



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:31 PM UTC

PDB ID : 3N4L / pdb_00003n4l
Title : BACE-1 in complex with ELN380842
Authors : Yao, N.H.
Deposited on : 2010-05-21
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

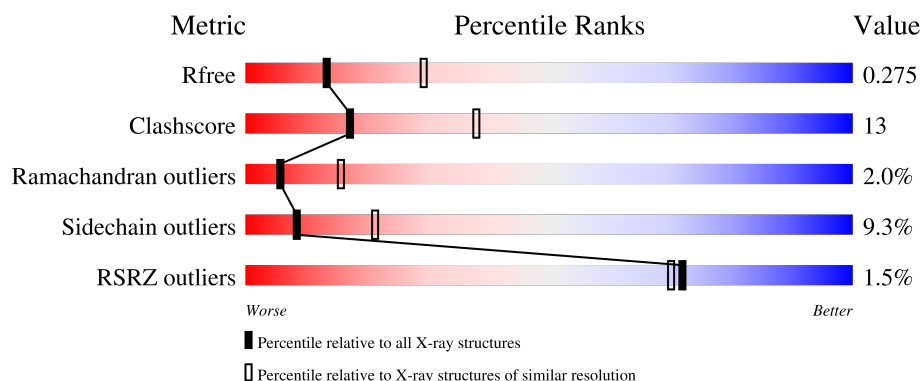
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	406	 2% 68% 23% 8%
1	B	406	 1% 61% 26% 5% 8%
1	C	406	 1% 57% 31% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8982 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	375	Total	C	N	O	S	0	0	0
			2953	1892	490	557	14			
1	B	375	Total	C	N	O	S	0	0	0
			2942	1887	490	551	14			
1	C	375	Total	C	N	O	S	0	0	0
			2947	1887	490	556	14			

There are 27 discrepancies between the modelled and reference sequences:

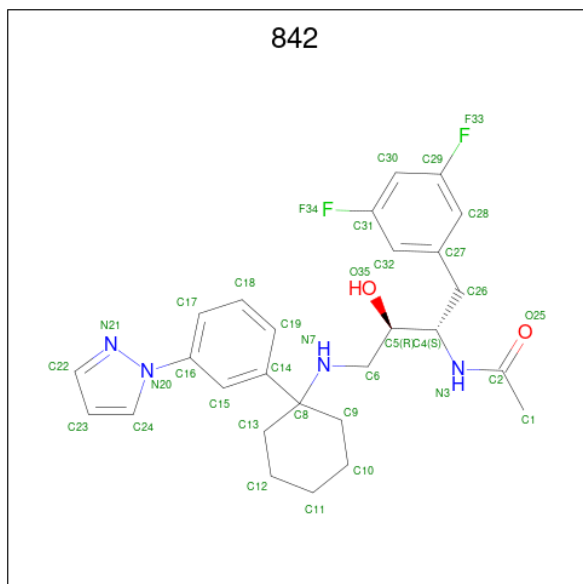
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P56817
A	399	ARG	-	expression tag	UNP P56817
A	400	SER	-	expression tag	UNP P56817
A	401	HIS	-	expression tag	UNP P56817
A	402	HIS	-	expression tag	UNP P56817
A	403	HIS	-	expression tag	UNP P56817
A	404	HIS	-	expression tag	UNP P56817
A	405	HIS	-	expression tag	UNP P56817
A	406	HIS	-	expression tag	UNP P56817
B	1	MET	-	initiating methionine	UNP P56817
B	399	ARG	-	expression tag	UNP P56817
B	400	SER	-	expression tag	UNP P56817
B	401	HIS	-	expression tag	UNP P56817
B	402	HIS	-	expression tag	UNP P56817
B	403	HIS	-	expression tag	UNP P56817
B	404	HIS	-	expression tag	UNP P56817
B	405	HIS	-	expression tag	UNP P56817
B	406	HIS	-	expression tag	UNP P56817
C	1	MET	-	initiating methionine	UNP P56817
C	399	ARG	-	expression tag	UNP P56817
C	400	SER	-	expression tag	UNP P56817
C	401	HIS	-	expression tag	UNP P56817
C	402	HIS	-	expression tag	UNP P56817

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Chain	Residue	Modelled	Actual	Comment	Reference
C	403	HIS	-	expression tag	UNP P56817
C	404	HIS	-	expression tag	UNP P56817
C	405	HIS	-	expression tag	UNP P56817
C	406	HIS	-	expression tag	UNP P56817

- Molecule 2 is N-[(1S,2R)-1-(3,5-difluorobenzyl)-2-hydroxy-3-({1-[3-(1H-pyrazol-1-yl)phenyl]cyclohexyl}amino)propyl]acetamide (CCD ID: 842) (formula: C₂₇H₃₂F₂N₄O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			35	27	2	4	2		
2	B	1	Total	C	F	N	O	0	0
			35	27	2	4	2		
2	C	1	Total	C	F	N	O	0	0
			35	27	2	4	2		

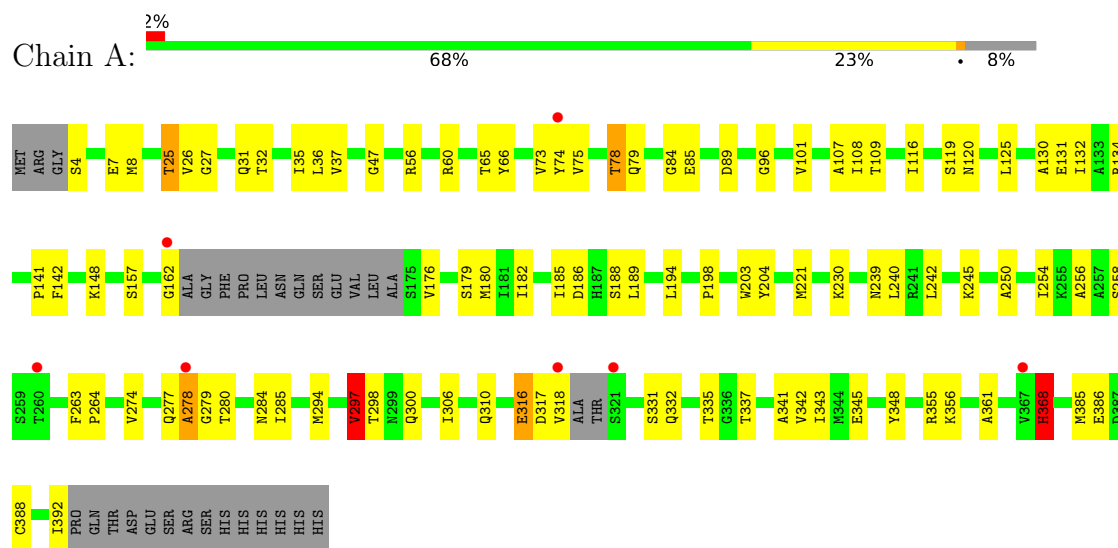
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total	O	0	0
			12	12		
3	B	14	Total	O	0	0
			14	14		
3	C	9	Total	O	0	0
			9	9		

