



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:22 AM UTC

PDB ID : 3H0B / pdb_00003h0b
Title : Discovery of aminoheterocycles as a novel beta-secretase inhibitor class
Authors : Allison, T.J.
Deposited on : 2009-04-08
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

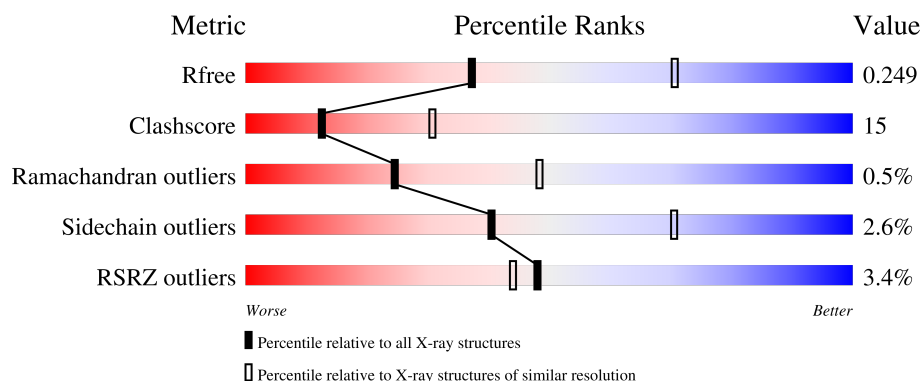
1 Overall quality at a glance

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	405	 3% 71% 20% 8%
1	B	405	 2% 65% 25% 8%
1	C	405	 4% 59% 32% 8%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9057 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.

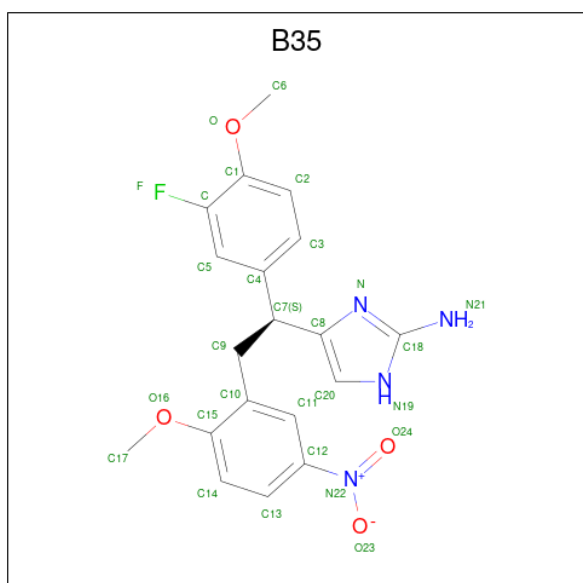
- Molecule 1 is a protein called Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	0	0
			2931	1877	488	552	14			
1	B	373	Total	C	N	O	S	0	0	0
			2935	1879	489	553	14			
1	C	373	Total	C	N	O	S	0	0	0
			2935	1879	489	553	14			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	429	MET	-	expression tag	UNP P56817
B	429	MET	-	expression tag	UNP P56817
C	429	MET	-	expression tag	UNP P56817

- Molecule 2 is 4-[(1S)-1-(3-fluoro-4-methoxyphenyl)-2-(2-methoxy-5-nitrophenyl)ethyl]-1H-imidazol-2-amine (CCD ID: B35) (formula: C₁₉H₁₉FN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			28	19	1	4	4		
2	B	1	Total	C	F	N	O	0	0
			28	19	1	4	4		
2	C	1	Total	C	F	N	O	0	0
			28	19	1	4	4		

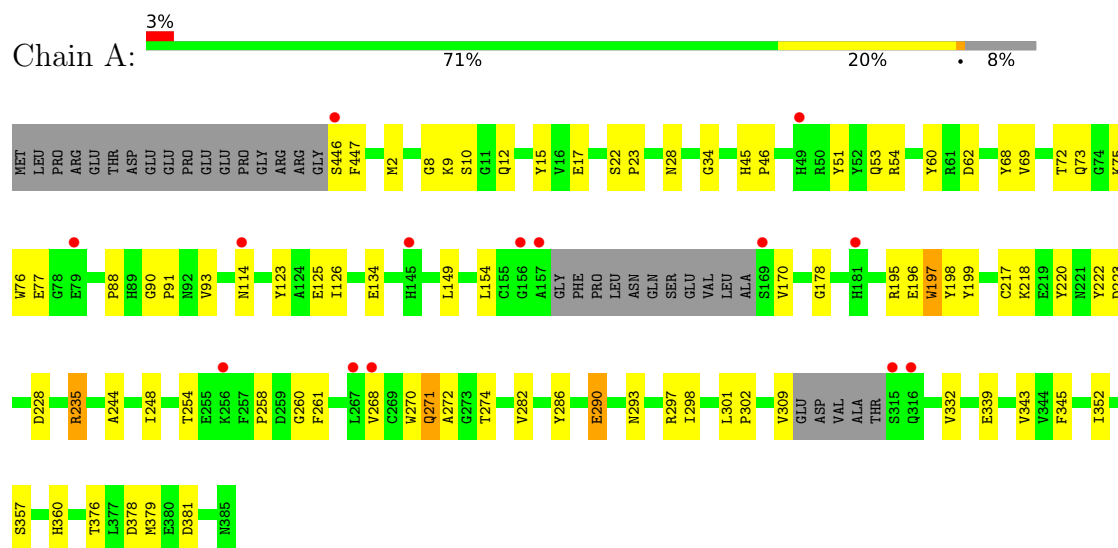
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	60	Total	O	0	0
			60	60		
3	B	77	Total	O	0	0
			77	77		
3	C	35	Total	O	0	0
			35	35		

