Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2024 – 05:23 AM EDT

PDB ID	:	3ZLQ
Title	:	BACE2 XAPERONE COMPLEX
Authors	:	Kuglstatter, A.; Stihle, M.
Deposited on	:	2013-02-04
Resolution	:	2.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

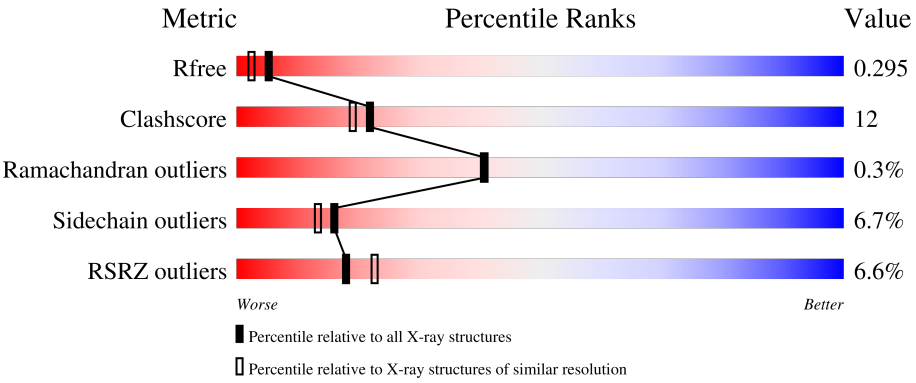
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	386	4% 66% 27% • 5%
1	B	386	11% 72% 21% • •
2	C	122	2% 70% 21% 8%
2	D	122	2% 68% 23% • 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7613 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	1	0
			2843	1827	455	548	13			
1	B	370	Total	C	N	O	S	0	2	0
			2878	1854	459	552	13			

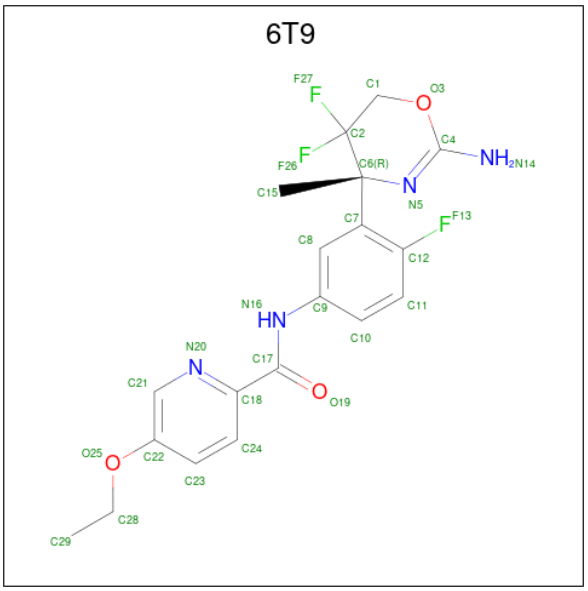
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	269	ALA	GLU	engineered mutation	UNP Q9Y5Z0
B	269	ALA	GLU	engineered mutation	UNP Q9Y5Z0

- Molecule 2 is a protein called XA4813.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	112	Total	C	N	O	S	0	0	0
			833	512	151	166	4			
2	D	112	Total	C	N	O	S	0	1	0
			842	517	153	168	4			

- Molecule 3 is 5-Ethoxy-pyridine-2-carboxylic acid [3-((R)-2-amino-5,5-difluoro-4-methyl-5,6-dihydro-4H-[1,3]oxazin-4-yl)-4-fluoro-phenyl]-amide (three-letter code: 6T9) (formula: $C_{19}H_{19}F_3N_4O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			29	19	3	4	3		
3	B	1	Total	C	F	N	O	0	0
			29	19	3	4	3		

- Molecule 4 is water.

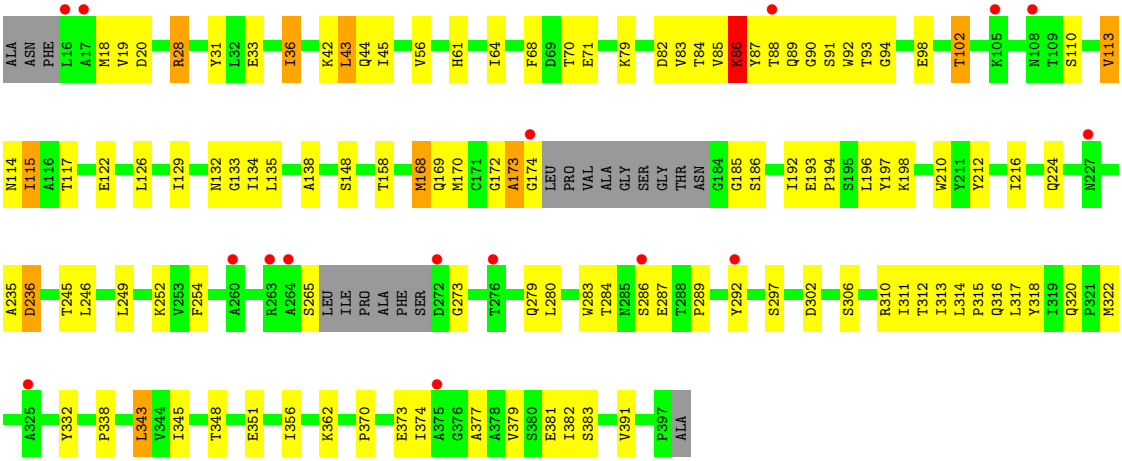
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	74	Total	O	0	0
			74	74		
4	B	51	Total	O	0	0
			51	51		
4	C	16	Total	O	0	0
			16	16		
4	D	18	Total	O	0	0
			18	18		

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.