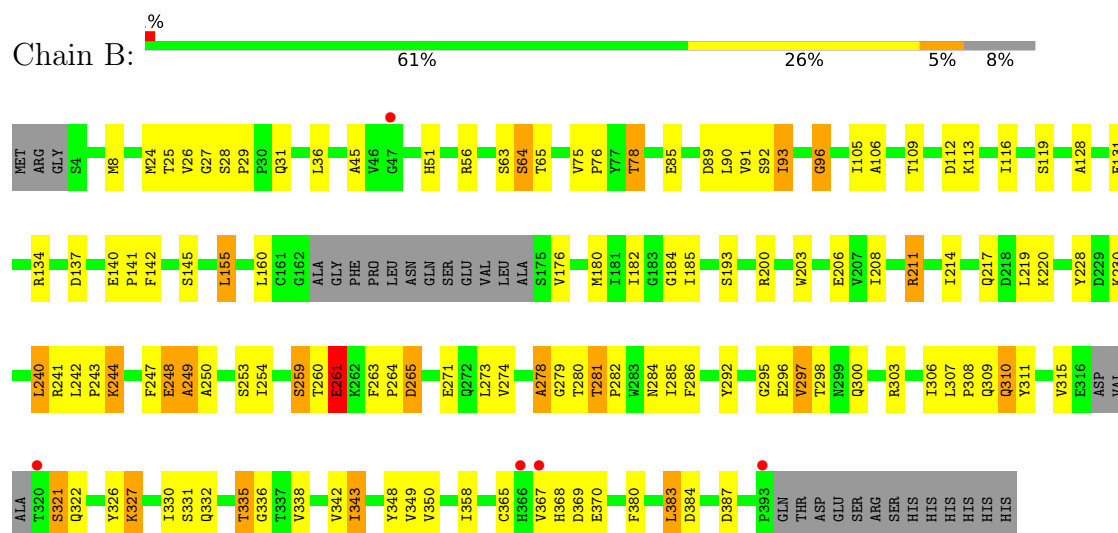
3 Residue-property plots [i](#)

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

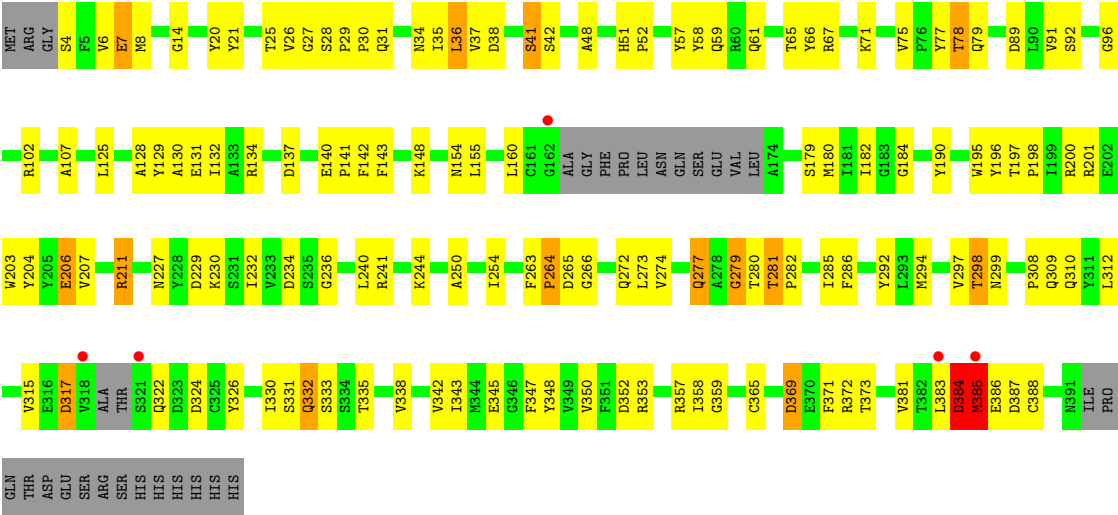


• Molecule 1: Beta-secretase 1



• Molecule 1: Beta-secretase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.05Å 105.58Å 101.58Å 90.00° 104.63° 90.00°	Depositor
Resolution (Å)	28.00 – 2.70 28.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.7 (28.00-2.70) 98.7 (28.00-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.223 , 0.283 0.216 , 0.275	Depositor DCC
R_{free} test set	2329 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	74.1	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 23.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8982	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
842

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	0.92	0/3027	1.10	5/4112 (0.1%)
1	B	0.94	0/3017	1.12	12/4100 (0.3%)
1	C	0.95	1/3021 (0.0%)	1.12	5/4105 (0.1%)
All	All	0.94	1/9065 (0.0%)	1.11	22/12317 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	347	PHE	CA-C	-5.08	1.46	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	388	CYS	N-CA-C	-8.50	103.35	114.31
1	A	239	ASN	N-CA-C	6.71	119.19	110.53
1	B	93	ILE	CA-C-N	6.63	126.88	119.32
1	B	93	ILE	C-N-CA	6.63	126.88	119.32
1	B	145	SER	N-CA-C	-6.63	103.98	111.07
1	B	96	GLY	CA-C-N	-6.42	114.16	120.52
1	B	96	GLY	C-N-CA	-6.42	114.16	120.52
1	B	51	HIS	N-CA-C	-6.22	102.31	110.39
1	A	316	GLU	N-CA-C	5.78	118.15	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	358	ILE	CB-CA-C	-5.78	102.08	110.63
1	C	385	MET	N-CA-C	-5.76	94.88	111.00
1	A	368	HIS	N-CA-C	5.45	118.35	107.62
1	A	297	VAL	CB-CA-C	5.33	118.57	110.90
1	B	368	HIS	N-CA-C	5.27	116.03	107.23
1	A	132	ILE	N-CA-C	5.25	116.58	111.91
1	C	279	GLY	N-CA-C	-5.21	100.82	113.18
1	C	57	TYR	N-CA-C	5.18	116.71	108.79
1	B	350	VAL	N-CA-C	5.13	115.48	107.99
1	B	286	PHE	CA-C-N	5.13	125.57	120.14
1	B	286	PHE	C-N-CA	5.13	125.57	120.14
1	B	349	VAL	N-CA-C	5.11	115.21	107.80
1	C	317	ASP	N-CA-C	5.01	118.12	110.36

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	384	ASP	Peptide
1	C	385	MET	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2953	0	2862	56	0
1	B	2942	0	2850	76	0
1	C	2947	0	2849	92	0
2	A	35	0	32	3	0
2	B	35	0	32	3	0
2	C	35	0	32	3	0
3	A	12	0	0	0	0
3	B	14	0	0	0	0
3	C	9	0	0	0	0
All	All	8982	0	8657	221	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 13.

