



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:30 PM UTC

PDB ID : 2G94 / pdb_00002g94
Title : Crystal structure of beta-secretase bound to a potent and highly selective inhibitor.
Authors : Hong, L.; Ghosh, A.; Tang, J.
Deposited on : 2006-03-05
Resolution : 1.86 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

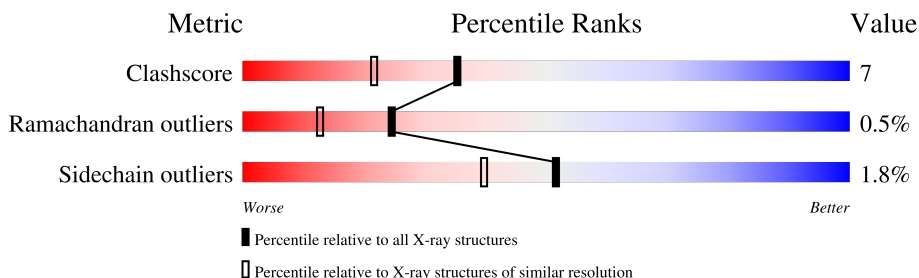
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	389	84% 13% .
1	B	389	86% 11% .
1	C	389	87% 11% .
1	D	389	85% 13% .

2 Entry composition [i](#)

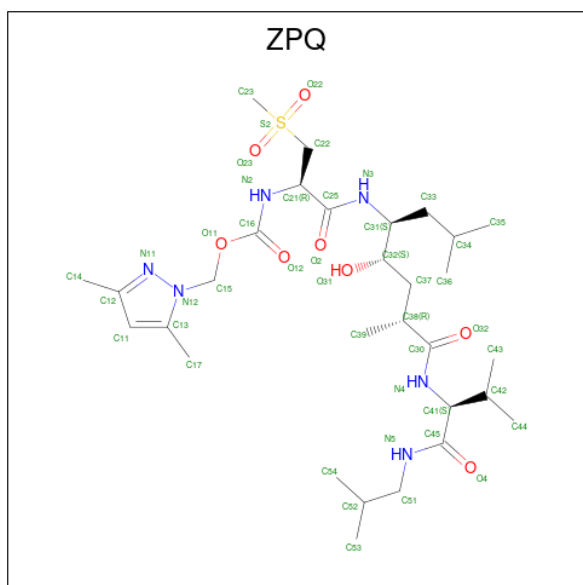
There are 3 unique types of molecules in this entry. The entry contains 13245 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2 -[(2R,4S,5S)-5-{[N-[(3,5-DIMETHYL-1H-PYRAZOL-1-YL)METHOXY]CARBONYL}-3-(METHYLSULFONYL)-L-ALANYL]AMINO}-4-HYDROXY-2,7-DIMETHYLOCTANOYL]-N-ISOBUTYL-L-VALINAMIDE (CCD ID: ZPQ) (formula: $C_{30}H_{54}N_6O_8S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			45	30	6	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			45	30	6	8	1		
2	C	1	Total	C	N	O	S	0	0
			45	30	6	8	1		
2	D	1	Total	C	N	O	S	0	0
			45	30	6	8	1		

- Molecule 3 is water.

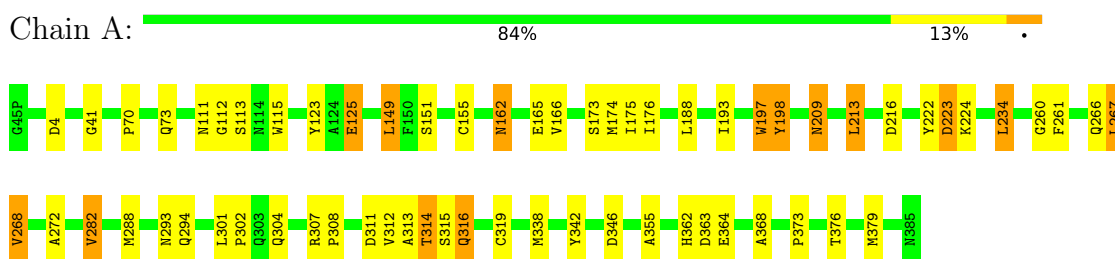
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	200	Total	O	0	0
			200	200		
3	B	212	Total	O	0	0
			212	212		
3	C	238	Total	O	0	0
			238	238		
3	D	203	Total	O	0	0
			203	203		

3 Residue-property plots [i](#)

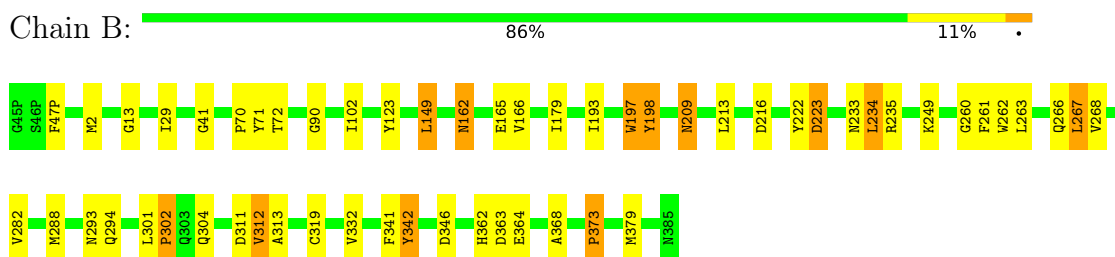
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