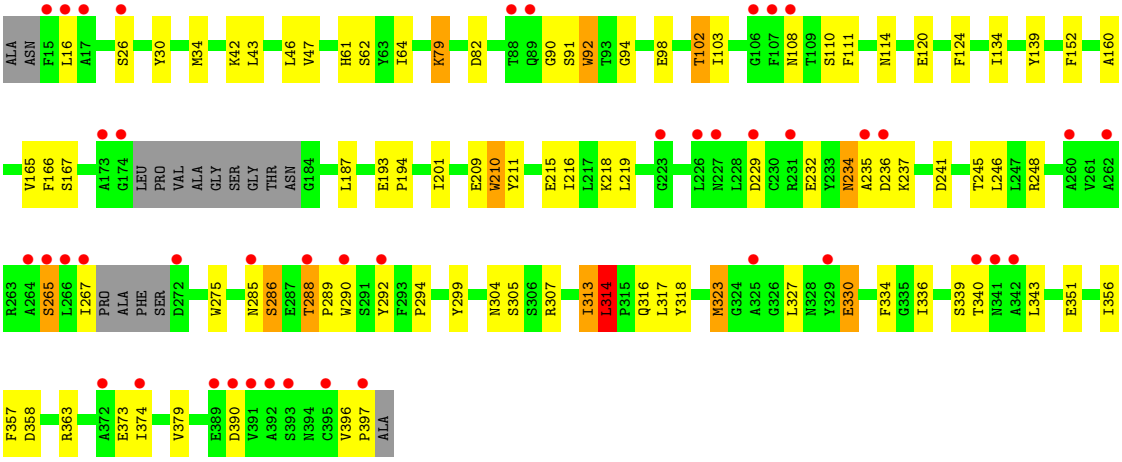
• Molecule 1: BETA-SECRETASE 2

Chain A:



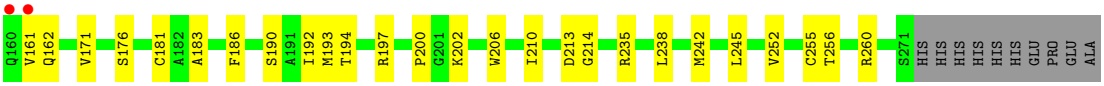
• Molecule 1: BETA-SECRETASE 2

Chain B:



• Molecule 2: XA4813

Chain C:



• Molecule 2: XA4813

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	46.78Å 210.98Å 53.30Å 90.00° 105.07° 90.00°	Depositor
Resolution (Å)	46.26 – 2.10 46.26 – 2.10	Depositor EDS
% Data completeness (in resolution range)	88.6 (46.26-2.10) 88.6 (46.26-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.238 , 0.296 0.236 , 0.295	Depositor DCC
R_{free} test set	2596 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	29.3	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7613	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 6T9

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	0.88	1/2912 (0.0%)	0.97	7/3959 (0.2%)
1	B	0.77	1/2948 (0.0%)	0.92	1/4008 (0.0%)
2	C	0.80	0/847	1.00	3/1146 (0.3%)
2	D	0.86	0/856	0.93	0/1158
All	All	0.83	2/7563 (0.0%)	0.95	11/10271 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	92	TRP	CB-CG	6.83	1.62	1.50
1	A	92	TRP	CB-CG	6.41	1.61	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	310	ARG	NE-CZ-NH2	-8.47	116.06	120.30
1	A	86	LYS	CB-CA-C	-6.19	98.03	110.40
2	C	193	MET	CG-SD-CE	6.17	110.06	100.20
1	A	310	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	28	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	302	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	19	VAL	N-CA-C	-5.71	95.58	111.00
1	A	135	LEU	CB-CG-CD1	-5.43	101.77	111.00
1	B	314	LEU	CA-CB-CG	5.32	127.53	115.30
2	C	213	ASP	CB-CG-OD1	5.22	123.00	118.30
2	C	213	ASP	CB-CG-OD2	-5.08	113.73	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2843	0	2757	73	0
1	B	2878	0	2798	69	1
2	C	833	0	814	14	0
2	D	842	0	821	19	0
3	A	29	0	19	3	0
3	B	29	0	19	4	0
4	A	74	0	0	7	0
4	B	51	0	0	4	0
4	C	16	0	0	0	0
4	D	18	0	0	2	0
All	All	7613	0	7228	174	1

