



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:53 PM UTC

PDB ID : 3ZKN / pdb_00003zkn
Title : BACE2 FAB INHIBITOR COMPLEX
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Deposited on : 2013-01-23
Resolution : 2.00 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

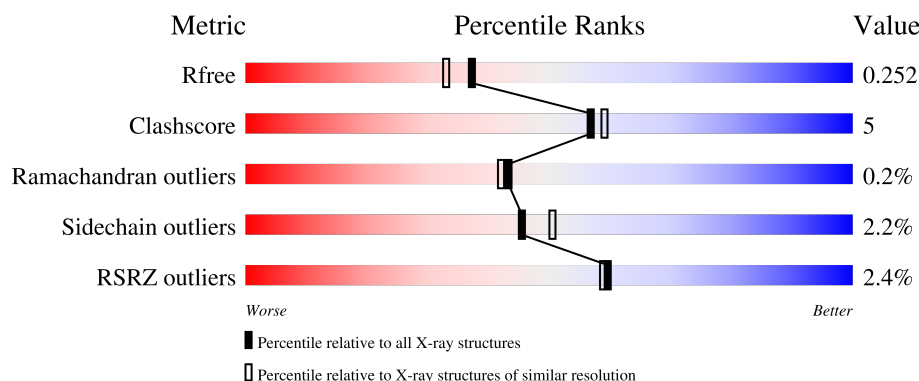
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	386	4% 81% 15% ..
1	B	386	3% 85% 12% ..
2	C	221	% 88% 10% .
2	H	221	% 90% 8% .
3	D	218	2% 89% 11%

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Mol	Chain	Length	Quality of chain
3	L	218	 92% 7%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13474 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	375	Total	C	N	O	S	0	4	0
			2942	1895	469	565	13			
1	B	375	Total	C	N	O	S	0	2	0
			2928	1888	466	561	13			

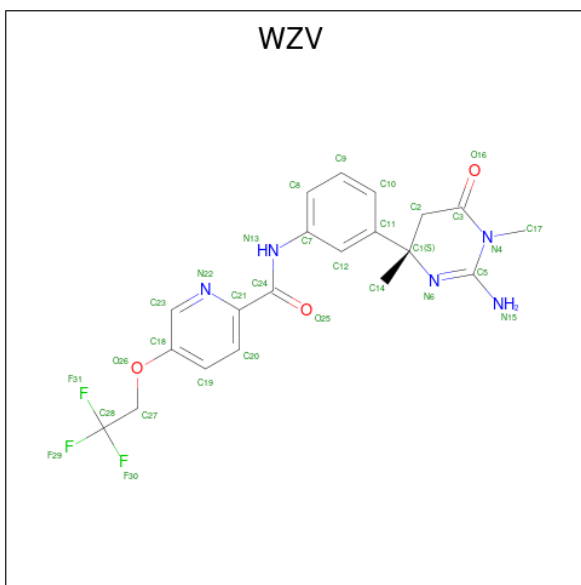
- Molecule 2 is a protein called FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	217	Total	C	N	O	S	0	1	1
			1640	1041	271	320	8			
2	H	217	Total	C	N	O	S	0	1	1
			1640	1041	271	320	8			

- Molecule 3 is a protein called FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	217	Total	C	N	O	S	0	2	0
			1688	1047	291	343	7			
3	L	217	Total	C	N	O	S	0	1	0
			1682	1044	290	342	6			

- Molecule 4 is 5-(2,2,2-Trifluoro-ethoxy)-pyridine-2-carboxylic acid [3-((S)-2-amino-1,4-dimethyl-6-oxo-1,4,5,6-tetrahydro-pyrimidin-4-yl)-phenyl]-amide (CCD ID: WZV) (formula: C₂₀H₂₀F₃N₅O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			31	20	3	5	3		
4	B	1	Total	C	F	N	O	0	0
			31	20	3	5	3		

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			6	3	3		
7	H	1	Total	C	O	0	0
			6	3	3		

