



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:09 pm BST

PDB ID : 2P4J
Title : Crystal structure of beta-secretase bound to an inhibitor with Isophthalamide Derivatives at P2-P3
Authors : Hong, L.; Ghosh, A.K.; Tang, J.
Deposited on : 2007-03-12
Resolution : 2.50 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 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 : 2.11
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) : 2.11

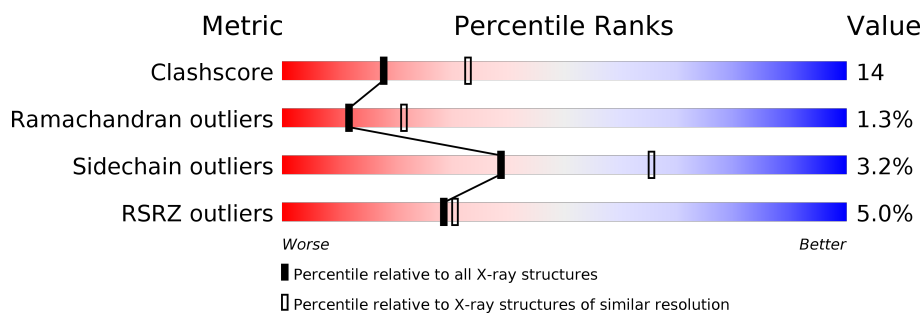
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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	389	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>.</div> </div> </div>
1	B	389	<div> <div>6%</div> <div> <div></div> <div>76%</div> <div>22%</div> <div>.</div> </div> </div>
1	C	389	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>24%</div> <div>.</div> </div> </div>
1	D	389	<div> <div>6%</div> <div> <div></div> <div>71%</div> <div>26%</div> <div>.</div> </div> </div>

2 Entry composition [i](#)

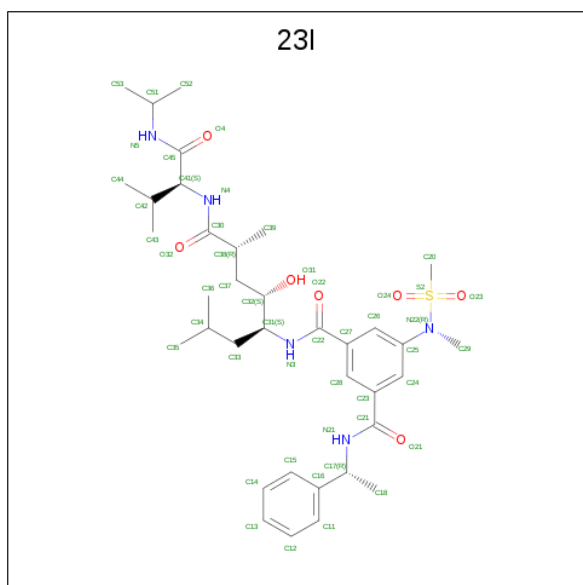
There are 3 unique types of molecules in this entry. The entry contains 12846 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	389	Total	C	N	O	S	0	0	0
			3053	1953	507	579	14			
1	B	389	Total	C	N	O	S	0	0	0
			3053	1953	507	579	14			
1	C	389	Total	C	N	O	S	0	0	0
			3053	1953	507	579	14			
1	D	389	Total	C	N	O	S	0	0	0
			3053	1953	507	579	14			

- Molecule 2 is N-[(1S,2S,4R)-2-HYDROXY-1-ISOBUTYL-5-({(1S)-1-[(ISOPROPYLAMINO)CARBONYL]-2-METHYLPROPYL}AMINO)-4-METHYL-5-OXOPENTYL]-5-[METHYL(METHYLSULFONYL)AMINO]-N'-[(1R)-1-PHENYLETHYL]ISOPHTHALAMIDE (three-letter code: 23I) (formula: C₃₆H₅₅N₅O₇S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			49	36	5	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total 49	C 36	N 5	O 7	S 1	0	0
2	C	1	Total 49	C 36	N 5	O 7	S 1	0	0
2	D	1	Total 49	C 36	N 5	O 7	S 1	0	0

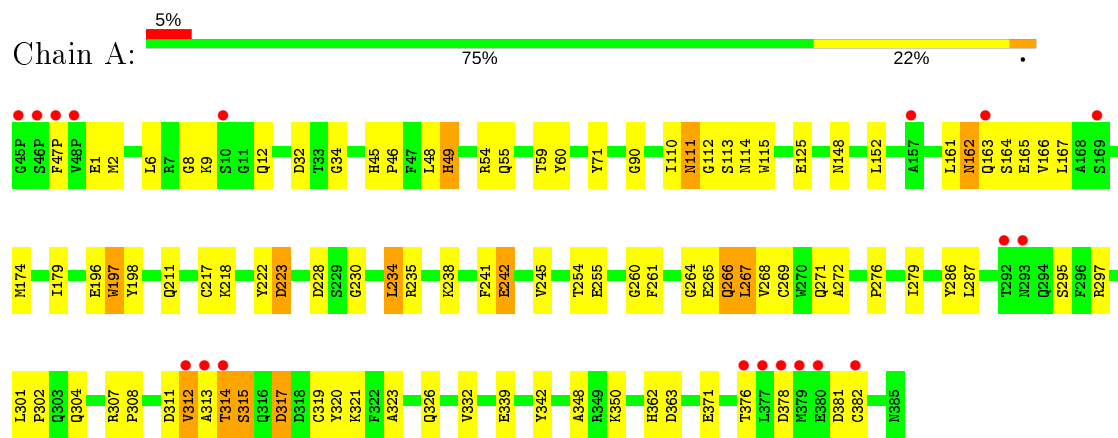
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	92	Total 92	O 92	0	0
3	B	109	Total 109	O 109	0	0
3	C	133	Total 133	O 133	0	0
3	D	104	Total 104	O 104	0	0

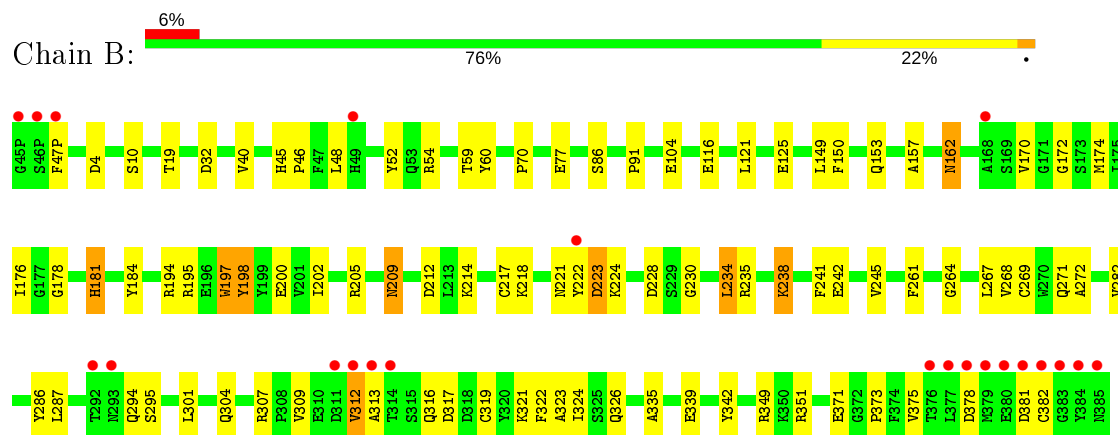
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