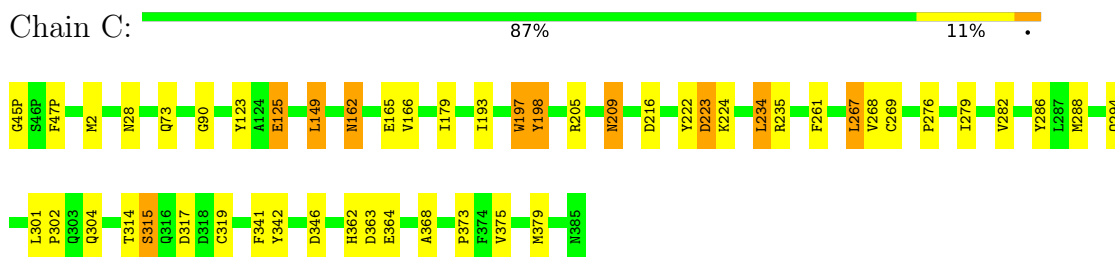
• Molecule 1: Beta-secretase 1



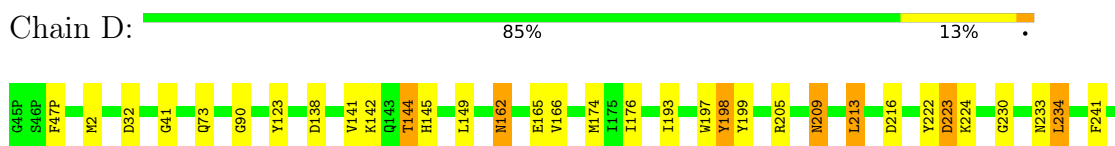
• Molecule 1: Beta-secretase 1

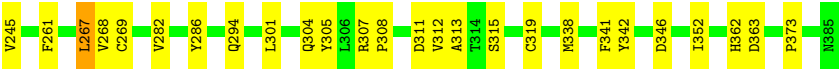


• Molecule 1: Beta-secretase 1



• Molecule 1: Beta-secretase 1





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.63Å 131.02Å 88.24Å 90.00° 97.39° 90.00°	Depositor
Resolution (Å)	46.38 – 1.86	Depositor
% Data completeness (in resolution range)	94.7 (46.38-1.86)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.199 , 0.227	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13245	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.47	0/3131	0.97	15/4256 (0.4%)
1	B	0.48	0/3131	0.97	14/4256 (0.3%)
1	C	0.49	0/3131	0.98	9/4256 (0.2%)
1	D	0.47	0/3131	0.98	15/4256 (0.4%)
All	All	0.48	0/12524	0.98	53/17024 (0.3%)

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	198	TYR	N-CA-C	-9.17	96.15	110.36
1	A	234	LEU	N-CA-C	-8.74	95.06	108.96
1	C	198	TYR	N-CA-C	-8.17	97.70	110.36
1	D	234	LEU	N-CA-C	-8.04	96.17	108.96
1	B	198	TYR	N-CA-C	-7.83	98.22	110.36
1	A	198	TYR	N-CA-C	-7.75	98.35	110.36
1	C	234	LEU	N-CA-C	-7.65	96.09	108.41
1	B	234	LEU	N-CA-C	-7.58	96.21	108.41
1	B	342	TYR	N-CA-C	-7.03	97.79	109.46
1	A	316	GLN	N-CA-C	-6.98	104.76	112.72
1	B	123	TYR	N-CA-C	6.98	119.98	110.55
1	C	123	TYR	N-CA-C	6.97	119.97	110.55
1	A	123	TYR	N-CA-C	6.93	119.91	110.55
1	D	342	TYR	N-CA-C	-6.77	98.23	109.46
1	A	216	ASP	N-CA-C	-6.64	100.21	110.10
1	A	342	TYR	N-CA-C	-6.39	98.86	109.46
1	B	193	ILE	N-CA-C	-6.34	98.40	107.98
1	D	144	THR	N-CA-C	-6.30	99.83	109.41
1	D	213	LEU	N-CA-C	-6.27	104.89	112.54
1	A	193	ILE	N-CA-C	-6.23	98.57	107.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	123	TYR	N-CA-C	6.20	118.91	110.55
1	C	216	ASP	N-CA-C	-6.19	100.88	110.10
1	D	216	ASP	N-CA-C	-6.17	100.90	110.10
1	D	233	ASN	N-CA-C	6.02	118.30	110.53
1	C	193	ILE	N-CA-C	-6.00	99.65	108.54
1	B	216	ASP	N-CA-C	-5.94	101.11	109.96
1	A	268	VAL	N-CA-C	-5.89	99.68	108.46
1	C	342	TYR	N-CA-C	-5.85	99.65	108.96
1	B	368	ALA	N-CA-C	-5.63	103.09	110.53
1	D	341	PHE	N-CA-C	5.61	118.21	109.52
1	D	41	GLY	N-CA-C	-5.58	104.83	111.36
1	A	213	LEU	N-CA-C	-5.57	105.75	112.54
1	A	368	ALA	N-CA-C	-5.54	103.22	110.53
1	D	338	MET	N-CA-C	5.40	117.92	111.71
1	C	341	PHE	N-CA-C	5.38	117.86	109.52
1	B	341	PHE	N-CA-C	5.35	117.81	109.52
1	B	13	GLY	N-CA-C	5.34	118.72	111.72
1	D	193	ILE	N-CA-C	-5.33	99.93	107.98
1	B	233	ASN	N-CA-C	5.33	117.40	110.53
1	A	41	GLY	N-CA-C	-5.28	105.18	111.36
1	A	282	VAL	N-CA-C	-5.28	104.30	110.05
1	D	305	TYR	N-CA-C	5.22	119.64	113.16
1	D	144	THR	CA-C-N	-5.21	114.90	122.86
1	D	144	THR	C-N-CA	-5.21	114.90	122.86
1	C	368	ALA	N-CA-C	-5.16	103.67	110.43
1	A	197	TRP	N-CA-C	-5.10	99.94	110.80
1	B	197	TRP	N-CA-C	-5.09	99.96	110.80
1	B	302	PRO	N-CA-C	-5.02	107.32	113.84
1	B	213	LEU	N-CA-C	-5.01	106.43	112.54
1	B	29	ILE	N-CA-C	5.01	115.06	107.75
1	A	155	CYS	N-CA-C	5.01	116.85	107.99
1	A	338	MET	N-CA-C	5.01	117.47	111.71
1	C	197	TRP	N-CA-C	-5.00	100.14	110.80

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	55	0
1	B	3053	0	2965	35	0
1	C	3053	0	2965	40	0
1	D	3053	0	2965	41	0
2	A	45	0	54	3	0
2	B	45	0	54	1	0
2	C	45	0	54	1	0
2	D	45	0	54	1	0
3	A	200	0	0	3	0
3	B	212	0	0	0	0
3	C	238	0	0	0	0
3	D	203	0	0	0	0
All	All	13245	0	12076	170	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 7.