All (221) 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:C:297:VAL:O	1:C:298:THR:HG22	1.39	1.18
1:B:211:ARG:HH11	1:B:211:ARG:HB2	1.22	1.03
1:C:385:MET:HE2	1:C:387:ASP:HB2	1.45	0.97
1:C:384:ASP:C	1:C:386:GLU:H	1.69	0.97
1:A:317:ASP:HA	1:A:318:VAL:HB	1.50	0.93
1:B:296:GLU:H	1:B:300:GLN:HE21	1.12	0.93
1:A:32:THR:HG22	1:A:56:ARG:HH12	1.42	0.85
1:A:180:MET:HE3	1:A:182:ILE:HD11	1.60	0.84
1:A:306:ILE:HD12	1:A:310:GLN:NE2	1.94	0.83
1:A:258:SER:HB2	1:A:285:ILE:HD12	1.61	0.82
1:C:297:VAL:O	1:C:298:THR:CG2	2.26	0.81
1:B:384:ASP:O	1:B:387:ASP:HB2	1.81	0.80
1:A:32:THR:HG22	1:A:56:ARG:NH1	1.96	0.80
1:C:36:LEU:HD23	1:C:36:LEU:C	2.06	0.80
1:C:384:ASP:C	1:C:386:GLU:N	2.34	0.79
1:B:327:LYS:HB2	1:B:327:LYS:NZ	1.98	0.79
1:C:384:ASP:CB	1:C:385:MET:HA	2.14	0.78
1:C:38:ASP:OD1	1:C:41:SER:HB3	1.84	0.77
1:A:230:LYS:NZ	1:A:335:THR:HB	1.99	0.77
1:C:155:LEU:HD12	1:C:352:ASP:HA	1.68	0.76
1:A:306:ILE:HD12	1:A:310:GLN:HE22	1.51	0.76
1:A:116:ILE:O	1:A:119:SER:HB2	1.88	0.73
1:B:8:MET:HG2	1:B:96:GLY:HA2	1.71	0.73
1:A:78:THR:HG22	2:A:407:842:H19	1.70	0.73
1:B:91:VAL:HG11	1:B:142:PHE:CE1	2.23	0.73
1:C:384:ASP:CB	1:C:385:MET:CA	2.67	0.72
1:C:155:LEU:HD23	1:C:184:GLY:HA2	1.71	0.71
1:B:78:THR:HG22	2:B:407:842:H19	1.71	0.71
1:A:185:ILE:HG23	1:A:348:TYR:HE2	1.55	0.71
1:A:8:MET:HG2	1:A:96:GLY:HA2	1.73	0.70
1:B:250:ALA:O	1:B:254:ILE:HG13	1.92	0.70
1:C:385:MET:HE2	1:C:387:ASP:CB	2.21	0.69
1:B:28:SER:O	1:B:63:SER:HA	1.94	0.68
1:C:385:MET:CE	1:C:387:ASP:HB2	2.21	0.68
1:B:296:GLU:N	1:B:300:GLN:HE21	1.88	0.67
1:C:36:LEU:HD23	1:C:37:VAL:N	2.08	0.67
1:A:306:ILE:HG13	1:A:343:ILE:HD13	1.76	0.67
1:B:24:MET:HE3	1:B:93:ILE:HG12	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:TYR:CD2	1:C:357:ARG:HG3	2.30	0.66
1:A:341:ALA:O	1:A:345:GLU:HG3	1.95	0.66
1:B:91:VAL:HG11	1:B:142:PHE:HE1	1.59	0.66
1:A:256:ALA:HB1	1:C:371:PHE:CD1	2.32	0.65
1:C:200:ARG:HB3	1:C:206:GLU:HG2	1.79	0.65
1:C:155:LEU:CD1	1:C:352:ASP:HA	2.28	0.64
1:A:36:LEU:HD23	1:A:36:LEU:C	2.24	0.62
1:B:211:ARG:NH2	1:C:385:MET:HG3	2.15	0.62
1:C:263:PHE:HD2	1:C:274:VAL:HG11	1.65	0.61
1:A:230:LYS:HZ1	1:A:335:THR:HB	1.64	0.61
1:B:230:LYS:O	1:B:336:GLY:HA3	2.01	0.61
1:C:180:MET:HE3	1:C:182:ILE:HD11	1.80	0.61
1:C:286:PHE:CE2	1:C:312:LEU:HD11	2.35	0.61
1:C:282:PRO:HB2	1:C:285:ILE:HG12	1.83	0.60
1:C:66:TYR:O	1:C:67:ARG:HG3	2.01	0.60
1:C:281:THR:HG21	1:C:326:TYR:CE1	2.37	0.59
1:C:211:ARG:HG2	1:C:292:TYR:CD1	2.37	0.59
1:A:73:VAL:HG22	1:A:74:TYR:N	2.16	0.59
1:C:282:PRO:O	1:C:285:ILE:HG12	2.02	0.59
1:B:214:ILE:HG13	1:B:219:LEU:HD21	1.85	0.59
1:C:89:ASP:O	1:C:102:ARG:HA	2.04	0.58
1:B:308:PRO:HG2	1:B:309:GLN:OE1	2.03	0.58
1:B:327:LYS:HB2	1:B:327:LYS:HZ2	1.67	0.58
1:A:78:THR:HG23	2:A:407:842:O25	2.03	0.57
1:C:25:THR:HA	1:C:31:GLN:O	2.05	0.57
1:C:385:MET:SD	1:C:385:MET:N	2.78	0.56
1:C:14:GLY:HA2	1:C:21:TYR:CE2	2.41	0.55
1:C:36:LEU:C	1:C:36:LEU:CD2	2.79	0.55
1:B:211:ARG:HB2	1:B:211:ARG:NH1	2.06	0.55
1:C:229:ASP:OD2	1:C:230:LYS:HG2	2.07	0.54
1:B:383:LEU:H	1:B:383:LEU:HD12	1.72	0.54
1:C:27:GLY:O	1:C:30:PRO:HA	2.07	0.54
1:B:240:LEU:HD22	1:B:343:ILE:HD11	1.89	0.54
1:A:75:VAL:HG22	1:A:134:ARG:HG3	1.89	0.54
1:C:59:GLN:HB3	1:C:61:GLN:NE2	2.23	0.54
1:A:317:ASP:HA	1:A:318:VAL:CB	2.31	0.53
1:A:368:HIS:H	1:A:368:HIS:CD2	2.25	0.53
1:A:36:LEU:HD23	1:A:37:VAL:N	2.24	0.53
1:A:73:VAL:CG2	1:A:74:TYR:N	2.70	0.53
1:B:327:LYS:HB2	1:B:327:LYS:HZ3	1.70	0.53
1:C:66:TYR:CG	1:C:67:ARG:N	2.77	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:SER:C	1:B:261:GLU:H	2.16	0.53
1:B:281:THR:HG21	1:B:326:TYR:CE1	2.43	0.53
1:B:282:PRO:HB2	1:B:285:ILE:HG12	1.91	0.53
1:A:385:MET:O	1:A:388:CYS:HB2	2.09	0.52
1:B:91:VAL:CG1	1:B:142:PHE:HE1	2.23	0.52
1:B:185:ILE:HG23	1:B:348:TYR:HE2	1.74	0.52
1:B:263:PHE:HD2	1:B:274:VAL:HG11	1.73	0.52
1:C:263:PHE:CD2	1:C:274:VAL:HG11	2.43	0.52
1:B:180:MET:HE3	1:B:182:ILE:HD11	1.92	0.52
1:C:130:ALA:O	1:C:131:GLU:C	2.53	0.51
1:A:368:HIS:H	1:A:368:HIS:HD2	1.58	0.51
1:B:306:ILE:HG13	1:B:343:ILE:HD13	1.92	0.51
1:C:28:SER:OG	1:C:65:THR:HG21	2.11	0.51
1:C:78:THR:HG22	2:C:407:842:H19	1.93	0.51
1:B:308:PRO:HA	1:B:311:TYR:CE2	2.46	0.51
2:B:407:842:H12A	2:B:407:842:C19	2.39	0.51
1:B:278:ALA:C	1:B:280:THR:H	2.19	0.50
1:C:38:ASP:OD2	1:C:236:GLY:HA3	2.11	0.50
1:B:28:SER:HA	1:B:29:PRO:C	2.36	0.50
1:B:309:GLN:NE2	1:B:369:ASP:HB3	2.27	0.50
1:B:292:TYR:CE2	1:B:303:ARG:HB3	2.47	0.50
1:B:297:VAL:HB	1:B:300:GLN:HG2	1.93	0.50
1:C:48:ALA:CB	1:C:107:ALA:HB1	2.42	0.50
1:C:198:PRO:HG2	1:C:294:MET:HE2	1.95	0.49
1:C:244:LYS:HG3	1:C:332:GLN:OE1	2.12	0.49
1:A:47:GLY:HA2	1:A:108:ILE:HB	1.94	0.49
1:C:42:SER:O	1:C:141:PRO:HB3	2.12	0.49
1:B:211:ARG:HH21	1:C:385:MET:HG3	1.77	0.49
1:B:296:GLU:H	1:B:300:GLN:NE2	1.95	0.49
1:C:132:ILE:HD13	1:C:204:TYR:CE1	2.48	0.49
1:C:206:GLU:HG3	1:C:207:VAL:N	2.28	0.49
1:A:194:LEU:HD23	1:A:361:ALA:HB2	1.95	0.49
1:A:306:ILE:CD1	1:A:310:GLN:HE22	2.23	0.49
1:C:20:TYR:CD1	1:C:20:TYR:N	2.80	0.49