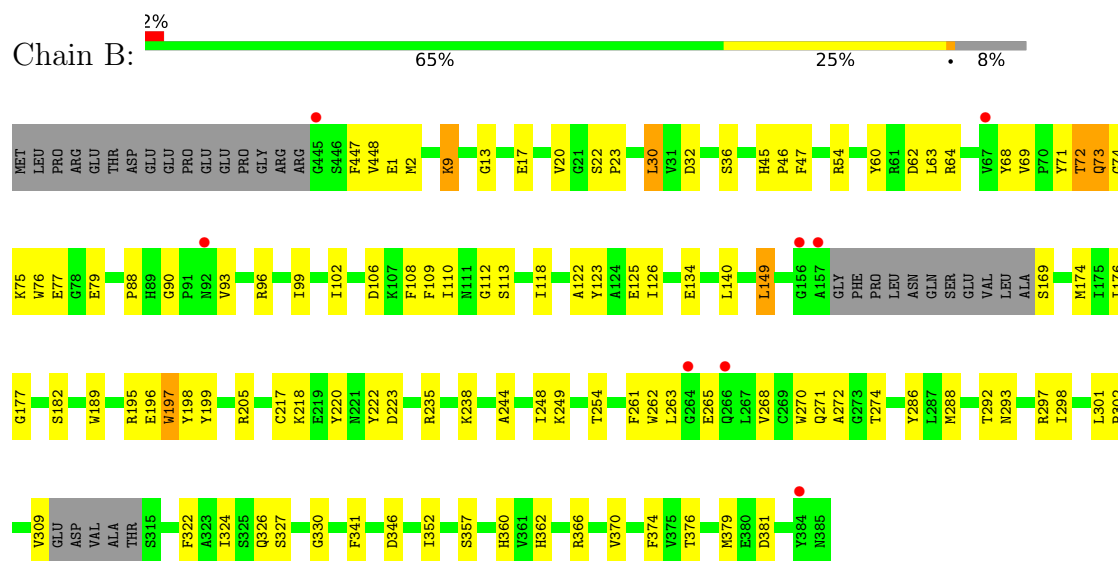
3 Residue-property plots [i](#)

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



MET	Q53	D130	I248	I352
LEU	R54	D131	I249	S357
PRO	Q55	S132	K249	H360
ARG	L56	L140	T254	T376
GLU	Y60	L149	P258	M379
ASP	L63	F150	D259	E380
GLU	G66	G156	G260	D381
PRO	Q67	A157	F261	M385
GLU	Y68	GLY	W262	
PRO	Y69	PHE	L263	
GLY	Y70	PRO	G264	
ARG	Y71	LEU	Q265	
G4445	Q73	ASN	Q266	
S4446	Q74	GLN	L267	
F4447	K75	SER	V268	
V448	W76	GLU	Q271	
E1	E77	VAL	A272	
M2	G81	LEU	N278	
V3	T82	ALA	I279	
D4	D83	V170	Y286	
R7	L84	I179	G289	
Q12	W85	D180	T292	
G13	P88	H181	N293	
E17	H89	S182	Q294	
V20	G90	R195	R297	
G21	P91	E196	I298	
S22	N92	W197	L301	
P23	V93	Y198	P302	
I29	I99	Y199	V309	
L30	A100	V204	GLU	
V31	A101	R205	ASP	
D32	I102	L213	VAL	
S35	D106	K214	ALA	
S36	I110	M215	THR	
R37	S113	D216	S315	
F38	M114	K217	Q316	
A39	W115	K218	F322	
V40	E116	E219	A323	
G41	G117	Y220	I324	
A42	T118	N221	S325	
A43	L119	Y222	Q326	
P44	A122	D223	S327	
H45	Y123	K224	T331	
P46	E125	S225	F341	
F47	A124	R235	Y342	
L48	I126	K238		
H49	R128	E242		
R50	P129	A243		
Y51		A244		
Y52				

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	221.18Å 107.44Å 65.08Å 90.00° 99.47° 90.00°	Depositor
Resolution (Å)	47.25 – 2.70 47.25 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.25-2.70) 99.8 (47.25-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.220 , 0.251 0.219 , 0.249	Depositor DCC
R_{free} test set	2072 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	52.9	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.3	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	0.93	EDS
Total number of atoms	9057	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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: B35

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	0.34	0/3005	0.71	0/4080
1	B	0.34	0/3009	0.73	0/4085
1	C	0.31	0/3009	0.73	0/4085
All	All	0.33	0/9023	0.72	0/12250

There are no bond length outliers.

There are no bond angle outliers.

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	2931	0	2843	64	0
1	B	2935	0	2846	92	0
1	C	2935	0	2846	122	0
2	A	28	0	19	0	0
2	B	28	0	19	1	0
2	C	28	0	19	4	0
3	A	60	0	0	2	0
3	B	77	0	0	6	0
3	C	35	0	0	6	0
All	All	9057	0	8592	267	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 15.