All (170) 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	1.35	0.91
1:A:311:ASP:HB2	1:A:319:CYS:SG	2.15	0.86
1:A:162:ASN:ND2	1:A:165:GLU:H	1.76	0.82
1:A:267:LEU:H	1:A:267:LEU:HD23	1.45	0.81
1:D:301:LEU:H	1:D:304:GLN:HE21	1.30	0.80
1:A:162:ASN:C	1:A:162:ASN:HD22	1.92	0.77
1:C:267:LEU:HD23	1:C:267:LEU:H	1.49	0.77
1:B:301:LEU:H	1:B:304:GLN:HE21	1.35	0.75
1:B:162:ASN:C	1:B:162:ASN:HD22	1.95	0.75
1:A:301:LEU:H	1:A:304:GLN:HE21	1.36	0.73
1:A:312:VAL:HG23	1:A:313:ALA:H	1.55	0.71
1:D:301:LEU:H	1:D:304:GLN:NE2	1.88	0.70
1:A:272:ALA:HB2	1:A:316:GLN:O	1.92	0.69
1:C:301:LEU:H	1:C:304:GLN:HE21	1.39	0.68
1:A:267:LEU:HD23	1:A:267:LEU:N	2.07	0.68
1:C:162:ASN:ND2	1:C:165:GLU:H	1.90	0.68
1:B:301:LEU:H	1:B:304:GLN:NE2	1.92	0.68
1:C:222:TYR:O	1:C:223:ASP:HB3	1.93	0.67
1:C:267:LEU:H	1:C:267:LEU:CD2	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:ASN:HD22	1:D:162:ASN:C	2.02	0.67
1:A:312:VAL:HG23	1:A:313:ALA:N	2.09	0.66
1:C:162:ASN:O	1:C:166:VAL:HG23	1.96	0.66
1:A:313:ALA:C	1:A:315:SER:H	2.05	0.65
1:C:261:PHE:CD1	1:C:268:VAL:HG23	2.32	0.65
1:C:162:ASN:HD22	1:C:162:ASN:C	2.05	0.65
1:A:301:LEU:H	1:A:304:GLN:NE2	1.96	0.63
1:D:141:VAL:O	1:D:144:THR:O	2.17	0.63
1:B:162:ASN:ND2	1:B:165:GLU:H	1.96	0.61
1:D:261:PHE:CD1	1:D:268:VAL:HG23	2.36	0.61
1:D:162:ASN:ND2	1:D:165:GLU:H	1.98	0.60
1:C:301:LEU:H	1:C:304:GLN:NE2	2.00	0.59
1:A:162:ASN:HD22	1:A:165:GLU:H	1.49	0.59
1:A:174:MET:HE3	1:A:176:ILE:HD11	1.85	0.58
1:D:73:GLN:HB2	2:D:4001:ZPQ:H222	1.84	0.58
1:B:311:ASP:HB2	1:B:319:CYS:SG	2.44	0.57
1:D:269:CYS:CB	1:D:319:CYS:HG	2.16	0.57
1:A:222:TYR:O	1:A:223:ASP:HB3	2.03	0.57
1:D:311:ASP:OD2	1:D:315:SER:OG	2.23	0.56
1:B:197:TRP:CG	1:B:198:TYR:H	2.24	0.56
1:D:311:ASP:HB2	1:D:319:CYS:SG	2.46	0.56
1:C:362:HIS:HD2	1:C:363:ASP:O	1.89	0.56
1:D:267:LEU:H	1:D:267:LEU:CD2	2.20	0.55
1:C:317:ASP:OD2	1:D:145:HIS:ND1	2.35	0.55
1:A:209:ASN:ND2	1:A:282:VAL:H	2.04	0.55
1:D:223:ASP:OD1	1:D:224:LYS:NZ	2.40	0.55
1:A:162:ASN:HD21	1:A:165:GLU:HG3	1.72	0.54
1:A:73:GLN:HB2	2:A:1001:ZPQ:H222	1.87	0.54
1:B:260:GLY:C	1:B:266:GLN:HG2	2.33	0.54
1:C:45(P):GLY:HA2	1:C:179:ILE:O	2.07	0.54
1:A:197:TRP:CG	1:A:198:TYR:H	2.26	0.54
1:B:364:GLU:HG2	1:B:364:GLU:O	2.06	0.54
1:C:364:GLU:HG2	1:C:364:GLU:O	2.07	0.54
1:B:222:TYR:O	1:B:223:ASP:CB	2.56	0.53
1:B:312:VAL:HG23	1:B:313:ALA:N	2.13	0.53
1:C:222:TYR:O	1:C:223:ASP:CB	2.57	0.52
1:A:301:LEU:HB3	1:A:302:PRO:HD2	1.90	0.52
1:C:197:TRP:CG	1:C:198:TYR:H	2.27	0.52
1:A:223:ASP:OD1	1:A:224:LYS:NZ	2.42	0.52
1:C:223:ASP:OD1	1:C:224:LYS:HG2	2.09	0.52
1:B:249:LYS:HE2	1:B:262:TRP:CD1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:MET:HG2	1:D:90:GLY:HA2	1.91	0.52
1:A:162:ASN:HD21	1:A:165:GLU:H	1.56	0.51
1:D:362:HIS:HD2	1:D:363:ASP:O	1.93	0.51
1:A:313:ALA:C	1:A:315:SER:N	2.67	0.51
1:D:197:TRP:CG	1:D:198:TYR:H	2.28	0.51
1:A:260:GLY:C	1:A:266:GLN:HG2	2.36	0.51
1:A:294:GLN:O	1:A:379:MET:HE1	2.10	0.51
1:C:209:ASN:ND2	1:C:282:VAL:H	2.09	0.51
1:C:162:ASN:HD22	1:C:165:GLU:H	1.56	0.50
1:B:261:PHE:CD1	1:B:268:VAL:HG23	2.47	0.50
1:C:125:GLU:O	1:C:125:GLU:HG3	2.11	0.50
1:D:223:ASP:OD1	1:D:224:LYS:HG2	2.11	0.50
1:B:209:ASN:ND2	1:B:282:VAL:H	2.09	0.50
1:A:162:ASN:ND2	1:A:165:GLU:HG3	2.27	0.49
1:B:162:ASN:C	1:B:162:ASN:ND2	2.68	0.49
1:D:47(P):PHE:HB3	1:D:2:MET:HE3	1.93	0.49
1:A:223:ASP:OD1	1:A:224:LYS:HG2	2.12	0.49
1:C:288:MET:HE2	1:C:379:MET:CB	2.42	0.49
1:D:222:TYR:O	1:D:223:ASP:HB3	2.12	0.49
1:B:162:ASN:O	1:B:166:VAL:HG23	2.13	0.49
1:C:269:CYS:HG	1:C:319:CYS:CB	2.20	0.49
1:A:314:THR:O	1:A:314:THR:HG22	2.13	0.48
1:B:293:ASN:HA	1:B:379:MET:HE2	1.94	0.48
1:A:224:LYS:CE	3:A:1198:HOH:O	2.61	0.48
1:D:313:ALA:C	1:D:315:SER:H	2.22	0.48
1:D:312:VAL:HG23	1:D:313:ALA:N	2.28	0.48
1:B:70:PRO:HG2	2:B:2001:ZPQ:H542	1.96	0.48
1:C:267:LEU:HD23	1:C:267:LEU:N	2.23	0.47