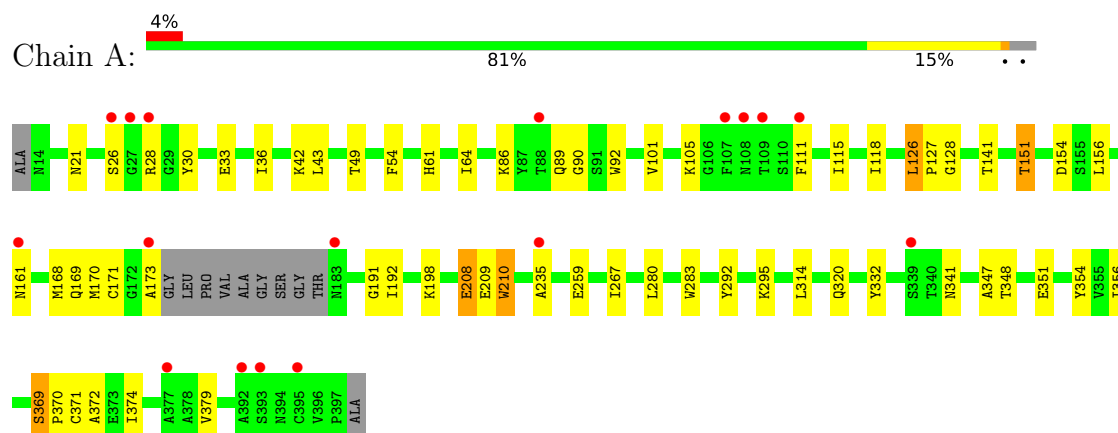
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	159	Total	O	0	0
			159	159		
8	B	161	Total	O	0	0
			161	161		
8	C	138	Total	O	0	0
			138	138		
8	D	126	Total	O	0	0
			126	126		
8	H	135	Total	O	0	0
			135	135		
8	L	123	Total	O	0	0
			123	123		

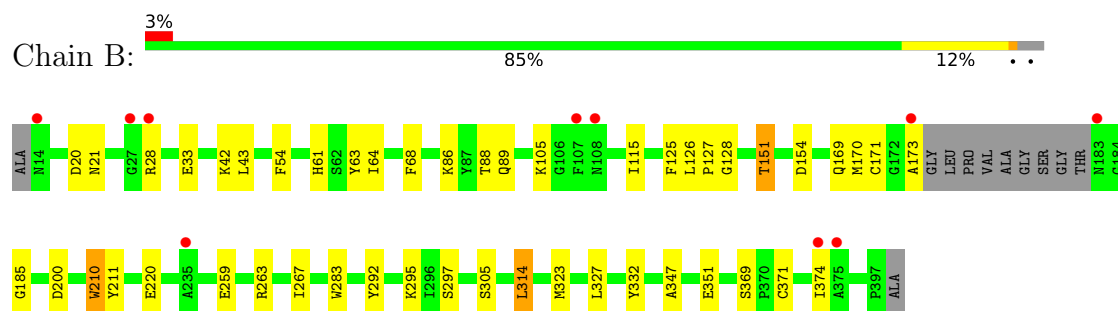
3 Residue-property plots [i](#)

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.

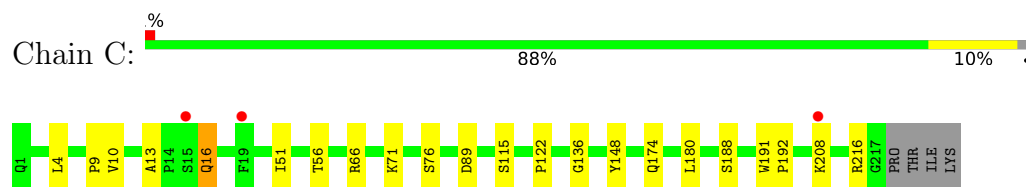
• Molecule 1: BETA-SECRETASE 2



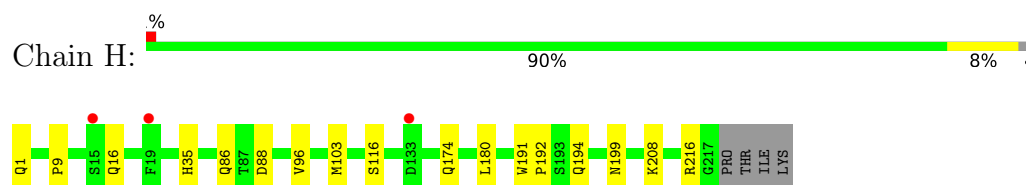
• Molecule 1: BETA-SECRETASE 2



• Molecule 2: FAB HEAVY CHAIN

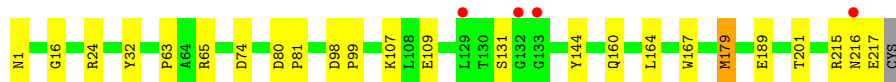


• Molecule 2: FAB HEAVY CHAIN



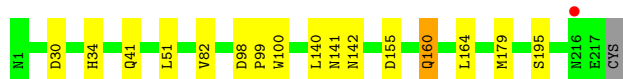
● Molecule 3: FAB LIGHT CHAIN

Chain D:  2% 89% 11%



● Molecule 3: FAB LIGHT CHAIN

Chain L:  92% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.93Å 68.14Å 160.85Å 90.00° 92.51° 90.00°	Depositor
Resolution (Å)	45.75 – 2.00 45.75 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.7 (45.75-2.00) 95.8 (45.75-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0027	Depositor
R, R_{free}	0.203 , 0.251 0.203 , 0.252	Depositor DCC
R_{free} test set	5999 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.098 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13474	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, WZV, DMS, GOL, PCA