All (267) 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:238:LYS:HG3	1:C:326:GLN:OE1	1.41	1.20
1:B:96:ARG:HG2	1:C:448:VAL:HG23	1.37	1.03
1:B:72:THR:O	1:B:73:GLN:HB3	1.65	0.94
1:C:261:PHE:CD1	1:C:268:VAL:HG23	2.06	0.90
1:B:64:ARG:HD2	3:C:477:HOH:O	1.76	0.86
1:B:71:TYR:O	1:B:72:THR:HG22	1.79	0.82
1:A:290:GLU:HG3	3:A:506:HOH:O	1.79	0.81
1:B:149:LEU:HD12	1:B:346:ASP:HA	1.62	0.80
1:B:72:THR:O	1:B:73:GLN:CB	2.28	0.80
1:C:149:LEU:HD23	1:C:149:LEU:C	2.06	0.80
1:B:64:ARG:CD	3:C:477:HOH:O	2.30	0.80
1:B:96:ARG:HG2	1:C:448:VAL:CG2	2.12	0.80
1:C:2:MET:HG2	1:C:90:GLY:HA2	1.65	0.79
1:B:2:MET:HG2	1:B:90:GLY:HA2	1.64	0.79
1:C:261:PHE:CD1	1:C:268:VAL:CG2	2.66	0.79
1:C:115:TRP:HH2	2:C:449:B35:H17A	1.50	0.77
1:A:2:MET:HG2	1:A:90:GLY:HA2	1.65	0.76
1:B:125:GLU:OE2	1:B:195:ARG:NH2	2.19	0.76
1:A:125:GLU:OE2	1:A:195:ARG:NH2	2.20	0.74
1:C:45:HIS:ND1	1:C:46:PRO:HD2	2.02	0.74
1:B:238:LYS:HD3	1:B:326:GLN:OE1	1.87	0.74
1:A:68:TYR:HD1	1:A:77:GLU:HG2	1.54	0.73
1:C:72:THR:OG1	1:C:73:GLN:N	2.21	0.72
1:A:244:ALA:O	1:A:248:ILE:HG13	1.90	0.71
1:B:45:HIS:ND1	1:B:46:PRO:HD2	2.04	0.71
1:C:115:TRP:CH2	2:C:449:B35:H17A	2.26	0.71
1:C:69:VAL:HG21	1:C:76:TRP:CZ2	2.27	0.70
1:C:130:ASP:OD2	1:C:132:SER:OG	2.09	0.70
1:B:249:LYS:HE2	1:B:262:TRP:CD1	2.27	0.70
1:C:156:GLY:O	1:C:170:VAL:HG12	1.91	0.69
1:A:45:HIS:ND1	1:A:46:PRO:HD2	2.07	0.69
1:C:38:PHE:HE1	1:C:85:VAL:HG21	1.58	0.68
1:B:96:ARG:CG	1:C:448:VAL:HG23	2.20	0.68
1:B:169:SER:N	3:B:509:HOH:O	2.26	0.67
1:C:45:HIS:CE1	1:C:46:PRO:HD2	2.29	0.67
1:B:79:GLU:HB2	3:B:512:HOH:O	1.94	0.67
1:B:447:PHE:HB3	1:B:2:MET:HE3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:GLU:CB	3:B:512:HOH:O	2.46	0.64
1:C:2:MET:CG	1:C:90:GLY:HA2	2.27	0.63
1:C:125:GLU:OE2	1:C:195:ARG:NH2	2.30	0.63
1:B:261:PHE:CD1	1:B:268:VAL:HG23	2.34	0.62
1:C:376:THR:HG22	1:C:379:MET:HG3	1.80	0.62
1:C:249:LYS:HE3	1:C:262:TRP:CD1	2.34	0.62
1:A:301:LEU:HB3	1:A:302:PRO:HD2	1.81	0.62
1:B:309:VAL:HG12	1:B:309:VAL:O	1.98	0.62
1:C:68:TYR:HD1	1:C:77:GLU:HG2	1.64	0.62
1:C:32:ASP:OD1	2:C:449:B35:H3	1.99	0.62
1:B:298:ILE:HG22	1:B:370:VAL:HG22	1.82	0.62
1:B:69:VAL:HG21	1:B:76:TRP:CZ2	2.35	0.61
1:B:2:MET:CG	1:B:90:GLY:HA2	2.31	0.61
1:C:68:TYR:CD1	1:C:77:GLU:HG2	2.35	0.61
1:A:68:TYR:CE1	1:A:75:LYS:HD3	2.36	0.60
1:C:301:LEU:HB3	1:C:302:PRO:HD2	1.84	0.60
1:B:13:GLY:HA3	1:B:30:LEU:HD11	1.82	0.60
1:A:8:GLY:C	1:A:170:VAL:HG22	2.26	0.60
1:C:293:ASN:HA	1:C:376:THR:O	2.01	0.59
1:C:376:THR:HG22	1:C:379:MET:CG	2.32	0.59
1:C:156:GLY:O	1:C:157:ALA:HB2	2.02	0.58
1:C:63:LEU:HD12	1:C:81:GLY:N	2.19	0.58
1:C:131:ASP:OD1	1:C:131:ASP:C	2.46	0.58
1:A:2:MET:CG	1:A:90:GLY:HA2	2.34	0.58
1:A:197:TRP:CG	1:A:198:TYR:H	2.22	0.58
1:C:205:ARG:HB3	1:C:286:TYR:HB2	1.85	0.58
1:A:261:PHE:CD1	1:A:268:VAL:HG23	2.40	0.57
1:C:52:TYR:OH	1:C:83:ASP:OD2	2.22	0.57
1:A:68:TYR:CD1	1:A:77:GLU:HG2	2.37	0.56
1:C:197:TRP:HD1	1:C:197:TRP:H	1.54	0.56
1:C:244:ALA:O	1:C:248:ILE:HG13	2.05	0.56
1:B:45:HIS:CE1	1:B:46:PRO:HD2	2.40	0.56
1:B:96:ARG:O	1:C:448:VAL:HG21	2.06	0.56
1:C:114:ASN:O	1:C:114:ASN:ND2	2.36	0.56
1:C:51:TYR:HE1	1:C:53:GLN:HG2	1.72	0.55
1:C:197:TRP:CG	1:C:198:TYR:H	2.23	0.55
1:B:197:TRP:CG	1:B:198:TYR:H	2.24	0.55
1:A:9:LYS:HD3	1:A:12:GLN:CD	2.32	0.55
1:B:235:ARG:HB3	1:B:327:SER:HB2	1.88	0.55
1:B:298:ILE:HB	1:B:341:PHE:CZ	2.41	0.55
1:B:357:SER:HB3	1:B:360:HIS:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:TYR:CZ	1:A:196:GLU:HG2	2.42	0.55
1:B:74:GLY:O	1:B:75:LYS:HB3	2.06	0.55
1:C:261:PHE:HD1	1:C:268:VAL:HG23	1.67	0.54
1:B:293:ASN:HA	1:B:376:THR:O	2.06	0.54
1:A:8:GLY:O	1:A:170:VAL:HG22	2.06	0.54
1:C:45:HIS:ND1	1:C:46:PRO:CD	2.70	0.54
1:C:235:ARG:HG2	1:C:325:SER:OG	2.07	0.54
1:C:197:TRP:H	1:C:197:TRP:CD1	2.25	0.54
1:C:357:SER:HB3	1:C:360:HIS:HB3	1.88	0.54
1:C:63:LEU:HG	1:C:81:GLY:HA2	1.89	0.54
1:C:45:HIS:HE1	1:C:47:PHE:CD1	2.26	0.53
1:C:13:GLY:HA3	1:C:30:LEU:HD11	1.91	0.53