1:C:26:VAL:HG22	1:C:91:VAL:HG22	1.95	0.49
1:C:78:THR:HG23	2:C:407:842:O25	2.12	0.49
1:A:85:GLU:OE1	1:A:109:THR:HG21	2.13	0.49
1:B:230:LYS:HZ3	1:B:335:THR:HB	1.77	0.49
1:C:240:LEU:HD22	1:C:343:ILE:HD11	1.95	0.49
1:C:365:CYS:O	1:C:365:CYS:SG	2.71	0.48
1:A:242:LEU:HD23	1:A:337:THR:HG23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:ARG:HB3	1:C:333:SER:HB2	1.95	0.48
1:B:155:LEU:HD21	1:B:184:GLY:HA2	1.95	0.48
1:A:130:ALA:O	1:A:131:GLU:C	2.56	0.48
1:B:45:ALA:HB2	1:B:106:ALA:HB3	1.94	0.48
1:A:203:TRP:CG	1:A:204:TYR:H	2.32	0.47
1:B:89:ASP:OD1	1:B:90:LEU:N	2.41	0.47
1:B:228:TYR:O	1:B:336:GLY:HA2	2.14	0.47
1:B:292:TYR:CD2	1:B:303:ARG:HB3	2.49	0.47
1:B:383:LEU:HD12	1:B:383:LEU:N	2.29	0.47
1:C:42:SER:OG	1:C:128:ALA:HB3	2.15	0.47
1:A:198:PRO:HG2	1:A:294:MET:HE3	1.97	0.47
1:A:186:ASP:HB3	1:A:189:LEU:HD12	1.96	0.47
1:A:240:LEU:HD13	1:A:343:ILE:HG13	1.97	0.47
1:C:240:LEU:HD23	1:C:330:ILE:HG12	1.95	0.47
1:C:240:LEU:HD12	1:C:338:VAL:O	2.15	0.47
1:C:250:ALA:O	1:C:254:ILE:HG13	2.15	0.47
1:C:232:ILE:HD12	1:C:234:ASP:HB2	1.97	0.47
1:A:27:GLY:HA2	1:A:89:ASP:OD1	2.15	0.47
1:A:204:TYR:CE1	2:A:407:842:H9A	2.50	0.47
1:B:307:LEU:H	1:B:310:GLN:NE2	2.13	0.46
1:C:77:TYR:CG	2:C:407:842:H28	2.50	0.46
1:C:200:ARG:CB	1:C:206:GLU:HG2	2.44	0.46
1:B:140:GLU:HA	1:B:141:PRO:HD3	1.75	0.46
1:C:154:ASN:ND2	1:C:353:ARG:HB3	2.30	0.46
1:B:116:ILE:HB	1:B:119:SER:HB3	1.97	0.46
1:B:203:TRP:NE1	1:B:206:GLU:OE1	2.35	0.46
1:A:250:ALA:O	1:A:254:ILE:HG13	2.16	0.46
1:C:142:PHE:O	1:C:143:PHE:C	2.57	0.46
1:C:308:PRO:O	1:C:310:GLN:N	2.49	0.46
1:C:201:ARG:O	1:C:203:TRP:HD1	1.99	0.46
1:A:185:ILE:HG23	1:A:348:TYR:CE2	2.44	0.45
1:B:112:ASP:OD2	1:B:113:LYS:HE2	2.15	0.45
1:B:25:THR:HA	1:B:31:GLN:O	2.16	0.45
1:C:28:SER:HA	1:C:29:PRO:C	2.40	0.45
1:C:14:GLY:HA2	1:C:21:TYR:HE2	1.82	0.45
1:B:85:GLU:OE1	1:B:109:THR:HG21	2.16	0.45
1:B:91:VAL:CG1	1:B:142:PHE:CE1	2.96	0.45
1:C:281:THR:CG2	1:C:326:TYR:HE1	2.29	0.45
1:A:25:THR:HA	1:A:31:GLN:O	2.17	0.45
1:A:119:SER:O	1:A:120:ASN:CB	2.65	0.45
1:C:264:PRO:O	1:C:266:GLY:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LYS:HZ3	1:A:335:THR:HB	1.81	0.44
1:C:4:SER:O	1:C:7:GLU:HG3	2.18	0.44
1:A:60:ARG:CD	1:A:66:TYR:CE1	3.00	0.44
1:B:248:GLU:O	1:B:249:ALA:C	2.60	0.44
1:C:195:TRP:O	1:C:359:GLY:HA2	2.17	0.44
1:B:264:PRO:O	1:B:265:ASP:C	2.60	0.44
1:B:365:CYS:SG	1:B:365:CYS:O	2.75	0.44
1:B:295:GLY:HA3	1:B:300:GLN:NE2	2.33	0.44
1:A:162:GLY:C	1:A:176:VAL:HG12	2.42	0.43
1:B:281:THR:CG2	1:B:326:TYR:HE1	2.31	0.43
2:B:407:842:H19	2:B:407:842:H12A	1.99	0.43
1:A:186:ASP:OD2	1:A:188:SER:OG	2.31	0.43
1:B:26:VAL:HG22	1:B:91:VAL:HG22	1.99	0.43
1:A:263:PHE:HD2	1:A:274:VAL:HG11	1.82	0.43
1:C:350:VAL:O	1:C:358:ILE:HA	2.19	0.43
1:A:221:MET:HE1	1:A:245:LYS:HB3	2.01	0.43
1:B:281:THR:HA	1:B:282:PRO:HD3	1.86	0.43
1:C:140:GLU:HA	1:C:141:PRO:HD3	1.94	0.43
1:C:308:PRO:C	1:C:310:GLN:N	2.77	0.43
1:B:63:SER:O	1:B:64:SER:C	2.61	0.43
1:B:200:ARG:HD2	1:B:208:ILE:HD11	2.01	0.43
1:C:8:MET:HG2	1:C:96:GLY:HA2	2.00	0.43
1:B:28:SER:HB2	1:B:64:SER:HB3	2.01	0.42
1:A:8:MET:CG	1:A:96:GLY:HA2	2.46	0.42
1:C:322:GLN:HG2	1:C:322:GLN:O	2.19	0.42
1:C:129:TYR:HD1	1:C:203:TRP:O	2.03	0.42
1:A:277:GLN:O	1:A:278:ALA:C	2.63	0.42
1:C:51:HIS:O	1:C:52:PRO:C	2.60	0.42
1:A:84:GLY:HA3	1:A:107:ALA:O	2.20	0.42
1:A:355:ARG:O	1:A:356:LYS:C	2.63	0.42
1:C:34:ASN:C	1:C:35:ILE:HD13	2.45	0.42
1:C:369:ASP:HB3	1:C:372:ARG:H	1.85	0.42
1:B:75:VAL:HG22	1:B:134:ARG:HB2	2.02	0.42
1:B:242:LEU:HB2	1:B:247:PHE:HB2	2.00	0.42
1:B:327:LYS:NZ	1:B:327:LYS:CB	2.76	0.42
1:C:282:PRO:HG2	1:C:285:ILE:HD11	2.02	0.42
1:B:230:LYS:NZ	1:B:335:THR:HB	2.35	0.41
1:C:281:THR:HA	1:C:282:PRO:HD3	1.91	0.41
1:B:27:GLY:HA2	1:B:89:ASP:OD1	2.21	0.41
1:C:190:TYR:CD1	1:C:348:TYR:CD2	3.09	0.41
1:C:332:GLN:HE21	1:C:332:GLN:HB2	1.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:PHE:CD2	1:B:274:VAL:HG11	2.55	0.41
1:A:141:PRO:O	1:A:142:PHE:C	2.64	0.41
1:B:380:PHE:HE2	1:C:298:THR:HG23	1.85	0.41
1:C:26:VAL:HG12	1:C:58:TYR:CE1	2.56	0.41
1:C:160:LEU:O	1:C:345:GLU:HA	2.20	0.41
1:C:385:MET:SD	1:C:387:ASP:HB2	2.60	0.41
1:B:241:ARG:HB2	1:B:338:VAL:HB	2.02	0.41
1:B:242:LEU:HD12	1:B:330:ILE:CG2	2.51	0.41
1:C:75:VAL:HG22	1:C:134:ARG:HG3	2.03	0.41
1:A:297:VAL:HG12	1:A:300:GLN:HB3	2.02	0.40
1:A:368:HIS:CD2	1:A:368:HIS:N	2.89	0.40
1:B:36:LEU:HD23	1:B:36:LEU:C	2.46	0.40
1:B:141:PRO:O	1:B:142:PHE:C	2.63	0.40
1:B:383:LEU:HD11	1:C:383:LEU:HD11	2.02	0.40
1:C:241:ARG:HA	1:C:331:SER:O	2.22	0.40
1:A:35:ILE:CG2	1:A:125:LEU:HB2	2.52	0.40
1:B:243:PRO:O	1:B:244:LYS:C	2.64	0.40
1:B:295:GLY:CA	1:B:300:GLN:NE2	2.84	0.40
1:C:279:GLY:O	1:C:280:THR:OG1	2.38	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	369/406 (91%)	346 (94%)	19 (5%)	4 (1%)	11	29
1	B	369/406 (91%)	323 (88%)	35 (10%)	11 (3%)	3	8
1	C	369/406 (91%)	322 (87%)	40 (11%)	7 (2%)	6	17
All	All	1107/1218 (91%)	991 (90%)	94 (8%)	22 (2%)	6	16