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

All (174) 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:79:LYS:HE2	2:D:190:SER:O	1.59	1.00
3:A:1398:6T9:O19	3:A:1398:6T9:H10	1.71	0.90
2:D:198:GLN:HG2	4:D:2006:HOH:O	1.75	0.84
1:B:26:SER:HB3	1:B:351:GLU:OE2	1.77	0.84
1:A:64:ILE:HG22	4:A:2015:HOH:O	1.82	0.80
1:A:283:TRP:HD1	1:A:287:GLU:OE1	1.63	0.80
1:B:46:LEU:HD23	1:B:134[B]:ILE:HG12	1.63	0.80
1:A:33:GLU:OE2	1:A:42:LYS:HD2	1.82	0.79
1:A:320:GLN:HE22	1:A:348:THR:HG21	1.48	0.78
1:A:245:THR:O	1:A:348:THR:HG23	1.83	0.77
1:B:245:THR:HG22	1:B:246:LEU:HD23	1.65	0.77
1:B:26:SER:HA	3:B:1398:6T9:H292	1.66	0.77
1:B:201:ILE:HD13	1:B:356:ILE:CD1	2.15	0.76
1:A:172:GLY:O	1:A:173:ALA:O	2.03	0.75
1:B:124:PHE:CZ	1:B:134[B]:ILE:HD12	2.23	0.74
2:D:242:MET:HE2	2:D:245:LEU:HD21	1.69	0.73
1:A:79:LYS:HE3	2:C:190:SER:O	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ARG:NH2	4:A:2003:HOH:O	2.23	0.72
1:B:26:SER:HB3	1:B:351:GLU:CD	2.10	0.72
1:B:241:ASP:OD2	3:B:1398:6T9:N14	2.24	0.71
2:D:161:VAL:HB	2:D:260:ARG:HD3	1.72	0.70
1:B:201:ILE:HD13	1:B:356:ILE:HD13	1.73	0.70
1:A:71:GLU:HB3	4:A:2018:HOH:O	1.93	0.68
1:A:283:TRP:CD1	1:A:287:GLU:OE1	2.47	0.68
1:B:79:LYS:CE	2:D:190:SER:O	2.39	0.67
3:B:1398:6T9:O19	3:B:1398:6T9:H10	1.94	0.66
1:B:139:TYR:CZ	1:B:209:GLU:HG2	2.31	0.66
1:A:289:PRO:HD2	4:A:2067:HOH:O	1.96	0.65
1:B:47:VAL:HG21	1:B:187:LEU:HD22	1.78	0.64
1:B:124:PHE:HZ	1:B:134[B]:ILE:HD12	1.62	0.64
1:A:84:THR:HG22	1:A:86:LYS:CE	2.27	0.64
2:D:261:ARG:NH1	2:D:262:GLY:O	2.31	0.64
1:A:82:ASP:HB2	1:A:94:GLY:O	1.98	0.63
2:C:194:THR:HB	2:C:256:THR:HG22	1.80	0.63
1:A:43:LEU:HD11	1:A:68:PHE:HB2	1.79	0.63
1:B:229:ASP:O	1:B:232:GLU:HG2	1.99	0.63
1:B:61:HIS:HB3	1:B:64:ILE:HG12	1.79	0.63
1:B:111:PHE:CE1	1:B:160:ALA:HB2	2.33	0.63
1:B:248:ARG:HH12	1:B:339:SER:HA	1.64	0.63
2:C:210:ILE:HD11	2:C:214:GLY:HA2	1.81	0.63
1:B:305:SER:HB3	4:B:2044:HOH:O	2.00	0.62
1:A:198:LYS:NZ	4:A:2053:HOH:O	2.12	0.62
1:B:82:ASP:HB2	1:B:94:GLY:O	1.99	0.62
1:A:314:LEU:HB3	1:A:315:PRO:HD2	1.82	0.61
2:D:198:GLN:NE2	2:D:202:LYS:O	2.32	0.61
1:B:30:TYR:OH	1:B:351:GLU:OE2	2.16	0.60
2:D:250:THR:O	2:D:251:ALA:HB2	2.02	0.60
1:B:193:GLU:OE2	1:B:194:PRO:HD2	2.03	0.59
1:A:56:VAL:HG13	1:A:115:ILE:HD11	1.84	0.58
1:A:316:GLN:HG2	1:A:374:ILE:HD12	1.85	0.58
1:B:290:TRP:CE3	1:B:316:GLN:HG3	2.39	0.58
1:B:165:VAL:HG13	1:B:358:ASP:HA	1.84	0.58
1:B:313:ILE:HB	1:B:317:LEU:HD12	1.86	0.57
3:B:1398:6T9:H152	3:B:1398:6T9:F13	1.94	0.57
1:A:45:ILE:CD1	1:A:133:GLY:HA3	2.34	0.57
1:B:61:HIS:ND1	1:B:62:SER:N	2.53	0.57
1:B:286:SER:C	1:B:288:THR:H	2.08	0.57