1:A:268:VAL:CG1	1:A:270:TRP:CH2	2.92	0.53
1:B:20:VAL:HG11	1:B:99:ILE:HD13	1.90	0.53
1:C:261:PHE:CD1	1:C:268:VAL:HG21	2.43	0.53
1:A:357:SER:HB3	1:A:360:HIS:HB3	1.91	0.52
1:C:4:ASP:CG	1:C:7:ARG:HH22	2.17	0.52
1:A:9:LYS:O	1:A:10:SER:C	2.51	0.52
1:A:69:VAL:HG21	1:A:76:TRP:CZ2	2.44	0.52
1:C:197:TRP:CD1	1:C:197:TRP:N	2.78	0.52
1:B:261:PHE:CD1	1:B:268:VAL:CG2	2.93	0.52
1:A:199:TYR:HB3	1:A:352:ILE:HD11	1.92	0.51
1:C:447:PHE:HB3	1:C:2:MET:HE3	1.91	0.51
1:C:68:TYR:CE1	1:C:75:LYS:CD	2.92	0.51
1:C:225:SER:N	3:C:479:HOH:O	2.11	0.51
1:B:288:MET:HE2	1:B:379:MET:HB3	1.92	0.51
1:C:29:ILE:HG21	1:C:119:LEU:HB2	1.93	0.51
1:C:113:SER:O	1:C:114:ASN:CB	2.57	0.51
1:A:9:LYS:HD3	1:A:12:GLN:NE2	2.26	0.51
1:A:45:HIS:CE1	1:A:46:PRO:HD2	2.45	0.51
1:A:218:LYS:HG3	1:A:381:ASP:O	2.10	0.51
1:A:309:VAL:HG12	1:A:309:VAL:O	2.09	0.51
1:B:123:TYR:CZ	1:B:196:GLU:HG2	2.46	0.51
1:B:301:LEU:HB3	1:B:302:PRO:HD2	1.92	0.51
1:C:68:TYR:CE1	1:C:75:LYS:HD2	2.46	0.51
1:C:149:LEU:HD23	1:C:150:PHE:N	2.26	0.51
1:A:446:SER:O	1:A:447:PHE:HB2	2.11	0.51
1:A:268:VAL:HG11	1:A:270:TRP:CH2	2.46	0.51
1:B:62:ASP:O	1:C:182:SER:HA	2.10	0.50
1:B:271:GLN:O	1:B:272:ALA:C	2.53	0.50
1:C:42:ALA:O	1:C:51:TYR:CD1	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:SER:HA	1:C:23:PRO:C	2.35	0.50
1:A:343:VAL:HG12	1:A:345:PHE:CE2	2.47	0.50
1:C:253:SER:HA	3:C:454:HOH:O	2.11	0.50
1:C:264:GLY:O	1:C:266:GLN:N	2.44	0.50
1:B:205:ARG:HB3	1:B:286:TYR:HB2	1.93	0.50
1:B:63:LEU:HD23	1:C:182:SER:HB3	1.94	0.50
1:B:174:MET:HE3	1:B:176:ILE:HD11	1.94	0.50
1:C:235:ARG:HB3	1:C:327:SER:HB2	1.93	0.49
1:B:74:GLY:HA3	1:B:106:ASP:O	2.12	0.49
1:A:197:TRP:N	1:A:197:TRP:CD1	2.81	0.49
1:A:290:GLU:CG	3:A:506:HOH:O	2.48	0.49
1:A:293:ASN:HA	1:A:376:THR:O	2.12	0.49
1:B:64:ARG:HD3	3:C:477:HOH:O	2.05	0.49
1:C:74:GLY:HA3	1:C:106:ASP:O	2.13	0.49
1:B:76:TRP:CE3	1:B:102:ILE:HG12	2.48	0.48
1:A:15:TYR:CE2	1:A:114:ASN:HB2	2.48	0.48
1:B:96:ARG:NE	3:B:518:HOH:O	2.13	0.48
1:B:68:TYR:HD1	1:B:77:GLU:HG3	1.78	0.48
1:C:322:PHE:CZ	1:C:324:ILE:HB	2.49	0.48
1:B:199:TYR:HB3	1:B:352:ILE:HD11	1.96	0.48
1:C:264:GLY:C	1:C:266:GLN:H	2.22	0.48
1:C:20:VAL:HG11	1:C:99:ILE:HD13	1.96	0.48
1:A:68:TYR:CE1	1:A:75:LYS:CD	2.97	0.47
1:B:125:GLU:CD	1:B:195:ARG:HH21	2.20	0.47
1:C:222:TYR:HA	1:C:223:ASP:HA	1.67	0.47
1:B:93:VAL:HG21	1:B:140:LEU:HD11	1.97	0.47
1:B:96:ARG:C	1:C:448:VAL:HG21	2.40	0.47
1:C:123:TYR:CZ	1:C:196:GLU:HG2	2.50	0.47
1:B:218:LYS:HG3	1:B:381:ASP:O	2.15	0.47
1:C:292:THR:O	1:C:293:ASN:HB2	2.14	0.47
1:C:36:SER:OG	1:C:122:ALA:HB3	2.14	0.47
1:A:222:TYR:HA	1:A:223:ASP:HA	1.66	0.47
1:B:22:SER:HA	1:B:23:PRO:C	2.39	0.47
1:B:32:ASP:OD1	2:B:449:B35:N	2.47	0.47
1:B:47:PHE:HD1	1:B:109:PHE:O	1.97	0.47
1:B:238:LYS:HD3	1:B:326:GLN:CD	2.40	0.47
1:C:45:HIS:HB3	1:C:48:LEU:HG	1.97	0.47
1:C:218:LYS:HG3	1:C:381:ASP:O	2.15	0.47
1:C:235:ARG:O	1:C:331:THR:HA	2.14	0.47
1:A:235:ARG:HG3	1:A:332:VAL:HB	1.97	0.47
1:B:297:ARG:HG2	1:B:374:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:VAL:O	1:C:205:ARG:HB2	2.15	0.47
1:C:238:LYS:HE3	1:C:242:GLU:OE1	2.15	0.47
1:A:22:SER:HA	1:A:23:PRO:C	2.40	0.46
1:B:362:HIS:HB2	1:B:366:ARG:O	2.15	0.46
1:C:29:ILE:HD12	1:C:117:GLY:HA3	1.98	0.46
1:C:149:LEU:C	1:C:149:LEU:CD2	2.79	0.46
1:A:197:TRP:HD1	1:A:197:TRP:H	1.62	0.46
1:B:197:TRP:N	1:B:197:TRP:CD1	2.82	0.46
1:A:271:GLN:O	1:A:274:THR:HG23	2.16	0.46
1:C:298:ILE:O	1:C:298:ILE:HG13	2.15	0.46
1:A:447:PHE:CZ	1:A:178:GLY:HA3	2.51	0.46
1:B:36:SER:OG	1:B:122:ALA:HB3	2.15	0.46
1:A:268:VAL:HG12	1:A:270:TRP:CZ3	2.51	0.46
1:C:41:GLY:HA2	1:C:102:ILE:HB	1.98	0.46
1:A:271:GLN:O	1:A:272:ALA:C	2.57	0.46
1:B:268:VAL:HG11	1:B:270:TRP:CH2	2.51	0.46
1:C:110:ILE:HB	1:C:113:SER:HB3	1.97	0.46
1:C:128:ARG:HA	1:C:129:PRO:C	2.42	0.45
1:A:197:TRP:CD1	1:A:197:TRP:H	2.35	0.45
1:C:199:TYR:HB3	1:C:352:ILE:HD11	1.99	0.45
1:A:17:GLU:O	1:A:88:PRO:HD2	2.16	0.45
1:A:62:ASP:O	1:B:182:SER:HA	2.17	0.45