1:D:205:ARG:HB3	1:D:286:TYR:HB2	1.97	0.47
1:A:312:VAL:CG2	1:A:313:ALA:H	2.26	0.47
1:D:174:MET:HE3	1:D:176:ILE:HD11	1.97	0.47
1:C:197:TRP:CD1	1:C:198:TYR:H	2.32	0.47
1:D:138:ASP:O	1:D:142:LYS:HG3	2.14	0.47
1:A:222:TYR:O	1:A:223:ASP:CB	2.62	0.47
1:A:4:ASP:H	1:A:173:SER:HG	1.61	0.46
1:C:47(P):PHE:N	1:C:47(P):PHE:CD1	2.83	0.46
1:A:261:PHE:CD1	1:A:268:VAL:HG23	2.50	0.46
1:B:294:GLN:CG	1:B:373:PRO:HB2	2.46	0.46
1:A:209:ASN:HD22	1:A:282:VAL:HG22	1.81	0.46
1:B:2:MET:HG2	1:B:90:GLY:HA2	1.98	0.46
1:A:294:GLN:CG	1:A:373:PRO:HB2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:GLN:HB2	2:C:3001:ZPQ:H222	1.98	0.46
1:C:294:GLN:CG	1:C:373:PRO:HB2	2.46	0.46
1:A:312:VAL:CG2	1:A:313:ALA:N	2.79	0.46
1:A:224:LYS:HE2	3:A:1198:HOH:O	2.15	0.45
1:D:199:TYR:HB3	1:D:352:ILE:HD11	1.98	0.45
1:D:222:TYR:O	1:D:223:ASP:CB	2.64	0.45
1:D:311:ASP:O	1:D:312:VAL:C	2.60	0.45
1:D:209:ASN:HD22	1:D:282:VAL:HG22	1.80	0.45
1:B:47(P):PHE:HB3	1:B:2:MET:HE3	1.99	0.45
1:D:162:ASN:C	1:D:162:ASN:ND2	2.74	0.45
1:B:364:GLU:CD	1:C:375:VAL:H	2.24	0.45
1:C:288:MET:HE2	1:C:379:MET:HB3	1.99	0.44
1:D:162:ASN:HD22	1:D:165:GLU:H	1.64	0.44
1:A:125:GLU:HG2	1:A:197:TRP:HB2	1.99	0.44
1:A:293:ASN:HA	1:A:376:THR:O	2.17	0.44
1:B:209:ASN:HD22	1:B:282:VAL:HG22	1.82	0.44
1:B:149:LEU:HB2	1:B:346:ASP:HA	1.99	0.44
2:A:1001:ZPQ:H533	3:A:1193:HOH:O	2.17	0.44
1:B:235:ARG:HG3	1:B:332:VAL:HB	1.98	0.44
1:C:47(P):PHE:HB3	1:C:2:MET:HE3	1.99	0.44
1:C:209:ASN:HD22	1:C:282:VAL:HG22	1.81	0.44
1:D:294:GLN:CG	1:D:373:PRO:HB2	2.48	0.44
1:A:149:LEU:HB2	1:A:346:ASP:HA	1.99	0.44
1:A:125:GLU:HG2	1:A:197:TRP:CB	2.48	0.44
1:A:313:ALA:O	1:A:315:SER:N	2.51	0.44
1:A:111:ASN:HD22	1:A:112:GLY:N	2.16	0.44
1:B:179:ILE:HG23	1:B:342:TYR:HE2	1.82	0.43
1:B:301:LEU:HB3	1:B:302:PRO:HD2	1.99	0.43
1:C:149:LEU:HB2	1:C:346:ASP:HA	2.00	0.43
1:D:149:LEU:HB2	1:D:346:ASP:HA	2.00	0.43
1:D:162:ASN:O	1:D:166:VAL:HG23	2.18	0.43
1:D:307:ARG:HA	1:D:308:PRO:HD3	1.91	0.43
1:B:222:TYR:O	1:B:223:ASP:HB2	2.18	0.43
1:C:314:THR:O	1:C:315:SER:O	2.36	0.43
1:B:41:GLY:HA2	1:B:102:ILE:HB	2.00	0.43
1:D:213:LEU:HD12	1:D:213:LEU:HA	1.86	0.43
1:A:307:ARG:HA	1:A:308:PRO:HD3	1.88	0.42
1:A:213:LEU:HD12	1:A:213:LEU:HA	1.89	0.42
1:C:294:GLN:HG2	1:C:373:PRO:HB2	2.01	0.42
1:C:209:ASN:HD22	1:C:209:ASN:HA	1.61	0.42
1:D:32:ASP:OD1	1:D:230:GLY:HA3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:ASN:ND2	1:D:282:VAL:H	2.16	0.42
1:D:241:PHE:CZ	1:D:245:VAL:HG21	2.55	0.42
1:A:70:PRO:HG2	2:A:1001:ZPQ:H542	2.02	0.42
1:B:362:HIS:HD2	1:B:363:ASP:O	2.01	0.42
1:D:267:LEU:H	1:D:267:LEU:HD22	1.84	0.42
1:B:209:ASN:HD22	1:B:209:ASN:HA	1.63	0.41
1:C:301:LEU:HB3	1:C:302:PRO:HD2	2.02	0.41
1:A:162:ASN:ND2	1:A:165:GLU:N	2.57	0.41
1:A:362:HIS:HD2	1:A:363:ASP:O	2.02	0.41
1:A:364:GLU:O	1:A:364:GLU:HG2	2.19	0.41
1:D:209:ASN:HD22	1:D:209:ASN:HA	1.59	0.41
1:C:276:PRO:O	1:C:279:ILE:HG12	2.20	0.41
1:A:188:LEU:HD23	1:A:355:ALA:HB2	2.02	0.41
1:A:113:SER:HB2	1:A:115:TRP:CD1	2.56	0.41
1:A:162:ASN:ND2	1:A:162:ASN:C	2.65	0.41
1:A:162:ASN:HD21	1:A:165:GLU:N	2.19	0.41
1:D:197:TRP:CD1	1:D:198:TYR:H	2.37	0.41
1:A:288:MET:HE2	1:A:379:MET:CB	2.51	0.41
1:B:71:TYR:O	1:B:72:THR:C	2.62	0.41
1:B:197:TRP:CD1	1:B:198:TYR:H	2.37	0.41
1:C:2:MET:HG2	1:C:90:GLY:HA2	2.01	0.41
1:C:261:PHE:CD1	1:C:268:VAL:CG2	3.03	0.41
1:B:267:LEU:H	1:B:267:LEU:CD2	2.34	0.40
1:B:288:MET:HE2	1:B:379:MET:HB3	2.03	0.40
1:A:151:SER:OG	1:A:175:ILE:HB	2.21	0.40
1:A:162:ASN:O	1:A:166:VAL:HG23	2.20	0.40
1:C:28:ASN:HD22	1:C:28:ASN:HA	1.71	0.40
1:C:205:ARG:HB3	1:C:286:TYR:HB2	2.03	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%)	373 (96%)	12 (3%)	2 (0%)	24	13
1	B	387/389 (100%)	374 (97%)	11 (3%)	2 (0%)	24	13
1	C	387/389 (100%)	375 (97%)	10 (3%)	2 (0%)	24	13
1	D	387/389 (100%)	372 (96%)	14 (4%)	1 (0%)	36	25
All	All	1548/1556 (100%)	1494 (96%)	47 (3%)	7 (0%)	24	13

