Full wwPDB X-ray Structure Validation Report (i)

Jun 26, 2024 – 12:05 AM EDT

PDB ID	:	7D5U
Title	:	BACE2 xaperone complex with N-{3-[(9S)-7-amino-2,2-difluoro-9-(prop-1-yn-1-yl)-6-oxa-8-azaspiro[3.5]non-7-en-9-yl]-4-fluorophenyl}-5-cyanopyridine-2-carboxamide
Authors	:	Fujimoto, K.; Yoshida, S.; Tadano, G.; Asada, N.; Fuchino, K.; Suzuki, S.; Matsuoka, E.; Yamamoto, T.; Yamamoto, S.; Ando, S.; Kanegawa, N.; Tonomura, Y.; Ito, H.; Moechars, D.; Rombouts, F.J.R.; Gijsen, H.J.M.; Kusakabe, K.I.
Deposited on	:	2020-09-28
Resolution	:	2.04 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 (i) 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 (i)) were used in the production of this report:

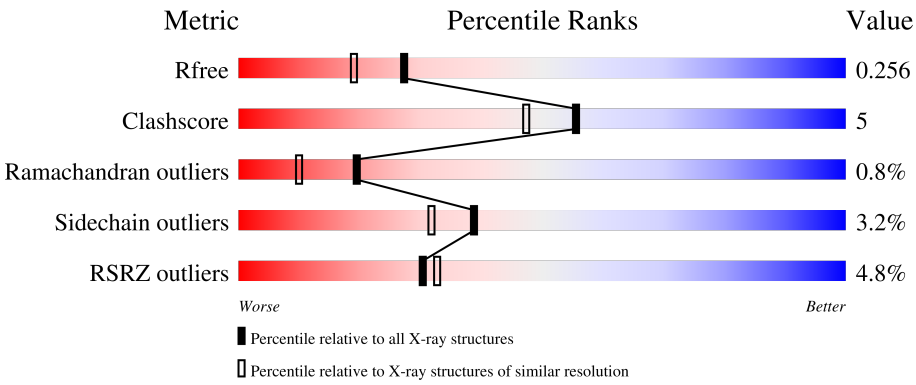
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)

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 2.04 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	5% 59% 32% 5% •
2	D	114	4% 63% 33% • •

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3815 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.

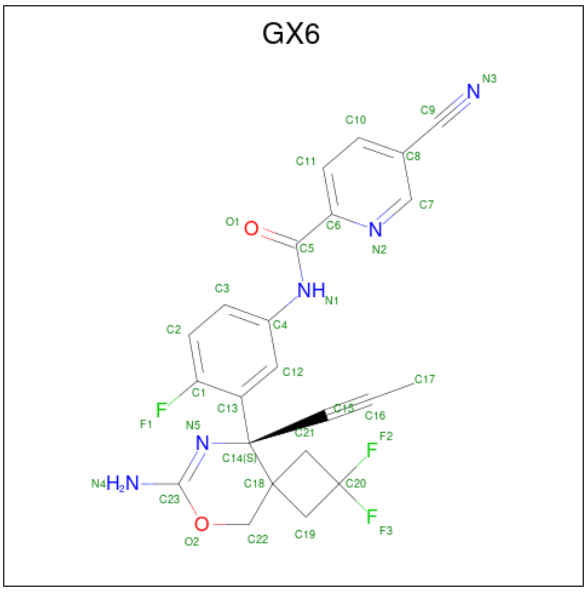
- Molecule 1 is a protein called Beta-secretase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	370	2815	1823	438	542	12	0	2	0

- Molecule 2 is a protein called xaperone.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	114	835	515	149	167	4	0	1	0

- Molecule 3 is N-[3-[(9S)-7-azanyl-2,2-bis(fluoranyl)-9-prop-1-ynyl-6-oxa-8-azaspiro[3.5]non-7-en-9-yl]-4-fluoranyl-phenyl]-5-cyano-pyridine-2-carboxamide (three-letter code: GX6) (formula: $C_{23}H_{18}F_3N_5O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
3	A	1	33	23	3	5	2	0	0

- Molecule 4 is water.