1:B:96:ARG:O	1:C:448:VAL:CG2	2.64	0.45
1:C:286:TYR:CZ	1:C:297:ARG:HD3	2.52	0.45
1:B:217:CYS:HA	1:B:220:TYR:CD1	2.51	0.45
1:C:289:GLY:HA3	1:C:294:GLN:O	2.16	0.45
1:A:91:PRO:HB2	1:A:93:VAL:HG22	1.98	0.45
1:B:45:HIS:ND1	1:B:46:PRO:CD	2.76	0.45
1:C:213:LEU:HD12	1:C:213:LEU:HA	1.87	0.45
1:C:271:GLN:O	1:C:272:ALA:C	2.60	0.45
1:A:45:HIS:CG	1:A:46:PRO:HD2	2.51	0.45
1:A:268:VAL:HG12	1:A:270:TRP:CH2	2.52	0.44
1:C:4:ASP:CG	1:C:7:ARG:NH2	2.75	0.44
1:C:12:GLN:OE1	1:C:113:SER:HA	2.17	0.44
1:C:93:VAL:HG21	1:C:140:LEU:HD11	1.99	0.44
1:C:122:ALA:CB	1:C:126:ILE:HD11	2.47	0.44
1:B:72:THR:O	1:B:72:THR:HG23	2.17	0.44
1:B:244:ALA:O	1:B:248:ILE:HG13	2.17	0.44
1:A:261:PHE:CD1	1:A:268:VAL:CG2	3.00	0.44
1:B:268:VAL:CG1	1:B:270:TRP:CH2	3.01	0.44
1:B:9:LYS:NZ	1:B:112:GLY:O	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:ILE:HG23	1:C:342:TYR:HE2	1.82	0.43
1:B:45:HIS:CG	1:B:46:PRO:HD2	2.53	0.43
1:B:122:ALA:CB	1:B:126:ILE:HD11	2.49	0.43
1:B:197:TRP:CD1	1:B:197:TRP:H	2.36	0.43
1:C:68:TYR:OH	1:C:75:LYS:HD3	2.18	0.43
1:A:72:THR:OG1	1:A:73:GLN:N	2.51	0.43
1:C:156:GLY:O	1:C:157:ALA:CB	2.67	0.43
1:B:169:SER:CA	3:B:509:HOH:O	2.65	0.43
1:B:197:TRP:H	1:B:197:TRP:HD1	1.66	0.43
1:C:17:GLU:O	1:C:88:PRO:HD2	2.18	0.43
1:A:54:ARG:HD2	1:A:60:TYR:CZ	2.54	0.43
1:C:217:CYS:HA	1:C:220:TYR:CD1	2.54	0.43
1:C:298:ILE:HB	1:C:341:PHE:CZ	2.54	0.43
1:B:68:TYR:CE1	1:B:75:LYS:HD2	2.54	0.43
1:B:271:GLN:O	1:B:274:THR:HG23	2.18	0.43
1:C:71:TYR:O	1:C:73:GLN:N	2.52	0.42
1:C:126:ILE:HG23	1:C:197:TRP:HB2	2.00	0.42
1:A:197:TRP:CG	1:A:198:TYR:N	2.87	0.42
1:A:286:TYR:CZ	1:A:297:ARG:HD3	2.55	0.42
1:B:222:TYR:HA	1:B:223:ASP:HA	1.67	0.42
1:B:322:PHE:CZ	1:B:324:ILE:HB	2.54	0.42
1:C:4:ASP:OD2	1:C:7:ARG:NH2	2.53	0.42
1:C:214:LYS:HE3	1:C:214:LYS:HB2	1.81	0.42
1:C:45:HIS:CE1	1:C:47:PHE:CD1	3.08	0.42
1:A:51:TYR:HE1	1:A:53:GLN:HG2	1.85	0.42
1:A:154:LEU:O	1:A:339:GLU:HA	2.20	0.42
1:A:282:VAL:HG12	1:A:301:LEU:HD23	2.00	0.42
1:A:126:ILE:HG23	1:A:197:TRP:HB2	2.02	0.41
1:A:217:CYS:HA	1:A:220:TYR:CD1	2.54	0.41
1:C:51:TYR:CD1	1:C:51:TYR:C	2.98	0.41
1:C:74:GLY:O	1:C:75:LYS:HB3	2.19	0.41
1:C:225:SER:OG	1:C:331:THR:HB	2.20	0.41
1:B:149:LEU:O	1:B:177:GLY:N	2.48	0.41
1:C:20:VAL:HG13	1:C:85:VAL:HG22	2.02	0.41
1:A:378:ASP:HB3	1:A:381:ASP:OD2	2.20	0.41
1:C:35:SER:CB	2:C:449:B35:H2	2.50	0.41
1:C:53:GLN:OE1	1:C:56:LEU:HD12	2.20	0.41
1:B:13:GLY:HA3	1:B:30:LEU:CD1	2.50	0.41
1:A:134:GLU:OE2	1:B:1:GLU:OE1	2.37	0.41
1:A:298:ILE:O	1:A:298:ILE:HG13	2.20	0.41
1:B:134:GLU:OE2	1:C:1:GLU:OE1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:TRP:CD1	1:B:370:VAL:HG12	2.54	0.41
1:B:238:LYS:HA	1:B:238:LYS:HD2	1.74	0.41
1:C:45:HIS:CG	1:C:46:PRO:HD2	2.56	0.41
1:A:376:THR:HG22	1:A:379:MET:HG2	2.02	0.41
1:C:76:TRP:CE3	1:C:102:ILE:HG12	2.55	0.41
1:A:34:GLY:HA3	1:A:228:ASP:OD1	2.20	0.41
1:C:29:ILE:CG2	1:C:119:LEU:HB2	2.50	0.41
1:C:54:ARG:HD2	1:C:60:TYR:CZ	2.56	0.41
1:C:376:THR:CG2	1:C:379:MET:CG	2.99	0.41
1:A:15:TYR:CD1	1:A:28:ASN:HB3	2.55	0.41
1:B:110:ILE:HB	1:B:113:SER:HB2	2.01	0.41
1:C:197:TRP:CG	1:C:198:TYR:N	2.88	0.41
1:C:215:MET:HE2	1:C:219:GLU:CB	2.50	0.41
1:B:68:TYR:CE1	1:B:75:LYS:CD	3.05	0.40
1:B:108:PHE:HZ	1:B:118:ILE:CD1	2.35	0.40
1:B:330:GLY:N	3:B:513:HOH:O	2.35	0.40
1:C:45:HIS:CG	1:C:46:PRO:CD	3.04	0.40
1:B:54:ARG:HD2	1:B:60:TYR:CZ	2.57	0.40
1:B:72:THR:O	1:B:73:GLN:CG	2.68	0.40
1:C:224:LYS:HA	3:C:479:HOH:O	2.21	0.40
1:C:258:PRO:C	1:C:260:GLY:N	2.78	0.40
1:A:258:PRO:C	1:A:260:GLY:N	2.79	0.40
1:B:17:GLU:O	1:B:88:PRO:HD2	2.21	0.40
1:B:263:LEU:HB2	1:B:265:GLU:HG3	2.02	0.40
1:C:235:ARG:HA	1:C:325:SER:O	2.21	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	366/405 (90%)	350 (96%)	16 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	367/405 (91%)	348 (95%)	18 (5%)	1 (0%)	36	60
1	C	367/405 (91%)	341 (93%)	22 (6%)	4 (1%)	11	29
All	All	1100/1215 (90%)	1039 (94%)	56 (5%)	5 (0%)	24	48