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	370	GLU
1	A	278	ALA
1	A	279	GLY
1	B	64	SER
1	B	128	ALA
1	C	265	ASP
1	C	277	GLN
1	C	309	GLN
1	A	284	ASN
1	B	260	THR
1	B	278	ALA
1	B	279	GLY
1	B	321	SER
1	C	298	THR
1	C	384	ASP
1	C	369	ASP
1	B	137	ASP
1	B	249	ALA
1	B	261	GLU
1	C	264	PRO
1	A	264	PRO
1	B	76	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	321/348 (92%)	300 (94%)	21 (6%)	15	37
1	B	318/348 (91%)	280 (88%)	38 (12%)	5	13
1	C	319/348 (92%)	289 (91%)	30 (9%)	8	21
All	All	958/1044 (92%)	869 (91%)	89 (9%)	8	21

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER

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Mol	Chain	Res	Type
1	A	7	GLU
1	A	25	THR
1	A	26	VAL
1	A	65	THR
1	A	78	THR
1	A	79	GLN
1	A	101	VAL
1	A	148	LYS
1	A	157	SER
1	A	179	SER
1	A	280	THR
1	A	297	VAL
1	A	298	THR
1	A	316	GLU
1	A	331	SER
1	A	332	GLN
1	A	342	VAL
1	A	368	HIS
1	A	386	GLU
1	A	392	ILE
1	B	56	ARG
1	B	65	THR
1	B	78	THR
1	B	92	SER
1	B	105	ILE
1	B	131	GLU
1	B	155	LEU
1	B	160	LEU
1	B	176	VAL
1	B	193	SER
1	B	211	ARG
1	B	217	GLN
1	B	220	LYS
1	B	240	LEU
1	B	244	LYS
1	B	248	GLU
1	B	253	SER
1	B	259	SER
1	B	261	GLU
1	B	265	ASP
1	B	271	GLU
1	B	273	LEU

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Mol	Chain	Res	Type
1	B	281	THR
1	B	284	ASN
1	B	297	VAL
1	B	298	THR
1	B	310	GLN
1	B	315	VAL
1	B	321	SER
1	B	322	GLN
1	B	327	LYS
1	B	331	SER
1	B	332	GLN
1	B	335	THR
1	B	342	VAL
1	B	343	ILE
1	B	367	VAL
1	B	383	LEU
1	C	6	VAL
1	C	7	GLU
1	C	36	LEU
1	C	41	SER
1	C	71	LYS
1	C	78	THR
1	C	79	GLN
1	C	92	SER
1	C	125	LEU
1	C	137	ASP
1	C	148	LYS
1	C	179	SER
1	C	197	THR
1	C	206	GLU
1	C	211	ARG
1	C	227	ASN
1	C	272	GLN
1	C	273	LEU
1	C	277	GLN
1	C	281	THR
1	C	299	ASN
1	C	315	VAL
1	C	317	ASP
1	C	324	ASP
1	C	332	GLN
1	C	335	THR

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Mol	Chain	Res	Type
1	C	342	VAL
1	C	373	THR
1	C	381	VAL
1	C	385	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	59	GLN
1	A	104	ASN
1	A	272	GLN
1	A	277	GLN
1	A	310	GLN
1	A	332	GLN
1	A	368	HIS
1	B	217	GLN
1	B	284	ASN
1	B	300	GLN
1	C	79	GLN
1	C	104	ASN
1	C	272	GLN
1	C	284	ASN
1	C	299	ASN
1	C	300	GLN
1	C	310	GLN
1	C	332	GLN

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

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	842	B	407	-	35,38,38	1.28	3 (8%)	46,53,53	1.84	10 (21%)
2	842	C	407	-	35,38,38	1.24	4 (11%)	46,53,53	1.98	16 (34%)
2	842	A	407	-	35,38,38	1.27	3 (8%)	46,53,53	1.70	9 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	842	B	407	-	-	14/28/38/38	0/4/4/4
2	842	C	407	-	-	8/28/38/38	0/4/4/4
2	842	A	407	-	-	7/28/38/38	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	407	842	C16-N20	-5.26	1.33	1.43
2	B	407	842	C16-N20	-5.14	1.33	1.43
2	C	407	842	C16-N20	-4.82	1.34	1.43
2	C	407	842	C32-C31	2.32	1.41	1.37
2	A	407	842	F34-C31	-2.22	1.31	1.36
2	B	407	842	N20-N21	2.21	1.39	1.36
2	C	407	842	C24-N20	-2.19	1.32	1.35
2	C	407	842	C28-C29	2.14	1.41	1.37
2	B	407	842	C28-C29	2.09	1.41	1.37
2	A	407	842	N20-N21	2.08	1.39	1.36