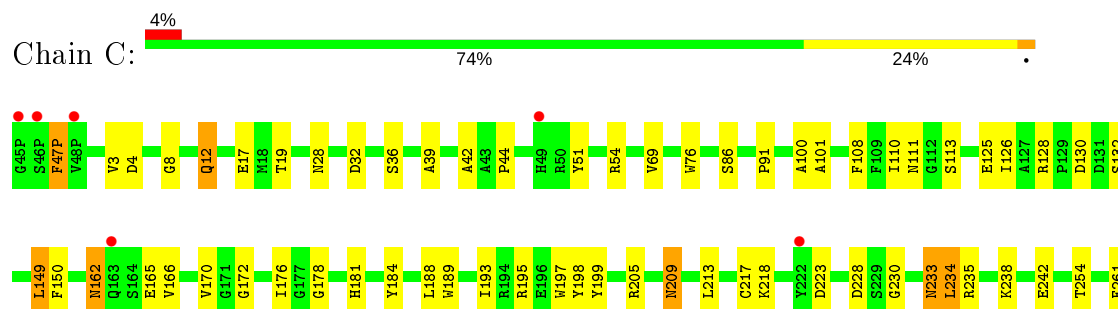
• Molecule 1: Beta-secretase 1

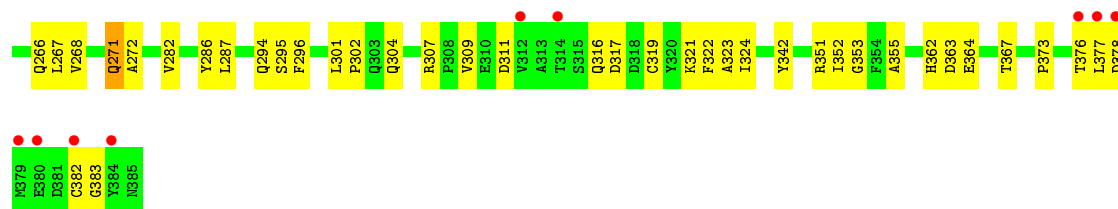


• Molecule 1: Beta-secretase 1

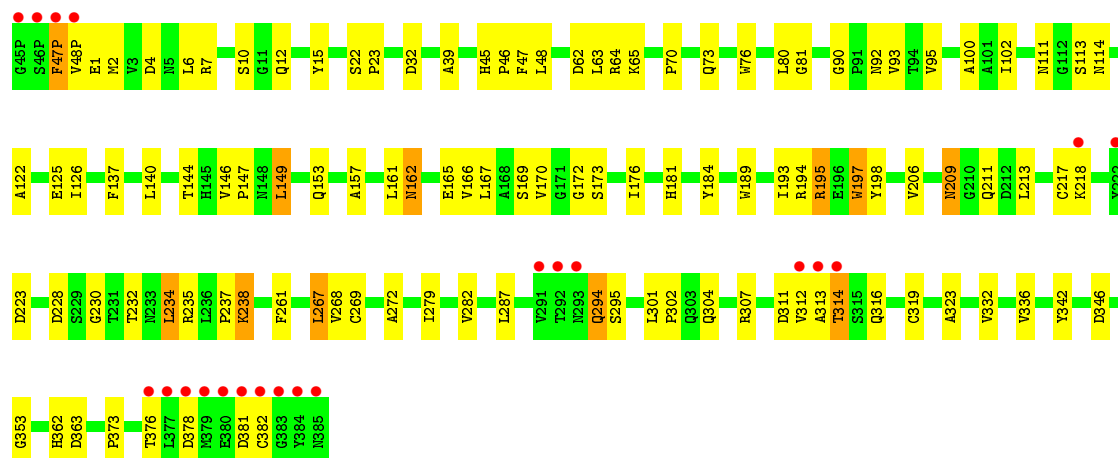


• Molecule 1: Beta-secretase 1





● Molecule 1: Beta-secretase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.93Å 129.97Å 87.48Å 90.00° 97.48° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 46.15 – 2.47	Depositor EDS
% Data completeness (in resolution range)	91.3 (50.00-2.50) 89.8 (46.15-2.47)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.201 , 0.259 0.197 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12846	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.21 % 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 4.4409e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: 23I

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	0.46	0/3131	0.71	2/4256 (0.0%)
1	B	0.44	0/3131	0.71	3/4256 (0.1%)
1	C	0.47	0/3131	0.71	3/4256 (0.1%)
1	D	0.46	0/3131	0.70	3/4256 (0.1%)
All	All	0.46	0/12524	0.71	11/17024 (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	234	LEU	N-CA-C	-6.78	92.69	111.00
1	B	234	LEU	N-CA-C	-6.50	93.44	111.00
1	B	342	TYR	N-CA-C	-5.61	95.85	111.00
1	C	234	LEU	N-CA-C	-5.58	95.92	111.00
1	D	342	TYR	N-CA-C	-5.35	96.55	111.00
1	C	342	TYR	N-CA-C	-5.31	96.67	111.00
1	B	198	TYR	N-CA-C	-5.22	96.89	111.00
1	D	198	TYR	N-CA-C	-5.17	97.04	111.00
1	D	234	LEU	N-CA-C	-5.15	97.09	111.00
1	A	198	TYR	N-CA-C	-5.14	97.11	111.00
1	C	198	TYR	N-CA-C	-5.05	97.35	111.00

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	3053	0	2965	76	0
1	B	3053	0	2965	71	0
1	C	3053	0	2965	84	0
1	D	3053	0	2965	90	0
2	A	49	0	55	1	0
2	B	49	0	55	3	0
2	C	49	0	55	2	0
2	D	49	0	55	4	0
3	A	92	0	0	3	0
3	B	109	0	0	4	0
3	C	133	0	0	10	0
3	D	104	0	0	5	0
All	All	12846	0	12080	319	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 14.

