR:HD2	1:B:355:ALA:HB1	1.85	0.42
1:C:14:TYR:CG	1:C:154:LEU:HD22	2.55	0.42
1:C:35:SER:O	1:C:122:ALA:N	2.47	0.42
1:C:45:HIS:C	1:C:47:PHE:H	2.28	0.42
1:C:63:LEU:HD12	1:C:81:GLY:HA2	2.02	0.42
1:B:67:VAL:HG11	1:B:100:ALA:HB1	2.01	0.41
1:B:283:ILE:HD12	1:B:305:TYR:CD2	2.55	0.41
1:B:234:LEU:HB2	1:B:336:VAL:HG22	1.99	0.41
1:C:154:LEU:HD12	1:C:338:MET:HB3	2.02	0.41
1:A:226:ILE:HD12	1:A:228:ASP:HB2	2.02	0.41
1:B:14:TYR:CZ	1:B:154:LEU:HB3	2.55	0.41
1:C:32:ASP:C	1:C:34:GLY:N	2.77	0.41
1:C:195:ARG:NH1	1:C:197:TRP:CD2	2.88	0.41
1:C:217:CYS:O	1:C:218:LYS:C	2.63	0.41
1:C:235:ARG:O	1:C:331:THR:HA	2.20	0.41
1:A:149:LEU:C	1:A:149:LEU:CD2	2.90	0.41
1:A:297:ARG:HG2	1:A:374:PHE:HE1	1.83	0.41
1:A:338:MET:O	1:A:340:GLY:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ASP:O	1:B:132:SER:N	2.54	0.41
1:C:137:PHE:O	1:C:141:VAL:HG23	2.19	0.41
1:C:297:ARG:NH1	1:C:374:PHE:CZ	2.88	0.41
1:C:346:ASP:HB3	1:C:351:ARG:O	2.21	0.41
1:A:146:VAL:CG1	1:A:177:GLY:HA3	2.50	0.41
1:A:212:ASP:OD1	1:A:214:LYS:N	2.48	0.41
1:A:241:PHE:CE1	1:A:325:SER:HA	2.55	0.41
1:B:216:ASP:O	1:B:218:LYS:N	2.53	0.41
1:C:200:GLU:HG3	1:C:201:VAL:N	2.34	0.41
1:A:201:VAL:O	1:A:202:ILE:HG13	2.21	0.41
1:B:300:ILE:HG22	1:B:341:PHE:HE1	1.86	0.41
1:A:203:ILE:N	1:A:203:ILE:HD12	2.36	0.41
1:A:386:ILE:HD12	3:A:527:HOH:O	2.20	0.41
1:B:32:ASP:C	1:B:34:GLY:H	2.28	0.41
1:B:235:ARG:NH1	1:B:327:SER:HB2	2.36	0.41
1:C:287:LEU:O	1:C:288:MET:C	2.62	0.41
1:A:179:ILE:HG23	1:A:342:TYR:CE2	2.52	0.41
1:B:-2:PHE:CD1	1:B:-2:PHE:N	2.87	0.41
1:B:189:TRP:O	1:B:353:GLY:HA2	2.21	0.41
1:B:293:ASN:HA	1:B:376:THR:O	2.21	0.41
1:C:232:THR:CG2	1:C:307:ARG:NE	2.83	0.41
1:B:234:LEU:C	1:B:234:LEU:CD2	2.94	0.41
1:C:179:ILE:HG23	1:C:342:TYR:HE2	1.86	0.41
1:C:212:ASP:OD1	1:C:213:LEU:N	2.54	0.41
1:B:362:HIS:ND1	1:B:362:HIS:N	2.70	0.40
1:C:60:TYR:C	1:C:61:ARG:HG2	2.46	0.40
1:C:283:ILE:CD1	1:C:305:TYR:CE2	3.04	0.40
1:A:237:PRO:HD3	1:A:331:THR:OG1	2.21	0.40
1:A:333:MET:HE2	1:A:337:ILE:HG21	2.04	0.40
1:B:96:ARG:NH1	1:B:96:ARG:HG3	2.36	0.40
1:C:70:PRO:HD2	1:C:128:ARG:CZ	2.50	0.40
1:C:71:TYR:HB3	2:C:503:009:HD2	2.03	0.40
1:C:189:TRP:O	1:C:353:GLY:CA	2.69	0.40
1:C:190:TYR:CD2	1:C:353:GLY:N	2.89	0.40
1:C:293:ASN:HB3	1:C:377:LEU:CD2	2.51	0.40
1:A:77:GLU:N	1:A:104:GLU:O	2.47	0.40
1:C:29:ILE:HD12	1:C:117:GLY:CA	2.48	0.40
1:C:54:ARG:HG2	1:C:60:TYR:CE1	2.56	0.40
1:C:309:VAL:O	1:C:310:GLU:C	2.63	0.40
1:A:356:VAL:HG22	1:A:369:ALA:HA	2.02	0.40
1:B:36:SER:HB3	1:B:127:ALA:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:VAL:HG21	1:B:140:LEU:HD11	2.02	0.40
1:C:38:PHE:CD2	1:C:38:PHE:C	3.00	0.40
1:C:47:PHE:HD1	1:C:109:PHE:O	2.05	0.40
1:A:-2:PHE:CD1	1:A:-2:PHE:N	2.90	0.40
1:A:26:THR:HG22	1:A:27:LEU:N	2.36	0.40
1:A:261:PHE:CD1	1:A:268:VAL:CG2	3.00	0.40
1:C:357:SER:HB3	1:C:360:HIS:HB3	2.03	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:68:TYR:OH	1:C:68:TYR:O[4_555]	2.04	0.16