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	73	GLN
1	C	72	THR
1	C	265	GLU
1	C	114	ASN
1	C	44	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	318/346 (92%)	312 (98%)	6 (2%)	50	77
1	B	318/346 (92%)	310 (98%)	8 (2%)	42	71
1	C	318/346 (92%)	307 (96%)	11 (4%)	32	61
All	All	954/1038 (92%)	929 (97%)	25 (3%)	40	70

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	LEU
1	A	197	TRP
1	A	235	ARG
1	A	254	THR
1	A	271	GLN
1	A	290	GLU
1	B	448	VAL
1	B	9	LYS
1	B	30	LEU

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Mol	Chain	Res	Type
1	B	72	THR
1	B	149	LEU
1	B	197	TRP
1	B	254	THR
1	B	292	THR
1	C	22	SER
1	C	30	LEU
1	C	40	VAL
1	C	72	THR
1	C	92	ASN
1	C	149	LEU
1	C	181	HIS
1	C	197	TRP
1	C	254	THR
1	C	279	ILE
1	C	292	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	89	HIS
1	A	385	ASN
1	B	98	ASN
1	C	73	GLN
1	C	233	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	B35	C	449	-	29,30,30	2.18	5 (17%)	32,42,42	1.13	2 (6%)
2	B35	B	449	-	29,30,30	2.15	5 (17%)	32,42,42	1.12	2 (6%)
2	B35	A	449	-	29,30,30	2.19	4 (13%)	32,42,42	1.11	2 (6%)

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	B35	C	449	-	-	6/18/20/20	0/3/3/3
2	B35	B	449	-	-	0/18/20/20	0/3/3/3
2	B35	A	449	-	-	0/18/20/20	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	449	B35	O24-N22	9.70	1.39	1.22
2	B	449	B35	O24-N22	9.70	1.39	1.22
2	A	449	B35	O24-N22	9.64	1.39	1.22
2	A	449	B35	C12-N22	-4.68	1.34	1.45
2	C	449	B35	C12-N22	-4.61	1.34	1.45
2	B	449	B35	C12-N22	-4.25	1.35	1.45
2	A	449	B35	O16-C15	-2.36	1.33	1.37
2	C	449	B35	O16-C15	-2.26	1.33	1.37
2	A	449	B35	O-C1	-2.26	1.33	1.37
2	C	449	B35	O-C1	-2.15	1.33	1.37
2	C	449	B35	C20-C8	2.11	1.39	1.36
2	B	449	B35	O-C1	-2.08	1.33	1.37
2	B	449	B35	C20-C8	2.05	1.39	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	449	B35	O16-C15	-2.00	1.33	1.37

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	449	B35	C20-C8-N	-4.00	105.58	110.75
2	B	449	B35	C20-C8-N	-3.86	105.75	110.75
2	A	449	B35	C20-C8-N	-3.69	105.97	110.75
2	C	449	B35	N21-C18-N19	2.78	126.79	122.68
2	B	449	B35	N21-C18-N19	2.60	126.53	122.68
2	A	449	B35	N21-C18-N19	2.54	126.44	122.68

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	449	B35	C-C1-O-C6
2	C	449	B35	C11-C12-N22-O24
2	C	449	B35	C13-C12-N22-O24
2	C	449	B35	C14-C15-O16-C17
2	C	449	B35	C10-C15-O16-C17
2	C	449	B35	C2-C1-O-C6

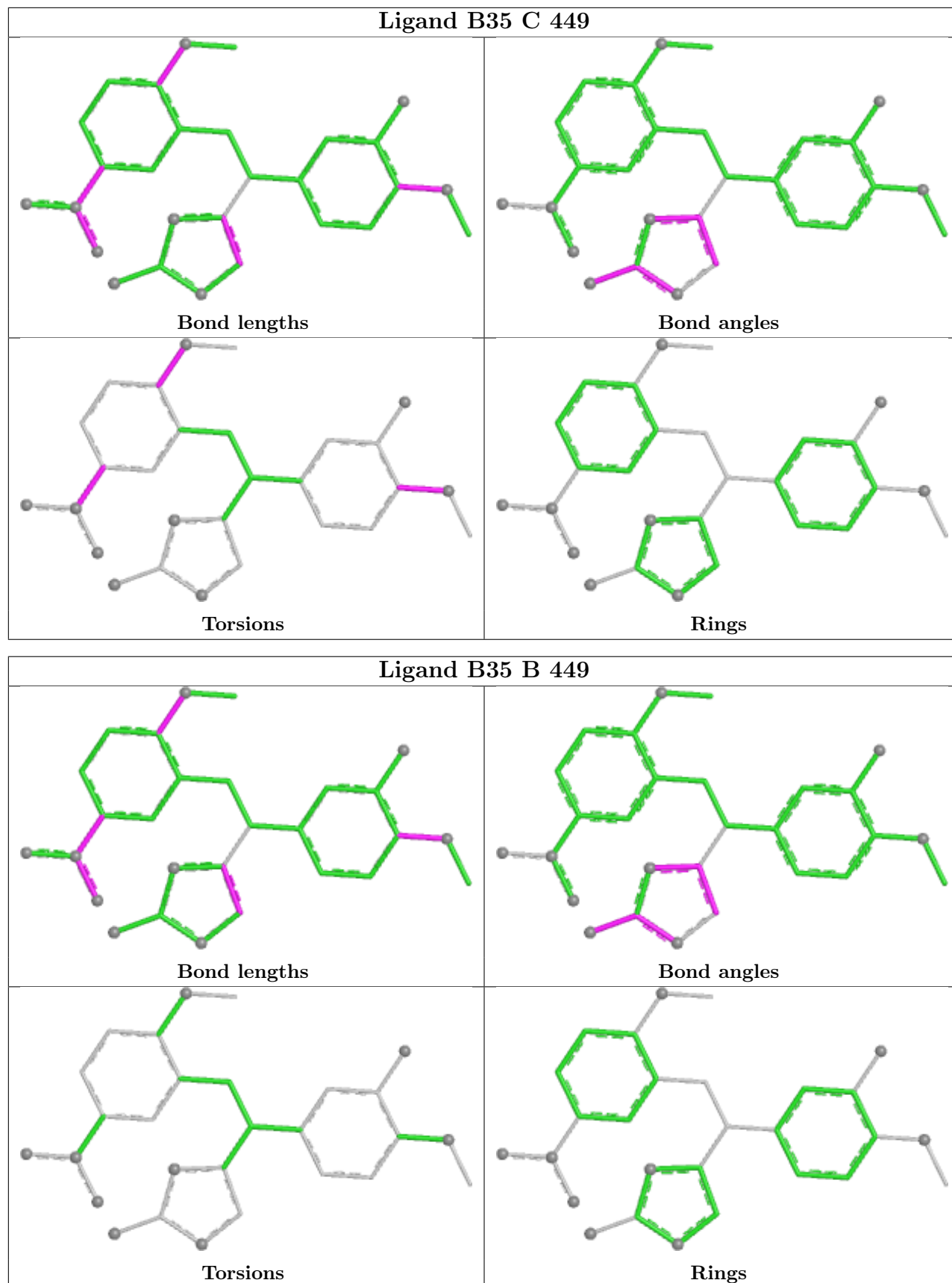
There are no ring outliers.