All (319) 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:312:VAL:HG23	1:B:313:ALA:H	1.29	0.96
1:C:162:ASN:HD21	1:C:165:GLU:HG3	1.32	0.94
1:A:12:GLN:HG2	1:A:110:ILE:HG21	1.50	0.93
1:A:164:SER:HA	1:A:167:LEU:HD12	1.54	0.89
1:A:267:LEU:H	1:A:267:LEU:HD23	1.40	0.86
1:A:267:LEU:CD2	1:A:267:LEU:H	1.89	0.86
1:A:301:LEU:H	1:A:304:GLN:NE2	1.77	0.82
1:C:162:ASN:ND2	1:C:165:GLU:HG3	1.94	0.81
1:A:312:VAL:HG23	1:A:313:ALA:H	1.46	0.80
1:B:238:LYS:O	1:B:242:GLU:HG2	1.81	0.80
1:A:162:ASN:ND2	1:A:165:GLU:HG3	1.96	0.79
1:A:152:LEU:CD2	1:A:174:MET:HG3	2.12	0.79
1:D:301:LEU:H	1:D:304:GLN:HE21	1.30	0.79
1:C:267:LEU:HD23	1:C:267:LEU:H	1.47	0.78
1:A:301:LEU:H	1:A:304:GLN:HE21	1.32	0.78
1:A:279:ILE:HA	1:D:211:GLN:HG3	1.68	0.76
1:B:238:LYS:HA	1:B:326:GLN:HG3	1.67	0.76
1:C:376:THR:HA	3:C:517:HOH:O	1.86	0.75
1:D:181:HIS:HA	1:D:184:TYR:HE1	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:PHE:HE1	1:D:176:ILE:HG23	1.52	0.74
1:B:378:ASP:HB3	1:B:381:ASP:OD2	1.88	0.73
1:D:162:ASN:ND2	1:D:165:GLU:H	1.87	0.73
1:B:301:LEU:H	1:B:304:GLN:HE21	1.35	0.73
1:A:162:ASN:HD21	1:A:165:GLU:HG3	1.52	0.72
1:A:162:ASN:C	1:A:162:ASN:HD22	1.92	0.72
1:D:169:SER:HB2	3:D:604:HOH:O	1.89	0.71
1:D:181:HIS:HA	1:D:184:TYR:CE1	2.25	0.70
1:A:238:LYS:HG3	1:A:326:GLN:NE2	2.06	0.69
1:B:47(P):PHE:CZ	1:B:178:GLY:HA3	2.27	0.69
1:D:70:PRO:HG2	2:D:504:23I:H533	1.73	0.69
1:A:152:LEU:HD21	1:A:174:MET:HG3	1.76	0.68
1:A:313:ALA:O	1:A:315:SER:N	2.26	0.68
1:B:267:LEU:HD23	1:B:321:LYS:HD3	1.75	0.68
1:D:166:VAL:HG12	3:D:602:HOH:O	1.92	0.68
1:B:261:PHE:CD1	1:B:268:VAL:HG23	2.29	0.67
1:B:301:LEU:H	1:B:304:GLN:NE2	1.93	0.67
1:D:4:ASP:H	1:D:173:SER:HB3	1.60	0.67
1:D:218:LYS:HD2	1:D:381:ASP:O	1.95	0.67
1:A:45:HIS:HB3	1:A:48:LEU:HD12	1.78	0.66
1:C:238:LYS:O	1:C:242:GLU:HG2	1.96	0.66
1:C:149:LEU:C	1:C:149:LEU:HD12	2.16	0.66
1:C:301:LEU:H	1:C:304:GLN:HE21	1.44	0.66
1:D:6:LEU:HG	1:D:173:SER:HA	1.77	0.66
1:B:312:VAL:HG23	1:B:313:ALA:N	2.07	0.65
1:B:205:ARG:HB3	1:B:286:TYR:HB2	1.78	0.65
1:A:315:SER:OG	1:A:317:ASP:HB2	1.97	0.65
1:B:10:SER:OG	1:B:157:ALA:HB3	1.97	0.64
1:D:4:ASP:N	1:D:173:SER:HB3	2.12	0.64
1:B:269:CYS:HG	1:B:319:CYS:HG	0.67	0.64
1:B:194:ARG:HB2	1:B:202:ILE:HD11	1.79	0.64
1:D:294:GLN:HG2	1:D:373:PRO:HB2	1.79	0.64
1:C:195:ARG:HD3	3:C:636:HOH:O	1.98	0.63
1:A:267:LEU:N	1:A:267:LEU:HD23	2.12	0.63
1:B:267:LEU:CD2	1:B:321:LYS:HD3	2.29	0.63
1:D:114:ASN:HB3	3:D:603:HOH:O	1.98	0.63
1:C:209:ASN:HD22	1:C:282:VAL:HG22	1.64	0.62
1:A:2:MET:HG2	1:A:90:GLY:HA2	1.82	0.62
1:B:272:ALA:HB2	1:B:316:GLN:HB3	1.82	0.62
1:B:209:ASN:ND2	1:B:282:VAL:H	1.98	0.61
1:A:269:CYS:HG	1:A:319:CYS:HG	0.61	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:ARG:HB3	1:B:200:GLU:HG2	1.82	0.60
1:A:217:CYS:CB	1:A:382:CYS:HG	2.13	0.60
1:B:4:ASP:OD1	1:B:170:VAL:HG21	2.01	0.60
1:A:241:PHE:O	1:A:245:VAL:HG23	2.00	0.60
1:D:261:PHE:CD1	1:D:268:VAL:HG23	2.35	0.60
1:D:272:ALA:HB2	1:D:316:GLN:O	2.01	0.60
1:C:362:HIS:HD2	1:C:363:ASP:O	1.85	0.60
1:C:233:ASN:N	1:C:233:ASN:HD22	1.99	0.60
1:B:267:LEU:CD2	1:B:309:VAL:HG21	2.32	0.59
1:C:311:ASP:OD2	1:C:317:ASP:HB2	2.02	0.59
1:C:47(P):PHE:CD1	1:C:47(P):PHE:N	2.71	0.59
1:B:54:ARG:HD2	1:B:60:TYR:CZ	2.38	0.58
1:D:45:HIS:HB3	1:D:48:LEU:HD12	1.86	0.58
1:A:12:GLN:HG2	1:A:110:ILE:CG2	2.27	0.58
1:D:47(P):PHE:O	1:D:1:GLU:N	2.37	0.58
1:A:218:LYS:HG3	1:A:381:ASP:O	2.04	0.58
1:A:307:ARG:NH2	1:A:339:GLU:OE1	2.37	0.58
1:D:63:LEU:HG	1:D:81:GLY:HA2	1.86	0.58
1:A:49:HIS:CE1	1:A:114:ASN:HA	2.39	0.57
1:C:267:LEU:HD13	1:C:309:VAL:HG21	1.85	0.57
1:D:39:ALA:HB2	1:D:100:ALA:HB3	1.85	0.57
1:A:312:VAL:HG23	1:A:313:ALA:N	2.18	0.57
1:C:12:GLN:HE21	1:C:113:SER:HA	1.70	0.57
1:D:301:LEU:H	1:D:304:GLN:NE2	2.02	0.57
1:C:267:LEU:CD2	1:C:267:LEU:H	2.17	0.57
1:A:32:ASP:OD1	1:A:230:GLY:HA3	2.04	0.57
1:B:241:PHE:O	1:B:245:VAL:HG23	2.03	0.57
1:C:162:ASN:HD22	1:C:162:ASN:C	2.08	0.57
1:A:12:GLN:CG	1:A:110:ILE:HG21	2.30	0.56
1:A:163:GLN:O	1:A:167:LEU:HG	2.04	0.56
1:B:267:LEU:HD22	1:B:309:VAL:HG21	1.87	0.56
1:C:162:ASN:O	1:C:166:VAL:HG23	2.04	0.56
1:A:152:LEU:HD23	1:A:174:MET:HG3	1.86	0.56
1:D:267:LEU:HD23	1:D:267:LEU:H	1.70	0.56
1:C:162:ASN:ND2	1:C:165:GLU:H	2.04	0.56
1:A:8:GLY:HA2	1:A:166:VAL:CG1	2.36	0.56
1:D:162:ASN:HD22	1:D:162:ASN:C	2.09	0.56
1:A:311:ASP:HB2	1:A:319:CYS:SG	2.46	0.55
1:A:314:THR:O	1:A:315:SER:C	2.44	0.55
1:B:209:ASN:HD22	1:B:282:VAL:HG22	1.72	0.55
1:D:122:ALA:HB1	1:D:126:ILE:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:ALA:CB	1:D:126:ILE:HD11	2.36	0.55
1:B:349:ARG:HD3	1:B:351:ARG:NH2	2.21	0.55
1:D:362:HIS:HD2	1:D:363:ASP:O	1.88	0.55
1:D:45:HIS:CG	1:D:46:PRO:HD2	2.42	0.55
1:A:54:ARG:HD2	1:A:60:TYR:CZ	2.42	0.55
1:A:235:ARG:HB2	1:A:332:VAL:HB	1.89	0.54
1:C:235:ARG:HD3	2:C:503:23I:O23	2.07	0.54
1:D:7:ARG:HB2	1:D:15:TYR:CE1	2.43	0.54
1:A:254:THR:HG23	3:A:571:HOH:O	2.08	0.54
1:A:179:ILE:HG23	1:A:342:TYR:HE2	1.73	0.54
1:C:188:LEU:HD23	1:C:355:ALA:HB2	1.91	0.53
1:C:209:ASN:ND2	1:C:282:VAL:H	2.06	0.53
1:D:10:SER:HB2	1:D:161:LEU:HB2	1.91	0.53
1:A:218:LYS:CG	1:A:381:ASP:O	2.56	0.53
1:D:73:GLN:NE2	3:D:597:HOH:O	2.29	0.52
1:C:130:ASP:OD2	1:C:132:SER:N	2.41	0.52
1:A:264:GLY:HA2	3:A:507:HOH:O	2.10	0.52
1:B:312:VAL:CG2	1:B:313:ALA:H	2.11	0.52
1:C:54:ARG:HG3	3:C:543:HOH:O	2.10	0.52
1:D:162:ASN:O	1:D:166:VAL:HG23	2.09	0.52
1:A:162:ASN:C	1:A:162:ASN:ND2	2.62	0.52
1:D:47(P):PHE:CD1	1:D:47(P):PHE:N	2.77	0.52
1:A:6:LEU:HD21	1:A:174:MET:HB2	1.91	0.51
1:B:235:ARG:HD2	3:B:599:HOH:O	2.10	0.51
1:C:39:ALA:HB2	1:C:100:ALA:HB3	1.92	0.51
1:D:125:GLU:HG2	1:D:197:TRP:HB3	1.92	0.51
1:B:307:ARG:HG3	1:B:323:ALA:HB2	1.92	0.51
1:D:197:TRP:HD1	1:D:197:TRP:H	1.57	0.51
1:C:362:HIS:CD2	1:C:367:THR:HG22	2.46	0.51
1:C:193:ILE:HG13	1:C:351:ARG:HA	1.92	0.51
1:D:45:HIS:ND1	1:D:46:PRO:HD2	2.26	0.51
1:C:364:GLU:HG2	1:C:364:GLU:O	2.09	0.51
1:C:294:GLN:HG3	1:C:373:PRO:HB2	1.92	0.51
1:D:12:GLN:OE1	1:D:12:GLN:HA	2.10	0.51
1:A:47(P):PHE:HD2	1:A:2:MET:CE	2.24	0.50
1:B:181:HIS:HA	1:B:184:TYR:CE1	2.46	0.50
1:B:322:PHE:CZ	1:B:324:ILE:HB	2.47	0.50
1:B:217:CYS:CB	1:B:382:CYS:HG	2.22	0.50
1:D:149:LEU:HD12	1:D:346:ASP:HA	1.94	0.50
1:D:162:ASN:HD21	1:D:165:GLU:HG3	1.76	0.50
1:D:269:CYS:HG	1:D:319:CYS:CB	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:LEU:HB2	1:D:346:ASP:HA	1.93	0.50
1:A:301:LEU:HB3	1:A:302:PRO:HD2	1.92	0.50
1:B:261:PHE:CD1	1:B:268:VAL:CG2	2.95	0.50
1:B:195:ARG:O	1:B:197:TRP:HD1	1.95	0.50
1:D:267:LEU:H	1:D:267:LEU:CD2	2.23	0.50
1:B:335:ALA:O	1:B:339:GLU:HG3	2.11	0.50
1:D:209:ASN:ND2	1:D:282:VAL:H	2.09	0.50
1:D:149:LEU:HD23	1:D:149:LEU:C	2.32	0.50
1:D:22:SER:HA	1:D:23:PRO:C	2.32	0.50
1:C:47(P):PHE:CZ	1:C:178:GLY:HA3	2.47	0.50
1:D:307:ARG:HG2	1:D:323:ALA:HB2	1.94	0.49
1:B:197:TRP:CG	1:B:198:TYR:N	2.79	0.49
1:D:307:ARG:CG	1:D:323:ALA:HB2	2.41	0.49
1:A:314:THR:O	1:A:315:SER:O	2.29	0.49
1:C:301:LEU:HB3	1:C:302:PRO:HD2	1.93	0.49
1:C:130:ASP:OD2	1:C:132:SER:HB3	2.12	0.49
1:B:121:LEU:HD13	1:B:150:PHE:CE2	2.48	0.49
1:B:181:HIS:HA	1:B:184:TYR:HE1	1.78	0.49
1:B:228:ASP:OD2	2:B:502:23I:H372	2.12	0.49
1:D:62:ASP:OD1	1:D:64:ARG:N	2.40	0.48