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	373/412 (90%)	320 (86%)	40 (11%)	13 (4%)	3	6
1	B	373/412 (90%)	328 (88%)	32 (9%)	13 (4%)	3	6
1	C	371/412 (90%)	309 (83%)	40 (11%)	22 (6%)	1	2
All	All	1117/1236 (90%)	957 (86%)	112 (10%)	48 (4%)	2	4

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	131	ASP
1	A	223	ASP
1	A	253	SER
1	B	223	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	253	SER
1	B	312	VAL
1	C	72	THR
1	C	123	TYR
1	C	125	GLU
1	C	133	LEU
1	C	223	ASP
1	C	238	LYS
1	C	253	SER
1	C	316	GLN
1	A	83	ASP
1	A	169	SER
1	A	217	CYS
1	B	214	LYS
1	B	259	ASP
1	B	310	GLU
1	B	311	ASP
1	C	56	LEU
1	C	194	ARG
1	C	214	LYS
1	C	350	LYS
1	A	339	GLU
1	C	136	PHE
1	C	196	GLU
1	C	347	ARG
1	A	272	ALA
1	B	131	ASP
1	B	197	TRP
1	C	64	ARG
1	C	83	ASP
1	C	98	ASN
1	C	140	LEU
1	C	346	ASP
1	A	149	LEU
1	B	70	PRO
1	B	156	GLY
1	C	46	PRO
1	A	156	GLY
1	A	278	ASN
1	B	181	HIS
1	B	217	CYS
1	C	276	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	237	PRO

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	321/353 (91%)	305 (95%)	16 (5%)	22	48
1	B	322/353 (91%)	298 (92%)	24 (8%)	12	31
1	C	322/353 (91%)	299 (93%)	23 (7%)	13	33
All	All	965/1059 (91%)	902 (94%)	63 (6%)	15	37

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	35	SER
1	A	61	ARG
1	A	125	GLU
1	A	130	ASP
1	A	141	VAL
1	A	149	LEU
1	A	188	LEU
1	A	191	THR
1	A	234	LEU
1	A	237	PRO
1	A	252	SER
1	A	304	GLN
1	A	329	THR
1	A	333	MET
1	A	336	VAL
1	B	30	LEU
1	B	56	LEU
1	B	65	LYS
1	B	72	THR
1	B	73	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	77	GLU
1	B	103	THR
1	B	104	GLU
1	B	105	SER
1	B	149	LEU
1	B	213	LEU
1	B	225	SER
1	B	226	ILE
1	B	234	LEU
1	B	278	ASN
1	B	310	GLU
1	B	311	ASP
1	B	325	SER
1	B	333	MET
1	B	336	VAL
1	B	362	HIS
1	B	373	PRO
1	B	375	VAL
1	B	380	GLU
1	C	55	GLN
1	C	68	TYR
1	C	94	THR
1	C	103	THR
1	C	149	LEU
1	C	155	CYS
1	C	234	LEU
1	C	242	GLU
1	C	245	VAL
1	C	246	LYS
1	C	254	THR
1	C	259	ASP
1	C	278	ASN
1	C	300	ILE
1	C	306	LEU
1	C	310	GLU
1	C	328	SER
1	C	329	THR
1	C	331	THR
1	C	336	VAL
1	C	341	PHE
1	C	377	LEU
1	C	386	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	28	ASN
1	A	49	HIS
1	A	111	ASN
1	A	114	ASN
1	A	266	GLN
1	A	271	GLN
1	A	278	ASN
1	A	316	GLN
1	A	326	GLN
1	A	362	HIS
1	B	28	ASN
1	B	55	GLN
1	B	73	GLN
1	B	98	ASN
1	B	111	ASN
1	B	211	GLN
1	B	278	ASN
1	B	294	GLN
1	B	304	GLN
1	B	316	GLN
1	B	326	GLN
1	C	25	GLN
1	C	28	ASN
1	C	45	HIS
1	C	55	GLN
1	C	73	GLN
1	C	111	ASN
1	C	114	ASN
1	C	181	HIS
1	C	211	GLN
1	C	304	GLN
1	C	316	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](#)

