



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2023 – 07:45 PM EDT

PDB ID : 4GID
Title : Structure of beta-secretase complexed with inhibitor
Authors : Ghosh, A.; Tang, J.; Venkateswara, R.K.; Yadav, N.; Anderson, D.; Gavande, N.; Huang, X.; Terzyan, S.
Deposited on : 2012-08-08
Resolution : 2.00 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

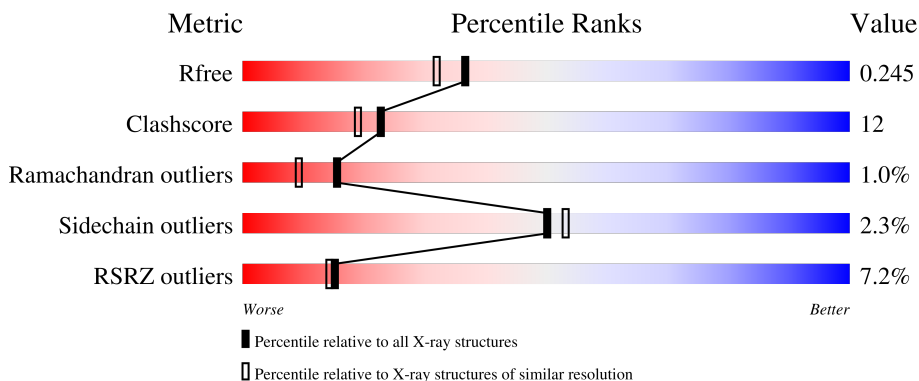
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	388	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div>
1	B	388	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div>
1	C	388	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div>
1	D	388	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div>

2 Entry composition i

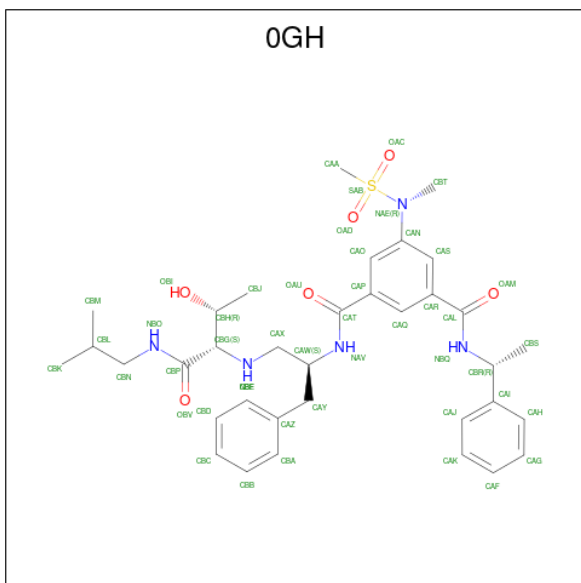
There are 4 unique types of molecules in this entry. The entry contains 13617 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	387	Total 3043	C 1948	N 505	O 576	S 14	6	0	0
1	B	387	Total 3043	C 1948	N 505	O 576	S 14	10	0	0
1	C	388	Total 3049	C 1951	N 506	O 578	S 14	14	0	0
1	D	387	Total 3043	C 1948	N 505	O 576	S 14	18	0	0

- Molecule 2 is N-[(2S)-1-({(2S,3R)-3-hydroxy-1-[(2-methylpropyl)amino]-1-oxobutan-2-yl}amino)-3-phenylpropan-2-yl]-5-[methyl(methylsulfonyl)amino]-N'-[(1R)-1-phenylethyl]benzene-1,3-dicarboxamide (three-letter code: 0GH) (formula: C₃₅H₄₇N₅O₆S).



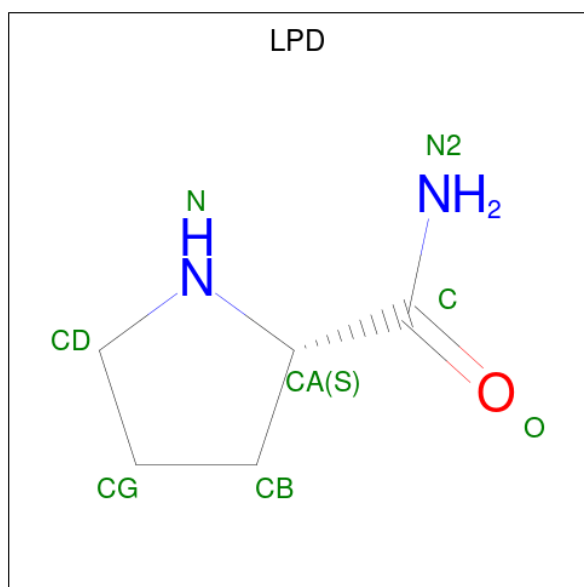
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	Total 47	C 35	N 5	O 6	S 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			47	35	5	6	1		
2	C	1	Total	C	N	O	S	0	0
			47	35	5	6	1		
2	D	1	Total	C	N	O	S	0	0
			47	35	5	6	1		

- Molecule 3 is L-PROLINAMIDE (three-letter code: LPD) (formula: C₅H₁₀N₂O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	5	2	1		
3	B	1	Total	C	N	O	0	0
			8	5	2	1		
3	C	1	Total	C	N	O	0	0
			8	5	2	1		
3	D	1	Total	C	N	O	0	0
			8	5	2	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	316	Total	O	0	0
			316	316		
4	B	279	Total	O	0	0
			279	279		

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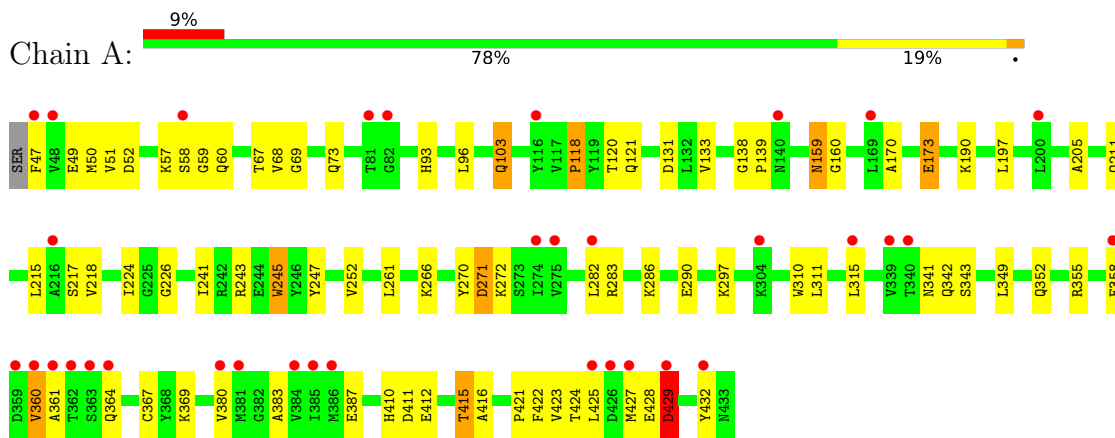
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	330	Total 330	O 330	0	0
4	D	294	Total 294	O 294	0	0

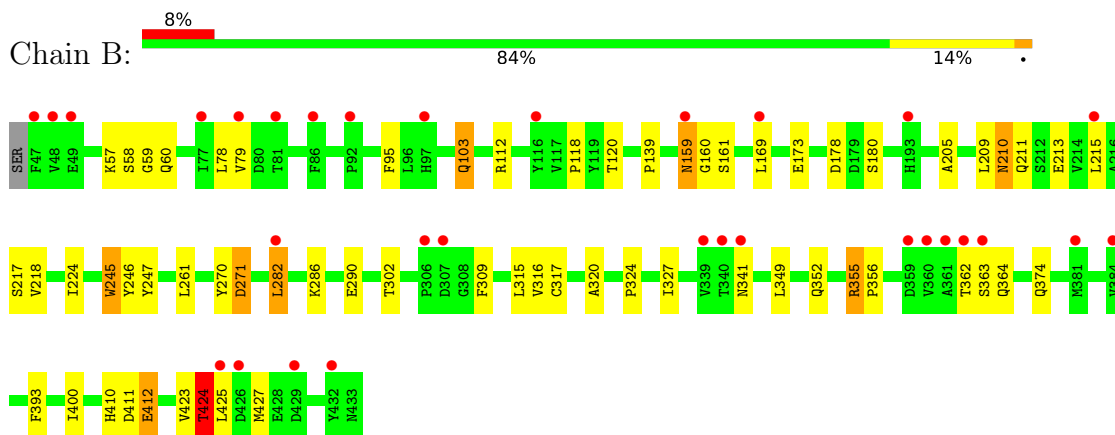
3 Residue-property plots [i](#)