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	0.62	0/3017	0.85	3/4106 (0.1%)
1	B	0.64	0/3003	0.88	1/4087 (0.0%)
2	C	0.74	1/1675 (0.1%)	0.87	0/2291
2	H	0.75	1/1675 (0.1%)	0.87	0/2291
3	D	0.69	0/1728	0.84	0/2351
3	L	0.68	0/1722	0.85	0/2343
All	All	0.68	2/12820 (0.0%)	0.86	4/17469 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	216	ARG	C-N	-6.71	1.24	1.33
2	H	216	ARG	C-N	-6.65	1.24	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	GLY	N-CA-C	5.49	117.99	110.58
1	B	305	SER	N-CA-C	5.35	117.80	111.33
1	A	341	ASN	N-CA-C	5.18	119.06	112.12
1	A	90	GLY	N-CA-C	5.03	117.89	110.80

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	2942	0	2848	43	0
1	B	2928	0	2839	30	0
2	C	1640	0	1611	12	0
2	H	1640	0	1611	7	1
3	D	1688	0	1599	14	0
3	L	1682	0	1596	10	0
4	A	31	0	20	3	0
4	B	31	0	20	2	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0
6	A	10	0	0	0	0
6	B	10	0	0	0	0
6	C	5	0	0	0	0
6	H	5	0	0	0	0
7	C	6	0	8	0	0
7	H	6	0	8	0	0
8	A	159	0	0	3	0
8	B	161	0	0	5	0
8	C	138	0	0	1	2
8	D	126	0	0	3	0
8	H	135	0	0	1	1
8	L	123	0	0	0	0
All	All	13474	0	12172	111	2

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 5.