3 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	009	B	502	-	48,49,49	1.49	7 (14%)	58,67,67	2.03	7 (12%)
2	009	C	503	-	48,49,49	1.63	10 (20%)	58,67,67	1.93	7 (12%)
2	009	A	501	-	48,49,49	1.68	12 (25%)	58,67,67	1.86	7 (12%)

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	009	B	502	-	-	6/37/51/51	0/5/5/5
2	009	C	503	-	-	10/37/51/51	0/5/5/5
2	009	A	501	-	-	8/37/51/51	0/5/5/5

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	503	009	C51-C30	4.07	1.60	1.55
2	A	501	009	C51-C30	3.77	1.60	1.55
2	A	501	009	C36-N34	2.96	1.51	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	009	C57-C56	2.88	1.44	1.38
2	A	501	009	C30-C	2.80	1.59	1.53
2	B	502	009	C36-N34	2.79	1.51	1.46
2	B	502	009	C35-C30	2.64	1.56	1.53
2	C	503	009	C57-C56	2.48	1.43	1.38
2	C	503	009	C51-C56	2.47	1.55	1.51
2	A	501	009	CA-N	2.44	1.50	1.46
2	B	502	009	C51-C30	2.43	1.58	1.55
2	A	501	009	C23-C24	2.41	1.43	1.38
2	C	503	009	C52-C57	2.34	1.42	1.38
2	A	501	009	C24-C25	2.30	1.43	1.39
2	C	503	009	C55-C56	2.23	1.43	1.38
2	A	501	009	C52-C57	2.20	1.42	1.38
2	C	503	009	C26-C21	2.20	1.43	1.39
2	A	501	009	C-N	2.19	1.38	1.34
2	B	502	009	C42-C41	2.18	1.43	1.38
2	B	502	009	C57-C56	2.16	1.43	1.38
2	C	503	009	C54-C55	2.16	1.42	1.38
2	A	501	009	C54-C55	2.14	1.42	1.38
2	A	501	009	C26-C21	2.12	1.42	1.39
2	C	503	009	CD2-CG	2.10	1.43	1.38
2	A	501	009	C55-C56	2.10	1.43	1.38
2	B	502	009	C26-C21	2.07	1.42	1.39
2	C	503	009	CA-N	2.06	1.49	1.46
2	B	502	009	C54-C53	2.02	1.42	1.38
2	C	503	009	C23-C24	2.01	1.42	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	503	009	C35-N34-C32	-8.40	100.77	111.51
2	B	502	009	C35-N34-C32	-8.08	101.19	111.51
2	A	501	009	C35-N34-C32	-8.03	101.25	111.51
2	C	503	009	C30-N31-C32	-7.97	107.59	113.51
2	A	501	009	C30-N31-C32	-7.89	107.65	113.51
2	B	502	009	C30-N31-C32	-7.25	108.12	113.51
2	B	502	009	N31-C32-N34	5.94	114.15	108.54
2	B	502	009	C41-C36-N34	5.72	122.15	113.15
2	C	503	009	N31-C32-N34	4.95	113.22	108.54
2	A	501	009	N31-C32-N34	4.82	113.09	108.54
2	C	503	009	C41-C36-N34	3.77	119.08	113.15
2	A	501	009	C41-C36-N34	3.60	118.81	113.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	503	009	C1-C2-N2	-3.31	107.61	111.95
2	B	502	009	C30-C51-C56	2.86	119.19	114.94
2	B	502	009	C51-C30-C	-2.82	105.30	109.64
2	B	502	009	CB-CA-N	-2.49	106.54	110.08
2	A	501	009	CG-CB-CA	-2.38	109.36	113.40
2	A	501	009	CB-CA-N	-2.22	106.93	110.08
2	C	503	009	C30-C-N	-2.17	112.83	116.55
2	C	503	009	C30-C51-C56	2.14	118.11	114.94
2	A	501	009	C30-C51-C56	2.12	118.08	114.94