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

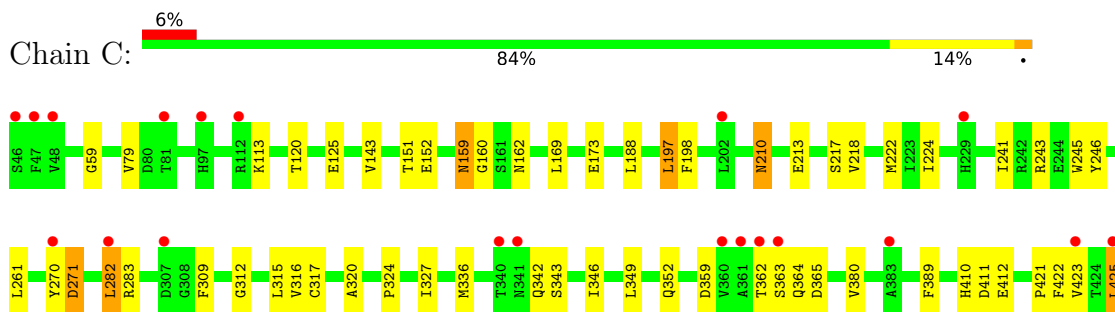
- Molecule 1: Beta-secretase 1

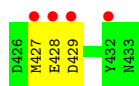


- Molecule 1: Beta-secretase 1

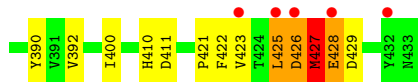
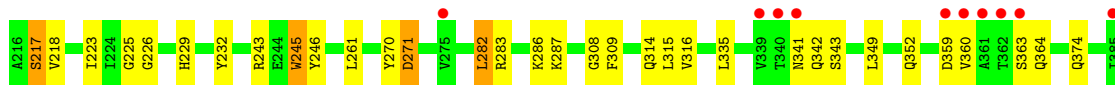
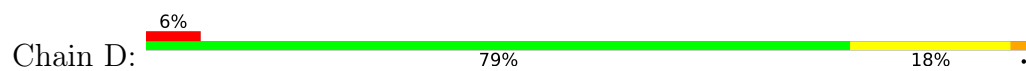


- Molecule 1: Beta-secretase 1





- Molecule 1: Beta-secretase 1



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.43Å 130.35Å 88.40Å 90.00° 97.50° 90.00°	Depositor
Resolution (Å)	34.49 – 2.00 34.49 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.1 (34.49-2.00) 95.1 (34.49-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.00Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.216 , 0.252 0.208 , 0.245	Depositor DCC
R_{free} test set	9185 reflections (7.04%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtrriage
Anisotropy	0.701	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.011 for l,-k,h	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13617	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.31 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4066e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 0GH, LPD