1:A:125:GLU:HG2	1:A:197:TRP:HB3	1.94	0.48
1:D:193:ILE:HG22	1:D:195:ARG:O	2.13	0.48
1:D:65:LYS:HE3	1:D:80:LEU:HD12	1.95	0.48
1:A:47(P):PHE:HD2	1:A:2:MET:HE1	1.79	0.48
1:B:349:ARG:HD3	1:B:351:ARG:HH21	1.78	0.48
1:B:153:GLN:O	1:B:172:GLY:HA3	2.12	0.48
1:C:32:ASP:OD1	1:C:230:GLY:HA3	2.13	0.48
1:D:301:LEU:HB3	1:D:302:PRO:HD2	1.96	0.48
1:B:48:LEU:HD22	1:B:116:GLU:HB3	1.94	0.48
2:B:502:23I:H12	3:B:609:HOH:O	2.13	0.48
1:A:307:ARG:O	1:A:320:TYR:HA	2.14	0.48
1:B:125:GLU:HG2	1:B:197:TRP:HB3	1.95	0.48
1:C:205:ARG:HB3	1:C:286:TYR:CG	2.49	0.47
1:B:149:LEU:HD23	1:B:149:LEU:C	2.34	0.47
1:B:202:ILE:HD12	1:B:202:ILE:N	2.29	0.47
1:C:218:LYS:HE3	1:C:383:GLY:O	2.14	0.47
1:D:7:ARG:NH1	1:D:167:LEU:O	2.48	0.47
1:B:19:THR:OG1	1:B:86:SER:HB2	2.15	0.47
1:D:237:PRO:O	1:D:238:LYS:C	2.53	0.47
1:C:170:VAL:HG12	1:C:172:GLY:H	1.79	0.47
1:C:110:ILE:HB	1:C:113:SER:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:ARG:HD2	3:D:506:HOH:O	2.13	0.47
1:B:218:LYS:HG3	1:B:381:ASP:O	2.15	0.47
1:D:189:TRP:O	1:D:353:GLY:HA2	2.15	0.47
1:D:311:ASP:HB2	1:D:319:CYS:SG	2.54	0.47
1:C:307:ARG:CG	1:C:323:ALA:HB2	2.44	0.46
1:D:170:VAL:HG12	1:D:172:GLY:H	1.80	0.46
1:A:162:ASN:ND2	1:A:165:GLU:H	2.13	0.46
1:B:205:ARG:HB3	1:B:286:TYR:CG	2.51	0.46
1:A:125:GLU:HG2	1:A:197:TRP:CB	2.46	0.46
1:B:221:ASN:HB3	3:B:562:HOH:O	2.14	0.46
1:B:269:CYS:CB	1:B:319:CYS:HG	2.24	0.46
1:C:205:ARG:HB3	1:C:286:TYR:HB2	1.97	0.46
1:C:42:ALA:HB2	1:C:101:ALA:HB1	1.97	0.46
1:D:149:LEU:HD23	1:D:149:LEU:O	2.15	0.46
1:C:19:THR:OG1	1:C:86:SER:HB2	2.16	0.46
1:D:47(P):PHE:C	1:D:1:GLU:H	2.19	0.46
1:D:32:ASP:OD1	1:D:230:GLY:HA3	2.16	0.46
1:B:40:VAL:HG21	1:B:52:TYR:HB2	1.97	0.46
1:B:198:TYR:CE2	1:B:224:LYS:HE3	2.51	0.46
1:D:162:ASN:HD21	1:D:165:GLU:CG	2.28	0.46
1:B:205:ARG:HB3	1:B:286:TYR:CB	2.44	0.45
1:C:267:LEU:HD12	1:C:319:CYS:HB3	1.98	0.45
1:A:9:LYS:HD3	1:A:161:LEU:HD11	1.99	0.45
1:B:264:GLY:O	1:B:321:LYS:HE3	2.16	0.45
1:C:91:PRO:HD3	1:C:176:ILE:HB	1.97	0.45
1:D:153:GLN:O	1:D:172:GLY:HA3	2.17	0.45
1:A:255:GLU:HG3	3:A:553:HOH:O	2.16	0.45
1:C:228:ASP:OD2	2:C:503:23I:H372	2.15	0.45
1:A:307:ARG:HA	1:A:308:PRO:HD3	1.69	0.45
1:B:287:LEU:O	1:B:295:SER:HB2	2.15	0.45
1:A:260:GLY:HA3	1:A:266:GLN:HG2	1.99	0.45
1:A:148:ASN:HB3	1:A:348:ALA:HB2	1.98	0.45
1:B:77:GLU:HB2	1:B:104:GLU:HB2	1.99	0.45
1:C:42:ALA:CB	1:C:101:ALA:HB1	2.47	0.45
1:C:217:CYS:HG	1:C:382:CYS:HG	0.61	0.45
1:B:235:ARG:HD3	2:B:502:23I:O23	2.17	0.45
1:C:301:LEU:H	1:C:304:GLN:NE2	2.12	0.44
1:D:39:ALA:CB	1:D:100:ALA:HB3	2.46	0.44
1:B:45:HIS:ND1	1:B:46:PRO:HD2	2.33	0.44
1:C:307:ARG:HG3	1:C:323:ALA:HB2	1.98	0.44
1:D:228:ASP:OD2	2:D:504:23I:H372	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:ARG:HD3	2:D:504:23I:O23	2.17	0.44
1:A:307:ARG:HG3	1:A:323:ALA:HB2	1.98	0.44
1:D:162:ASN:HD21	1:D:165:GLU:H	1.65	0.44
1:A:265:GLU:O	1:A:321:LYS:HE2	2.16	0.44
1:C:217:CYS:SG	1:C:382:CYS:HA	2.57	0.44
1:A:238:LYS:O	1:A:242:GLU:HG2	2.17	0.44
1:B:271:GLN:O	1:B:272:ALA:C	2.56	0.44
1:C:28:ASN:ND2	3:C:604:HOH:O	2.50	0.44
1:B:375:VAL:N	1:C:364:GLU:OE2	2.40	0.44
1:A:1:GLU:H	1:A:1:GLU:HG2	1.58	0.44
1:A:261:PHE:CD1	1:A:268:VAL:HG23	2.52	0.44
1:C:36:SER:OG	1:C:126:ILE:HG13	2.18	0.43
1:D:209:ASN:HD22	1:D:282:VAL:HG22	1.83	0.43
1:A:315:SER:C	1:A:317:ASP:N	2.68	0.43
1:B:162:ASN:C	1:B:162:ASN:HD22	2.21	0.43
1:B:267:LEU:HD23	1:B:321:LYS:CD	2.45	0.43
1:B:294:GLN:HG2	1:B:373:PRO:HB2	2.01	0.43
1:D:47:PHE:CE2	1:D:111:ASN:HB2	2.53	0.43
1:B:222:TYR:O	1:B:223:ASP:CB	2.66	0.43
1:C:130:ASP:OD2	1:C:132:SER:CB	2.66	0.43
1:A:287:LEU:O	1:A:295:SER:HB2	2.18	0.43
1:C:233:ASN:N	1:C:233:ASN:ND2	2.65	0.43
1:C:322:PHE:CE2	1:C:324:ILE:HB	2.54	0.43
1:D:235:ARG:HD3	2:D:504:23I:H292	2.00	0.43
1:B:371:GLU:HG2	3:B:547:HOH:O	2.18	0.43
1:D:162:ASN:ND2	1:D:165:GLU:HB2	2.33	0.43
1:B:212:ASP:CG	1:B:214:LYS:H	2.23	0.42
1:C:69:VAL:HG22	1:C:128:ARG:HB2	2.01	0.42
1:D:10:SER:OG	1:D:157:ALA:HB3	2.18	0.42
1:D:161:LEU:HB2	1:D:166:VAL:HG22	2.01	0.42
1:C:287:LEU:O	1:C:295:SER:HB2	2.19	0.42
1:A:71:TYR:HB3	2:A:501:23I:H31	2.01	0.42
1:A:286:TYR:CD2	1:A:297:ARG:HB3	2.55	0.42
1:C:189:TRP:O	1:C:353:GLY:HA2	2.20	0.42
1:C:193:ILE:HG22	1:C:195:ARG:O	2.18	0.42
1:A:222:TYR:O	1:A:223:ASP:CB	2.67	0.42
1:A:362:HIS:HD2	1:A:363:ASP:O	2.01	0.42
1:C:272:ALA:HB2	1:C:316:GLN:O	2.19	0.42
1:D:235:ARG:HB2	1:D:332:VAL:HB	2.02	0.42
1:B:4:ASP:CG	1:B:170:VAL:HG11	2.40	0.42
1:C:76:TRP:HD1	1:C:108:PHE:CD1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:TRP:CD1	1:D:197:TRP:N	2.88	0.42
1:A:45:HIS:CG	1:A:46:PRO:HD2	2.55	0.42
1:C:12:GLN:HG3	1:C:110:ILE:HG21	2.01	0.42
1:C:321:LYS:HB3	3:C:600:HOH:O	2.19	0.42
1:C:218:LYS:HA	1:C:382:CYS:O	2.20	0.42
1:D:311:ASP:O	1:D:313:ALA:N	2.53	0.42
1:D:4:ASP:H	1:D:173:SER:CB	2.30	0.42
1:A:276:PRO:O	1:A:279:ILE:HG12	2.19	0.42
1:C:12:GLN:HG3	1:C:110:ILE:CG2	2.50	0.42
1:D:12:GLN:HB2	1:D:113:SER:HB3	2.02	0.42
1:C:209:ASN:HA	1:C:209:ASN:HD22	1.66	0.41
1:D:47(P):PHE:C	1:D:1:GLU:N	2.73	0.41
1:C:149:LEU:C	1:C:149:LEU:CD1	2.86	0.41
1:C:235:ARG:HD2	3:C:507:HOH:O	2.20	0.41
1:D:137:PHE:CE1	1:D:176:ILE:HG23	2.42	0.41
1:C:261:PHE:CD1	1:C:268:VAL:HG23	2.54	0.41
1:C:377:LEU:N	3:C:541:HOH:O	2.49	0.41
1:C:47(P):PHE:HD1	1:C:47(P):PHE:N	2.16	0.41
1:D:2:MET:HG2	1:D:90:GLY:HA2	2.03	0.41
1:B:32:ASP:OD1	1:B:230:GLY:HA3	2.19	0.41
1:C:17:GLU:HB2	3:C:604:HOH:O	2.20	0.41
1:C:254:THR:HG23	3:C:550:HOH:O	2.20	0.41
1:D:76:TRP:HB2	1:D:102:ILE:HG23	2.02	0.41
1:B:91:PRO:HD3	1:B:176:ILE:HB	2.02	0.41
1:D:217:CYS:HG	1:D:382:CYS:CB	2.29	0.41
1:B:174:MET:CE	1:B:176:ILE:HD11	2.51	0.41
1:C:286:TYR:HA	1:C:296:PHE:O	2.21	0.41
1:D:287:LEU:O	1:D:295:SER:HB2	2.21	0.41
1:C:149:LEU:HD12	1:C:150:PHE:N	2.36	0.41
1:C:44:PRO:HD3	1:C:51:TYR:CZ	2.56	0.41
1:A:34:GLY:HA3	1:A:228:ASP:OD1	2.21	0.41
1:C:4:ASP:CG	1:C:170:VAL:HG11	2.41	0.40
1:C:8:GLY:HA2	3:C:632:HOH:O	2.21	0.40
1:D:93:VAL:HG11	1:D:144:THR:HG21	2.03	0.40
1:D:206:VAL:CG1	1:D:213:LEU:HD22	2.52	0.40
1:B:195:ARG:HB3	1:B:197:TRP:CD1	2.56	0.40
1:D:232:THR:O	1:D:336:VAL:HG23	2.20	0.40
1:D:95:VAL:HG11	1:D:140:LEU:HD12	2.02	0.40
1:A:313:ALA:C	1:A:315:SER:H	2.24	0.40
1:C:181:HIS:HA	1:C:184:TYR:CE1	2.56	0.40
1:C:199:TYR:HB3	1:C:352:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:GLN:HG3	1:D:279:ILE:HA	2.03	0.40
1:A:113:SER:HB2	1:A:115:TRP:CD1	2.56	0.40
1:A:196:GLU:HG3	1:A:350:LYS:HE3	2.02	0.40
1:A:271:GLN:O	1:A:272:ALA:C	2.60	0.40
1:C:213:LEU:HD12	1:C:213:LEU:HA	1.84	0.40
1:D:146:VAL:HA	1:D:147:PRO:HD3	1.93	0.40
1:A:111:ASN:HD22	1:A:112:GLY:N	2.19	0.40
1:A:267:LEU:CD2	1:A:267:LEU:N	2.65	0.40
1:B:194:ARG:HB2	1:B:202:ILE:CD1	2.49	0.40
1:C:193:ILE:HG13	1:C:351:ARG:CA	2.52	0.40
1:C:271:GLN:HG2	1:C:271:GLN:H	1.56	0.40
1:C:3:VAL:O	1:C:4:ASP:HB2	2.21	0.40
1:D:95:VAL:HG11	1:D:140:LEU:CD1	2.52	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	387/389 (100%)	353 (91%)	29 (8%)	5 (1%)	12	21
1	B	387/389 (100%)	357 (92%)	24 (6%)	6 (2%)	9	17
1	C	387/389 (100%)	361 (93%)	25 (6%)	1 (0%)	41	61
1	D	387/389 (100%)	355 (92%)	24 (6%)	8 (2%)	7	11
All	All	1548/1556 (100%)	1426 (92%)	102 (7%)	20 (1%)	12	21