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	ASP
1	B	223	ASP
1	B	312	VAL
1	C	223	ASP
1	C	315	SER
1	D	223	ASP
1	A	314	THR

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%)	325 (98%)	6 (2%)	51	40
1	B	331/331 (100%)	324 (98%)	7 (2%)	47	33
1	C	331/331 (100%)	324 (98%)	7 (2%)	47	33
1	D	331/331 (100%)	327 (99%)	4 (1%)	63	55
All	All	1324/1324 (100%)	1300 (98%)	24 (2%)	51	40

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	GLU
1	A	149	LEU
1	A	162	ASN
1	A	209	ASN

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Mol	Chain	Res	Type
1	A	234	LEU
1	A	267	LEU
1	B	149	LEU
1	B	162	ASN
1	B	209	ASN
1	B	234	LEU
1	B	263	LEU
1	B	267	LEU
1	B	373	PRO
1	C	125	GLU
1	C	149	LEU
1	C	162	ASN
1	C	209	ASN
1	C	234	LEU
1	C	235	ARG
1	C	267	LEU
1	D	162	ASN
1	D	209	ASN
1	D	234	LEU
1	D	267	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	111	ASN
1	A	162	ASN
1	A	163	GLN
1	A	209	ASN
1	A	293	ASN
1	A	304	GLN
1	A	326	GLN
1	A	362	HIS
1	A	385	ASN
1	B	28	ASN
1	B	49	HIS
1	B	73	GLN
1	B	111	ASN
1	B	162	ASN
1	B	209	ASN
1	B	211	GLN
1	B	304	GLN

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Mol	Chain	Res	Type
1	B	326	GLN
1	B	362	HIS
1	B	385	ASN
1	C	28	ASN
1	C	55	GLN
1	C	89	HIS
1	C	111	ASN
1	C	162	ASN
1	C	163	GLN
1	C	209	ASN
1	C	304	GLN
1	C	326	GLN
1	C	362	HIS
1	D	28	ASN
1	D	98	ASN
1	D	111	ASN
1	D	162	ASN
1	D	181	HIS
1	D	209	ASN
1	D	266	GLN
1	D	304	GLN
1	D	326	GLN
1	D	362	HIS
1	D	385	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	ZPQ	A	1001	-	45,45,45	3.55	9 (20%)	58,63,63	2.36	15 (25%)
2	ZPQ	B	2001	-	45,45,45	3.58	9 (20%)	58,63,63	2.28	14 (24%)
2	ZPQ	C	3001	-	45,45,45	3.49	7 (15%)	58,63,63	2.34	16 (27%)
2	ZPQ	D	4001	-	45,45,45	3.56	8 (17%)	58,63,63	2.31	14 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ZPQ	A	1001	-	-	7/55/55/55	0/1/1/1
2	ZPQ	B	2001	-	-	6/55/55/55	0/1/1/1
2	ZPQ	C	3001	-	-	5/55/55/55	0/1/1/1
2	ZPQ	D	4001	-	-	4/55/55/55	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	ZPQ	C12-N11	18.79	1.59	1.33
2	D	4001	ZPQ	C12-N11	18.72	1.59	1.33
2	B	2001	ZPQ	C12-N11	18.65	1.59	1.33
2	C	3001	ZPQ	C12-N11	18.32	1.58	1.33
2	B	2001	ZPQ	C13-N12	10.56	1.46	1.35
2	A	1001	ZPQ	C13-N12	10.41	1.46	1.35
2	C	3001	ZPQ	C13-N12	10.32	1.46	1.35
2	D	4001	ZPQ	C13-N12	10.10	1.46	1.35
2	C	3001	ZPQ	C11-C12	6.31	1.51	1.40
2	A	1001	ZPQ	C11-C12	6.18	1.50	1.40
2	B	2001	ZPQ	C11-C12	6.16	1.50	1.40
2	D	4001	ZPQ	C11-C12	6.16	1.50	1.40
2	D	4001	ZPQ	C22-C21	4.13	1.56	1.53
2	B	2001	ZPQ	C22-C21	3.75	1.56	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	ZPQ	C33-C31	3.60	1.58	1.53
2	A	1001	ZPQ	C22-C21	2.80	1.55	1.53
2	A	1001	ZPQ	C33-C31	2.79	1.57	1.53
2	A	1001	ZPQ	C15-N12	2.74	1.50	1.46
2	C	3001	ZPQ	C33-C31	2.72	1.56	1.53
2	C	3001	ZPQ	C15-N12	2.68	1.49	1.46
2	C	3001	ZPQ	C22-C21	2.54	1.55	1.53
2	D	4001	ZPQ	C45-N5	2.52	1.39	1.33
2	A	1001	ZPQ	C45-N5	2.47	1.39	1.33
2	D	4001	ZPQ	C33-C31	2.44	1.56	1.53
2	B	2001	ZPQ	C45-N5	2.37	1.39	1.33
2	D	4001	ZPQ	C25-N3	2.37	1.39	1.34
2	B	2001	ZPQ	C25-N3	2.35	1.39	1.34
2	B	2001	ZPQ	C15-N12	2.28	1.49	1.46
2	D	4001	ZPQ	O11-C15	-2.25	1.41	1.44
2	A	1001	ZPQ	C25-N3	2.25	1.38	1.34
2	C	3001	ZPQ	C32-C31	2.19	1.57	1.53
2	B	2001	ZPQ	C41-N4	2.16	1.50	1.45
2	A	1001	ZPQ	N12-N11	2.11	1.40	1.36