All (111) 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:89:GLN:HB2	4:B:1398:WZV:H23	1.39	1.03
1:A:171:CYS:HG	1:A:371:CYS:HG	1.03	1.01
1:B:151:THR:HG21	8:B:2061:HOH:O	1.59	1.00
1:A:169:GLN:HE21	1:A:369:SER:HB3	1.27	0.96
1:A:170:MET:HE1	1:A:347:ALA:HB1	1.48	0.93
1:A:151:THR:HG22	1:A:154:ASP:H	1.33	0.93
1:A:126:LEU:HD11	4:A:1398:WZV:H19	1.52	0.92
1:B:126:LEU:HD11	4:B:1398:WZV:H19	1.54	0.89
1:A:89:GLN:HB2	4:A:1398:WZV:H23	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:CYS:HG	1:B:371:CYS:HG	0.94	0.86
2:C:174:GLN:HE21	3:D:164:LEU:HD21	1.44	0.82
1:B:28:ARG:HE	1:B:128:GLY:HA3	1.44	0.81
1:A:151:THR:HG21	8:A:2059:HOH:O	1.85	0.76
1:A:170:MET:HE1	1:A:347:ALA:CB	2.18	0.74
2:H:174:GLN:HE21	3:L:164:LEU:HD21	1.54	0.73
1:A:151:THR:HG23	8:A:2058:HOH:O	1.91	0.70
1:A:30:TYR:CE1	1:A:170:MET:HE3	2.27	0.70
1:A:169:GLN:NE2	1:A:369:SER:HB3	2.06	0.70
1:A:61:HIS:HB3	1:A:64:ILE:HG12	1.72	0.69
1:B:151:THR:HG22	1:B:154:ASP:H	1.55	0.69
1:A:170:MET:CE	1:A:347:ALA:HB1	2.22	0.67
3:L:140:LEU:HD13	3:L:179:MET:HE2	1.76	0.67
1:A:126:LEU:CD1	4:A:1398:WZV:H19	2.26	0.64
3:D:109:GLU:OE2	3:D:144:TYR:OH	2.14	0.62
1:B:151:THR:HG23	8:B:2060:HOH:O	1.99	0.62
1:B:169:GLN:HE21	1:B:369:SER:HB3	1.66	0.60
1:A:170:MET:HE2	1:A:351:GLU:HG3	1.83	0.60
1:A:161[B]:ASN:O	1:A:161[B]:ASN:CG	2.46	0.59
2:C:9:PRO:HG3	8:C:2013:HOH:O	2.04	0.57
3:D:1:ASN:HA	8:D:2001:HOH:O	2.03	0.57
1:A:33:GLU:CD	1:A:42:LYS:HD2	2.30	0.57
1:B:295:LYS:HG2	1:B:314:LEU:HD22	1.87	0.55
1:A:26:SER:HB3	1:A:351:GLU:OE2	2.06	0.55
1:A:36:ILE:HG12	1:A:101:VAL:HG22	1.88	0.54
2:H:9:PRO:HG3	8:H:2013:HOH:O	2.08	0.53
1:B:33:GLU:CD	1:B:42:LYS:HD2	2.33	0.53
3:D:131:SER:HB2	8:D:2090:HOH:O	2.07	0.53
2:H:86:GLN:HG3	2:H:88:ASP:OD1	2.09	0.53
2:C:13:ALA:O	2:C:16:GLN:HB2	2.08	0.53
2:C:51:ILE:HD13	2:C:71:LYS:HG2	1.90	0.53
1:B:63:TYR:HD2	1:B:125:PHE:O	1.91	0.52
1:A:30:TYR:HE1	1:A:170:MET:HE3	1.74	0.52
1:B:88:THR:HG22	1:B:89:GLN:HG3	1.91	0.52
1:A:192:ILE:HG23	1:A:354:TYR:HE2	1.75	0.52
1:A:283:TRP:HH2	1:A:292:TYR:HE2	1.58	0.51
2:C:122:PRO:HB3	2:C:148:TYR:HB3	1.92	0.51
1:A:28:ARG:HE	1:A:128:GLY:HA3	1.76	0.51
1:B:54:PHE:CE2	1:B:115:ILE:HD12	2.45	0.51
1:A:42:LYS:O	1:A:43[A]:LEU:HD23	2.10	0.51
1:B:169:GLN:NE2	1:B:369:SER:HB3	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ALA:HB3	8:A:2094:HOH:O	2.10	0.49
1:B:28:ARG:HB2	8:B:2003:HOH:O	2.11	0.49
1:A:49:THR:CG2	1:A:168:MET:HE1	2.42	0.49
1:B:332:TYR:HB2	3:D:32:TYR:OH	2.13	0.49
2:C:136:GLY:O	2:C:188:SER:HB3	2.12	0.49
1:B:170:MET:HE1	1:B:347:ALA:HB1	1.97	0.47
1:B:210:TRP:CG	1:B:211:TYR:H	2.33	0.47
2:C:174:GLN:HG2	3:D:164:LEU:HD11	1.97	0.47
2:C:51:ILE:CD1	2:C:71:LYS:HG2	2.44	0.46
2:H:96:VAL:HG12	2:H:103:MET:HB3	1.97	0.46
3:L:41:GLN:HB2	3:L:51:LEU:HD11	1.97	0.46
1:A:21:ASN:HA	1:A:105:LYS:HD3	1.97	0.46
3:L:30:ASP:HA	3:L:34:HIS:O	2.15	0.46
1:B:61:HIS:HB3	1:B:64:ILE:HG12	1.98	0.46
1:A:283:TRP:CH2	1:A:292:TYR:HE2	2.33	0.45
1:B:151:THR:CG2	8:B:2061:HOH:O	2.37	0.45
1:A:320:GLN:O	1:A:332:TYR:HA	2.16	0.45
1:B:63:TYR:CE2	1:B:127:PRO:HD3	2.51	0.45
1:B:173:ALA:O	1:B:374:ILE:HD11	2.16	0.45
1:B:323:MET:HB3	1:B:327:LEU:HD12	1.99	0.45
3:D:167:TRP:CD2	3:D:179:MET:HG3	2.52	0.45
3:D:24:ARG:NE	3:D:74:ASP:OD1	2.50	0.45
8:B:2124:HOH:O	2:C:56:THR:HG21	2.16	0.45
1:A:198:LYS:HD2	1:A:370:PRO:HG3	1.98	0.44
2:C:66:ARG:HH22	2:C:89:ASP:CG	2.25	0.44
1:A:111:PHE:CZ	1:A:156:LEU:HD13	2.53	0.44
3:D:215:ARG:C	3:D:217:GLU:H	2.26	0.43
2:H:96:VAL:CG1	2:H:103:MET:HB3	2.48	0.43
2:H:191:TRP:CG	2:H:192:PRO:HA	2.53	0.43
1:A:54:PHE:CE2	1:A:115:ILE:HD12	2.52	0.43
1:B:21:ASN:HA	1:B:105:LYS:HD3	2.00	0.43
3:L:155:ASP:HA	3:L:195:SER:OG	2.18	0.43
3:D:107:LYS:NZ	8:D:2067:HOH:O	2.51	0.43
3:L:141:ASN:HB3	3:L:142:ASN:HD22	1.83	0.43
1:A:372:ALA:O	1:A:379:VAL:HG22	2.19	0.43
3:D:80:ASP:HA	3:D:81:PRO:HA	1.94	0.43
1:B:43[A]:LEU:HD11	1:B:68:PHE:HB2	2.01	0.43
2:C:4:LEU:HD12	2:C:4:LEU:N	2.34	0.43
1:A:295:LYS:HG2	1:A:314:LEU:HD22	2.00	0.42
1:A:92:TRP:CE3	1:A:118:ILE:HG12	2.54	0.42
2:C:191:TRP:CG	2:C:192:PRO:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:98:ASP:HA	3:L:99:PRO:C	2.44	0.42
3:L:160:GLN:HE21	3:L:160:GLN:HB2	1.57	0.42
1:B:220:GLU:HB3	1:B:297:SER:HB2	2.00	0.42
1:B:283:TRP:HH2	1:B:292:TYR:HE2	1.67	0.42
1:A:208:GLU:HG2	1:A:210:TRP:CD1	2.55	0.42
3:L:140:LEU:HD13	3:L:179:MET:CE	2.46	0.42
1:B:20:ASP:HA	1:B:185:GLY:O	2.20	0.42
1:A:173:ALA:O	1:A:374:ILE:HD11	2.20	0.41
1:A:141:THR:HG21	1:A:209:GLU:O	2.20	0.41
1:B:259:GLU:HG2	1:B:263:ARG:HH12	1.85	0.41
1:A:374:ILE:HG12	1:A:379:VAL:HG11	2.02	0.41
3:D:98:ASP:HA	3:D:99:PRO:C	2.46	0.41
2:H:35:HIS:CE1	3:L:100:TRP:CH2	3.08	0.41
1:A:168:MET:HE3	1:A:168:MET:HB2	1.87	0.41
1:A:267:ILE:HD12	1:A:280:LEU:HD21	2.02	0.41
3:D:16:GLY:HA2	3:D:81:PRO:HB2	2.03	0.40
3:D:63:PRO:HB2	3:D:65:ARG:HG3	2.03	0.40
1:A:126:LEU:HB3	1:A:127:PRO:HD2	2.02	0.40
1:A:354:TYR:CD2	1:A:356:ILE:HD11	2.57	0.40
1:B:170:MET:HE1	1:B:347:ALA:HA	2.03	0.40