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	ASP
1	A	314	THR

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Mol	Chain	Res	Type
1	B	223	ASP
1	B	317	ASP
1	C	223	ASP
1	D	223	ASP
1	A	315	SER
1	B	181	HIS
1	B	312	VAL
1	D	48(P)	VAL
1	D	92	ASN
1	D	194	ARG
1	D	238	LYS
1	A	378	ASP
1	D	314	THR
1	D	378	ASP
1	B	238	LYS
1	D	312	VAL
1	B	70	PRO
1	A	312	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	331/331 (100%)	318 (96%)	13 (4%)	32	57
1	B	331/331 (100%)	326 (98%)	5 (2%)	65	85
1	C	331/331 (100%)	318 (96%)	13 (4%)	32	57
1	D	331/331 (100%)	320 (97%)	11 (3%)	38	64
All	All	1324/1324 (100%)	1282 (97%)	42 (3%)	39	65

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	55	GLN
1	A	59	THR

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Mol	Chain	Res	Type
1	A	111	ASN
1	A	162	ASN
1	A	197	TRP
1	A	234	LEU
1	A	242	GLU
1	A	266	GLN
1	A	267	LEU
1	A	317	ASP
1	A	371	GLU
1	A	376	THR
1	B	59	THR
1	B	162	ASN
1	B	197	TRP
1	B	209	ASN
1	B	234	LEU
1	C	47(P)	PHE
1	C	12	GLN
1	C	111	ASN
1	C	125	GLU
1	C	149	LEU
1	C	162	ASN
1	C	197	TRP
1	C	209	ASN
1	C	233	ASN
1	C	234	LEU
1	C	266	GLN
1	C	271	GLN
1	C	378	ASP
1	D	47(P)	PHE
1	D	149	LEU
1	D	162	ASN
1	D	195	ARG
1	D	197	TRP
1	D	209	ASN
1	D	234	LEU
1	D	267	LEU
1	D	294	GLN
1	D	314	THR
1	D	376	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	111	ASN
1	A	162	ASN
1	A	294	GLN
1	A	304	GLN
1	A	326	GLN
1	A	362	HIS
1	B	28	ASN
1	B	111	ASN
1	B	114	ASN
1	B	162	ASN
1	B	209	ASN
1	B	304	GLN
1	B	362	HIS
1	C	12	GLN
1	C	28	ASN
1	C	55	GLN
1	C	111	ASN
1	C	162	ASN
1	C	209	ASN
1	C	233	ASN
1	C	304	GLN
1	C	362	HIS
1	D	28	ASN
1	D	98	ASN
1	D	111	ASN
1	D	162	ASN
1	D	209	ASN
1	D	304	GLN
1	D	362	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	23I	B	502	-	49,50,50	2.48	9 (18%)	67,71,71	1.91	10 (14%)
2	23I	D	504	-	49,50,50	2.56	8 (16%)	67,71,71	1.90	6 (8%)
2	23I	C	503	-	49,50,50	2.44	9 (18%)	67,71,71	1.88	9 (13%)
2	23I	A	501	-	49,50,50	2.43	9 (18%)	67,71,71	1.89	8 (11%)