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	407	842	C27-C28-C29	5.01	123.11	118.75
2	B	407	842	C4-N3-C2	4.47	128.89	122.90
2	C	407	842	C26-C4-N3	-3.92	104.52	110.08
2	C	407	842	C27-C26-C4	-3.84	106.89	113.40
2	B	407	842	C24-N20-N21	3.82	115.02	111.83
2	A	407	842	C16-C15-C14	3.79	124.98	120.39
2	A	407	842	C27-C26-C4	-3.74	107.06	113.40
2	B	407	842	C17-C16-N20	3.67	124.07	119.58
2	A	407	842	C17-C16-N20	3.48	123.84	119.58
2	A	407	842	C23-C24-N20	-3.41	103.95	106.76
2	B	407	842	C23-C24-N20	-3.39	103.97	106.76
2	C	407	842	C17-C16-N20	3.39	123.73	119.58
2	C	407	842	C16-N20-C24	-3.39	121.00	128.39
2	B	407	842	C27-C28-C29	3.32	121.64	118.75
2	C	407	842	C18-C17-C16	3.20	123.48	119.68
2	A	407	842	C16-N20-C24	-3.01	121.83	128.39
2	C	407	842	C26-C4-C5	2.96	116.47	111.66
2	B	407	842	C13-C12-C11	-2.90	106.84	111.35
2	C	407	842	C23-C24-N20	-2.76	104.49	106.76
2	B	407	842	C16-C15-C14	2.74	123.70	120.39
2	B	407	842	C30-C29-C28	-2.69	120.24	123.50
2	C	407	842	C16-N20-N21	2.50	125.35	121.08
2	C	407	842	C30-C29-C28	-2.43	120.55	123.50
2	A	407	842	C24-N20-N21	2.41	113.84	111.83
2	C	407	842	F33-C29-C28	2.32	121.58	118.28
2	C	407	842	C32-C27-C28	-2.30	115.88	119.01
2	C	407	842	F34-C31-C32	2.30	121.55	118.28
2	C	407	842	C16-C15-C14	2.21	123.06	120.39
2	A	407	842	C26-C4-C5	2.18	115.20	111.66
2	A	407	842	C26-C4-N3	-2.17	107.00	110.08
2	B	407	842	C18-C17-C16	2.13	122.22	119.68
2	C	407	842	C5-C6-N7	2.12	113.53	110.73
2	C	407	842	C27-C32-C31	2.11	120.59	118.75
2	B	407	842	C19-C14-C8	2.04	124.10	121.09
2	A	407	842	F34-C31-C32	2.03	121.17	118.28

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	407	842	C15-C14-C8-N7
2	A	407	842	C19-C14-C8-N7
2	B	407	842	O35-C5-C6-N7

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Mol	Chain	Res	Type	Atoms
2	B	407	842	C15-C14-C8-N7
2	B	407	842	C19-C14-C8-N7
2	C	407	842	C15-C14-C8-N7
2	C	407	842	C19-C14-C8-N7
2	B	407	842	C1-C2-N3-C4
2	B	407	842	C26-C4-C5-O35
2	A	407	842	C15-C16-N20-C24
2	B	407	842	O25-C2-N3-C4
2	A	407	842	C15-C16-N20-N21
2	B	407	842	C5-C6-N7-C8
2	A	407	842	C17-C16-N20-C24
2	C	407	842	C15-C16-N20-C24
2	B	407	842	C4-C5-C6-N7
2	C	407	842	C15-C16-N20-N21
2	C	407	842	C17-C16-N20-C24
2	B	407	842	C17-C16-N20-N21
2	B	407	842	C15-C16-N20-N21
2	B	407	842	N3-C4-C5-C6
2	A	407	842	C17-C16-N20-N21
2	B	407	842	C17-C16-N20-C24
2	B	407	842	C15-C16-N20-C24
2	C	407	842	C1-C2-N3-C4
2	A	407	842	C15-C14-C8-C13
2	B	407	842	C19-C14-C8-C13
2	C	407	842	C15-C14-C8-C13
2	C	407	842	C17-C16-N20-N21

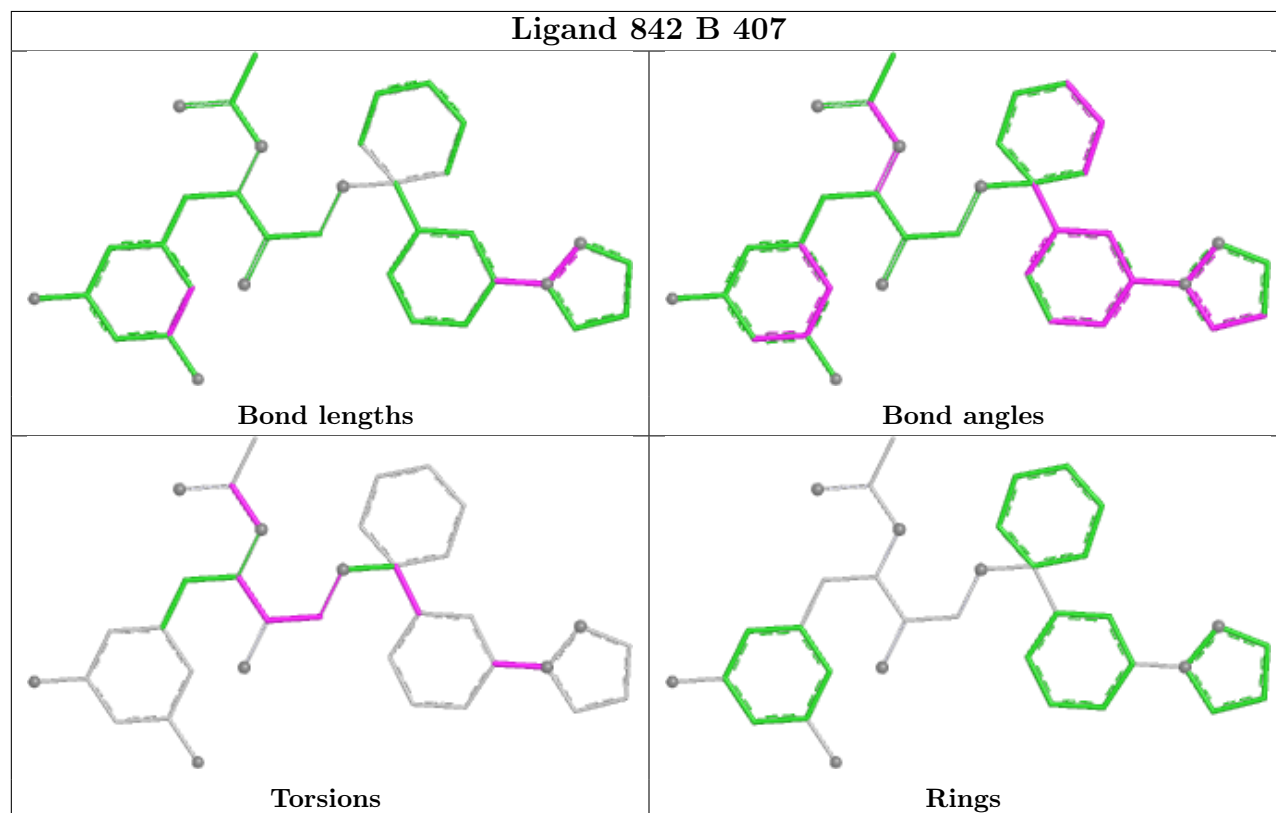
There are no ring outliers.