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	503	009	CA-C1-C2-N2
2	C	503	009	OG-C1-C2-N2
2	C	503	009	C35-C30-C51-C56
2	B	502	009	C24-C25-N27-C29
2	B	502	009	C26-C25-N27-C28
2	C	503	009	C24-C25-N27-C29
2	C	503	009	C26-C25-N27-C28
2	B	502	009	C24-C25-N27-C28
2	B	502	009	C26-C25-N27-C29
2	C	503	009	C24-C25-N27-C28
2	C	503	009	C26-C25-N27-C29
2	A	501	009	C24-C25-N27-C29
2	A	501	009	C26-C25-N27-C28
2	A	501	009	C24-C25-N27-C28
2	A	501	009	C26-C25-N27-C29
2	A	501	009	C41-C36-N34-C35
2	C	503	009	C41-C36-N34-C35
2	C	503	009	C21-C20-N2-C2
2	A	501	009	CA-C1-C2-N2
2	C	503	009	C-C30-C51-C56
2	B	502	009	CA-C1-C2-N2
2	A	501	009	C21-C20-N2-C2
2	A	501	009	OG-C1-C2-N2
2	B	502	009	OG-C1-C2-N2

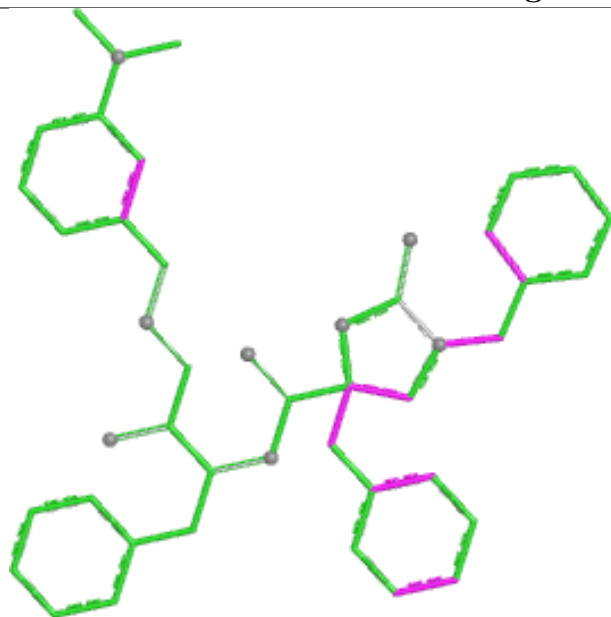
There are no ring outliers.

3 monomers are involved in 7 short contacts:

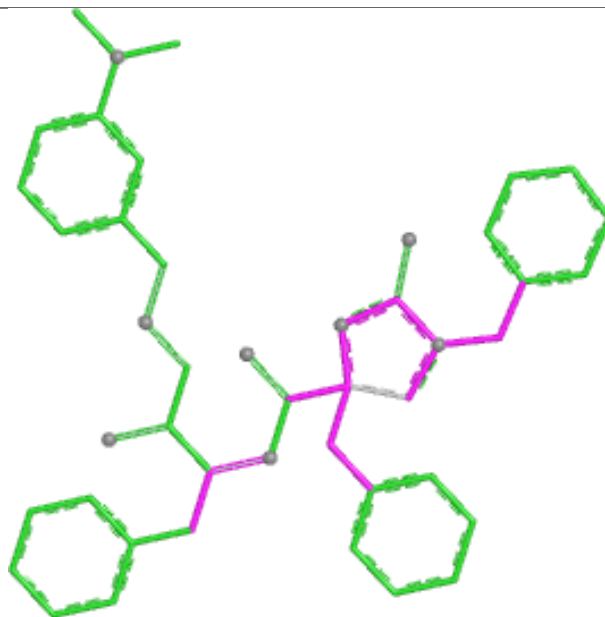
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	009	2	0
2	C	503	009	1	0
2	A	501	009	4	0

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.