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	ZPQ	C11-C12-N11	-8.55	102.77	111.11
2	D	4001	ZPQ	C11-C12-N11	-8.48	102.85	111.11
2	C	3001	ZPQ	C11-C12-N11	-8.38	102.94	111.11
2	B	2001	ZPQ	C11-C12-N11	-8.18	103.13	111.11
2	B	2001	ZPQ	C11-C13-N12	6.70	110.23	105.95
2	A	1001	ZPQ	C11-C13-N12	6.32	109.99	105.95
2	C	3001	ZPQ	C11-C13-N12	6.27	109.96	105.95
2	D	4001	ZPQ	C11-C13-N12	6.24	109.94	105.95
2	C	3001	ZPQ	C21-C22-S2	5.31	116.46	113.51
2	C	3001	ZPQ	C15-N12-N11	5.12	127.40	119.50
2	B	2001	ZPQ	C15-N12-N11	5.04	127.28	119.50
2	A	1001	ZPQ	C21-C22-S2	4.96	116.27	113.51
2	D	4001	ZPQ	C13-C11-C12	4.93	110.76	106.75
2	A	1001	ZPQ	C13-C11-C12	4.86	110.70	106.75
2	B	2001	ZPQ	C21-C22-S2	4.83	116.20	113.51
2	D	4001	ZPQ	C15-N12-N11	4.81	126.92	119.50
2	D	4001	ZPQ	C21-C22-S2	4.76	116.16	113.51
2	C	3001	ZPQ	C13-C11-C12	4.67	110.55	106.75
2	D	4001	ZPQ	C17-C13-N12	4.65	127.39	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	ZPQ	C15-N12-N11	4.65	126.68	119.50
2	A	1001	ZPQ	C17-C13-N12	4.57	127.31	122.81
2	B	2001	ZPQ	C17-C13-N12	4.36	127.11	122.81
2	C	3001	ZPQ	C17-C13-N12	4.34	127.09	122.81
2	B	2001	ZPQ	C17-C13-C11	-4.33	122.66	129.90
2	D	4001	ZPQ	C17-C13-C11	-4.33	122.66	129.90
2	A	1001	ZPQ	C17-C13-C11	-4.30	122.70	129.90
2	B	2001	ZPQ	C13-C11-C12	4.30	110.25	106.75
2	C	3001	ZPQ	C17-C13-C11	-4.15	122.95	129.90
2	B	2001	ZPQ	C21-N2-C16	3.46	129.53	120.93
2	C	3001	ZPQ	C21-N2-C16	3.44	129.49	120.93
2	A	1001	ZPQ	C21-N2-C16	3.43	129.46	120.93
2	D	4001	ZPQ	C21-N2-C16	3.40	129.39	120.93
2	A	1001	ZPQ	C14-C12-C11	3.36	133.65	128.62
2	C	3001	ZPQ	C14-C12-C11	3.21	133.43	128.62
2	D	4001	ZPQ	C25-C21-N2	-3.11	102.69	111.11
2	D	4001	ZPQ	C14-C12-C11	3.10	133.27	128.62
2	B	2001	ZPQ	C14-C12-C11	3.08	133.23	128.62
2	C	3001	ZPQ	C25-C21-N2	-3.05	102.87	111.11
2	A	1001	ZPQ	O23-S2-C23	2.99	111.65	108.87
2	B	2001	ZPQ	O23-S2-C23	2.98	111.64	108.87
2	B	2001	ZPQ	C25-C21-N2	-2.96	103.11	111.11
2	A	1001	ZPQ	C13-N12-N11	-2.90	110.51	112.32
2	D	4001	ZPQ	C14-C12-N11	2.89	123.89	120.24
2	A	1001	ZPQ	C25-C21-N2	-2.87	103.35	111.11
2	C	3001	ZPQ	O23-S2-C23	2.79	111.46	108.87
2	D	4001	ZPQ	C32-C31-N3	2.77	115.17	109.97
2	B	2001	ZPQ	C14-C12-N11	2.70	123.64	120.24
2	A	1001	ZPQ	C32-C31-N3	2.69	115.02	109.97
2	C	3001	ZPQ	C14-C12-N11	2.69	123.63	120.24
2	A	1001	ZPQ	C14-C12-N11	2.65	123.58	120.24
2	C	3001	ZPQ	C13-N12-N11	-2.60	110.70	112.32
2	C	3001	ZPQ	O22-S2-C22	-2.59	106.84	108.73
2	C	3001	ZPQ	C32-C31-N3	2.58	114.80	109.97
2	A	1001	ZPQ	O22-S2-C22	-2.48	106.92	108.73
2	B	2001	ZPQ	C32-C31-N3	2.45	114.57	109.97
2	D	4001	ZPQ	O23-S2-C23	2.44	111.14	108.87
2	B	2001	ZPQ	C13-N12-N11	-2.43	110.80	112.32
2	D	4001	ZPQ	C13-N12-N11	-2.27	110.90	112.32
2	C	3001	ZPQ	C31-N3-C25	-2.08	119.63	123.25

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	ZPQ	N12-C15-O11-C16
2	B	2001	ZPQ	N2-C21-C22-S2
2	D	4001	ZPQ	N2-C21-C22-S2
2	B	2001	ZPQ	C21-C22-S2-O22
2	A	1001	ZPQ	N2-C21-C25-O2
2	A	1001	ZPQ	C21-C22-S2-O22
2	C	3001	ZPQ	C21-C22-S2-O22
2	D	4001	ZPQ	C21-C22-S2-O22
2	A	1001	ZPQ	C22-C21-C25-O2
2	C	3001	ZPQ	C22-C21-C25-O2
2	C	3001	ZPQ	N2-C21-C25-O2
2	D	4001	ZPQ	N2-C21-C25-O2
2	B	2001	ZPQ	N5-C'51-C'52-C'54
2	A	1001	ZPQ	N2-C21-C25-N3
2	B	2001	ZPQ	N2-C21-C25-O2
2	C	3001	ZPQ	N2-C21-C25-N3
2	A	1001	ZPQ	N2-C21-C22-S2
2	A	1001	ZPQ	C21-C22-S2-O23
2	B	2001	ZPQ	C21-C22-S2-O23
2	C	3001	ZPQ	C21-C22-S2-O23
2	D	4001	ZPQ	C21-C22-S2-O23
2	B	2001	ZPQ	C21-C22-S2-C23