3 monomers are involved in 9 short contacts:

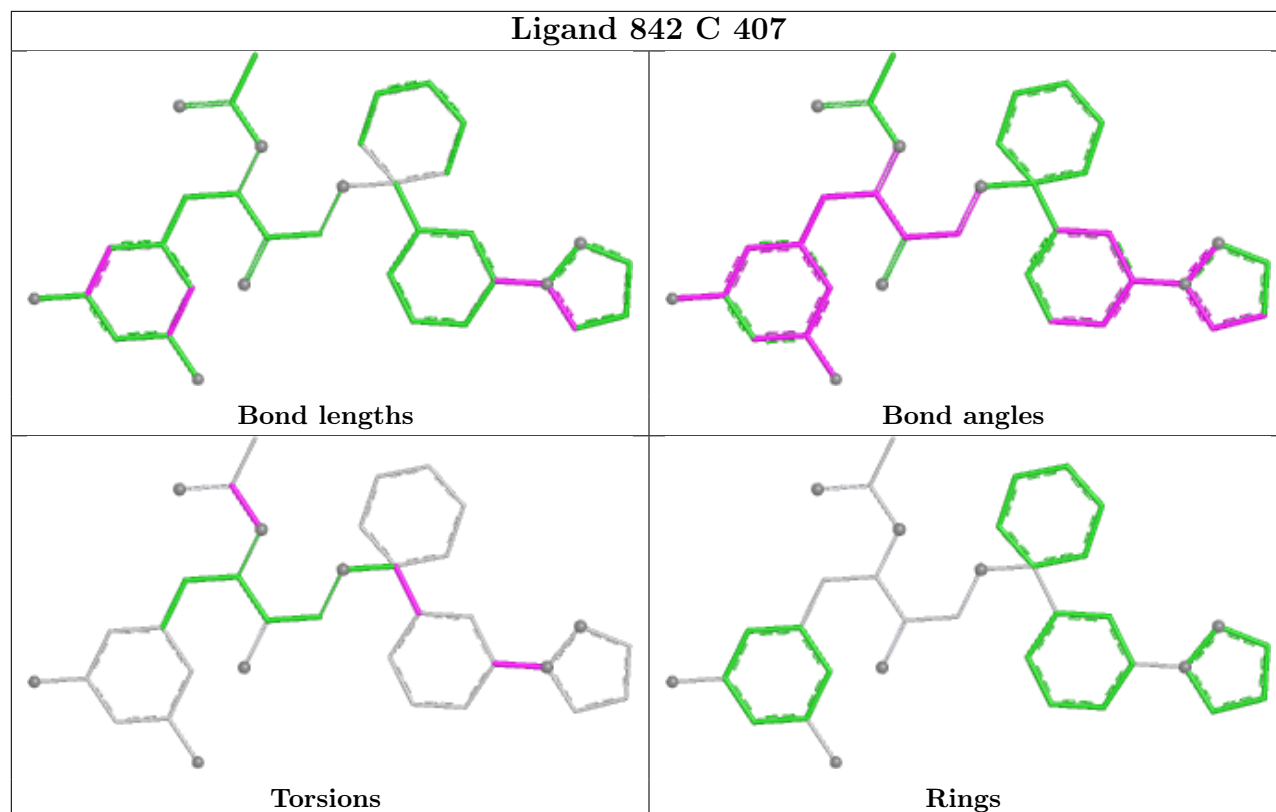
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	407	842	3	0
2	C	407	842	3	0
2	A	407	842	3	0

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

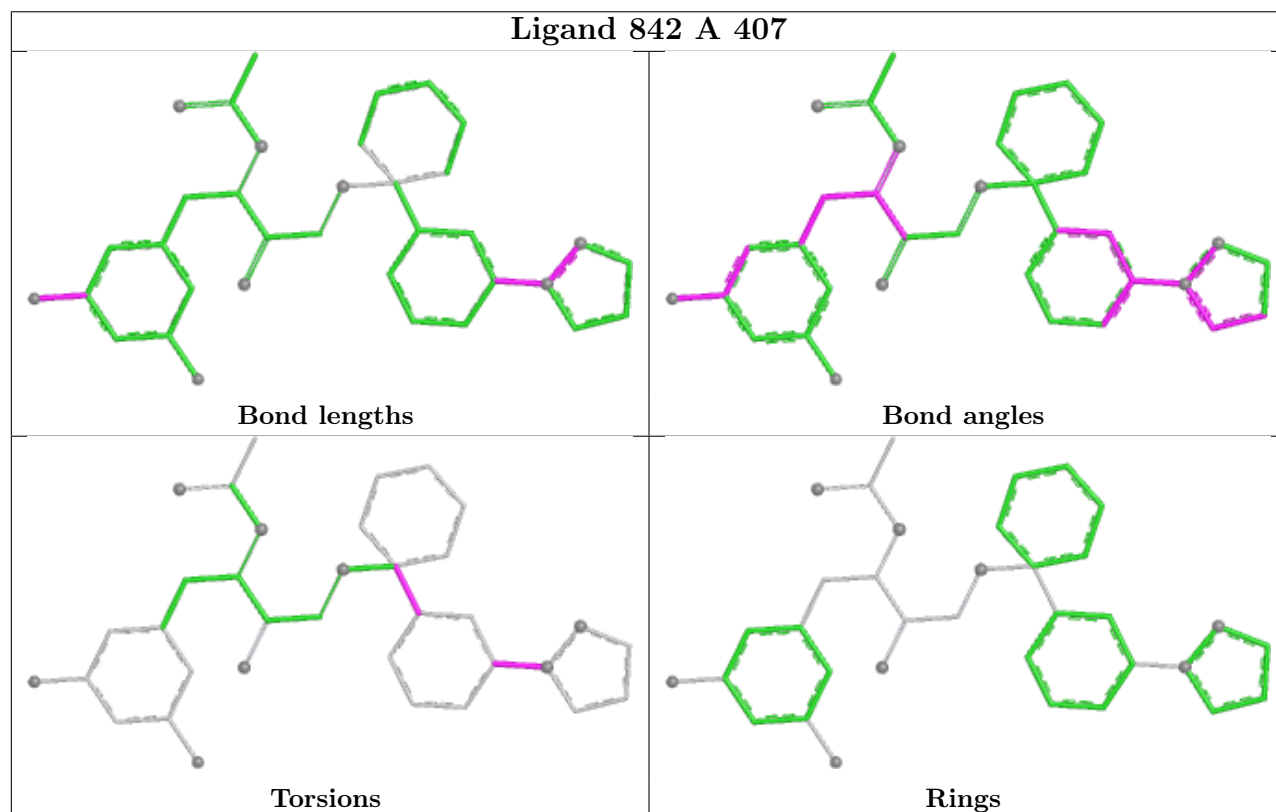
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand 842 C 407



Ligand 842 A 407



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	375/406 (92%)	-0.04	7 (1%) 66 63	43, 66, 99, 111	0
1	B	375/406 (92%)	-0.07	5 (1%) 75 73	44, 67, 99, 114	0
1	C	375/406 (92%)	-0.09	5 (1%) 75 73	45, 66, 99, 112	0
All	All	1125/1218 (92%)	-0.07	17 (1%) 72 70	43, 66, 99, 114	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	318	VAL	4.4
1	B	367	VAL	4.0
1	C	318	VAL	3.3
1	C	383	LEU	3.1
1	B	393	PRO	3.1
1	B	366	HIS	2.9
1	C	162	GLY	2.7
1	C	385	MET	2.5
1	A	74	TYR	2.5
1	A	367	VAL	2.5
1	A	162	GLY	2.4
1	A	260	THR	2.3
1	A	278	ALA	2.3
1	B	320	THR	2.3
1	B	47	GLY	2.2
1	C	321	SER	2.2
1	A	321	SER	2.1

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

There are no oligosaccharides in this entry.