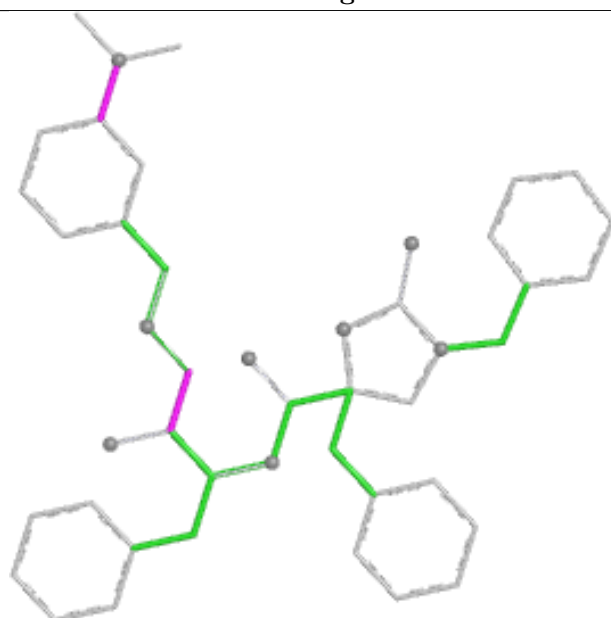
Ligand 009 B 502



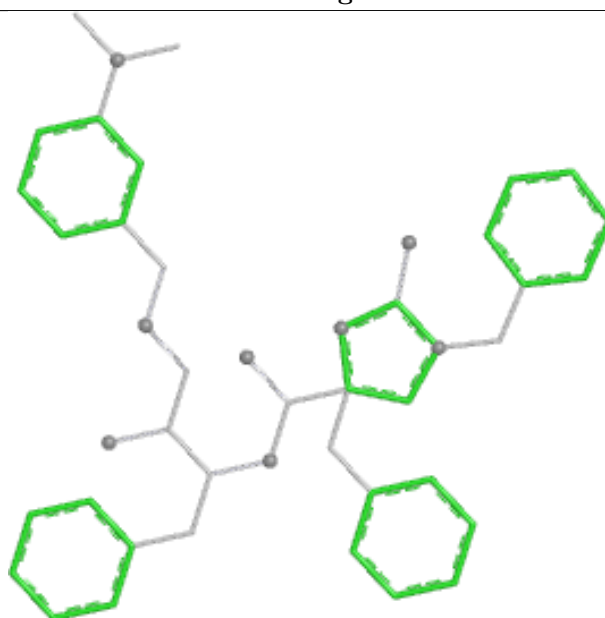
Bond lengths



Bond angles

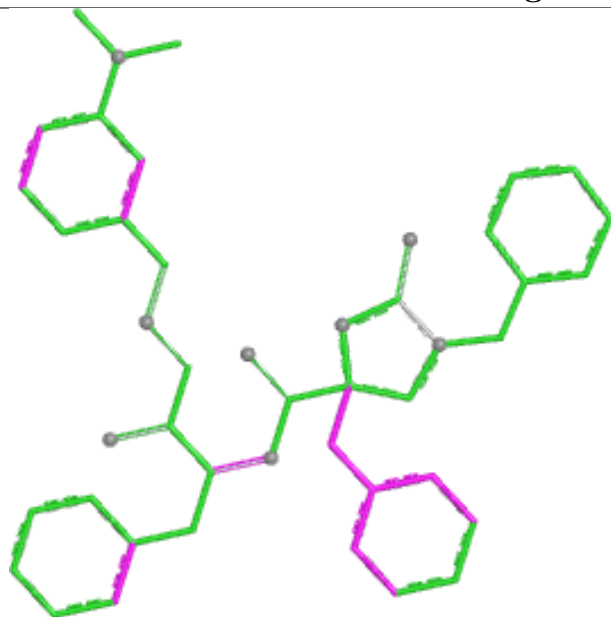


Torsions

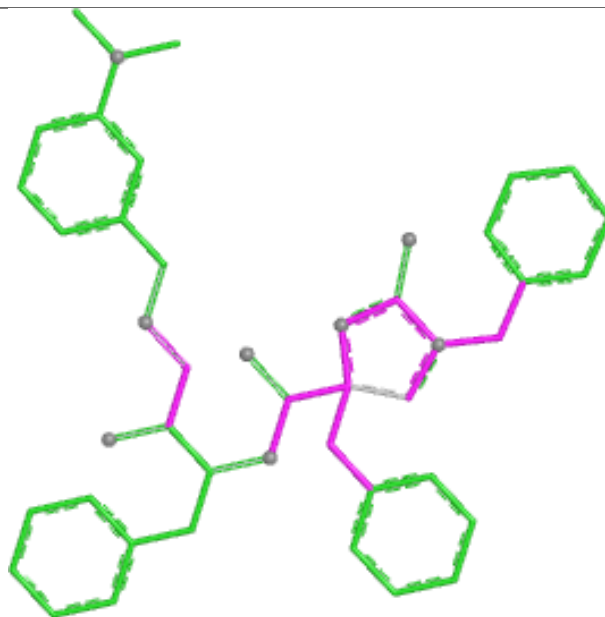


Rings

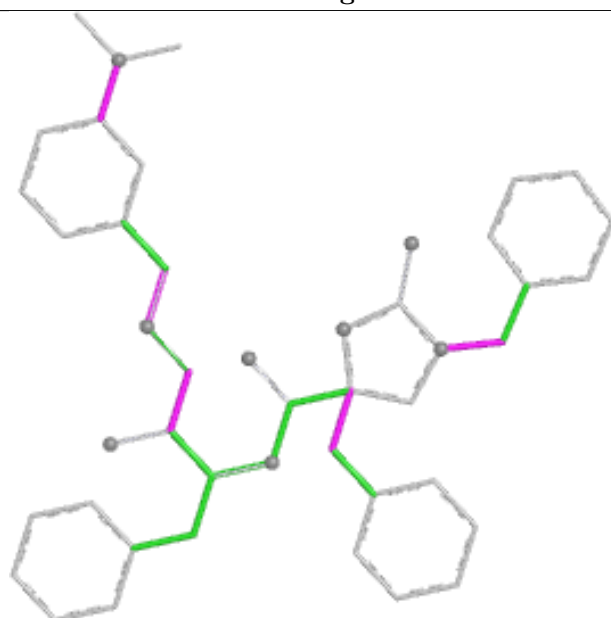
Ligand 009 C 503



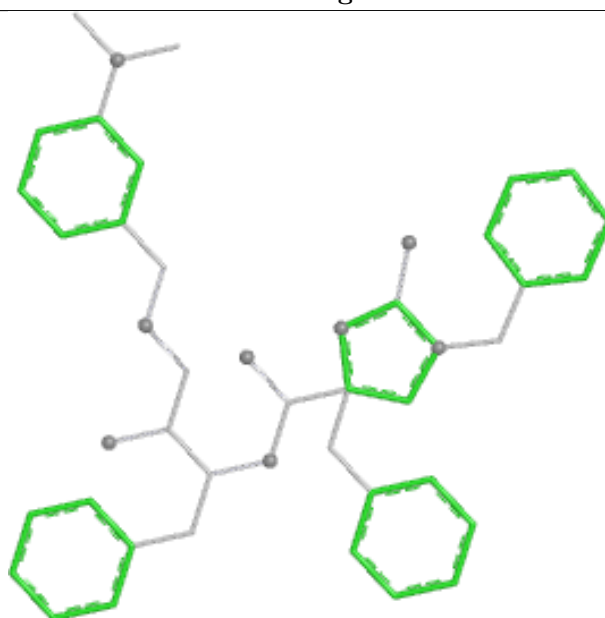
Bond lengths



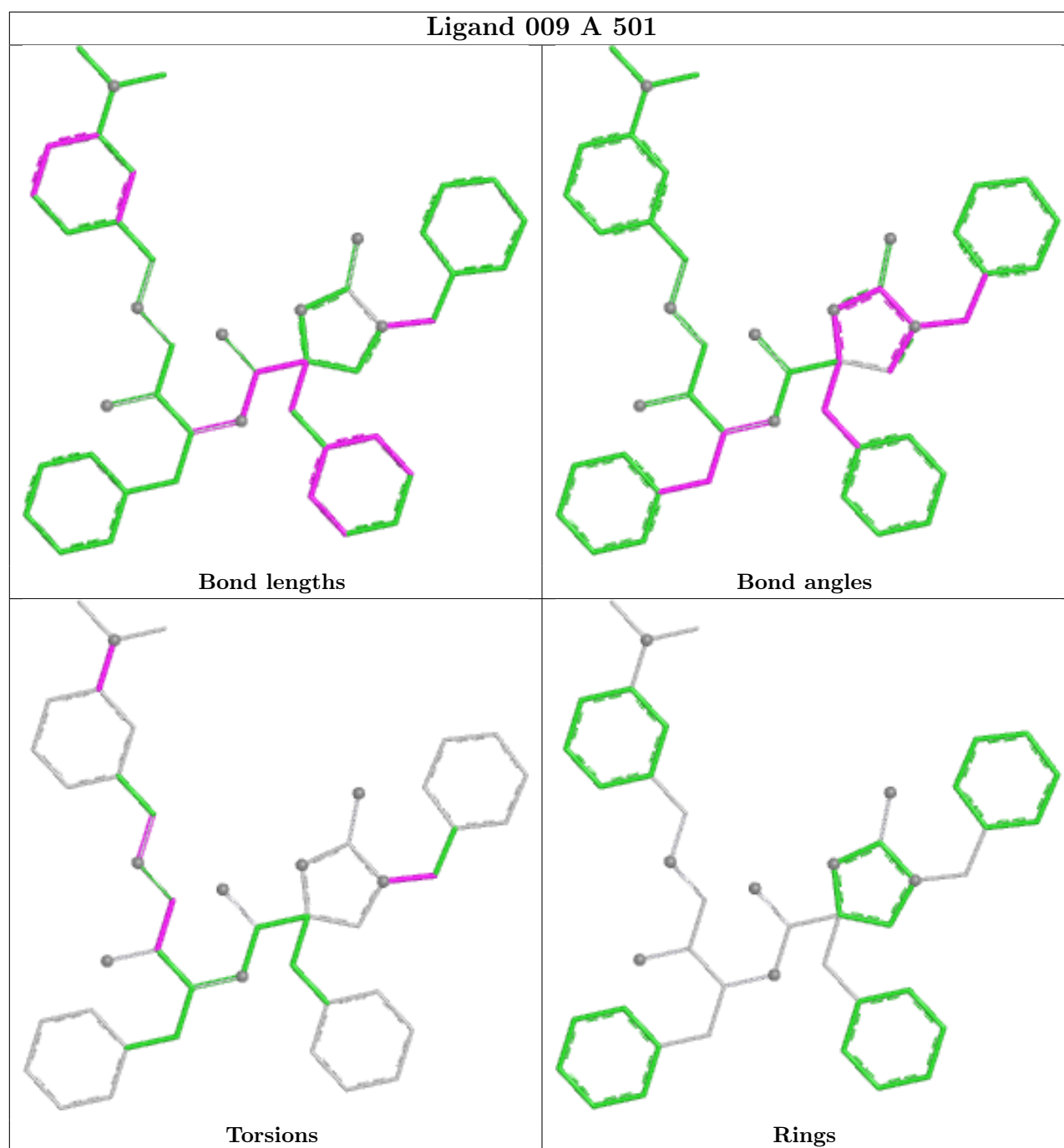
Bond angles



Torsions



Rings