All (2) 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)
8:C:2015:HOH:O	8:H:2122:HOH:O[2_656]	1.34	0.86
2:H:194:GLN:OE1	8:C:2015:HOH:O[2_646]	2.03	0.17

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	375/386 (97%)	359 (96%)	16 (4%)	0	100	100
1	B	373/386 (97%)	360 (96%)	13 (4%)	0	100	100
2	C	216/221 (98%)	207 (96%)	8 (4%)	1 (0%)	24	21
2	H	216/221 (98%)	209 (97%)	6 (3%)	1 (0%)	24	21
3	D	217/218 (100%)	207 (95%)	9 (4%)	1 (0%)	24	21
3	L	216/218 (99%)	209 (97%)	7 (3%)	0	100	100
All	All	1613/1650 (98%)	1551 (96%)	59 (4%)	3 (0%)	43	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	16	GLN
2	C	16	GLN
3	D	216	ASN

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	319/320 (100%)	311 (98%)	8 (2%)	42	45
1	B	317/320 (99%)	310 (98%)	7 (2%)	45	50
2	C	188/191 (98%)	183 (97%)	5 (3%)	39	42
2	H	188/191 (98%)	184 (98%)	4 (2%)	47	52
3	D	191/190 (100%)	187 (98%)	4 (2%)	47	52
3	L	190/190 (100%)	188 (99%)	2 (1%)	65	73
All	All	1393/1402 (99%)	1363 (98%)	30 (2%)	45	50

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LYS
1	A	126	LEU

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Mol	Chain	Res	Type
1	A	151	THR
1	A	208	GLU
1	A	210	TRP
1	A	259	GLU
1	A	348	THR
1	A	369	SER
1	B	86	LYS
1	B	151	THR
1	B	200	ASP
1	B	210	TRP
1	B	267	ILE
1	B	314	LEU
1	B	351	GLU
2	C	10	VAL
2	C	76	SER
2	C	115	SER
2	C	180	LEU
2	C	208	LYS
3	D	160	GLN
3	D	179	MET
3	D	189	GLU
3	D	201	THR
2	H	116	SER
2	H	180	LEU
2	H	199	ASN
2	H	208	LYS
3	L	82	VAL
3	L	160	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	169	GLN
1	A	227	ASN
1	A	251	GLN
1	A	285	ASN
1	A	341	ASN
1	B	169	GLN
1	B	251	GLN
1	B	285	ASN
2	C	174	GLN