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	0.57	0/3121	0.81	3/4243 (0.1%)
1	B	0.57	0/3121	0.79	2/4243 (0.0%)
1	C	0.59	0/3127	0.81	3/4251 (0.1%)
1	D	0.58	0/3121	0.80	3/4243 (0.1%)
All	All	0.58	0/12490	0.80	11/16980 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	429	ASP	N-CA-C	-8.10	89.12	111.00
1	B	282	LEU	N-CA-C	-6.49	93.47	111.00
1	A	282	LEU	N-CA-C	-6.47	93.52	111.00
1	C	282	LEU	N-CA-C	-6.36	93.82	111.00
1	D	282	LEU	N-CA-C	-6.20	94.27	111.00
1	D	427	MET	N-CA-C	5.51	125.87	111.00
1	D	390	TYR	N-CA-C	-5.38	96.49	111.00
1	A	241	ILE	N-CA-C	-5.37	96.50	111.00
1	C	246	TYR	N-CA-C	-5.20	96.97	111.00
1	B	246	TYR	N-CA-C	-5.16	97.07	111.00
1	C	241	ILE	N-CA-C	-5.02	97.45	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3043	0	2951	80	0
1	B	3043	0	2951	64	0
1	C	3049	0	2956	59	0
1	D	3043	0	2951	71	0
2	A	47	0	47	5	0
2	B	47	0	47	4	0
2	C	47	0	47	4	0
2	D	47	0	47	8	0
3	A	8	0	10	3	0
3	B	8	0	10	3	0
3	C	8	0	10	2	0
3	D	8	0	10	2	0
4	A	316	0	0	7	0
4	B	279	0	0	10	0
4	C	330	0	0	5	0
4	D	294	0	0	7	0
All	All	13617	0	12037	281	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (281) 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)
2:D:501:0GH:CBN	2:D:501:0GH:CBL	1.76	1.56
1:A:425:LEU:HD22	1:A:427:MET:HE3	1.32	1.11
1:A:360:VAL:HG12	1:A:361:ALA:H	1.29	0.96
1:B:60:GLN:HE21	1:B:161:SER:HA	1.33	0.93
1:A:103:GLN:H	1:A:103:GLN:HE21	1.16	0.93
1:B:103:GLN:H	1:B:103:GLN:HE21	1.18	0.91
1:A:343:SER:HB3	1:A:427:MET:CE	2.02	0.89
1:B:57:LYS:HE3	4:B:806:HOH:O	1.70	0.89
1:A:355:ARG:HH21	1:A:369:LYS:HD3	1.39	0.88
1:A:425:LEU:HD12	1:A:425:LEU:O	1.76	0.85
1:B:412:GLU:H	1:B:412:GLU:CD	1.77	0.85
1:B:159:ASN:HD22	1:B:160:GLY:N	1.77	0.82
1:A:266:LYS:HG3	1:A:429:ASP:O	1.79	0.82
1:C:422:PHE:O	1:C:425:LEU:HD11	1.80	0.80
1:C:210:ASN:HD22	1:C:210:ASN:C	1.85	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:MET:HG2	1:A:138:GLY:HA2	1.63	0.80
1:A:343:SER:HB3	1:A:427:MET:HE3	1.63	0.80
1:D:210:ASN:ND2	1:D:213:GLU:H	1.81	0.79
1:A:355:ARG:NH2	1:A:369:LYS:HD3	1.98	0.79
1:D:270:TYR:O	1:D:271:ASP:HB3	1.83	0.78
1:C:210:ASN:ND2	1:C:213:GLU:HG3	1.97	0.78
2:D:501:0GH:CBL	2:D:501:0GH:NBO	2.49	0.76
1:C:120:THR:OG1	2:C:501:0GH:H14	1.85	0.76
1:D:210:ASN:C	1:D:210:ASN:HD22	1.89	0.75
2:B:501:0GH:H15	4:B:879:HOH:O	1.87	0.74
1:D:243:ARG:HD3	4:D:718:HOH:O	1.87	0.74
2:D:501:0GH:CBN	2:D:501:0GH:CBM	2.64	0.74
1:A:349:LEU:H	1:A:352:GLN:HE21	1.36	0.73
1:A:103:GLN:H	1:A:103:GLN:NE2	1.86	0.73
1:A:415:THR:HG23	1:A:416:ALA:O	1.88	0.73
1:D:425:LEU:HD22	1:D:427:MET:SD	2.29	0.73
1:D:120:THR:OG1	2:D:501:0GH:H14	1.87	0.73
1:A:315:LEU:HD23	1:A:315:LEU:H	1.54	0.72
1:A:360:VAL:HG12	1:A:361:ALA:N	2.03	0.72
1:B:286:LYS:NZ	1:B:374:GLN:HE22	1.87	0.72
1:A:343:SER:HB3	1:A:427:MET:HE1	1.69	0.71
1:A:286:LYS:HE3	1:A:290:GLU:OE2	1.90	0.71
1:B:112:ARG:NH1	4:B:770:HOH:O	2.22	0.70
1:D:343:SER:OG	1:D:425:LEU:HD23	1.90	0.70
1:B:286:LYS:HZ3	1:B:374:GLN:HE22	1.37	0.70
1:B:217:SER:HB3	3:B:502:LPD:H	1.56	0.69
1:C:359:ASP:OD2	1:C:365:ASP:HB2	1.91	0.69
1:A:120:THR:OG1	2:A:501:0GH:H14	1.93	0.68
1:B:210:ASN:C	1:B:210:ASN:HD22	1.97	0.68
1:D:349:LEU:H	1:D:352:GLN:HE21	1.40	0.68
1:B:349:LEU:H	1:B:352:GLN:HE21	1.41	0.68
1:C:349:LEU:H	1:C:352:GLN:HE21	1.41	0.68
1:D:270:TYR:O	1:D:271:ASP:CB	2.42	0.67
1:A:410:HIS:HD2	1:A:411:ASP:O	1.78	0.66
1:D:426:ASP:O	1:D:427:MET:HB2	1.95	0.65
1:D:193:HIS:H	1:D:193:HIS:CD2	2.14	0.65
1:B:120:THR:OG1	2:B:501:0GH:H14	1.96	0.64
1:B:210:ASN:ND2	1:B:213:GLU:HG3	2.12	0.64
1:B:60:GLN:HE21	1:B:161:SER:CA	2.07	0.64
1:B:423:VAL:HG23	1:B:424:THR:N	2.13	0.63
1:D:349:LEU:H	1:D:352:GLN:NE2	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:GLN:O	1:A:215:LEU:HG	1.98	0.63
2:C:501:OGH:H15	4:C:701:HOH:O	1.98	0.63
1:A:60:GLN:HA	1:A:60:GLN:NE2	2.14	0.62
1:A:271:ASP:OD1	1:A:272:LYS:HG2	2.00	0.62
1:C:428:GLU:HG3	1:C:429:ASP:OD1	2.00	0.61
1:D:55:ARG:HH21	1:D:215:LEU:HA	1.65	0.61
1:A:217:SER:HB3	3:A:502:LPD:H	1.64	0.61
1:B:423:VAL:HG23	1:B:424:THR:H	1.65	0.61
1:D:55:ARG:HD3	4:D:760:HOH:O	1.99	0.61
1:B:349:LEU:H	1:B:352:GLN:NE2	1.98	0.61
1:D:341:ASN:O	1:D:425:LEU:HD11	2.00	0.61
1:D:342:GLN:HG3	1:D:421:PRO:HB2	1.83	0.61
1:A:159:ASN:HD22	1:A:160:GLY:N	1.99	0.61
1:A:349:LEU:H	1:A:352:GLN:NE2	1.99	0.61
1:C:343:SER:HB3	1:C:425:LEU:HD13	1.83	0.61
1:B:410:HIS:HD2	1:B:411:ASP:O	1.83	0.60
1:C:349:LEU:H	1:C:352:GLN:NE2	1.99	0.60
1:B:286:LYS:HD3	1:B:374:GLN:OE1	2.02	0.60
1:D:217:SER:HB2	3:D:502:LPD:H	1.66	0.60
1:C:309:PHE:CD1	1:C:316:VAL:HG23	2.37	0.60
1:C:218:VAL:O	3:C:502:LPD:HA	2.02	0.59
1:D:218:VAL:O	3:D:502:LPD:HA	2.02	0.59
1:C:343:SER:HB3	1:C:427:MET:CE	2.33	0.58
1:D:229:HIS:HA	1:D:232:TYR:CE1	2.38	0.58
1:B:103:GLN:HE21	1:B:103:GLN:N	1.96	0.58
1:C:210:ASN:ND2	1:C:213:GLU:H	2.02	0.58
1:A:139:PRO:HD3	1:A:224:ILE:HB	1.86	0.57
1:B:210:ASN:HD21	1:B:213:GLU:HG3	1.69	0.57
1:C:210:ASN:C	1:C:210:ASN:ND2	2.57	0.57
1:B:218:VAL:O	3:B:502:LPD:HA	2.05	0.56
1:C:113:LYS:NZ	4:C:703:HOH:O	2.33	0.56
1:A:341:ASN:O	1:A:425:LEU:HD11	2.06	0.56
1:A:422:PHE:O	1:A:425:LEU:HD21	2.05	0.56
1:D:193:HIS:H	1:D:193:HIS:HD2	1.53	0.56
1:D:213:GLU:O	1:D:217:SER:OG	2.23	0.56
1:B:393:PHE:HE2	4:B:817:HOH:O	1.89	0.56
1:A:315:LEU:HD12	1:A:367:CYS:HB3	1.88	0.56
1:A:360:VAL:CG1	1:A:361:ALA:H	2.12	0.56
1:B:159:ASN:HD22	1:B:159:ASN:C	2.08	0.56
1:A:358:GLU:HG3	1:A:360:VAL:O	2.05	0.55
1:D:425:LEU:N	1:D:425:LEU:HD12	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:LEU:C	1:D:197:LEU:HD23	2.26	0.55
1:D:93:HIS:CG	1:D:94:PRO:HD2	2.42	0.55
1:B:60:GLN:NE2	1:B:161:SER:HA	2.13	0.55
2:A:501:OGH:H15	4:A:692:HOH:O	2.07	0.55
1:C:197:LEU:HD23	1:C:197:LEU:C	2.27	0.55
1:D:422:PHE:O	1:D:425:LEU:HD21	2.07	0.55
1:D:210:ASN:HD21	1:D:213:GLU:H	1.54	0.54
1:C:428:GLU:HG3	1:C:429:ASP:N	2.23	0.54
1:B:363:SER:HB2	4:B:749:HOH:O	2.08	0.53
1:B:412:GLU:CD	1:B:412:GLU:N	2.55	0.53
1:D:176:ARG:HD2	4:D:752:HOH:O	2.08	0.53
1:A:270:TYR:O	1:A:271:ASP:HB3	2.09	0.53
1:C:312:GLY:HA3	4:C:725:HOH:O	2.08	0.53
1:C:359:ASP:OD2	1:C:363:SER:OG	2.26	0.53
1:A:315:LEU:H	1:A:315:LEU:CD2	2.21	0.53
1:B:103:GLN:H	1:B:103:GLN:NE2	1.97	0.53
1:D:286:LYS:HD3	1:D:374:GLN:OE1	2.08	0.53
1:B:362:THR:HG22	1:B:362:THR:O	2.09	0.53
1:A:103:GLN:HE21	1:A:103:GLN:N	1.98	0.53
1:A:205:ALA:HB2	3:A:502:LPD:HB3	1.90	0.53
1:A:297:LYS:HE2	1:A:310:TRP:CD1	2.44	0.53
1:C:343:SER:HB3	1:C:427:MET:HE1	1.91	0.53
1:D:428:GLU:N	4:D:787:HOH:O	2.42	0.53
2:B:501:OGH:CBJ	4:B:879:HOH:O	2.51	0.52
1:C:243:ARG:HD3	4:C:780:HOH:O	2.07	0.52
1:A:173:GLU:OE2	1:A:243:ARG:NH1	2.43	0.52
1:D:423:VAL:HG12	1:D:423:VAL:O	2.10	0.52
1:B:320:ALA:HB2	1:B:364:GLN:O	2.09	0.52
1:A:60:GLN:HG3	4:A:849:HOH:O	2.10	0.51
1:A:364:GLN:OE1	1:A:364:GLN:HA	2.11	0.51
1:C:410:HIS:HD2	1:C:411:ASP:O	1.93	0.51
1:B:60:GLN:NE2	1:B:160:GLY:O	2.44	0.51
1:C:197:LEU:HD23	1:C:198:PHE:N	2.26	0.51
1:C:336:MET:HA	1:C:427:MET:CE	2.40	0.50
1:D:93:HIS:ND1	1:D:94:PRO:HD2	2.26	0.50
1:B:247:TYR:HB3	1:B:400:ILE:HD11	1.92	0.50
1:D:335:LEU:O	1:D:343:SER:HB2	2.11	0.50
1:C:315:LEU:HD13	1:C:317:CYS:SG	2.51	0.50
1:D:79:VAL:HG13	1:D:169:LEU:HD11	1.94	0.50
1:D:48:VAL:HG23	1:D:49:GLU:N	2.27	0.50
1:B:178:ASP:OD2	1:B:180:SER:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:GLN:O	1:B:215:LEU:HG	2.12	0.49
1:D:210:ASN:ND2	1:D:210:ASN:C	2.63	0.49
1:D:199:SER:OG	1:D:223:ILE:HB	2.13	0.49
1:A:59:GLY:C	1:A:60:GLN:HE21	2.15	0.49
1:C:222:MET:SD	1:C:224:ILE:HD11	2.52	0.49
1:D:286:LYS:CD	1:D:374:GLN:OE1	2.60	0.49
1:C:362:THR:O	1:C:362:THR:HG22	2.12	0.49
1:C:423:VAL:HG12	1:C:423:VAL:O	2.12	0.49
1:B:95:PHE:CE1	1:B:159:ASN:HB2	2.47	0.48
1:D:98:ARG:HG2	1:D:164:GLU:OE2	2.12	0.48
1:A:50:MET:CG	1:A:138:GLY:HA2	2.38	0.48
1:C:59:GLY:C	2:C:501:0GH:H44	2.33	0.48
1:D:309:PHE:CD1	1:D:316:VAL:HG23	2.48	0.48
1:C:270:TYR:O	1:C:271:ASP:CB	2.61	0.48
2:D:501:0GH:CBN	2:D:501:0GH:CBK	2.80	0.48
1:C:210:ASN:HD21	1:C:213:GLU:HG3	1.75	0.48
1:D:47:PHE:CZ	1:D:226:GLY:HA3	2.49	0.48
2:D:501:0GH:H15	4:D:713:HOH:O	2.13	0.48
1:B:58:SER:HA	4:B:739:HOH:O	2.13	0.47
1:A:270:TYR:O	1:A:271:ASP:CB	2.62	0.47
1:B:178:ASP:OD2	1:B:180:SER:CB	2.63	0.47
1:C:342:GLN:HG2	1:C:421:PRO:HB2	1.97	0.47
1:A:159:ASN:HD22	1:A:160:GLY:H	1.63	0.47
1:B:57:LYS:NZ	1:B:209:LEU:H	2.12	0.47
1:D:308:GLY:C	1:D:314:GLN:HG2	2.35	0.47
1:C:125:GLU:OE2	1:C:152:GLU:OE1	2.33	0.47
1:D:261:LEU:HD12	1:D:261:LEU:HA	1.79	0.47
1:A:423:VAL:N	1:C:412:GLU:OE2	2.36	0.47
1:B:59:GLY:H	2:B:501:0GH:H45	1.79	0.47
1:B:302:THR:HG23	4:B:702:HOH:O	2.15	0.47
1:B:315:LEU:HD13	1:B:317:CYS:SG	2.54	0.47
1:B:210:ASN:ND2	1:B:213:GLU:H	2.13	0.47
1:C:79:VAL:HG13	1:C:169:LEU:CD1	2.45	0.47
1:D:79:VAL:HG13	1:D:169:LEU:CD1	2.44	0.47
1:D:410:HIS:HD2	1:D:411:ASP:O	1.97	0.47
1:B:324:PRO:O	1:B:327:ILE:HG12	2.15	0.47
1:D:161:SER:HB2	1:D:163:TRP:CD1	2.50	0.47
1:D:197:LEU:HD23	1:D:198:PHE:N	2.30	0.47
1:A:59:GLY:O	1:A:60:GLN:NE2	2.47	0.46
1:A:60:GLN:HB3	4:A:672:HOH:O	2.15	0.46
1:A:93:HIS:HB3	1:A:96:LEU:HG	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:LEU:HD12	1:C:261:LEU:HA	1.78	0.46
1:C:283:ARG:HB2	1:C:380:VAL:HB	1.97	0.46
1:D:55:ARG:NH2	1:D:215:LEU:O	2.48	0.46
1:A:218:VAL:O	3:A:502:LPD:HA	2.16	0.46
1:A:173:GLU:HG2	1:A:245:TRP:HB2	1.97	0.46
1:A:342:GLN:HG3	1:A:421:PRO:HB2	1.98	0.46
1:A:422:PHE:O	1:A:425:LEU:CD2	2.64	0.46
1:C:343:SER:CB	1:C:425:LEU:HD13	2.45	0.46
1:C:336:MET:HA	1:C:427:MET:HE1	1.99	0.45
1:A:360:VAL:CG1	1:A:361:ALA:N	2.77	0.45
1:B:57:LYS:HG2	1:B:60:GLN:OE1	2.16	0.45
1:C:422:PHE:HB2	1:C:425:LEU:HD21	1.96	0.45
1:D:211:GLN:O	1:D:215:LEU:HG	2.16	0.45
1:A:315:LEU:HD23	1:A:315:LEU:N	2.29	0.45
1:A:383:ALA:O	1:A:387:GLU:HG3	2.16	0.45
1:B:79:VAL:HG13	1:B:169:LEU:CD1	2.46	0.45
1:B:425:LEU:N	1:B:425:LEU:CD1	2.79	0.45
1:D:178:ASP:OD1	1:D:180:SER:OG	2.25	0.45
1:C:346:ILE:HB	1:C:389:PHE:CZ	2.51	0.45
1:A:57:LYS:HG2	1:A:58:SER:N	2.32	0.45
1:A:252:VAL:HG21	1:A:427:MET:CE	2.47	0.45
1:B:364:GLN:C	4:B:769:HOH:O	2.55	0.45
1:A:69:GLY:HA2	1:A:131:ASP:OD1	2.16	0.45
1:C:151:THR:O	1:C:152:GLU:HG3	2.16	0.45
1:D:59:GLY:C	2:D:501:OGH:H44	2.37	0.44
1:D:283:ARG:HD2	2:D:501:OGH:H33	1.99	0.44
1:A:49:GLU:HG2	4:A:798:HOH:O	2.18	0.44
1:D:359:ASP:OD2	1:D:363:SER:OG	2.35	0.44
1:A:266:LYS:NZ	1:A:429:ASP:O	2.46	0.44
1:D:173:GLU:O	1:D:173:GLU:HG3	2.15	0.44
1:B:270:TYR:O	1:B:271:ASP:CB	2.65	0.44
1:C:217:SER:HB2	3:C:502:LPD:H	1.83	0.44
1:D:193:HIS:CD2	1:D:193:HIS:N	2.83	0.44
1:B:178:ASP:OD2	1:B:180:SER:HB3	2.18	0.44
1:D:161:SER:O	1:D:162:ASN:HB2	2.18	0.44
1:A:283:ARG:HD2	2:A:501:OGH:H33	1.98	0.44
1:C:315:LEU:C	1:C:315:LEU:HD12	2.38	0.43
1:B:261:LEU:HD12	1:B:261:LEU:HA	1.91	0.43
1:D:427:MET:HB3	1:D:428:GLU:H	1.38	0.43
1:A:121:GLN:O	2:A:501:OGH:H27	2.19	0.43
1:D:359:ASP:OD1	1:D:360:VAL:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:LEU:H	1:A:425:LEU:HG	1.49	0.43
1:B:423:VAL:CG2	1:B:424:THR:H	2.30	0.43
1:B:425:LEU:N	1:B:425:LEU:HD12	2.33	0.43
1:D:47:PHE:HD2	1:D:50:MET:CE	2.31	0.43
1:D:425:LEU:O	1:D:426:ASP:O	2.36	0.43
1:B:173:GLU:HG2	1:B:245:TRP:HB3	2.00	0.43
1:B:341:ASN:HA	1:B:427:MET:HE3	2.00	0.43
1:C:428:GLU:HG3	1:C:429:ASP:H	1.82	0.43
1:D:245:TRP:CG	1:D:246:TYR:N	2.87	0.43
1:D:392:VAL:O	1:D:400:ILE:HA	2.19	0.43
1:A:432:TYR:HB2	4:A:892:HOH:O	2.19	0.42
1:B:423:VAL:CG2	1:B:424:THR:N	2.81	0.42
1:A:51:VAL:O	1:A:52:ASP:HB2	2.19	0.42
1:B:355:ARG:HA	1:B:356:PRO:HD3	1.67	0.42
1:C:423:VAL:O	1:C:423:VAL:CG1	2.67	0.42
1:A:283:ARG:HB2	1:A:380:VAL:HB	2.02	0.42
1:A:412:GLU:CD	1:C:423:VAL:H	2.22	0.42
1:B:270:TYR:O	1:B:271:ASP:HB2	2.19	0.42
1:A:261:LEU:HD12	1:A:261:LEU:HA	1.94	0.42
1:B:423:VAL:O	1:B:424:THR:C	2.57	0.42
1:C:159:ASN:HD22	1:C:160:GLY:N	2.18	0.42
1:B:309:PHE:CD1	1:B:316:VAL:HG23	2.53	0.42
1:C:270:TYR:O	1:C:271:ASP:HB3	2.20	0.42
1:C:324:PRO:O	1:C:327:ILE:HG12	2.19	0.42
1:A:59:GLY:N	2:A:501:0GH:H45	2.35	0.42
1:B:205:ALA:HB2	3:B:502:LPD:HB3	2.02	0.42
1:B:374:GLN:HG2	4:B:783:HOH:O	2.20	0.42
1:C:320:ALA:HB2	1:C:364:GLN:O	2.20	0.42
1:D:210:ASN:HD22	1:D:213:GLU:H	1.62	0.42
1:D:183:PRO:HB2	1:D:186:ASP:OD1	2.19	0.42
1:A:68:VAL:HG12	1:A:133:VAL:HG22	2.01	0.42
1:B:79:VAL:HG13	1:B:169:LEU:HD12	2.02	0.42
1:D:96:LEU:HD21	1:D:157:PHE:CD1	2.54	0.42
1:A:67:THR:HA	1:A:73:GLN:O	2.20	0.41
1:A:197:LEU:HD23	1:A:197:LEU:C	2.40	0.41
1:A:424:THR:HG23	1:C:412:GLU:OE1	2.21	0.41
1:B:286:LYS:NZ	1:B:290:GLU:OE2	2.47	0.41
1:A:60:GLN:NE2	1:A:60:GLN:CA	2.82	0.41
1:C:79:VAL:HG13	1:C:169:LEU:HD11	2.01	0.41
1:D:55:ARG:NH2	4:D:869:HOH:O	2.53	0.41
1:A:47:PHE:CZ	1:A:226:GLY:HA3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LYS:HG2	4:A:892:HOH:O	2.19	0.41
1:C:143:VAL:HG11	1:C:188:LEU:HD12	2.02	0.41
1:C:429:ASP:OD1	1:C:429:ASP:N	2.52	0.41
1:D:197:LEU:O	1:D:225:GLY:N	2.53	0.41
1:C:342:GLN:CG	1:C:421:PRO:HB2	2.51	0.41
2:C:501:0GH:CBJ	4:C:701:HOH:O	2.63	0.41
1:A:118:PRO:O	1:A:118:PRO:HG2	2.21	0.41
1:D:427:MET:O	1:D:428:GLU:C	2.59	0.41
1:D:47:PHE:CD1	1:D:47:PHE:N	2.88	0.41
1:A:170:ALA:HA	1:A:247:TYR:CE2	2.55	0.40
1:A:355:ARG:HH21	1:A:369:LYS:CD	2.23	0.40
1:C:173:GLU:OE2	1:C:243:ARG:NH1	2.54	0.40
1:C:315:LEU:HD12	1:C:315:LEU:O	2.21	0.40
1:D:210:ASN:HD21	1:D:212:SER:HB2	1.85	0.40
1:A:190:LYS:NZ	4:A:746:HOH:O	2.55	0.40
1:C:422:PHE:O	1:C:425:LEU:CD1	2.62	0.40
1:D:287:LYS:HE3	4:D:839:HOH:O	2.21	0.40
1:A:311:LEU:HD23	1:A:311:LEU:HA	1.93	0.40
1:B:139:PRO:HD3	1:B:224:ILE:HB	2.02	0.40
1:D:342:GLN:CG	1:D:421:PRO:HB2	2.51	0.40