2:C:161:VAL:HB	2:C:260:ARG:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:242:MET:HE2	2:C:245:LEU:HD21	1.87	0.56
1:A:68:PHE:CE2	1:A:70:THR:HG22	2.42	0.55
1:B:79:LYS:HE3	1:B:98:GLU:OE2	2.06	0.55
3:A:1398:6T9:O19	3:A:1398:6T9:C10	2.35	0.55
1:A:31:TYR:CD2	1:A:44[B]:GLN:HB3	2.42	0.54
1:A:84:THR:HG22	1:A:86:LYS:HE2	1.89	0.54
1:B:34:MET:HE1	1:B:152:PHE:CE2	2.43	0.54
1:B:139:TYR:CE1	1:B:209:GLU:HG2	2.42	0.54
2:C:235:ARG:HG3	2:C:235:ARG:HH11	1.72	0.54
1:A:174:GLY:HA2	1:A:374:ILE:HD13	1.89	0.54
1:B:265:SER:HB3	1:B:292:TYR:O	2.08	0.54
1:B:290:TRP:CD2	1:B:316:GLN:HG3	2.42	0.54
1:B:316:GLN:HB3	1:B:374:ILE:HD12	1.89	0.54
1:A:88:THR:HB	1:A:89:GLN:OE1	2.07	0.54
1:A:84:THR:CG2	1:A:86:LYS:HE2	2.38	0.54
1:A:345:ILE:HG22	1:A:345:ILE:O	2.08	0.53
2:C:238:LEU:HD23	2:C:255:CYS:HB2	1.91	0.53
1:A:43:LEU:HD23	1:A:132:ASN:ND2	2.24	0.52
1:A:45:ILE:HD12	1:A:133:GLY:HA3	1.90	0.52
1:B:210:TRP:CD1	1:B:211:TYR:N	2.78	0.52
2:C:161:VAL:HB	2:C:260:ARG:CD	2.40	0.52
1:B:201:ILE:HD13	1:B:356:ILE:HD11	1.89	0.52
1:A:102:THR:HG22	1:A:110:SER:HB3	1.92	0.51
1:B:314:LEU:HG	1:B:379:VAL:C	2.30	0.51
1:B:103:ILE:HD11	1:B:152:PHE:HZ	1.75	0.51
1:A:70:THR:CG2	1:A:117:THR:HG21	2.40	0.51
2:D:194:THR:HG23	2:D:209:THR:OG1	2.11	0.51
2:D:199:ALA:HB3	2:D:202:LYS:HB2	1.92	0.51
1:A:36:ILE:HG13	1:A:43:LEU:CD1	2.41	0.51
1:B:234:ASN:HB3	4:B:2038:HOH:O	2.11	0.50
1:A:317:LEU:HD22	1:A:351:GLU:HG3	1.94	0.50
1:A:98:GLU:HG2	2:C:192:ILE:HD11	1.93	0.50
1:B:218:LYS:HB3	1:B:299:TYR:HB2	1.93	0.50
1:B:46:LEU:CD2	1:B:134[B]:ILE:HG12	2.38	0.49
1:A:83:VAL:O	1:A:93:THR:HA	2.12	0.49
1:B:134[A]:ILE:HG23	1:B:134[A]:ILE:O	2.12	0.49
1:B:267:ILE:HB	1:B:275:TRP:CZ2	2.48	0.49
1:B:294:PRO:HD2	1:B:318:TYR:OH	2.14	0.48
1:A:169:GLN:OE1	1:A:196:LEU:HD22	2.13	0.48
1:A:235:ALA:HA	1:A:236:ASP:HA	1.54	0.48
1:A:312:THR:HB	1:A:381:GLU:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:ASN:O	1:B:288:THR:HG23	2.14	0.47
1:A:56:VAL:HG21	1:A:68:PHE:HB3	1.96	0.47
1:A:192:ILE:HD11	1:A:356:ILE:HG21	1.96	0.47
1:B:103:ILE:HD11	1:B:152:PHE:CZ	2.50	0.47
1:B:215:GLU:HG3	1:B:396:VAL:HG23	1.97	0.47
2:D:161:VAL:HB	2:D:260:ARG:CD	2.43	0.47
1:B:234:ASN:O	1:B:397:PRO:HD2	2.15	0.47
2:C:242:MET:CE	2:C:245:LEU:HD21	2.45	0.47
1:A:297:SER:OG	1:A:312:THR:OG1	2.28	0.47
1:B:90:GLY:O	1:B:91:SER:HB3	2.14	0.46
1:A:374:ILE:HG13	1:A:379:VAL:HG11	1.96	0.46
1:B:98:GLU:OE2	2:D:212:SER:HB3	2.14	0.46
1:A:158:THR:O	2:C:206:TRP:HB2	2.16	0.46
1:B:166:PHE:CE1	1:B:357:PHE:CD2	3.04	0.46
1:A:61:HIS:HB3	1:A:64:ILE:HG12	1.97	0.46
1:A:90:GLY:O	1:A:91:SER:HB3	2.16	0.46
1:B:323:MET:HG3	1:B:330:GLU:OE1	2.16	0.46