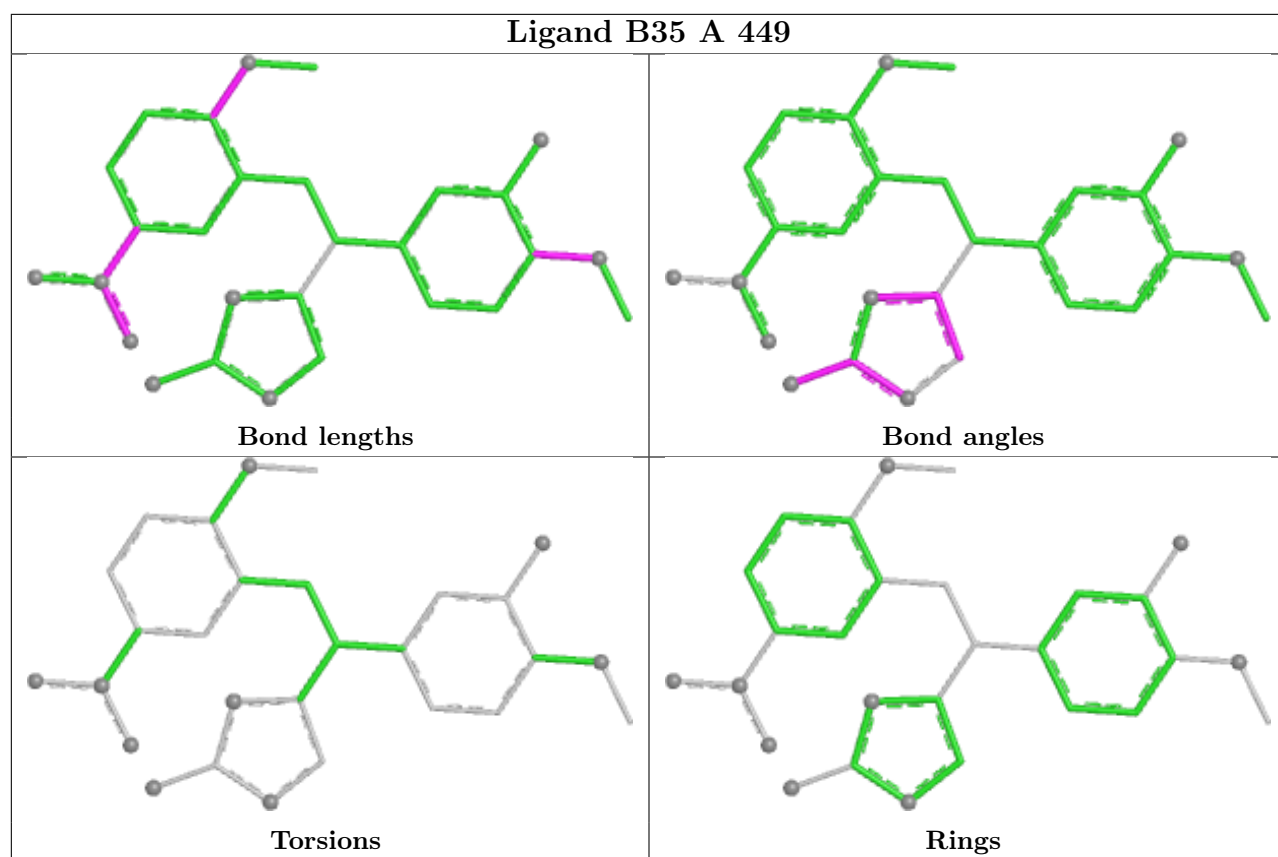
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	449	B35	4	0
2	B	449	B35	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

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	372/405 (91%)	0.31	14 (3%) 44 40	36, 51, 72, 92	0
1	B	373/405 (92%)	0.31	8 (2%) 63 61	36, 51, 72, 92	0
1	C	373/405 (92%)	0.52	16 (4%) 40 36	36, 52, 72, 92	0
All	All	1118/1215 (92%)	0.38	38 (3%) 48 44	36, 52, 72, 92	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	157	ALA	5.9
1	B	157	ALA	4.9
1	C	278	ASN	4.2
1	C	157	ALA	3.6
1	A	315	SER	3.5
1	C	68	TYR	3.2
1	A	49	HIS	3.1
1	C	42	ALA	3.1
1	B	92	ASN	2.9
1	C	445	GLY	2.9
1	C	181	HIS	2.8
1	A	267	LEU	2.6
1	C	264	GLY	2.6
1	A	316	GLN	2.6
1	B	384	TYR	2.5
1	B	266	GLN	2.5
1	C	316	GLN	2.5
1	A	79	GLU	2.5
1	C	66	GLY	2.4
1	A	156	GLY	2.4
1	A	169	SER	2.4
1	A	145	HIS	2.3
1	B	156	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	41	GLY	2.3
1	C	50	ARG	2.3
1	C	40	VAL	2.3
1	A	181	HIS	2.2
1	C	315	SER	2.2
1	B	445	GLY	2.2
1	A	446	SER	2.2
1	B	264	GLY	2.2
1	C	101	ALA	2.1
1	A	256	LYS	2.1
1	A	268	VAL	2.1
1	A	114	ASN	2.1
1	C	67	VAL	2.1
1	B	67	VAL	2.1
1	C	309	VAL	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