There are no symmetry-related clashes.

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	385/388 (99%)	369 (96%)	11 (3%)	5 (1%)	12 6
1	B	385/388 (99%)	372 (97%)	10 (3%)	3 (1%)	19 13
1	C	386/388 (100%)	373 (97%)	12 (3%)	1 (0%)	41 37
1	D	385/388 (99%)	370 (96%)	9 (2%)	6 (2%)	9 4
All	All	1541/1552 (99%)	1484 (96%)	42 (3%)	15 (1%)	15 9

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	271	ASP
1	A	360	VAL
1	A	428	GLU
1	A	429	ASP
1	B	271	ASP
1	B	424	THR
1	C	271	ASP
1	D	271	ASP
1	D	426	ASP
1	D	427	MET
1	D	428	GLU
1	D	429	ASP
1	D	48	VAL
1	B	118	PRO
1	A	118	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	330/331 (100%)	325 (98%)	5 (2%)	65 69
1	B	330/331 (100%)	321 (97%)	9 (3%)	44 46
1	C	331/331 (100%)	324 (98%)	7 (2%)	53 57
1	D	330/331 (100%)	320 (97%)	10 (3%)	41 41
All	All	1321/1324 (100%)	1290 (98%)	31 (2%)	50 53

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	159	ASN
1	A	173	GLU
1	A	245	TRP
1	A	415	THR