1:A:273:GLY:HA3	1:A:279:GLN:OE1	2.16	0.45
1:A:168:MET:HA	1:A:186:SER:O	2.16	0.45
1:B:267:ILE:HB	1:B:275:TRP:HZ2	1.80	0.45
1:B:16:LEU:HD23	1:B:16:LEU:O	2.16	0.45
1:A:235:ALA:HB3	4:A:2060:HOH:O	2.15	0.45
1:A:320:GLN:NE2	1:A:348:THR:HG21	2.24	0.45
1:A:280:LEU:HD13	1:A:322:MET:HG3	1.98	0.45
1:A:320:GLN:O	1:A:332:TYR:HA	2.16	0.45
1:A:374:ILE:HG13	1:A:379:VAL:CG1	2.47	0.45
1:A:284:THR:O	1:A:287:GLU:HB2	2.17	0.44
1:B:167:SER:HB3	4:B:2033:HOH:O	2.16	0.44
1:B:288:THR:HA	1:B:289:PRO:HD2	1.67	0.44
1:A:113:VAL:HG23	1:A:114:ASN:O	2.18	0.44
1:A:265:SER:CB	1:A:292:TYR:O	2.65	0.44
1:B:79:LYS:NZ	1:B:114:ASN:OD1	2.51	0.44
1:B:248:ARG:NH1	1:B:339:SER:HA	2.30	0.44
1:A:20:ASP:HA	1:A:185:GLY:O	2.18	0.44
1:A:193:GLU:HA	1:A:194:PRO:HD2	1.82	0.43
2:D:161:VAL:HG13	2:D:186:PHE:CE1	2.53	0.43
1:A:31:TYR:HD2	1:A:44[B]:GLN:HB3	1.81	0.43
1:A:246:LEU:HD12	4:A:2063:HOH:O	2.18	0.43
1:B:216:ILE:CD1	1:B:343:LEU:HD22	2.48	0.43
2:D:161:VAL:HA	2:D:186:PHE:CD1	2.53	0.43
1:A:174:GLY:HA2	1:A:374:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:TRP:CG	1:B:211:TYR:N	2.84	0.43
1:B:334:PHE:CE2	1:B:336:ILE:HB	2.54	0.43
2:C:197:ARG:HA	2:C:252:VAL:O	2.17	0.43
1:A:197:TYR:HA	1:A:370:PRO:HD2	2.00	0.43
1:A:216:ILE:CD1	1:A:343:LEU:HD22	2.48	0.43
2:C:183:ALA:HB1	2:C:186:PHE:CE1	2.54	0.43
1:A:84:THR:HG22	1:A:86:LYS:HE3	1.99	0.43
1:A:313:ILE:HD12	1:A:318:TYR:HB3	2.00	0.42
1:A:85:VAL:O	1:A:91:SER:HB2	2.20	0.42
1:B:330:GLU:OE1	1:B:330:GLU:HA	2.20	0.42
2:D:165:GLU:HA	2:D:180:SER:O	2.20	0.42
1:A:138:ALA:HA	1:A:212:TYR:CE2	2.55	0.42
1:B:290:TRP:CE2	1:B:316:GLN:HA	2.55	0.42
2:D:196:VAL:HG12	2:D:206:TRP:HA	2.00	0.42
2:C:235:ARG:HG3	2:C:235:ARG:NH1	2.34	0.42
1:A:33:GLU:HG3	1:A:44[A]:GLN:HE22	1.83	0.42
1:B:285:ASN:O	1:B:288:THR:CG2	2.68	0.42
1:A:126:LEU:O	1:A:129:ILE:HG12	2.20	0.41
2:D:184:SER:HB3	4:D:2004:HOH:O	2.18	0.41
1:B:46:LEU:HB3	1:B:134[B]:ILE:HG12	2.03	0.41
1:B:216:ILE:HD12	1:B:343:LEU:HD22	2.02	0.41
1:B:235:ALA:HA	1:B:236:ASP:HA	1.82	0.41
1:B:356:ILE:HG23	4:B:2033:HOH:O	2.19	0.41
1:A:170:MET:HB2	1:A:351:GLU:HA	2.03	0.41
2:D:227:PHE:HB3	2:D:240:LEU:HD11	2.01	0.41
1:A:249:LEU:HD23	1:A:343:LEU:HG	2.02	0.41
1:B:42:LYS:C	1:B:43:LEU:HD12	2.41	0.41
2:D:242:MET:HE1	2:D:267:VAL:HG11	2.02	0.41
1:A:311:ILE:HG22	1:A:382:ILE:HD12	2.03	0.41
1:A:348:THR:HA	1:A:351:GLU:OE2	2.22	0.40
1:A:373:GLU:HA	1:A:377:ALA:O	2.22	0.40
1:B:102:THR:HG22	1:B:110:SER:HB3	2.02	0.40
1:A:254:PHE:CE2	1:A:338:PRO:HG3	2.56	0.40
3:A:1398:6T9:H152	3:A:1398:6T9:F13	2.11	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:GLU:OE2	1:B:363:ARG:NH2[1_455]	2.10	0.10