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Mol	Chain	Res	Type
3	D	1	ASN
3	D	41	GLN
3	D	46	GLN
3	D	141	ASN
3	D	142	ASN
3	D	160	GLN
2	H	174	GLN
3	L	46	GLN
3	L	141	ASN
3	L	142	ASN
3	L	160	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	PCA	H	1	2	7,8,9	0.72	0	9,10,12	1.02	1 (11%)
2	PCA	C	1	2	7,8,9	0.60	0	9,10,12	0.94	0

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	PCA	H	1	2	-	0/0/11/13	0/1/1/1
2	PCA	C	1	2	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	PCA	O-C-CA	-2.01	119.61	124.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	$\# Z > 2$
6	SO4	A	1401	-	4,4,4	0.45	0	6,6,6	0.19	0
6	SO4	B	1400	-	4,4,4	0.43	0	6,6,6	0.16	0
5	DMS	A	1399	-	3,3,3	0.55	0	3,3,3	0.59	0
6	SO4	H	1217	-	4,4,4	0.45	0	6,6,6	0.21	0
5	DMS	B	1399	-	3,3,3	0.55	0	3,3,3	0.56	0
6	SO4	C	1217	-	4,4,4	0.43	0	6,6,6	0.20	0
4	WZV	A	1398	-	32,33,33	0.89	1 (3%)	42,49,49	1.53	7 (16%)
6	SO4	A	1400	-	4,4,4	0.43	0	6,6,6	0.29	0
4	WZV	B	1398	-	32,33,33	0.87	2 (6%)	42,49,49	1.59	6 (14%)
6	SO4	B	1401	-	4,4,4	0.50	0	6,6,6	0.22	0
7	GOL	C	1218	-	5,5,5	0.33	0	5,5,5	0.52	0
7	GOL	H	1218	-	5,5,5	0.26	0	5,5,5	0.69	0

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
7	GOL	C	1218	-	-	0/4/4/4	-
7	GOL	H	1218	-	-	0/4/4/4	-
4	WZV	A	1398	-	-	7/20/38/38	0/3/3/3
4	WZV	B	1398	-	-	11/20/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1398	WZV	C3-N4	-2.72	1.34	1.38
4	B	1398	WZV	C2-C3	2.50	1.53	1.50
4	B	1398	WZV	C3-N4	-2.45	1.35	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1398	WZV	C3-N4-C5	-5.28	118.43	124.20
4	A	1398	WZV	C3-N4-C5	-5.21	118.50	124.20
4	B	1398	WZV	C2-C3-N4	3.22	120.19	117.25
4	B	1398	WZV	C23-N22-C21	2.97	122.11	117.46
4	B	1398	WZV	C21-C24-N13	2.91	121.29	113.99
4	A	1398	WZV	C12-C11-C1	2.62	123.93	120.24
4	A	1398	WZV	C10-C11-C1	-2.56	117.67	121.03
4	A	1398	WZV	C21-C24-N13	2.43	120.09	113.99
4	A	1398	WZV	C23-N22-C21	2.37	121.16	117.46
4	B	1398	WZV	C27-O26-C18	2.18	124.39	117.80
4	B	1398	WZV	O25-C24-C21	-2.17	116.29	121.08
4	A	1398	WZV	C7-N13-C24	-2.10	121.07	126.61
4	A	1398	WZV	C18-C23-N22	-2.09	120.09	122.67

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1398	WZV	C23-C18-O26-C27
4	B	1398	WZV	O26-C27-C28-F31
4	B	1398	WZV	O26-C27-C28-F30
4	A	1398	WZV	N22-C21-C24-O25