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Mol	Chain	Res	Type
1	B	78	LEU
1	B	103	GLN
1	B	159	ASN
1	B	210	ASN
1	B	245	TRP
1	B	282	LEU
1	B	355	ARG
1	B	412	GLU
1	B	424	THR
1	C	159	ASN
1	C	162	ASN
1	C	197	LEU
1	C	210	ASN
1	C	245	TRP
1	C	282	LEU
1	C	425	LEU
1	D	78	LEU
1	D	173	GLU
1	D	193	HIS
1	D	210	ASN
1	D	217	SER
1	D	245	TRP
1	D	282	LEU
1	D	315	LEU
1	D	364	GLN
1	D	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	76	ASN
1	A	103	GLN
1	A	159	ASN
1	A	352	GLN
1	A	410	HIS
1	B	60	GLN
1	B	76	ASN
1	B	103	GLN
1	B	159	ASN
1	B	210	ASN
1	B	352	GLN

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Mol	Chain	Res	Type
1	B	374	GLN
1	B	410	HIS
1	C	76	ASN
1	C	159	ASN
1	C	210	ASN
1	C	352	GLN
1	C	410	HIS
1	D	60	GLN
1	D	76	ASN
1	D	97	HIS
1	D	121	GLN
1	D	193	HIS
1	D	210	ASN
1	D	259	GLN
1	D	352	GLN
1	D	410	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	0GH	D	501	-	48,49,49	2.36	9 (18%)	63,68,68	2.01	8 (12%)
3	LPD	C	502	-	8,8,8	0.81	0	10,10,10	1.96	1 (10%)
2	0GH	B	501	-	48,49,49	2.18	7 (14%)	63,68,68	1.64	5 (7%)
2	0GH	A	501	-	48,49,49	2.19	7 (14%)	63,68,68	1.60	6 (9%)
3	LPD	B	502	-	8,8,8	1.24	1 (12%)	10,10,10	1.47	1 (10%)
3	LPD	A	502	-	8,8,8	1.10	1 (12%)	10,10,10	1.49	1 (10%)
3	LPD	D	502	-	8,8,8	0.88	1 (12%)	10,10,10	1.88	1 (10%)
2	0GH	C	501	-	48,49,49	2.14	7 (14%)	63,68,68	1.48	5 (7%)

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	0GH	D	501	-	-	9/52/52/52	0/3/3/3
3	LPD	C	502	-	-	3/4/11/11	0/1/1/1
2	0GH	B	501	-	-	11/52/52/52	0/3/3/3
2	0GH	A	501	-	-	9/52/52/52	0/3/3/3
3	LPD	B	502	-	-	3/4/11/11	0/1/1/1
3	LPD	A	502	-	-	3/4/11/11	0/1/1/1
3	LPD	D	502	-	-	3/4/11/11	0/1/1/1
2	0GH	C	501	-	-	9/52/52/52	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	0GH	OAD-SAB	6.56	1.53	1.43
2	D	501	0GH	OAC-SAB	6.52	1.53	1.43
2	D	501	0GH	OAD-SAB	6.50	1.53	1.43
2	C	501	0GH	OAC-SAB	6.50	1.53	1.43
2	B	501	0GH	OAD-SAB	6.48	1.53	1.43
2	A	501	0GH	OAC-SAB	6.44	1.53	1.43
2	B	501	0GH	OAC-SAB	6.41	1.53	1.43
2	A	501	0GH	CBP-NBO	6.41	1.47	1.33
2	C	501	0GH	OAD-SAB	6.40	1.53	1.43
2	D	501	0GH	CBP-NBO	6.40	1.47	1.33
2	B	501	0GH	CBP-NBO	6.30	1.47	1.33
2	C	501	0GH	CBP-NBO	5.65	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	0GH	CBN-CBL	5.47	1.76	1.50
2	A	501	0GH	CAR-CAL	-5.16	1.39	1.50
2	C	501	0GH	CAR-CAL	-5.10	1.39	1.50
2	B	501	0GH	CAR-CAL	-5.07	1.39	1.50
2	D	501	0GH	CAR-CAL	-5.05	1.39	1.50
2	C	501	0GH	CAP-CAT	-5.04	1.39	1.50
2	A	501	0GH	CAP-CAT	-5.03	1.39	1.50
2	D	501	0GH	CAP-CAT	-5.01	1.39	1.50
2	B	501	0GH	CAP-CAT	-4.96	1.39	1.50
2	B	501	0GH	CAY-CAZ	-4.95	1.39	1.51
2	C	501	0GH	CAI-CBR	-4.89	1.39	1.52
2	D	501	0GH	CAI-CBR	-4.88	1.39	1.52
2	C	501	0GH	CAY-CAZ	-4.88	1.39	1.51
2	B	501	0GH	CAI-CBR	-4.86	1.39	1.52
2	D	501	0GH	CAY-CAZ	-4.80	1.39	1.51
2	A	501	0GH	CAI-CBR	-4.79	1.39	1.52
2	A	501	0GH	CAY-CAZ	-4.76	1.39	1.51
2	D	501	0GH	CBN-NBO	3.14	1.55	1.46
3	B	502	LPD	C-N2	2.68	1.39	1.32
3	A	502	LPD	C-N2	2.62	1.39	1.32
3	D	502	LPD	C-N2	2.01	1.38	1.32

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	0GH	CBN-NBO-CBP	-10.59	102.45	122.67
2	B	501	0GH	CBN-NBO-CBP	-8.62	106.21	122.67
2	A	501	0GH	CBN-NBO-CBP	-6.78	109.72	122.67
2	A	501	0GH	OAD-SAB-OAC	-6.59	109.19	118.59
2	B	501	0GH	OAD-SAB-OAC	-6.42	109.44	118.59
2	C	501	0GH	CBN-NBO-CBP	-6.16	110.91	122.67
2	D	501	0GH	OAD-SAB-OAC	-6.16	109.81	118.59
2	C	501	0GH	OAD-SAB-OAC	-5.99	110.06	118.59
3	C	502	LPD	CB-CA-C	5.83	119.90	111.18
3	D	502	LPD	CB-CA-C	5.60	119.55	111.18
2	D	501	0GH	CBL-CBN-NBO	-4.95	97.18	113.72
2	D	501	0GH	OAD-SAB-NAE	4.51	112.51	107.08
2	A	501	0GH	CBT-NAE-SAB	-4.48	110.61	117.86
2	D	501	0GH	CBT-NAE-SAB	-4.40	110.74	117.86
3	B	502	LPD	CB-CA-C	4.27	117.56	111.18
3	A	502	LPD	CB-CA-C	4.25	117.53	111.18
2	C	501	0GH	OAD-SAB-NAE	3.52	111.31	107.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	0GH	CBT-NAE-SAB	-3.43	112.31	117.86
2	C	501	0GH	CBT-NAE-SAB	-3.40	112.35	117.86
2	A	501	0GH	OAD-SAB-NAE	3.30	111.06	107.08
2	B	501	0GH	OAD-SAB-NAE	2.80	110.45	107.08
2	B	501	0GH	OAC-SAB-NAE	2.68	110.30	107.08
2	A	501	0GH	OAC-SAB-NAE	2.63	110.25	107.08
2	D	501	0GH	CBG-CBP-NBO	-2.51	112.08	116.41
2	D	501	0GH	OAC-SAB-NAE	2.49	110.07	107.08
2	C	501	0GH	OAC-SAB-NAE	2.47	110.06	107.08
2	A	501	0GH	CBG-CBP-NBO	-2.33	112.39	116.41
2	D	501	0GH	OBI-CBH-CBG	2.28	113.71	109.13

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	0GH	CAW-CAX-NBF-CBG
2	A	501	0GH	CAO-CAN-NAE-SAB
2	A	501	0GH	CAS-CAN-NAE-SAB
2	B	501	0GH	CAW-CAX-NBF-CBG
2	B	501	0GH	CAO-CAN-NAE-SAB
2	B	501	0GH	CAS-CAN-NAE-SAB
2	B	501	0GH	CAN-NAE-SAB-OAC
2	B	501	0GH	CBT-NAE-SAB-OAD
2	C	501	0GH	CAW-CAX-NBF-CBG
2	C	501	0GH	CAO-CAN-NAE-SAB
2	C	501	0GH	CAS-CAN-NAE-SAB
2	D	501	0GH	CAW-CAX-NBF-CBG
2	D	501	0GH	CAO-CAN-NAE-SAB
2	D	501	0GH	CAS-CAN-NAE-SAB
3	A	502	LPD	O-C-CA-CB
3	A	502	LPD	N2-C-CA-N
3	B	502	LPD	O-C-CA-CB
3	B	502	LPD	N2-C-CA-N
3	C	502	LPD	O-C-CA-CB
3	C	502	LPD	N2-C-CA-N
3	C	502	LPD	N2-C-CA-CB
3	D	502	LPD	O-C-CA-CB
3	D	502	LPD	N2-C-CA-N
3	D	502	LPD	N2-C-CA-CB
2	B	501	0GH	OBV-CBP-NBO-CBN
2	A	501	0GH	CAW-CAY-CAZ-CBE

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Mol	Chain	Res	Type	Atoms
3	A	502	LPD	N2-C-CA-CB
3	B	502	LPD	N2-C-CA-CB
2	A	501	0GH	CAN-NAE-SAB-OAC
2	A	501	0GH	CAN-NAE-SAB-OAD
2	B	501	0GH	CAN-NAE-SAB-OAD
2	C	501	0GH	CAN-NAE-SAB-OAC
2	C	501	0GH	CAN-NAE-SAB-OAD
2	D	501	0GH	CAN-NAE-SAB-OAC
2	D	501	0GH	CAN-NAE-SAB-OAD
2	B	501	0GH	CBP-CBG-CBH-CBJ
2	C	501	0GH	OAM-CAL-CAR-CAS
2	D	501	0GH	OAM-CAL-CAR-CAS
2	D	501	0GH	CAW-CAY-CAZ-CBE
2	A	501	0GH	CAW-CAY-CAZ-CBA
2	B	501	0GH	CAW-CAY-CAZ-CBE
2	B	501	0GH	CAW-CAY-CAZ-CBA
2	A	501	0GH	CBP-CBG-CBH-CBJ
2	B	501	0GH	CBT-NAE-SAB-CAA
2	C	501	0GH	CBP-CBG-CBH-CBJ
2	D	501	0GH	CBP-CBG-CBH-CBJ
2	D	501	0GH	CAW-CAY-CAZ-CBA
2	A	501	0GH	OBV-CBP-NBO-CBN
2	C	501	0GH	CAW-CAY-CAZ-CBE
2	C	501	0GH	CAW-CAY-CAZ-CBA