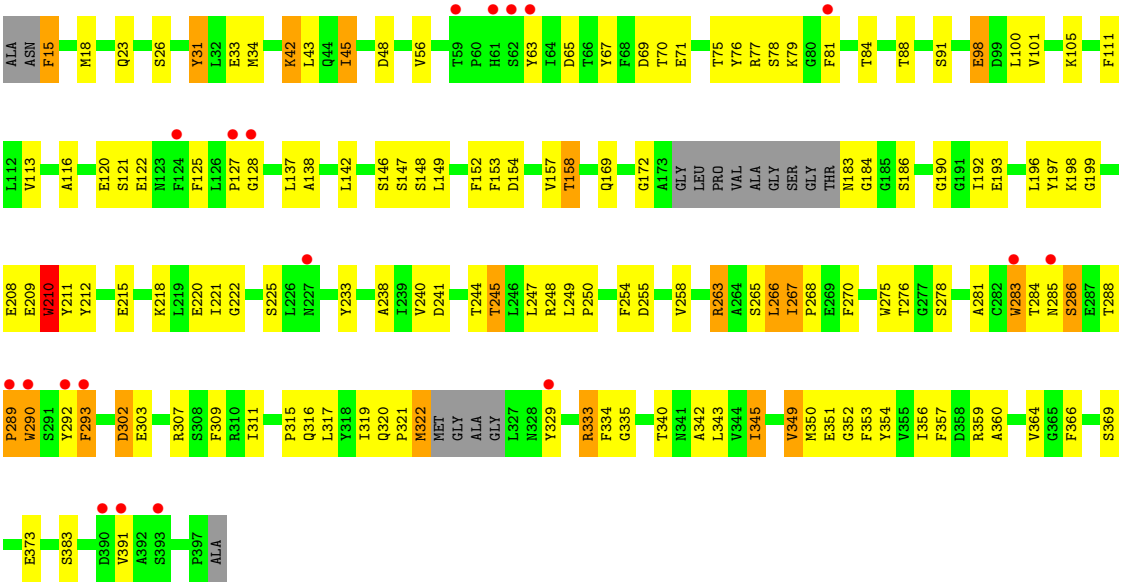
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	85	85	85	0	0
			Total	O		
4	D	47	47	47	0	0

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.

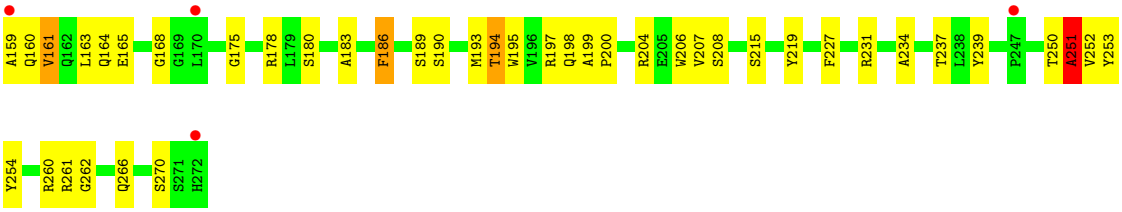
- Molecule 1: Beta-secretase 2

Chain A:



- Molecule 2: xaperone

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	62.93Å 74.34Å 108.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.31 – 2.04 43.91 – 2.04	Depositor EDS
% Data completeness (in resolution range)	96.0 (61.31-2.04) 96.0 (43.91-2.04)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.207 , 0.254 0.211 , 0.256	Depositor DCC
R_{free} test set	1745 reflections (5.49%)	wwPDB-VP
Wilson B-factor (Å^2)	45.1	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 66.3	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	0.96	EDS
Total number of atoms	3815	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GX6

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	2.26	115/2886 (4.0%)	1.66	48/3935 (1.2%)
2	D	2.39	36/849 (4.2%)	1.76	14/1152 (1.2%)
All	All	2.29	151/3735 (4.0%)	1.68	62/5087 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
2	D	0	3
All	All	0	8