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	379/412 (91%)	-0.00	2 (0%) 87 86	19, 41, 69, 114	0
1	B	377/412 (91%)	0.08	7 (1%) 66 63	25, 45, 79, 99	0
1	C	377/412 (91%)	0.61	24 (6%) 25 22	27, 64, 89, 132	0
All	All	1133/1236 (91%)	0.23	33 (2%) 53 50	19, 48, 84, 132	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	313	ALA	6.6
1	C	222	TYR	3.9
1	B	386	ILE	3.3
1	C	82	THR	3.1
1	B	113	SER	3.1
1	C	384	TYR	3.0
1	A	377	LEU	2.9
1	B	171	GLY	2.8
1	C	314	THR	2.8
1	C	66	GLY	2.7
1	B	359	CYS	2.6
1	C	141	VAL	2.6
1	C	202	ILE	2.4
1	B	112	GLY	2.4
1	C	102	ILE	2.4
1	B	312	VAL	2.4
1	C	221	ASN	2.3
1	C	240	VAL	2.3
1	C	41	GLY	2.2
1	A	380	GLU	2.2
1	B	155	CYS	2.2
1	C	260	GLY	2.2
1	C	126	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	63	LEU	2.1
1	C	386	ILE	2.1
1	C	80	LEU	2.1
1	C	49	HIS	2.1
1	C	201	VAL	2.1
1	C	67	VAL	2.1
1	C	115	TRP	2.0
1	C	315	SER	2.0
1	C	383	GLY	2.0
1	C	68	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