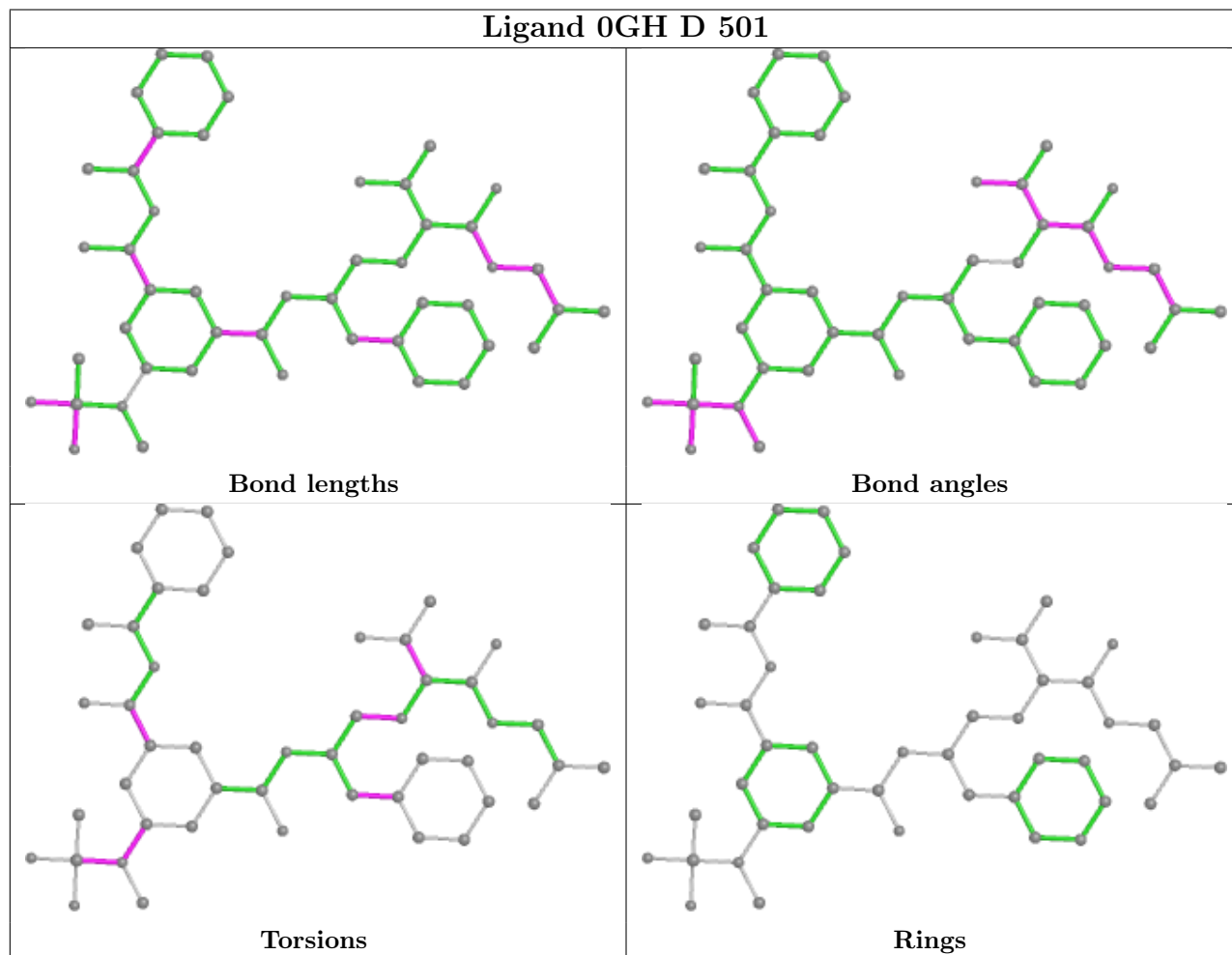
There are no ring outliers.

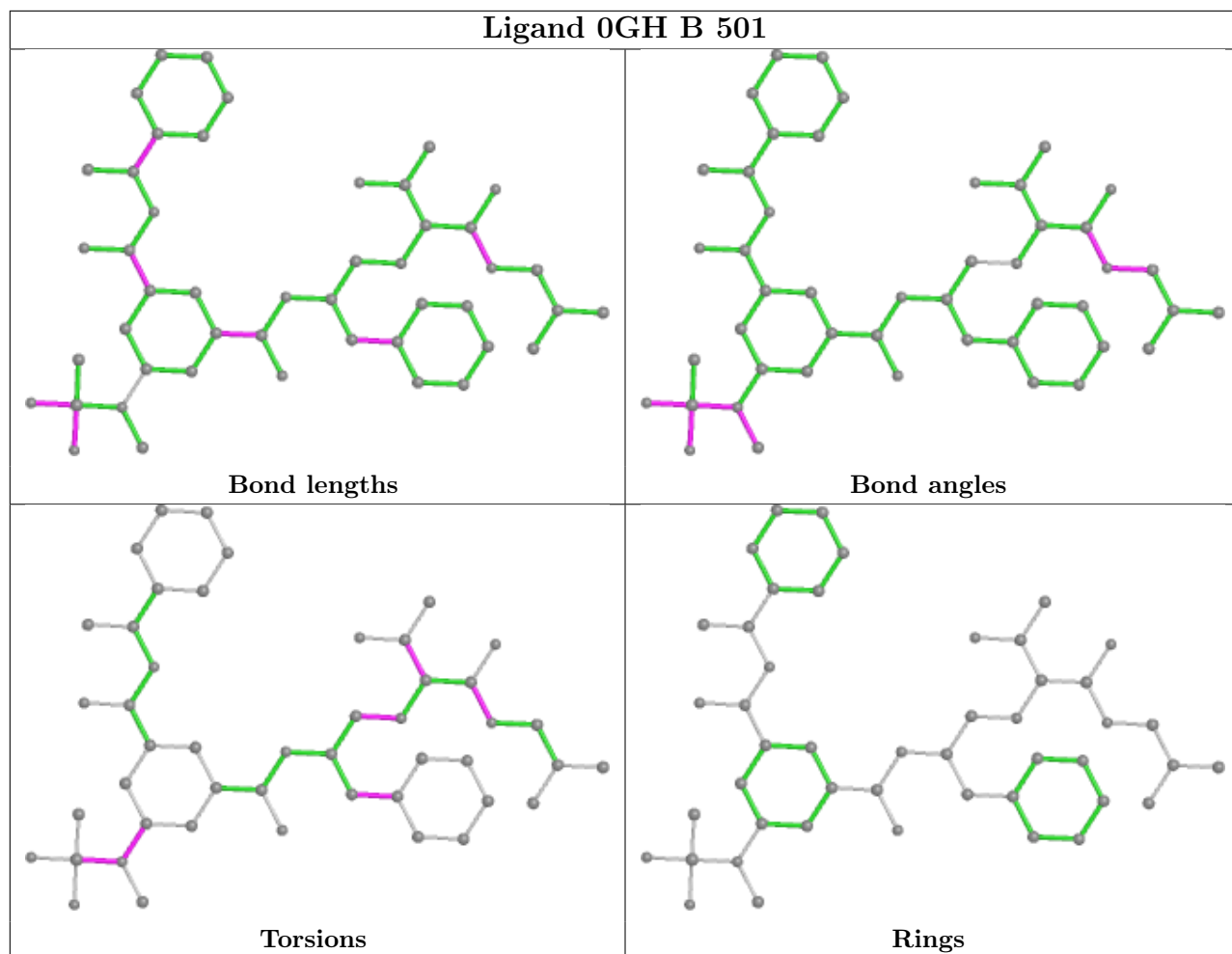
8 monomers are involved in 31 short contacts:

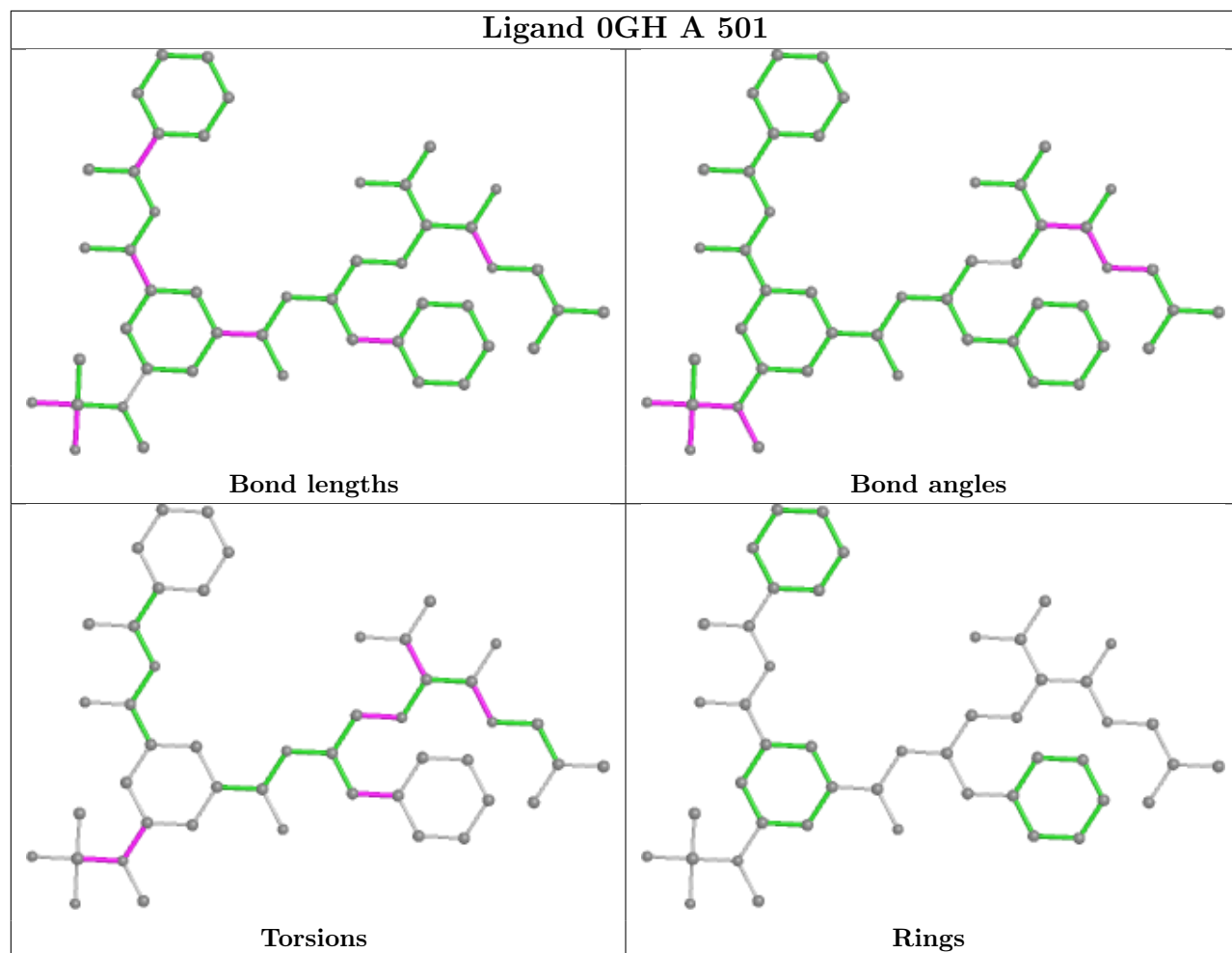
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	0GH	8	0
3	C	502	LPD	2	0
2	B	501	0GH	4	0
2	A	501	0GH	5	0
3	B	502	LPD	3	0
3	A	502	LPD	3	0
3	D	502	LPD	2	0
2	C	501	0GH	4	0

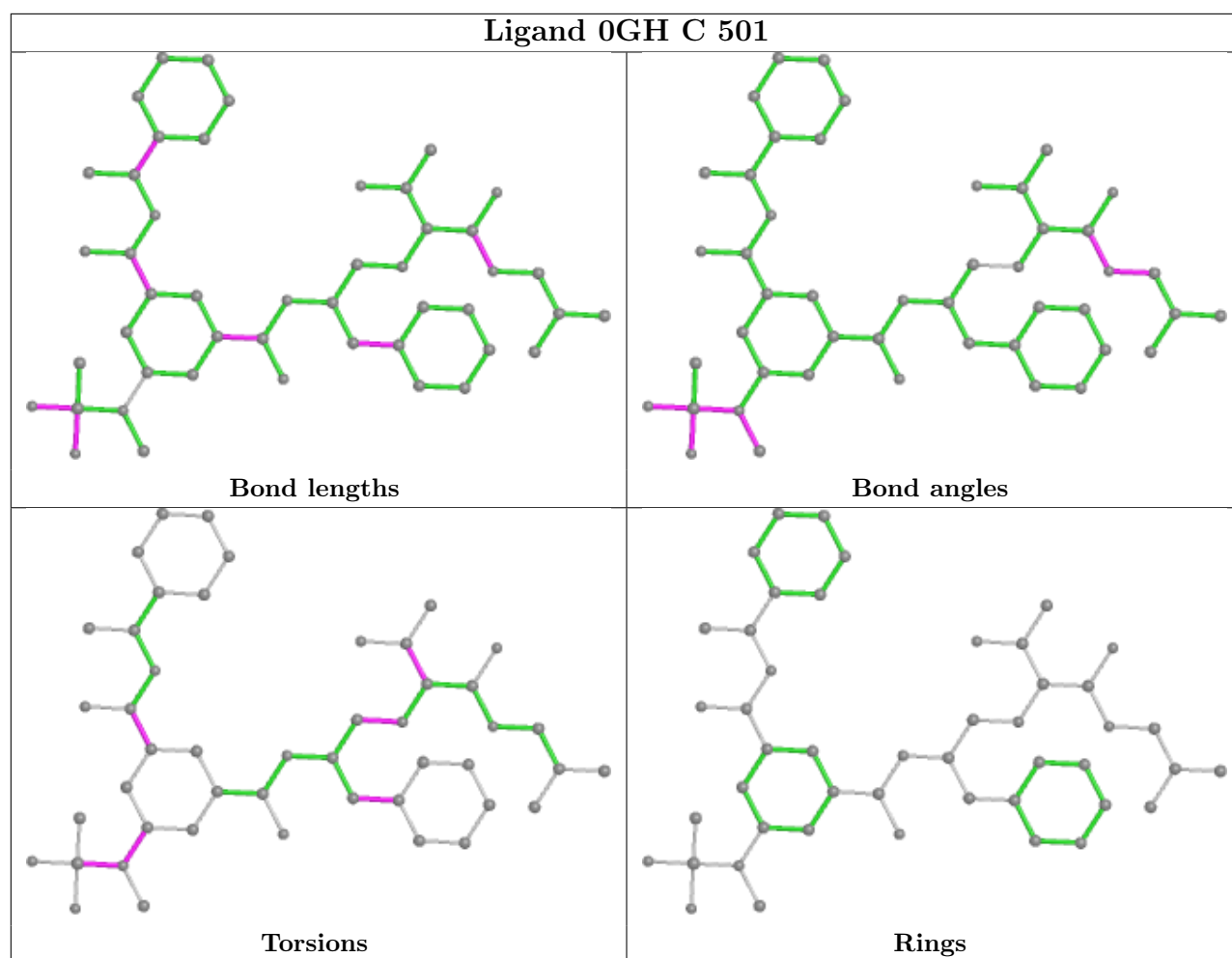
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.









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	387/388 (99%)	0.42	34 (8%) 10 9	17, 28, 43, 60	3 (0%)
1	B	387/388 (99%)	0.37	31 (8%) 12 11	18, 28, 44, 59	8 (2%)
1	C	388/388 (100%)	0.25	24 (6%) 20 19	16, 25, 41, 58	7 (1%)
1	D	387/388 (99%)	0.26	22 (5%) 23 23	18, 27, 42, 58	7 (1%)
All	All	1549/1552 (99%)	0.33	111 (7%) 15 14	16, 27, 44, 60	25 (1%)

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	362	THR	14.9
1	A	360	VAL	11.0
1	B	362	THR	10.8
1	B	360	VAL	10.6
1	C	360	VAL	8.4
1	D	362	THR	8.0
1	B	361	ALA	7.7
1	A	359	ASP	7.3
1	A	362	THR	6.4
1	D	48	VAL	5.9
1	C	361	ALA	5.9
1	C	46	SER	5.4
1	B	47	PHE	5.2
1	A	48	VAL	5.0
1	B	48	VAL	4.9
1	A	425	LEU	4.9
1	C	425	LEU	4.9
1	A	429	ASP	4.9
1	D	360	VAL	4.7
1	A	315	LEU	4.5
1	C	48	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	193	HIS	4.1
1	D	361	ALA	4.1
1	A	361	ALA	4.1
1	D	425	LEU	4.0
1	C	363	SER	3.9
1	D	340	THR	3.9
1	A	47	PHE	3.8
1	A	432	TYR	3.7
1	D	426	ASP	3.6
1	D	432	TYR	3.5
1	D	339	VAL	3.4
1	D	47	PHE	3.3
1	C	307	ASP	3.3
1	B	340	THR	3.3
1	A	340	THR	3.2
1	C	428	GLU	3.2
1	D	428	GLU	3.1
1	A	275	VAL	3.1
1	A	282	LEU	3.1
1	C	202	LEU	3.1
1	B	363	SER	3.0
1	D	423	VAL	3.0
1	C	429	ASP	2.9
1	C	341	ASN	2.9
1	C	383	ALA	2.9
1	A	363	SER	2.9
1	C	340	THR	2.9
1	C	423	VAL	2.9
1	D	341	ASN	2.9
1	A	358	GLU	2.9
1	B	169	LEU	2.9
1	B	215	LEU	2.9
1	D	97	HIS	2.9
1	B	282	LEU	2.8
1	C	47	PHE	2.8
1	A	426	ASP	2.8
1	D	116	TYR	2.7
1	A	304	LYS	2.7
1	A	381	MET	2.6
1	C	432	TYR	2.6
1	B	429	ASP	2.6
1	B	341	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	426	ASP	2.6
1	A	384	VAL	2.6
1	D	202	LEU	2.6
1	B	432	TYR	2.5
1	C	427	MET	2.5
1	B	359	ASP	2.5
1	A	385	ILE	2.5
1	B	81	THR	2.4
1	A	169	LEU	2.4
1	A	364	GLN	2.4
1	B	425	LEU	2.4
1	B	339	VAL	2.4
1	B	159	ASN	2.4
1	B	116	TYR	2.4
1	A	58	SER	2.4
1	A	116	TYR	2.3
1	D	275	VAL	2.3
1	D	200	LEU	2.3
1	A	81	THR	2.3
1	A	427	MET	2.3
1	A	140	ASN	2.3
1	C	270	TYR	2.3
1	C	81	THR	2.2
1	B	307	ASP	2.2
1	A	274	ILE	2.2
1	A	386	MET	2.2
1	B	381	MET	2.2
1	D	385	ILE	2.2
1	A	339	VAL	2.2
1	A	82	GLY	2.2
1	C	112	ARG	2.1
1	B	193	HIS	2.1
1	C	97	HIS	2.1
1	B	306	PRO	2.1
1	C	282	LEU	2.1
1	A	380	VAL	2.1
1	B	384	VAL	2.1
1	D	363	SER	2.1
1	B	92	PRO	2.1
1	B	77	ILE	2.1
1	D	359	ASP	2.1
1	B	79	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	229	HIS	2.0
1	B	49	GLU	2.0
1	A	200	LEU	2.0
1	A	216	ALA	2.0
1	B	97	HIS	2.0
1	B	86	PHE	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 monosaccharides in this entry.