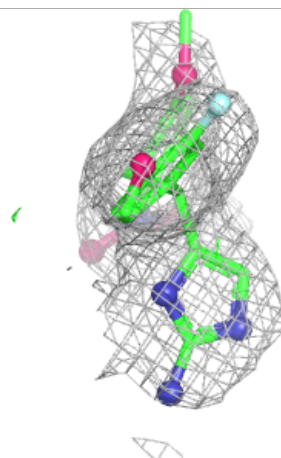
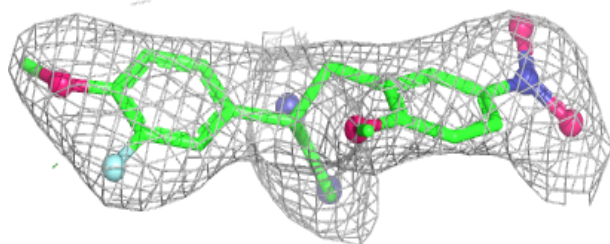
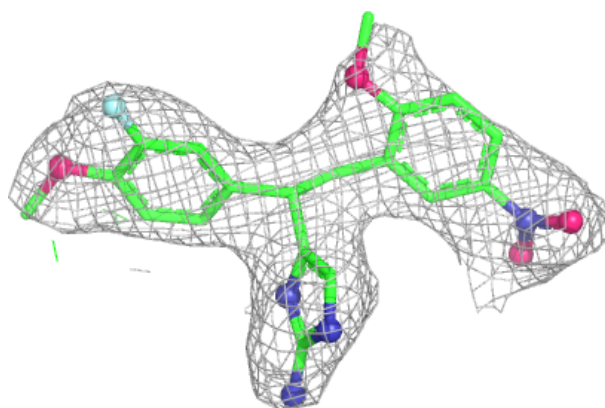
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	B35	C	449	28/28	0.91	0.12	71,73,74,74	0
2	B35	B	449	28/28	0.94	0.08	41,42,45,45	0
2	B35	A	449	28/28	0.94	0.09	37,39,44,44	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.

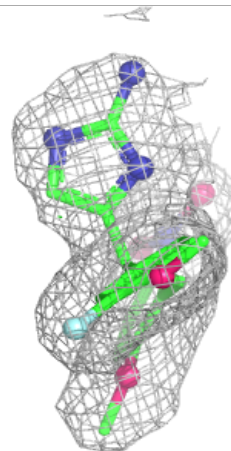
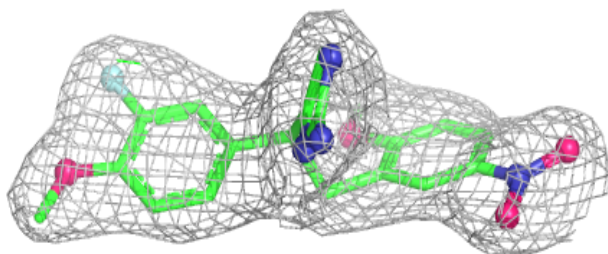
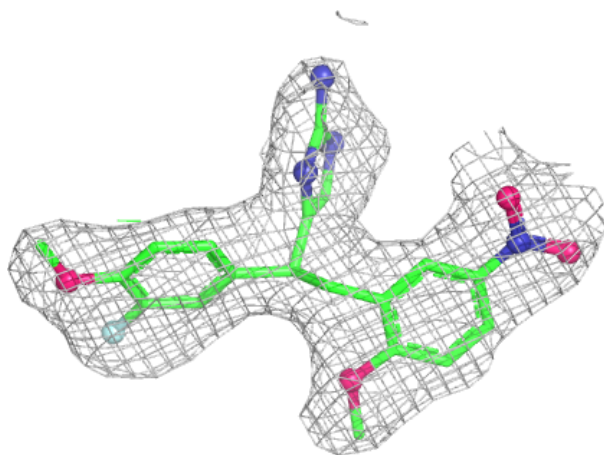
Electron density around B35 C 449:

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



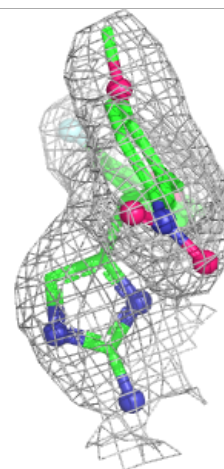
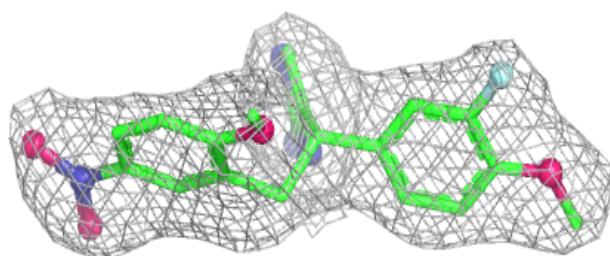
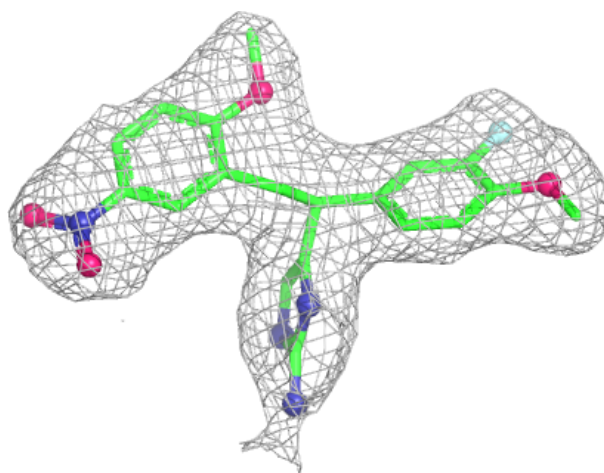
Electron density around B35 B 449:

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



Electron density around B35 A 449:

$2mF_o-DF_c$ (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.