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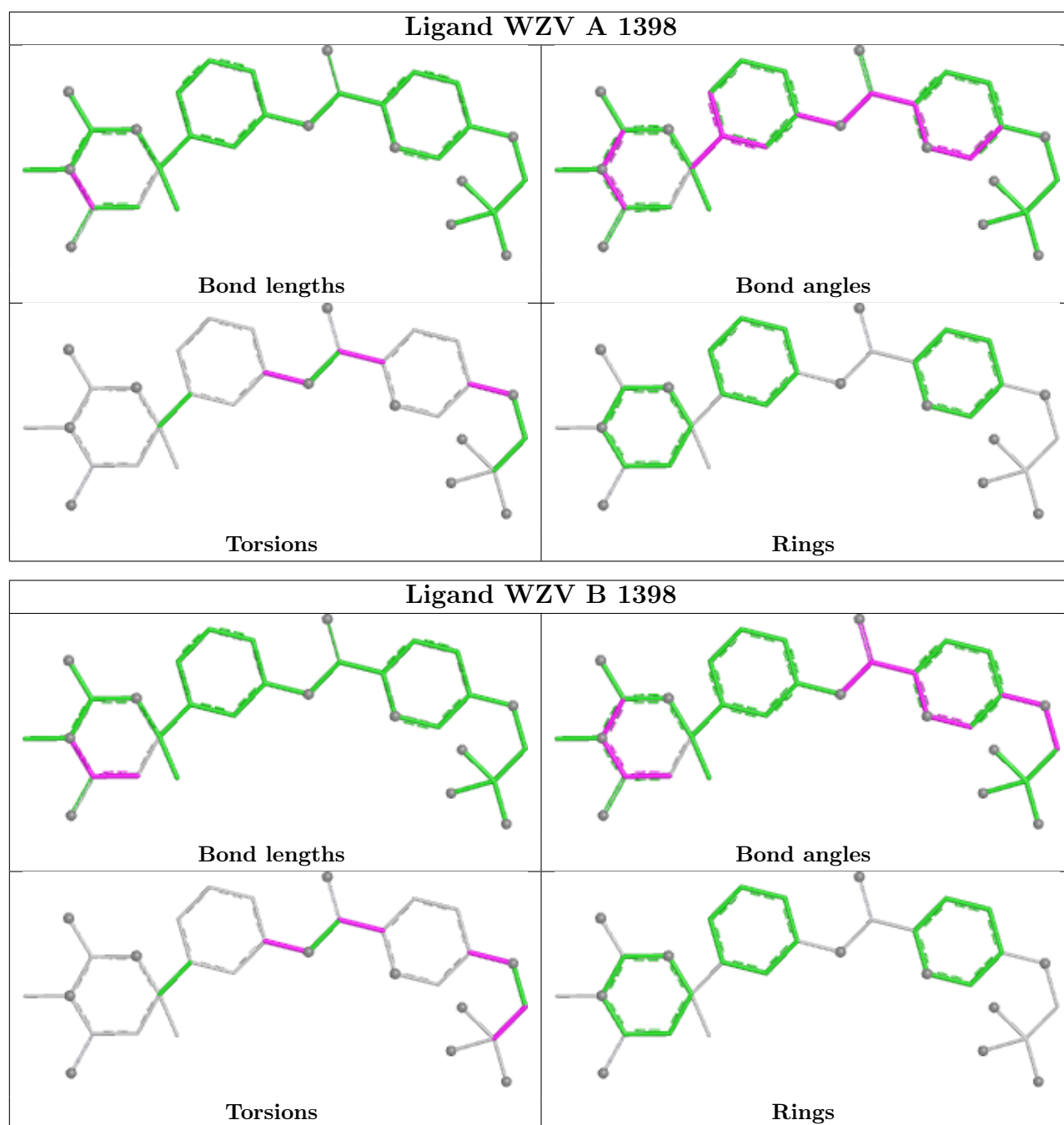
Mol	Chain	Res	Type	Atoms
4	B	1398	WZV	N22-C21-C24-O25
4	A	1398	WZV	C20-C21-C24-O25
4	B	1398	WZV	C20-C21-C24-O25
4	B	1398	WZV	N22-C21-C24-N13
4	A	1398	WZV	N22-C21-C24-N13
4	A	1398	WZV	C20-C21-C24-N13
4	B	1398	WZV	C20-C21-C24-N13
4	B	1398	WZV	O26-C27-C28-F29
4	A	1398	WZV	C19-C18-O26-C27
4	B	1398	WZV	C23-C18-O26-C27
4	B	1398	WZV	C19-C18-O26-C27
4	B	1398	WZV	C8-C7-N13-C24
4	B	1398	WZV	C12-C7-N13-C24
4	A	1398	WZV	C8-C7-N13-C24