6.4 Ligands

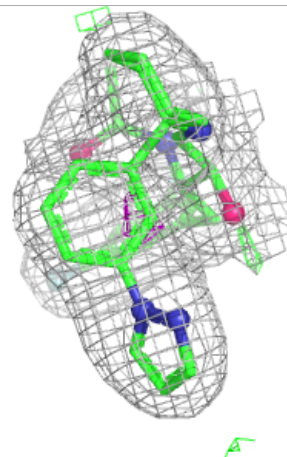
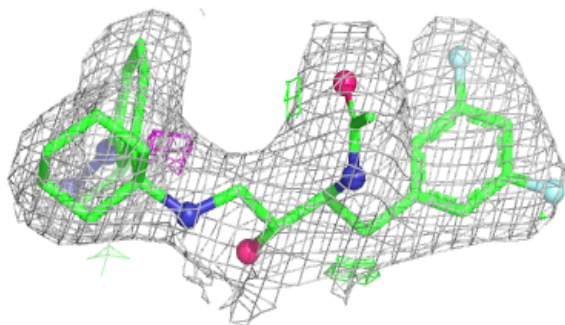
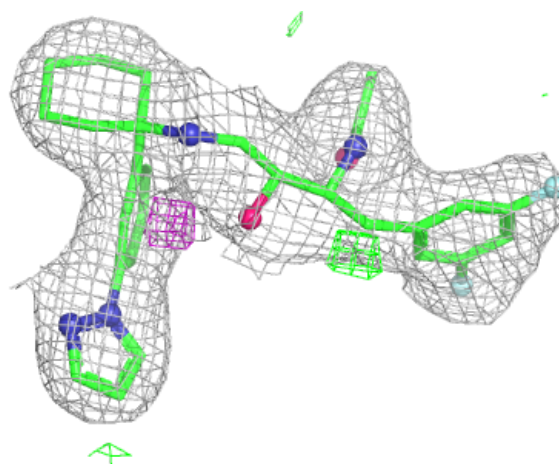
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	842	C	407	35/35	0.95	0.08	44,49,63,66	0
2	842	B	407	35/35	0.96	0.07	44,50,63,65	0
2	842	A	407	35/35	0.96	0.07	44,50,61,63	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.

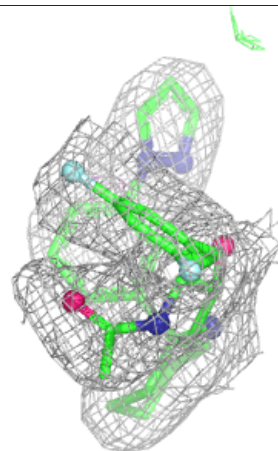
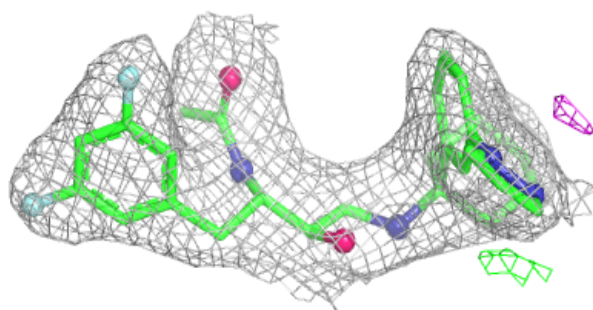
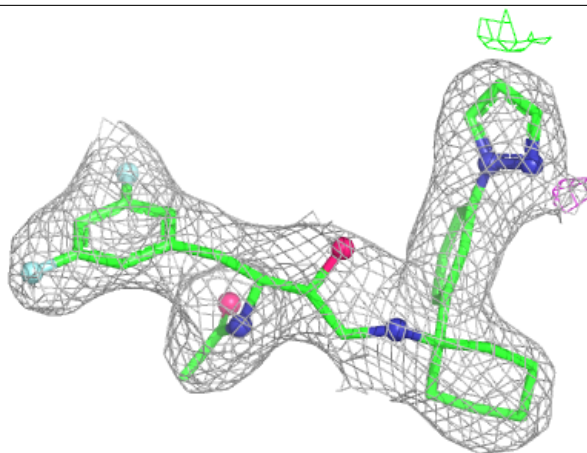
Electron density around 842 C 407:

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



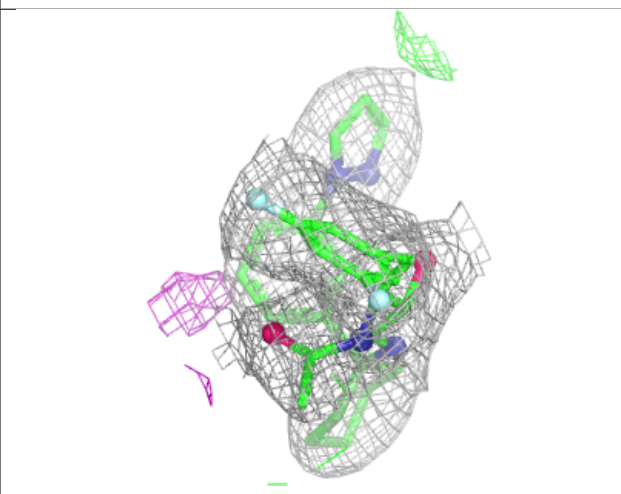
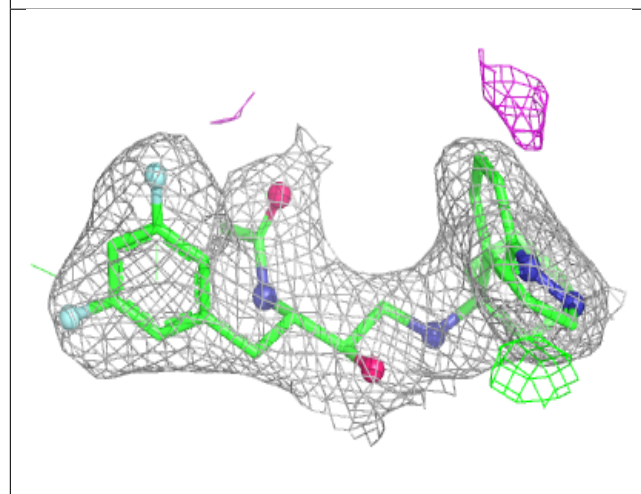
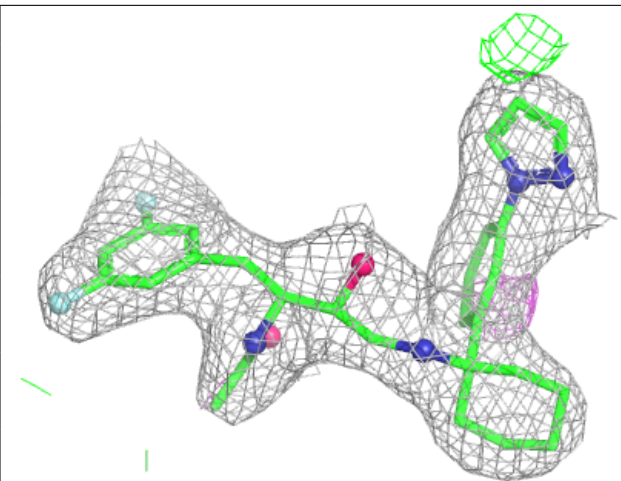
Electron density around 842 B 407:

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



Electron density around 842 A 407:

$2mF_o-DF_c$ (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.