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	23I	B	502	-	-	8/62/62/62	0/2/2/2
2	23I	D	504	-	-	9/62/62/62	0/2/2/2
2	23I	C	503	-	-	8/62/62/62	0/2/2/2
2	23I	A	501	-	-	8/62/62/62	0/2/2/2

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	504	23I	O24-S2	10.69	1.59	1.43
2	B	502	23I	O24-S2	10.19	1.59	1.43
2	C	503	23I	O24-S2	10.10	1.59	1.43
2	D	504	23I	O23-S2	9.41	1.57	1.43
2	A	501	23I	O23-S2	9.35	1.57	1.43
2	A	501	23I	O24-S2	9.35	1.57	1.43
2	C	503	23I	O23-S2	8.12	1.55	1.43
2	B	502	23I	O23-S2	8.11	1.55	1.43
2	C	503	23I	S2-N22	6.24	1.78	1.64
2	A	501	23I	S2-N22	6.18	1.77	1.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	23I	S2-N22	6.13	1.77	1.64
2	D	504	23I	S2-N22	6.03	1.77	1.64
2	B	502	23I	C15-C16	3.93	1.45	1.39
2	C	503	23I	C15-C16	3.60	1.44	1.39
2	D	504	23I	C15-C16	3.19	1.44	1.39
2	A	501	23I	C33-C31	3.11	1.57	1.52
2	D	504	23I	C24-C25	2.99	1.44	1.39
2	C	503	23I	C24-C23	2.69	1.43	1.39
2	A	501	23I	C11-C16	2.69	1.43	1.39
2	D	504	23I	C24-C23	2.67	1.43	1.39
2	B	502	23I	C26-C25	2.61	1.44	1.39
2	C	503	23I	C11-C16	2.58	1.43	1.39
2	B	502	23I	C33-C31	2.53	1.56	1.52
2	C	503	23I	C26-C27	2.44	1.43	1.39
2	B	502	23I	C11-C16	2.40	1.42	1.39
2	A	501	23I	C24-C25	2.34	1.43	1.39
2	D	504	23I	C11-C16	2.34	1.42	1.39
2	A	501	23I	C15-C16	2.34	1.42	1.39
2	C	503	23I	C26-C25	2.33	1.43	1.39
2	C	503	23I	C24-C25	2.33	1.43	1.39
2	A	501	23I	C26-C25	2.24	1.43	1.39
2	B	502	23I	C41-C45	2.17	1.58	1.52
2	A	501	23I	C41-C45	2.17	1.58	1.52
2	D	504	23I	C41-C45	2.13	1.58	1.52
2	B	502	23I	C24-C25	2.04	1.43	1.39

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	504	23I	O24-S2-O23	-9.34	105.28	118.59
2	A	501	23I	O24-S2-O23	-9.17	105.52	118.59
2	B	502	23I	O24-S2-O23	-9.07	105.66	118.59
2	C	503	23I	O24-S2-O23	-8.85	105.98	118.59
2	D	504	23I	O24-S2-N22	6.74	115.19	107.08
2	A	501	23I	O24-S2-N22	6.39	114.77	107.08
2	C	503	23I	O24-S2-N22	6.13	114.46	107.08
2	B	502	23I	O24-S2-N22	6.09	114.41	107.08
2	B	502	23I	C29-N22-S2	-5.84	108.41	117.86
2	C	503	23I	C29-N22-S2	-5.57	108.85	117.86
2	D	504	23I	C29-N22-S2	-5.40	109.12	117.86
2	A	501	23I	C29-N22-S2	-5.19	109.47	117.86
2	D	504	23I	C33-C31-N3	-4.12	104.86	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	503	23I	C33-C31-N3	-3.68	105.42	110.18
2	A	501	23I	C33-C31-N3	-3.61	105.51	110.18
2	B	502	23I	C33-C31-N3	-3.50	105.65	110.18
2	C	503	23I	O23-S2-N22	2.85	110.50	107.08
2	A	501	23I	O23-S2-N22	2.77	110.42	107.08
2	B	502	23I	C23-C28-C27	2.73	123.62	120.44
2	B	502	23I	O23-S2-N22	2.69	110.32	107.08
2	A	501	23I	C23-C28-C27	2.63	123.50	120.44
2	D	504	23I	O23-S2-N22	2.47	110.06	107.08
2	C	503	23I	C23-C28-C27	2.45	123.30	120.44
2	B	502	23I	C20-S2-N22	2.34	109.40	106.79
2	B	502	23I	C27-C26-C25	2.31	122.22	119.59
2	A	501	23I	C18-C17-N21	-2.21	105.16	109.05
2	D	504	23I	C23-C28-C27	2.20	123.01	120.44
2	C	503	23I	C32-C31-N3	2.15	114.06	109.92
2	C	503	23I	C42-C41-C45	2.13	116.71	111.38
2	A	501	23I	C42-C41-C45	2.07	116.56	111.38
2	C	503	23I	C27-C26-C25	2.07	121.95	119.59
2	B	502	23I	C42-C41-C45	2.06	116.51	111.38
2	B	502	23I	C32-C31-N3	2.01	113.80	109.92

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	502	23I	C24-C25-N22-S2
2	B	502	23I	C26-C25-N22-S2
2	B	502	23I	C25-N22-S2-O23
2	B	502	23I	C29-N22-S2-O24
2	D	504	23I	N3-C31-C33-C34
2	D	504	23I	C24-C25-N22-S2
2	D	504	23I	C26-C25-N22-S2
2	D	504	23I	C25-N22-S2-O23
2	D	504	23I	C29-N22-S2-O24
2	A	501	23I	C24-C25-N22-S2
2	A	501	23I	C26-C25-N22-S2
2	A	501	23I	C25-N22-S2-O23
2	A	501	23I	C29-N22-S2-O24
2	C	503	23I	C24-C25-N22-S2
2	C	503	23I	C26-C25-N22-S2
2	C	503	23I	C25-N22-S2-O23
2	C	503	23I	C31-C33-C34-C36

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Mol	Chain	Res	Type	Atoms
2	C	503	23I	C31-C33-C34-C35
2	D	504	23I	C31-C33-C34-C35
2	D	504	23I	C31-C33-C34-C36
2	B	502	23I	O31-C32-C37-C38
2	C	503	23I	O31-C32-C37-C38
2	A	501	23I	C29-N22-S2-C20
2	A	501	23I	N3-C31-C33-C34
2	B	502	23I	C31-C32-C37-C38
2	D	504	23I	C31-C32-C37-C38
2	C	503	23I	C31-C32-C37-C38
2	D	504	23I	O31-C32-C37-C38
2	A	501	23I	O31-C32-C37-C38
2	C	503	23I	C25-N22-S2-O24
2	B	502	23I	N3-C31-C33-C34
2	A	501	23I	C31-C32-C37-C38
2	B	502	23I	C29-N22-S2-C20

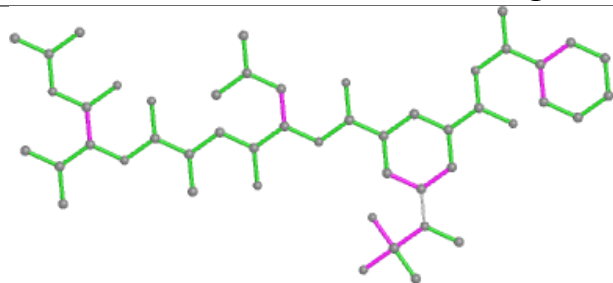
There are no ring outliers.

4 monomers are involved in 10 short contacts:

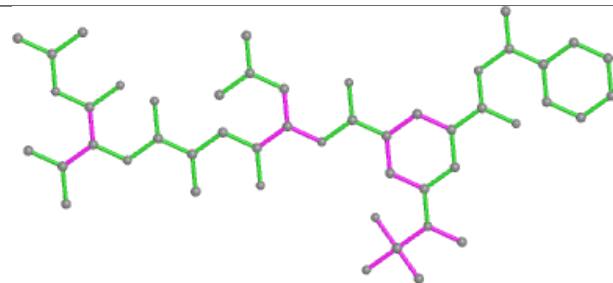
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	23I	3	0
2	D	504	23I	4	0
2	C	503	23I	2	0
2	A	501	23I	1	0

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.