6.4 Ligands [i](#)

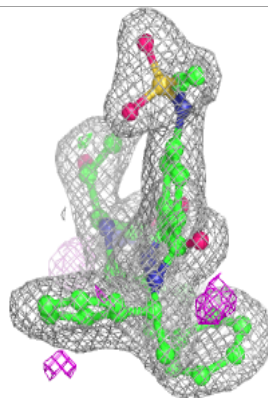
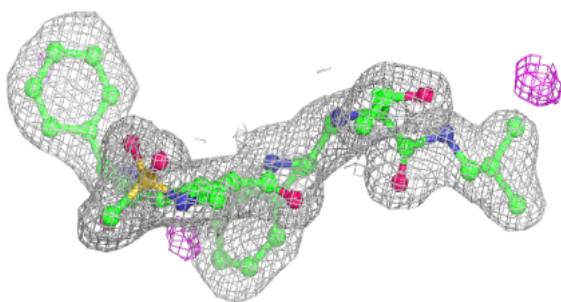
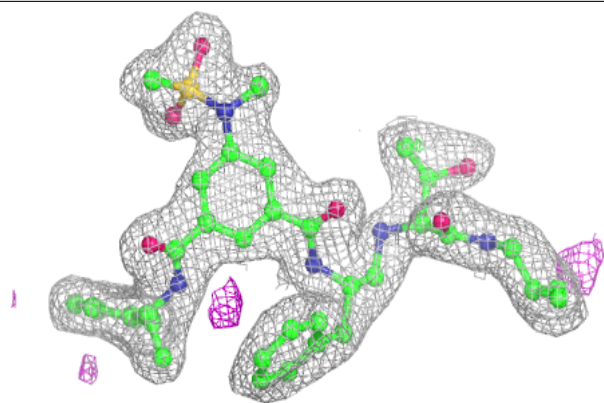
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	LPD	A	502	8/8	0.46	0.34	49,49,50,50	0
3	LPD	B	502	8/8	0.62	0.26	42,42,43,43	0
3	LPD	D	502	8/8	0.62	0.29	38,38,38,39	0
3	LPD	C	502	8/8	0.73	0.24	35,36,36,36	0
2	0GH	A	501	47/47	0.94	0.14	22,26,29,31	0
2	0GH	C	501	47/47	0.95	0.13	20,23,27,28	0
2	0GH	D	501	47/47	0.95	0.12	22,25,29,30	0
2	0GH	B	501	47/47	0.95	0.15	20,25,29,30	0

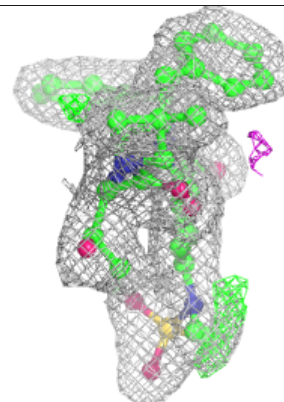
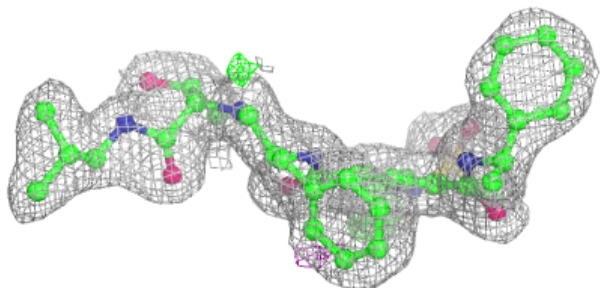
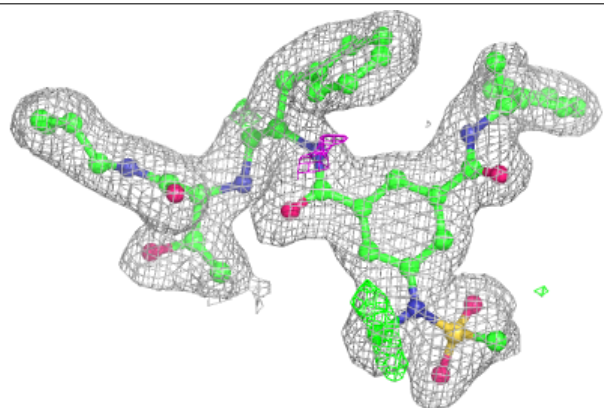
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 0GH 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)

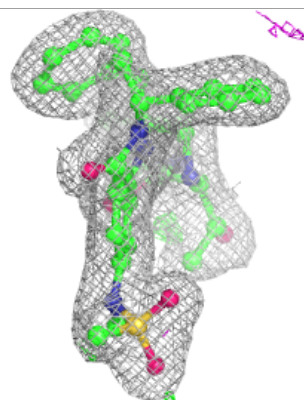
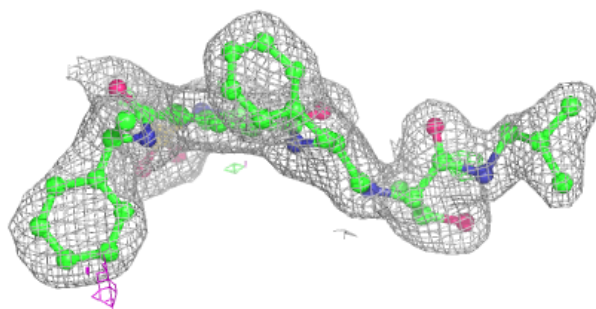
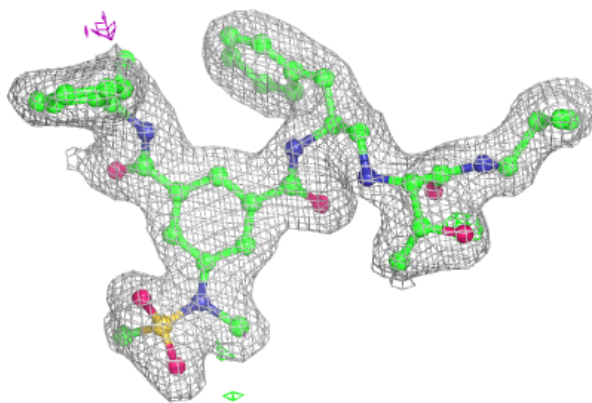
**Electron density around 0GH C 501:**

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

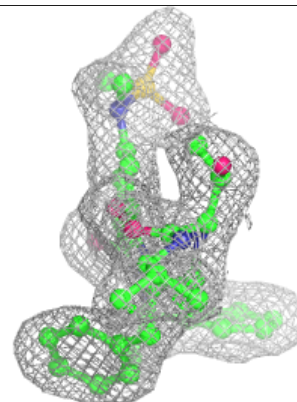
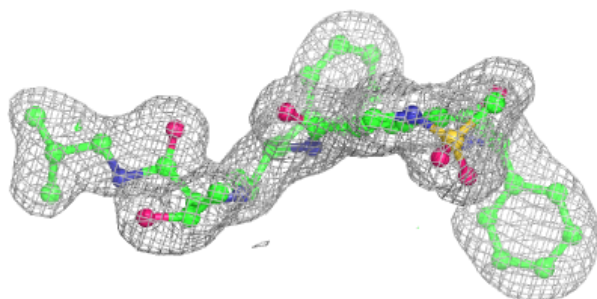
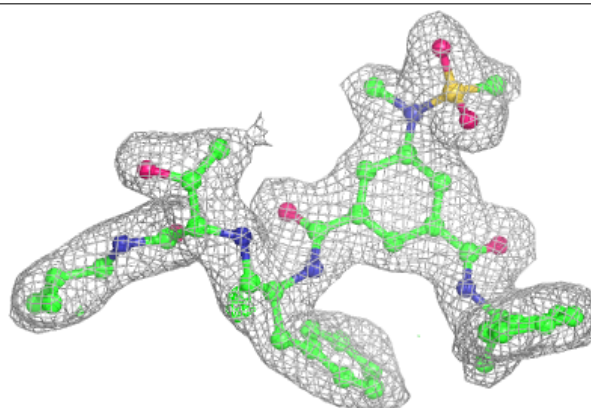


Electron density around 0GH D 501:

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

**Electron density around 0GH B 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 [i](#)

There are no such residues in this entry.