All (151) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	253	TYR	CG-CD2	-11.53	1.24	1.39
2	D	262	GLY	C-O	10.97	1.41	1.23
2	D	190	SER	CB-OG	10.64	1.56	1.42
1	A	215	GLU	CD-OE2	10.01	1.36	1.25
1	A	78	SER	CA-CB	9.83	1.67	1.52
1	A	222	GLY	N-CA	9.73	1.60	1.46
2	D	239	TYR	C-O	9.34	1.41	1.23
1	A	254	PHE	CE2-CZ	9.25	1.54	1.37
2	D	195	TRP	C-O	9.09	1.40	1.23
1	A	275	TRP	NE1-CE2	-8.64	1.26	1.37
1	A	208	GLU	CD-OE1	-8.55	1.16	1.25
1	A	275	TRP	CD2-CE2	8.39	1.51	1.41
1	A	208	GLU	CD-OE2	-8.24	1.16	1.25
1	A	121	SER	CA-CB	-7.96	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	239	TYR	CE1-CZ	7.86	1.48	1.38
1	A	334	PHE	CG-CD2	7.75	1.50	1.38
2	D	237	THR	C-O	7.60	1.37	1.23
1	A	209	GLU	CD-OE1	7.59	1.33	1.25
1	A	357	PHE	CG-CD1	7.56	1.50	1.38
2	D	215	SER	CB-OG	7.55	1.52	1.42
1	A	342	ALA	N-CA	7.45	1.61	1.46
2	D	254	TYR	CG-CD2	7.45	1.48	1.39
2	D	252	VAL	CA-CB	-7.18	1.39	1.54
1	A	373	GLU	CD-OE1	7.18	1.33	1.25
1	A	352	GLY	N-CA	7.14	1.56	1.46
1	A	157	VAL	CB-CG1	7.06	1.67	1.52
2	D	270	SER	CA-CB	7.05	1.63	1.52
1	A	290	TRP	CD2-CE2	7.00	1.49	1.41
1	A	210	TRP	CG-CD1	7.00	1.46	1.36
1	A	210	TRP	CE2-CZ2	-6.97	1.27	1.39
1	A	148	SER	CB-OG	-6.94	1.33	1.42
1	A	125	PHE	CG-CD2	6.92	1.49	1.38
1	A	210	TRP	CD2-CE2	6.90	1.49	1.41
2	D	168	GLY	N-CA	6.85	1.56	1.46
1	A	366	PHE	CG-CD2	6.78	1.49	1.38
1	A	142	LEU	C-O	6.73	1.36	1.23
1	A	311	ILE	C-O	6.72	1.36	1.23
1	A	248	ARG	CZ-NH2	-6.70	1.24	1.33
2	D	200	PRO	N-CA	-6.70	1.35	1.47
1	A	111	PHE	CB-CG	-6.62	1.40	1.51
1	A	154	ASP	CG-OD1	-6.57	1.10	1.25
1	A	78	SER	C-O	-6.53	1.10	1.23
2	D	195	TRP	CB-CG	6.51	1.61	1.50
1	A	120	GLU	CG-CD	6.46	1.61	1.51
1	A	76	TYR	CB-CG	6.43	1.61	1.51
1	A	369	SER	CA-CB	6.40	1.62	1.52
2	D	261	ARG	CZ-NH2	6.39	1.41	1.33
1	A	212	TYR	CD1-CE1	-6.31	1.29	1.39
1	A	127	PRO	C-O	6.24	1.35	1.23
1	A	292	TYR	CG-CD2	6.23	1.47	1.39
1	A	258	VAL	CB-CG2	6.18	1.65	1.52
1	A	70	THR	C-O	-6.18	1.11	1.23
2	D	175	GLY	C-O	6.07	1.33	1.23
1	A	15	PHE	N-CA	6.06	1.58	1.46
1	A	266	LEU	N-CA	6.03	1.58	1.46
2	D	165	GLU	N-CA	-6.02	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221	ILE	N-CA	6.01	1.58	1.46
1	A	303	GLU	CD-OE2	6.01	1.32	1.25
1	A	220	GLU	CG-CD	6.00	1.60	1.51
1	A	212	TYR	CG-CD1	5.99	1.47	1.39
2	D	219	TYR	CZ-OH	5.99	1.48	1.37
1	A	369	SER	CB-OG	5.96	1.50	1.42
2	D	254	TYR	CE1-CZ	5.96	1.46	1.38
2	D	194	THR	CB-CG2	5.96	1.72	1.52
2	D	262	GLY	N-CA	-5.96	1.37	1.46
1	A	350	MET	N-CA	5.96	1.58	1.46
1	A	42	LYS	CB-CG	5.94	1.68	1.52
1	A	190	GLY	N-CA	-5.94	1.37	1.46
1	A	364	VAL	CA-CB	-5.94	1.42	1.54
1	A	233	TYR	CD2-CE2	-5.92	1.30	1.39
1	A	383	SER	CB-OG	-5.89	1.34	1.42
1	A	172	GLY	N-CA	5.88	1.54	1.46
1	A	186	SER	CB-OG	-5.84	1.34	1.42
1	A	359	ARG	NE-CZ	-5.84	1.25	1.33
2	D	198	GLN	N-CA	5.83	1.58	1.46
1	A	197	TYR	CB-CG	-5.79	1.43	1.51
1	A	210	TRP	NE1-CE2	-5.76	1.30	1.37
1	A	98	GLU	N-CA	-5.73	1.34	1.46
1	A	335	GLY	C-O	5.70	1.32	1.23
1	A	31	TYR	CG-CD1	5.70	1.46	1.39