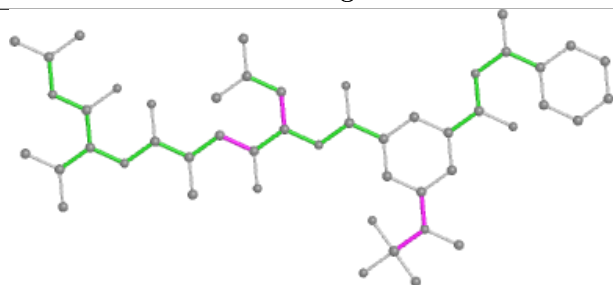
Ligand 23I B 502



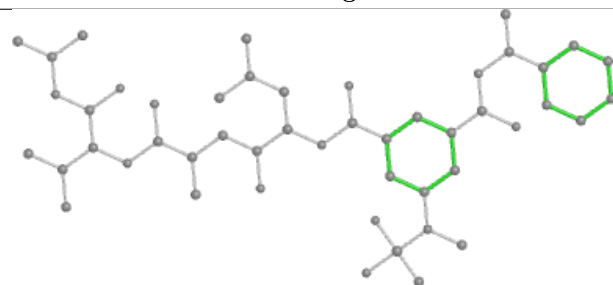
Bond lengths



Bond angles

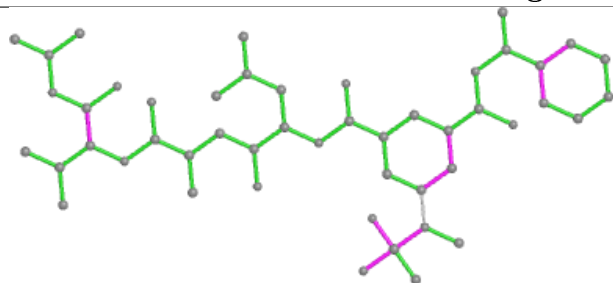


Torsions

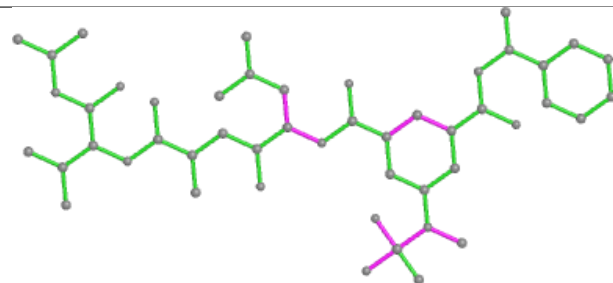


Rings

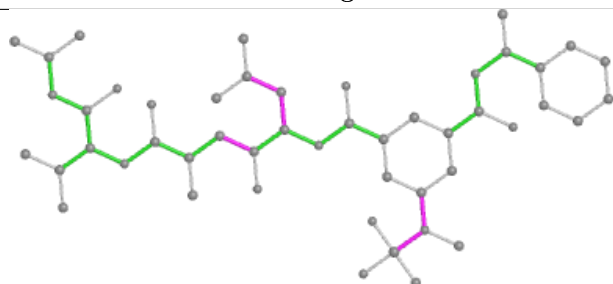
Ligand 23I D 504



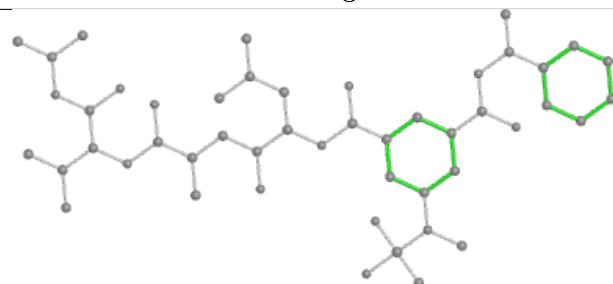
Bond lengths



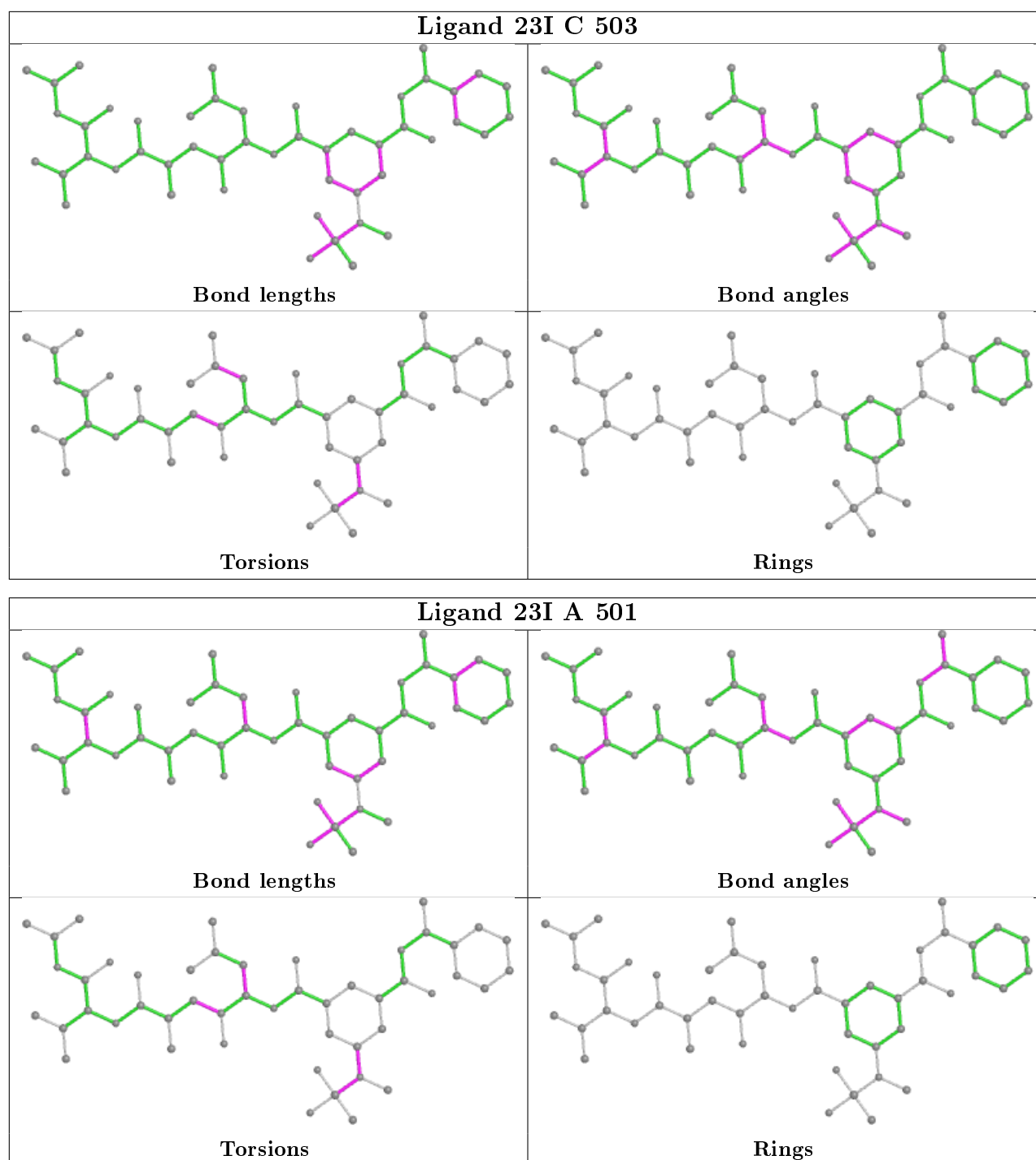
Bond angles



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	389/389 (100%)	0.16	19 (4%)	29	31	21, 36, 71, 88	0
1	B	389/389 (100%)	0.18	22 (5%)	23	25	22, 38, 68, 91	0
1	C	389/389 (100%)	0.00	15 (3%)	39	42	18, 32, 63, 87	0
1	D	389/389 (100%)	0.17	22 (5%)	23	25	20, 39, 62, 93	0
All	All	1556/1556 (100%)	0.13	78 (5%)	28	30	18, 36, 68, 93	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	312	VAL	10.7
1	A	46(P)	SER	8.7
1	B	314	THR	8.0
1	B	45(P)	GLY	7.6
1	B	46(P)	SER	6.2
1	D	378	ASP	5.6
1	A	314	THR	5.6
1	B	378	ASP	5.5
1	D	380	GLU	5.3
1	D	379	MET	5.1
1	C	312	VAL	5.1
1	A	377	LEU	4.9
1	D	377	LEU	4.9
1	D	313	ALA	4.9
1	A	378	ASP	4.8
1	A	313	ALA	4.7
1	D	314	THR	4.6
1	C	46(P)	SER	4.5
1	A	379	MET	4.5
1	B	377	LEU	4.5
1	A	45(P)	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	46(P)	SER	4.4
1	A	380	GLU	4.2
1	C	376	THR	4.2
1	C	377	LEU	4.2
1	B	380	GLU	4.0
1	C	380	GLU	4.0
1	C	378	ASP	3.9
1	A	376	THR	3.8
1	B	379	MET	3.7
1	B	381	ASP	3.6
1	C	379	MET	3.6
1	D	384	TYR	3.6
1	A	10	SER	3.5
1	C	384	TYR	3.5
1	B	384	TYR	3.5
1	A	293	ASN	3.4
1	B	312	VAL	3.3
1	B	382	CYS	3.3
1	D	381	ASP	3.2
1	A	312	VAL	3.2
1	D	376	THR	3.2
1	B	376	THR	3.1
1	D	48(P)	VAL	3.1
1	B	383	GLY	3.1
1	C	314	THR	3.0
1	B	311	ASP	3.0
1	A	47(P)	PHE	2.9
1	D	382	CYS	2.7
1	D	45(P)	GLY	2.7
1	A	157	ALA	2.6
1	B	313	ALA	2.6
1	D	218	LYS	2.6
1	C	45(P)	GLY	2.6
1	D	383	GLY	2.6
1	B	385	ASN	2.5
1	B	293	ASN	2.5
1	B	292	THR	2.5
1	D	385	ASN	2.5
1	A	163	GLN	2.4
1	B	47(P)	PHE	2.4
1	D	222	TYR	2.4
1	D	293	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	382	CYS	2.3
1	D	292	THR	2.3
1	A	169	SER	2.3
1	C	48(P)	VAL	2.2
1	A	382	CYS	2.2
1	C	222	TYR	2.2
1	A	48(P)	VAL	2.2
1	D	291	VAL	2.1
1	C	163	GLN	2.1
1	A	292	THR	2.1
1	D	47(P)	PHE	2.1
1	B	168	ALA	2.0
1	C	49	HIS	2.0
1	B	222	TYR	2.0
1	B	49	HIS	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 carbohydrates in this entry.