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	362/386 (94%)	338 (93%)	23 (6%)	1 (0%)	41 41
1	B	366/386 (95%)	343 (94%)	21 (6%)	2 (0%)	29 26
2	C	110/122 (90%)	105 (96%)	5 (4%)	0	100 100
2	D	111/122 (91%)	106 (96%)	5 (4%)	0	100 100
All	All	949/1016 (93%)	892 (94%)	54 (6%)	3 (0%)	41 41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	ALA
1	B	265	SER
1	B	288	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	307/319 (96%)	285 (93%)	22 (7%)	14 11
1	B	311/319 (98%)	292 (94%)	19 (6%)	18 16
2	C	90/99 (91%)	84 (93%)	6 (7%)	16 13
2	D	91/99 (92%)	84 (92%)	7 (8%)	13 9
All	All	799/836 (96%)	745 (93%)	54 (7%)	16 13

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	MET
1	A	36	ILE
1	A	43	LEU
1	A	86	LYS
1	A	87	TYR
1	A	102	THR
1	A	113	VAL
1	A	115	ILE
1	A	122	GLU
1	A	134	ILE
1	A	148	SER
1	A	168	MET
1	A	210	TRP
1	A	224	GLN
1	A	236	ASP
1	A	252	LYS
1	A	286	SER
1	A	306	SER
1	A	343	LEU
1	A	362	LYS
1	A	383	SER
1	A	391	VAL
1	B	79	LYS
1	B	92	TRP
1	B	102	THR
1	B	108	ASN
1	B	210	TRP
1	B	219	LEU
1	B	234	ASN
1	B	237	LYS
1	B	286	SER
1	B	304	ASN
1	B	307	ARG
1	B	313	ILE
1	B	314	LEU
1	B	323	MET
1	B	327	LEU
1	B	330	GLU
1	B	340	THR
1	B	373	GLU
1	B	390	ASP
2	C	162	GLN
2	C	171	VAL

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Mol	Chain	Res	Type
2	C	176	SER
2	C	181	CYS
2	C	200	PRO
2	C	202	LYS
2	D	162[A]	GLN
2	D	162[B]	GLN
2	D	176	SER
2	D	178	ARG
2	D	224	LYS
2	D	257	SER
2	D	260	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	B	108	ASN
1	B	224	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
3	6T9	A	1398	-	27,31,31	1.11	1 (3%)	36,46,46	1.91	11 (30%)
3	6T9	B	1398	-	27,31,31	1.08	2 (7%)	36,46,46	1.78	9 (25%)

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
3	6T9	A	1398	-	-	2/16/37/37	0/3/3/3
3	6T9	B	1398	-	-	1/16/37/37	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1398	6T9	C8-C7	-3.55	1.34	1.39
3	A	1398	6T9	C8-C7	-2.49	1.35	1.39
3	B	1398	6T9	C21-N20	-2.26	1.29	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1398	6T9	C15-C6-N5	4.80	113.57	108.81
3	A	1398	6T9	C22-C21-N20	-4.37	117.28	122.67
3	A	1398	6T9	F27-C2-F26	4.17	113.95	105.43
3	B	1398	6T9	C21-N20-C18	3.66	123.19	117.46
3	A	1398	6T9	C9-N16-C17	-3.63	117.06	126.61
3	B	1398	6T9	C22-C21-N20	-3.23	118.69	122.67
3	A	1398	6T9	F26-C2-C6	-3.04	101.81	109.87
3	B	1398	6T9	C17-C18-N20	-2.97	113.95	117.42
3	A	1398	6T9	C23-C22-C21	2.84	122.47	119.75
3	A	1398	6T9	C21-N20-C18	2.73	121.73	117.46
3	A	1398	6T9	C8-C7-C12	2.64	120.46	116.82
3	A	1398	6T9	O3-C4-N14	2.61	115.55	111.61
3	B	1398	6T9	C24-C18-C17	2.61	123.80	119.57
3	A	1398	6T9	C23-C24-C18	-2.59	115.24	118.89
3	B	1398	6T9	O3-C4-N14	2.57	115.49	111.61
3	A	1398	6T9	C15-C6-N5	2.43	111.22	108.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1398	6T9	C8-C7-C12	2.40	120.14	116.82
3	A	1398	6T9	C11-C12-C7	-2.28	120.45	123.46
3	B	1398	6T9	C10-C9-C8	2.27	122.40	119.66
3	B	1398	6T9	C23-C24-C18	-2.07	115.97	118.89

There are no chirality outliers.

All (3) torsion outliers are listed below:

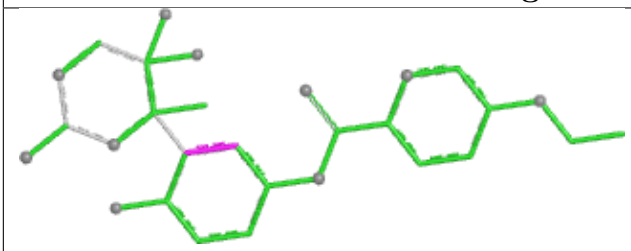
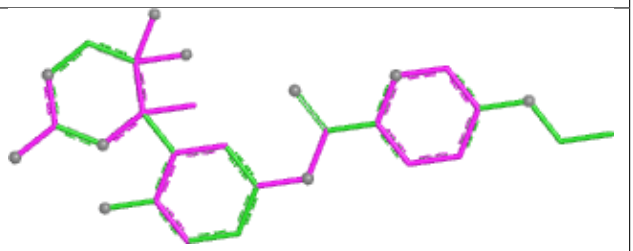
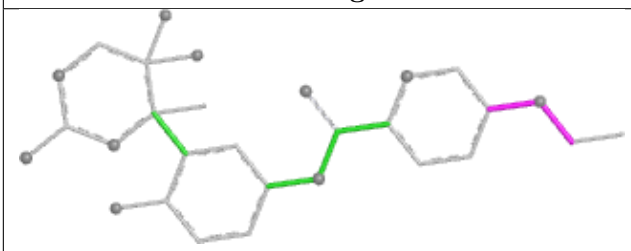
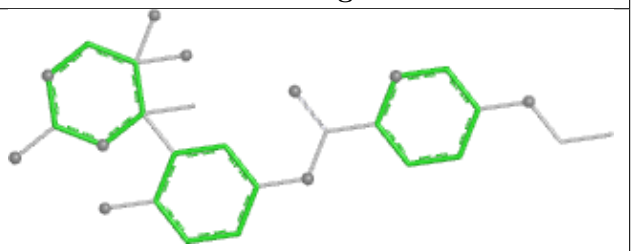
Mol	Chain	Res	Type	Atoms
3	A	1398	6T9	C29-C28-O25-C22
3	B	1398	6T9	C29-C28-O25-C22
3	A	1398	6T9	C23-C22-O25-C28

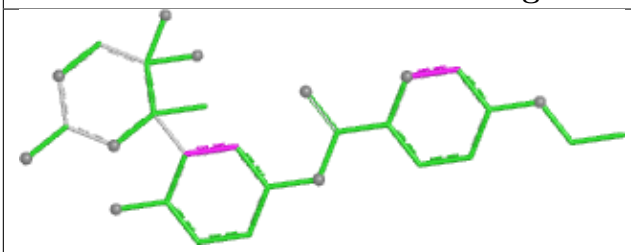
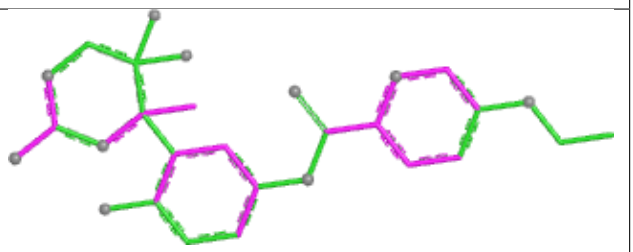
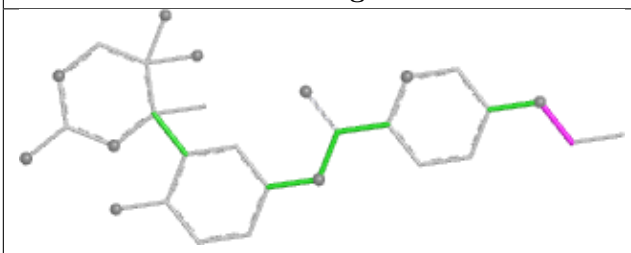
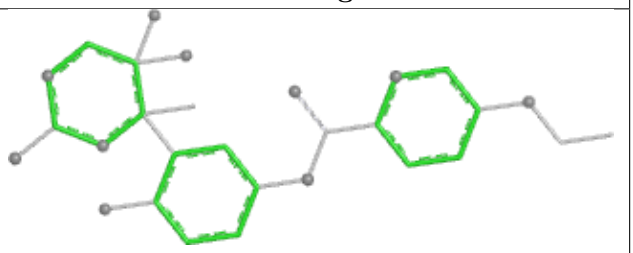
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1398	6T9	3	0
3	B	1398	6T9	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 6T9 A 1398	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 6T9 B 1398	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	367/386 (95%)	0.46	16 (4%) 34 40	15, 26, 48, 58	11 (2%)
1	B	370/386 (95%)	0.75	43 (11%) 4 6	16, 30, 60, 85	12 (3%)
2	C	112/122 (91%)	0.28	2 (1%) 68 72	16, 25, 42, 66	3 (2%)
2	D	112/122 (91%)	0.18	2 (1%) 68 72	16, 25, 40, 57	1 (0%)
All	All	961/1016 (94%)	0.52	63 (6%) 18 23	15, 27, 53, 85	27 (2%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	88	THR	5.2
1	A	227	ASN	4.9
1	A	88	THR	4.7
1	B	227	ASN	4.6
1	B	390	ASP	4.3
1	B	292	TYR	4.2
1	A	264	ALA	4.1
1	B	226	LEU	4.1
1	B	235	ALA	4.0
1	A	16	LEU	3.9
1	B	236	ASP	3.9
2	D	201	GLY	3.9
1	B	265	SER	3.8
1	B	15	PHE	3.8
1	B	266	LEU	3.7
1	B	395	CYS	3.7
1	B	393	SER	3.5
2	D	161	VAL	3.5
1	B	89	GLN	3.3
1	B	342	ALA	3.2
1	A	263	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	325	ALA	3.1
1	B	26	SER	3.0
1	A	17	ALA	3.0
1	B	267	ILE	3.0
1	B	231	ARG	2.9
1	A	375	ALA	2.9
1	B	17	ALA	2.8
1	B	329	TYR	2.8
1	B	223	GLY	2.7
1	B	391	VAL	2.7
1	B	374	ILE	2.7
1	A	105	LYS	2.6
1	A	108	ASN	2.6
1	B	285	ASN	2.6
1	B	260	ALA	2.5
1	B	397	PRO	2.5
1	B	372	ALA	2.5
1	B	392	ALA	2.5
2	C	161	VAL	2.4
1	B	106	GLY	2.4
1	B	262	ALA	2.4
1	B	272	ASP	2.3
1	B	341	ASN	2.3
1	A	174	GLY	2.3
1	A	325	ALA	2.3
1	B	108	ASN	2.3
1	B	290	TRP	2.3
1	B	229	ASP	2.2
1	A	272	ASP	2.2
1	B	16	LEU	2.2
1	B	107	PHE	2.2
1	B	288	THR	2.2
1	A	292	TYR	2.1
1	B	174	GLY	2.1
1	B	340	THR	2.1
1	A	276	THR	2.1
1	B	389	GLU	2.1
1	A	286	SER	2.1
1	B	173	ALA	2.0
1	A	260	ALA	2.0
1	B	264	ALA	2.0
2	C	160	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