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1398	WZV	3	0
4	B	1398	WZV	2	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	375/386 (97%)	0.34	17 (4%) 38 37	9, 32, 52, 71	11 (2%)
1	B	375/386 (97%)	0.18	10 (2%) 56 55	9, 29, 50, 66	8 (2%)
2	C	216/221 (97%)	0.12	3 (1%) 73 73	14, 26, 45, 58	7 (3%)
2	H	216/221 (97%)	-0.16	3 (1%) 73 73	12, 23, 38, 53	7 (3%)
3	D	217/218 (99%)	-0.06	4 (1%) 67 67	12, 24, 45, 65	4 (1%)
3	L	217/218 (99%)	-0.09	1 (0%) 87 87	12, 25, 46, 64	3 (1%)
All	All	1616/1650 (97%)	0.10	38 (2%) 59 59	9, 28, 49, 71	40 (2%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	235	ALA	4.9
1	A	235	ALA	4.7
1	A	108	ASN	3.7
1	B	28	ARG	3.6
1	A	28	ARG	3.3
1	B	108	ASN	3.2
3	D	129	LEU	3.0
1	A	27	GLY	2.9
2	C	15	SER	2.8
3	L	216	ASN	2.8
1	A	173	ALA	2.8
2	H	15	SER	2.8
1	A	111	PHE	2.8
1	B	27	GLY	2.7
2	C	19[A]	PHE	2.7
3	D	216	ASN	2.7
2	H	19[A]	PHE	2.6
3	D	132	GLY	2.6
1	A	109	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	183	ASN	2.4
1	B	374	ILE	2.4
1	B	173	ALA	2.4
2	C	208	LYS	2.3
2	H	133	ASP	2.2
1	A	392	ALA	2.2
3	D	133	GLY	2.2
1	B	107	PHE	2.2
1	A	183	ASN	2.2
1	B	375	ALA	2.2
1	A	161[A]	ASN	2.2
1	A	107	PHE	2.1
1	A	339	SER	2.1
1	B	14	ASN	2.1
1	A	88	THR	2.1
1	A	393	SER	2.1
1	A	395	CYS	2.1
1	A	26	SER	2.1
1	A	377	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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	PCA	H	1	8/9	0.94	0.06	20,23,23,25	0
2	PCA	C	1	8/9	0.97	0.06	21,23,24,25	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

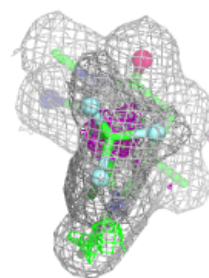
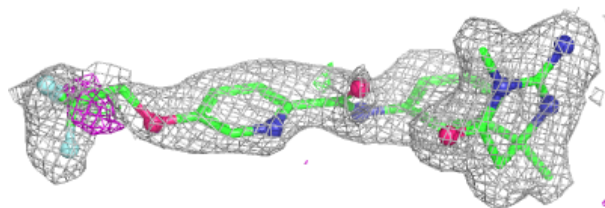
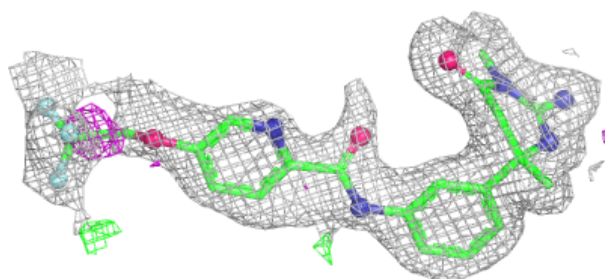
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	B	1401	5/5	0.77	0.12	68,71,76,77	0
6	SO4	C	1217	5/5	0.81	0.16	66,67,71,71	5
6	SO4	A	1401	5/5	0.83	0.11	73,76,77,79	0
6	SO4	A	1400	5/5	0.86	0.13	54,57,60,61	5
6	SO4	H	1217	5/5	0.88	0.20	49,51,53,57	5
5	DMS	A	1399	4/4	0.89	0.16	43,43,45,50	0
5	DMS	B	1399	4/4	0.89	0.17	48,53,54,56	0
6	SO4	B	1400	5/5	0.89	0.13	67,68,69,70	5
4	WZV	B	1398	31/31	0.90	0.11	21,28,74,74	0
4	WZV	A	1398	31/31	0.91	0.12	20,28,95,99	0
7	GOL	C	1218	6/6	0.94	0.08	27,28,29,30	0
7	GOL	H	1218	6/6	0.94	0.09	32,33,35,35	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.

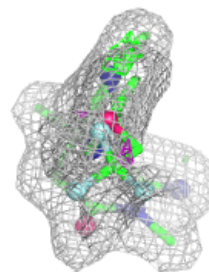
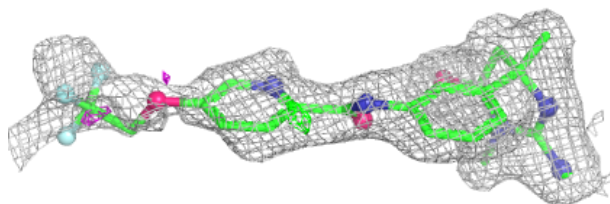
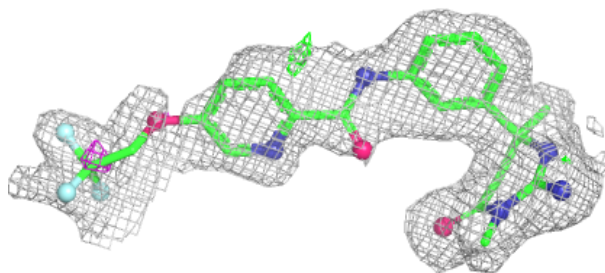
Electron density around WZV B 1398:

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



Electron density around WZV 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.