6.4 Ligands [i](#)

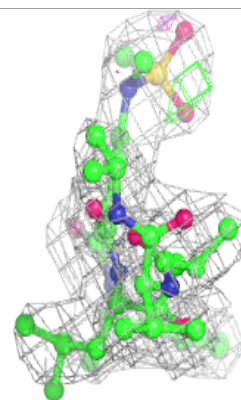
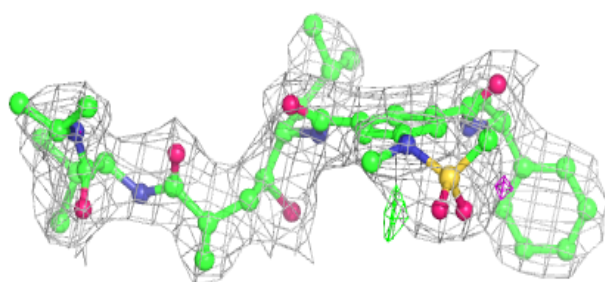
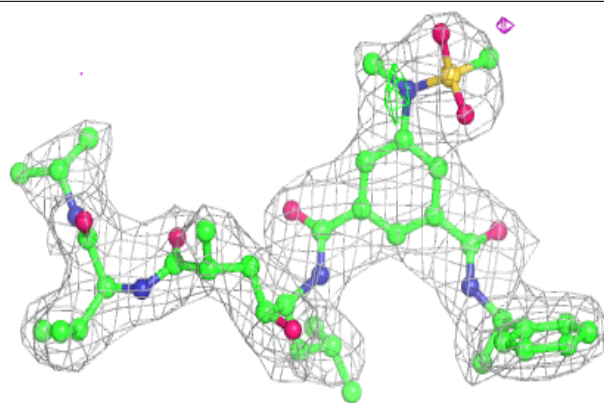
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	23I	A	501	49/49	0.95	0.18	26,31,35,36	0
2	23I	D	504	49/49	0.96	0.18	25,30,40,42	0
2	23I	B	502	49/49	0.96	0.17	25,31,35,35	0
2	23I	C	503	49/49	0.96	0.19	24,30,37,42	0

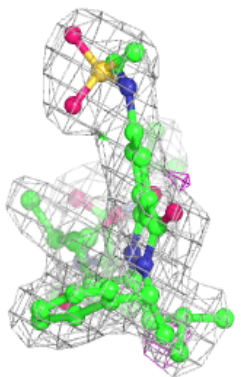
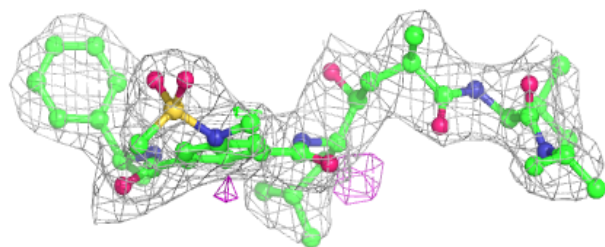
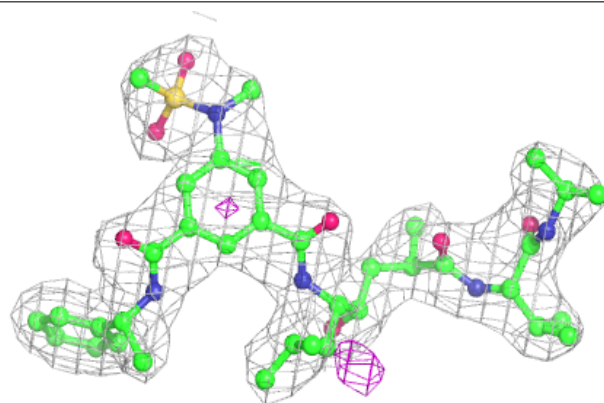
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 23I 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)

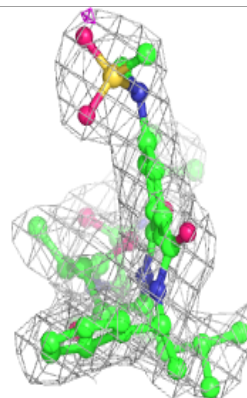
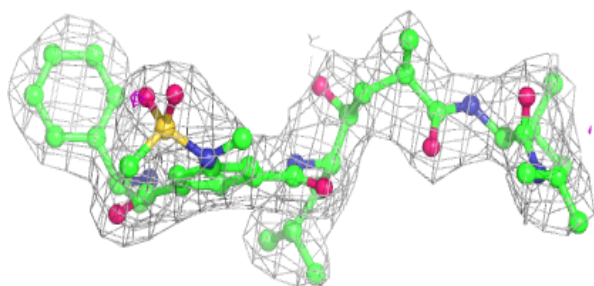
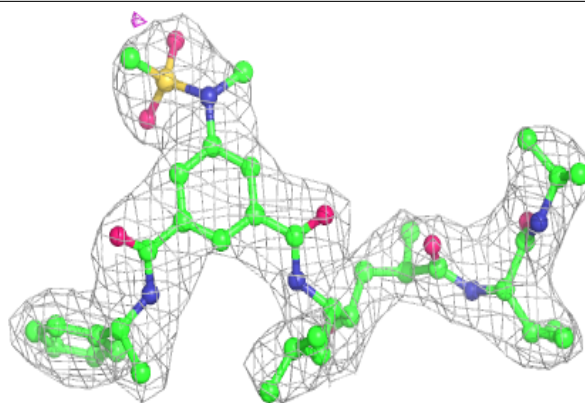
**Electron density around 23I D 504:**

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

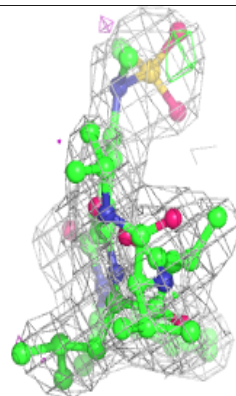
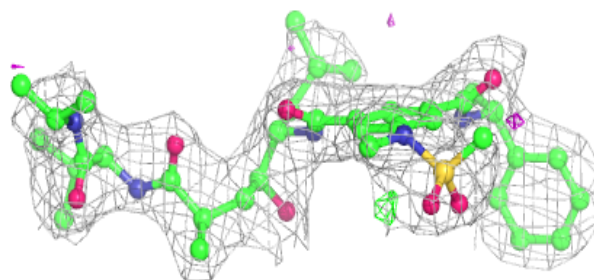
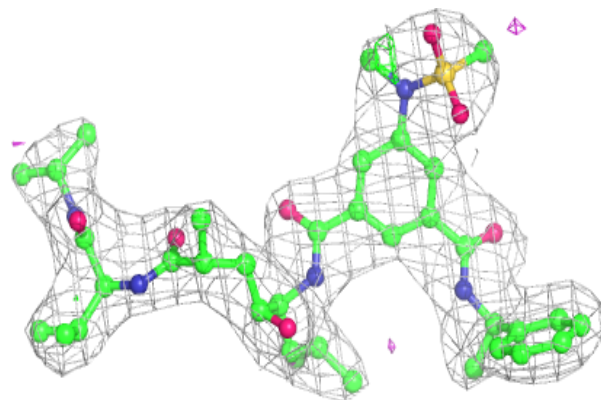


Electron density around 23I B 502:

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

**Electron density around 23I 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.