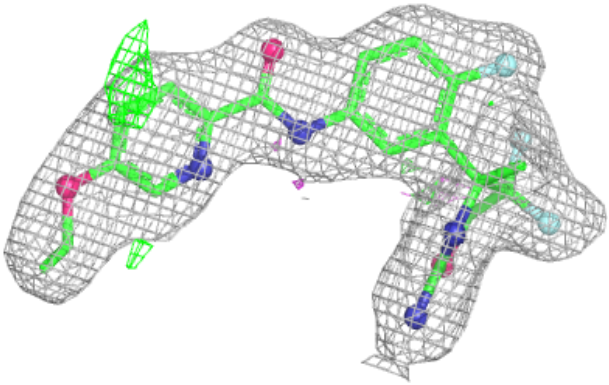
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

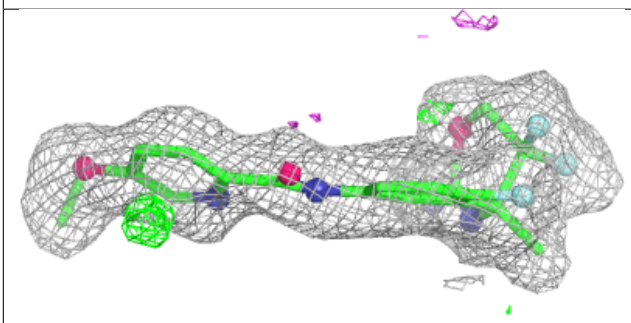
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	6T9	A	1398	29/29	0.93	0.14	19,24,27,30	0
3	6T9	B	1398	29/29	0.93	0.14	24,26,31,33	0

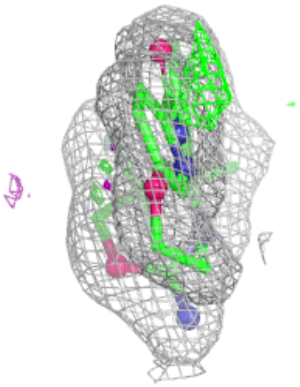
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 6T9 A 1398:

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

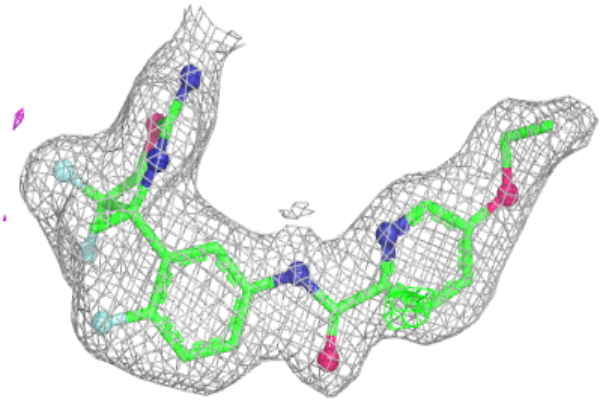


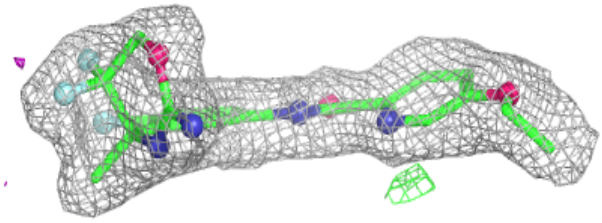


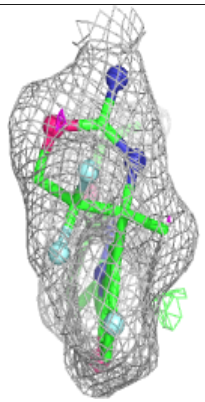


Electron density around 6T9 B 1398:

$2mF_o$-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.