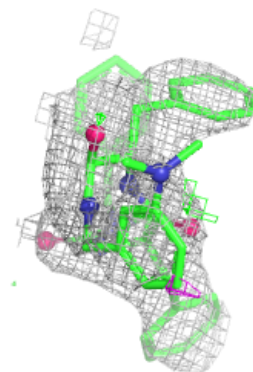
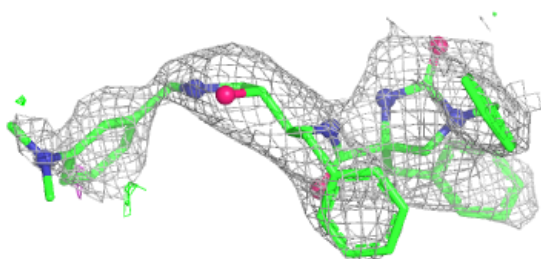
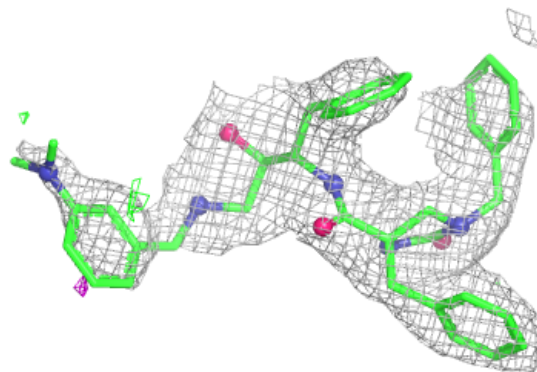
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	009	C	503	45/45	0.83	0.14	69,72,82,83	0
2	009	B	502	45/45	0.87	0.12	42,48,55,56	0
2	009	A	501	45/45	0.88	0.11	38,45,56,56	0

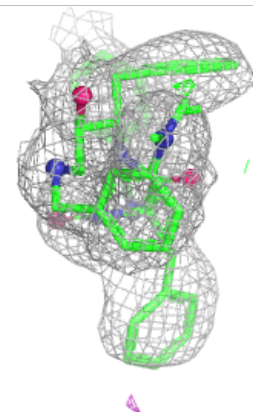
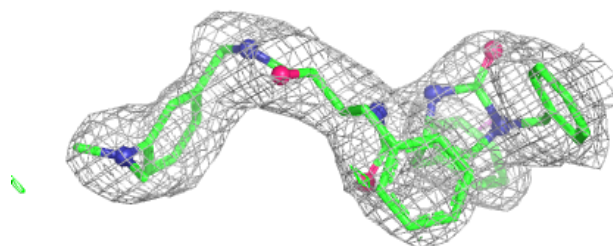
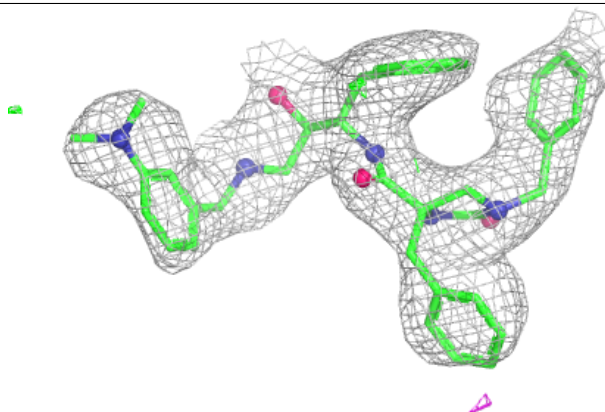
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 009 C 503:

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

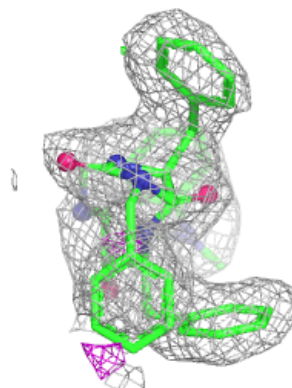
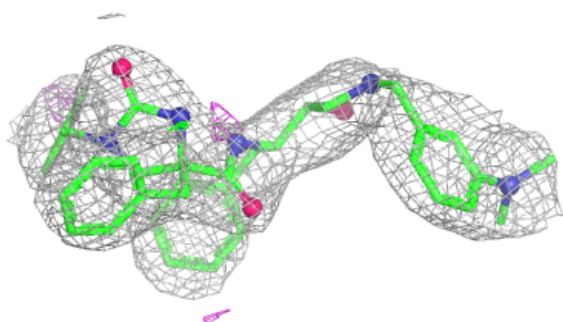
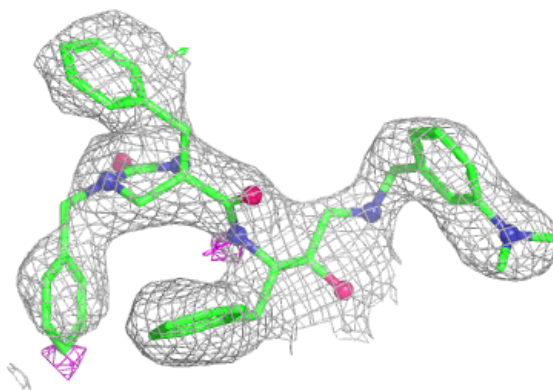
**Electron density around 009 B 502:**

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



Electron density around 009 A 501:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.