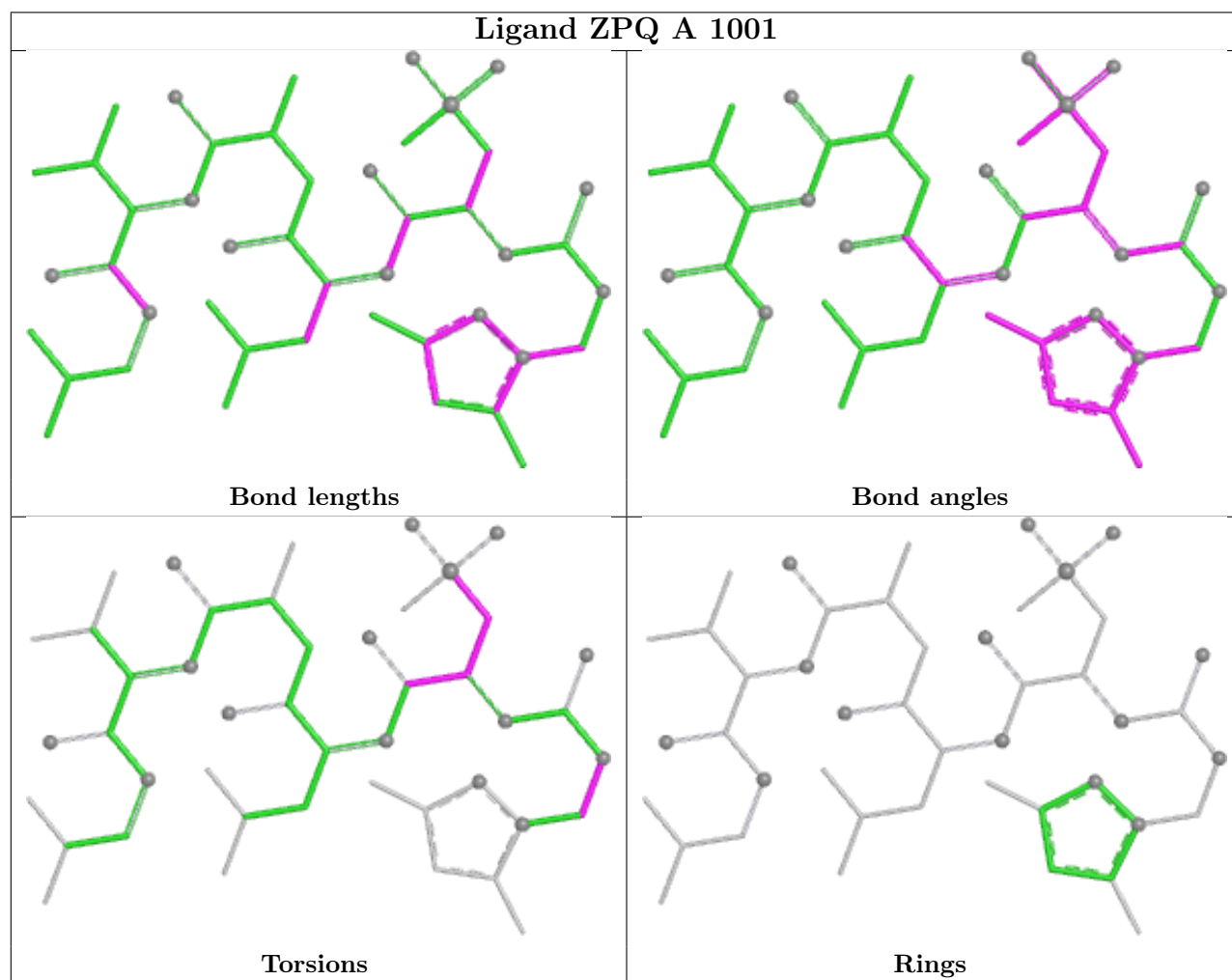
There are no ring outliers.

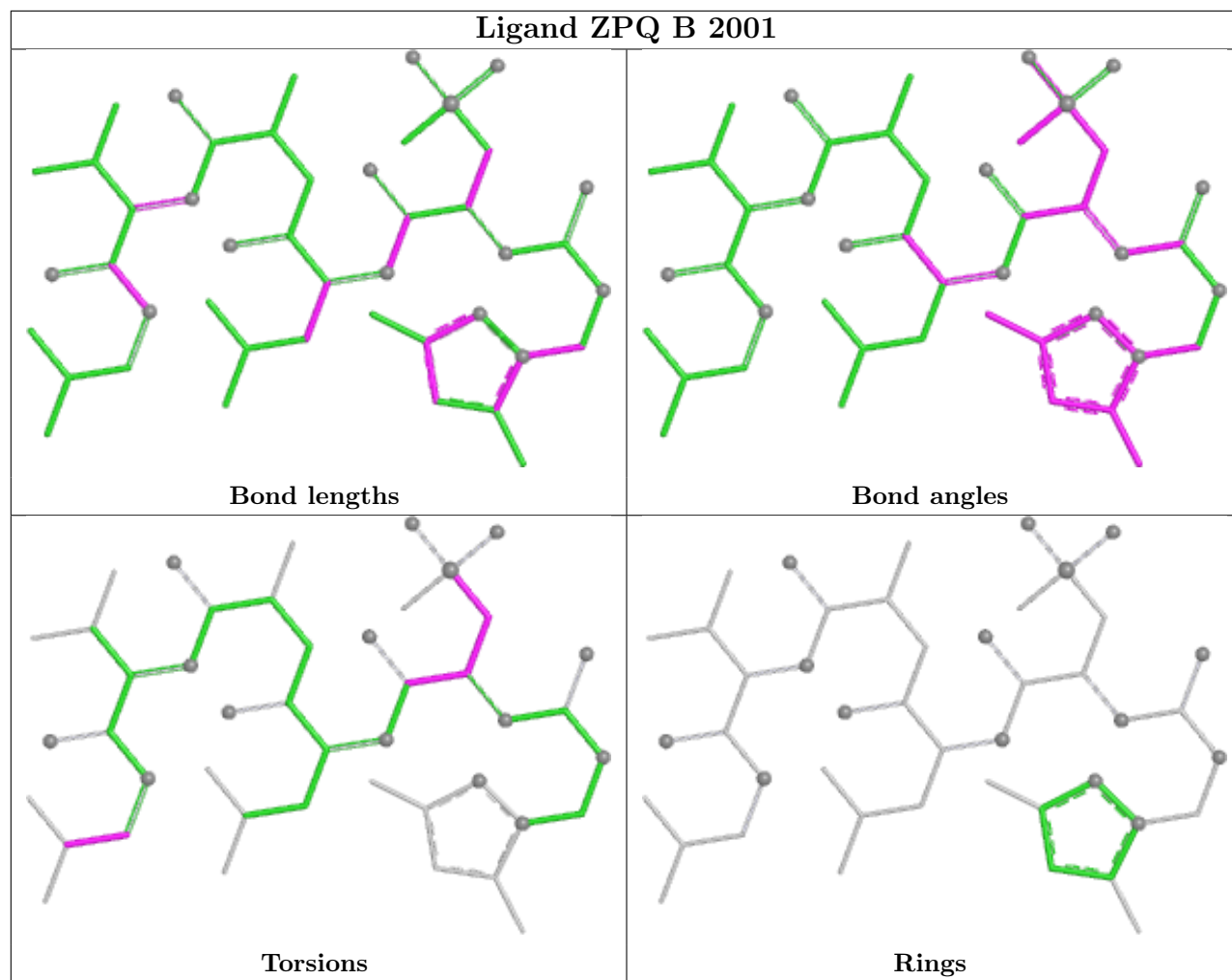
4 monomers are involved in 6 short contacts:

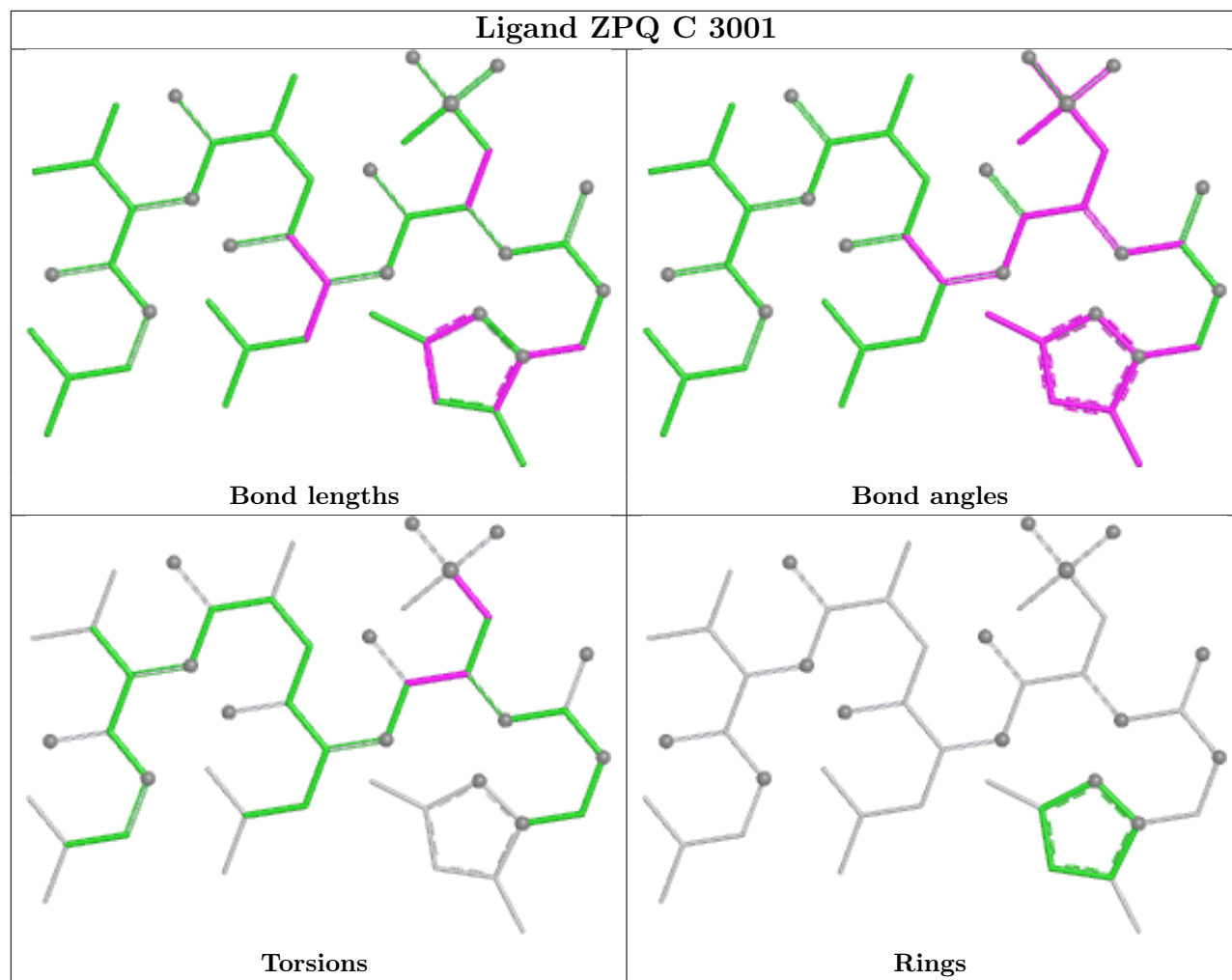
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	ZPQ	3	0
2	B	2001	ZPQ	1	0
2	C	3001	ZPQ	1	0
2	D	4001	ZPQ	1	0

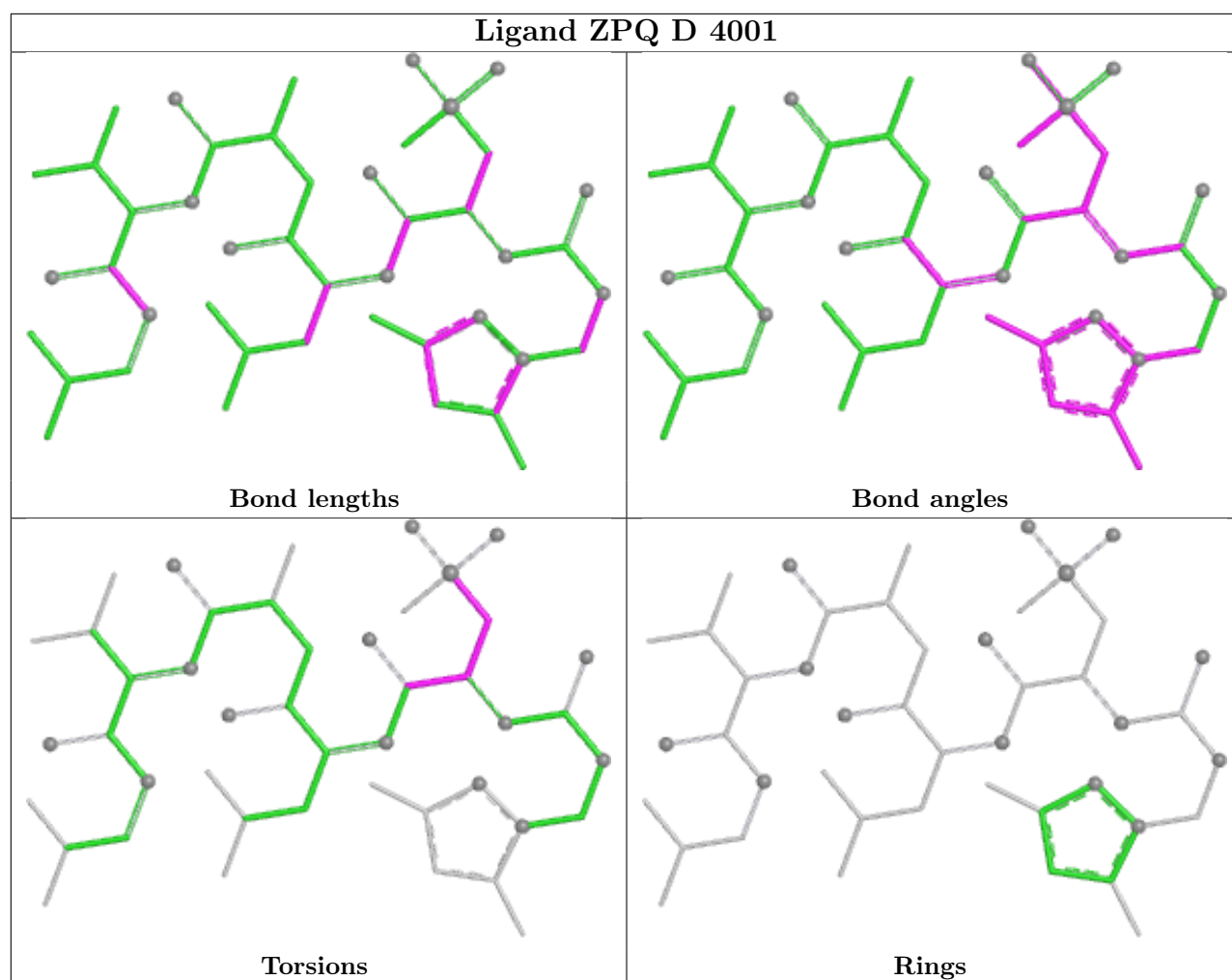
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.