1	A	356	ILE	N-CA	5.66	1.57	1.46
2	D	206	TRP	C-O	-5.66	1.12	1.23
1	A	360	ALA	C-O	-5.66	1.12	1.23
2	D	164	GLN	N-CA	5.66	1.57	1.46
1	A	245	THR	C-O	-5.64	1.12	1.23
1	A	309	PHE	CG-CD1	-5.63	1.30	1.38
2	D	231	ARG	CZ-NH2	5.62	1.40	1.33
1	A	63	TYR	CA-C	5.60	1.67	1.52
1	A	245	THR	N-CA	5.59	1.57	1.46
1	A	98	GLU	CG-CD	5.58	1.60	1.51
2	D	234	ALA	CA-CB	5.57	1.64	1.52
1	A	138	ALA	C-O	-5.56	1.12	1.23
1	A	289	PRO	CA-C	5.54	1.64	1.52
1	A	105	LYS	N-CA	5.54	1.57	1.46
1	A	303	GLU	N-CA	5.52	1.57	1.46
1	A	349	VAL	CB-CG1	-5.48	1.41	1.52
1	A	81	PHE	CD1-CE1	5.47	1.50	1.39
1	A	169	GLN	CD-OE1	5.47	1.35	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	SER	CA-CB	5.47	1.61	1.52
1	A	283	TRP	CD2-CE2	5.46	1.48	1.41
1	A	31	TYR	CD1-CE1	5.46	1.47	1.39
1	A	158	THR	C-O	-5.39	1.13	1.23
2	D	254	TYR	CA-CB	-5.39	1.42	1.53
1	A	329	TYR	CG-CD2	5.37	1.46	1.39
1	A	152	PHE	CG-CD1	-5.37	1.30	1.38
1	A	276	THR	C-O	-5.36	1.13	1.23
1	A	152	PHE	CE2-CZ	-5.35	1.27	1.37
2	D	165	GLU	CD-OE2	-5.35	1.19	1.25
1	A	76	TYR	CG-CD2	-5.33	1.32	1.39
1	A	211	TYR	CZ-OH	-5.32	1.28	1.37
1	A	153	PHE	CE1-CZ	-5.30	1.27	1.37
1	A	218	LYS	N-CA	5.26	1.56	1.46
2	D	189	SER	CA-CB	5.26	1.60	1.52
1	A	215	GLU	CG-CD	5.26	1.59	1.51
1	A	255	ASP	C-O	-5.25	1.13	1.23
1	A	303	GLU	C-O	-5.24	1.13	1.23
1	A	153	PHE	CE2-CZ	5.24	1.47	1.37
1	A	351	GLU	CD-OE2	-5.23	1.19	1.25
1	A	317	LEU	N-CA	5.23	1.56	1.46
2	D	254	TYR	CD1-CE1	5.23	1.47	1.39
1	A	77	ARG	CD-NE	5.21	1.55	1.46
1	A	293	PHE	CB-CG	-5.21	1.42	1.51
1	A	147	SER	CB-OG	-5.21	1.35	1.42
1	A	71	GLU	CD-OE1	5.19	1.31	1.25
1	A	120	GLU	CD-OE1	5.19	1.31	1.25
1	A	315	PRO	CA-CB	5.16	1.63	1.53
1	A	263	ARG	C-O	-5.15	1.13	1.23
1	A	75	THR	CB-CG2	5.15	1.69	1.52
1	A	244	THR	CB-OG1	-5.14	1.32	1.43
1	A	353	PHE	CG-CD2	5.14	1.46	1.38
2	D	253	TYR	CE1-CZ	-5.13	1.31	1.38
1	A	98	GLU	CA-CB	5.13	1.65	1.53
2	D	207	VAL	CB-CG2	-5.13	1.42	1.52
1	A	128	GLY	N-CA	5.12	1.53	1.46
2	D	266	GLN	N-CA	5.12	1.56	1.46
1	A	211	TYR	CB-CG	-5.12	1.44	1.51
2	D	186	PHE	CG-CD1	5.12	1.46	1.38
1	A	220	GLU	CB-CG	-5.11	1.42	1.52
2	D	208	SER	C-O	-5.11	1.13	1.23
1	A	45	ILE	CA-CB	-5.10	1.43	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	240	VAL	CB-CG2	-5.10	1.42	1.52
1	A	88	THR	C-O	5.09	1.33	1.23
1	A	290	TRP	CE2-CZ2	5.08	1.48	1.39
1	A	212	TYR	CE1-CZ	5.06	1.45	1.38
1	A	359	ARG	CD-NE	-5.06	1.37	1.46
2	D	183	ALA	N-CA	5.05	1.56	1.46
1	A	354	TYR	CA-CB	-5.03	1.42	1.53
1	A	281	ALA	CA-CB	5.03	1.63	1.52
1	A	198	LYS	C-O	5.03	1.32	1.23
1	A	351	GLU	C-O	-5.01	1.13	1.23
1	A	290	TRP	CG-CD1	5.00	1.43	1.36

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	178	ARG	NE-CZ-NH1	-14.62	112.99	120.30
2	D	261	ARG	NE-CZ-NH1	-12.05	114.28	120.30
1	A	248	ARG	NE-CZ-NH1	10.23	125.42	120.30
2	D	197	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	A	154	ASP	CB-CG-OD1	-9.34	109.89	118.30
2	D	261	ARG	NE-CZ-NH2	9.34	124.97	120.30
1	A	154	ASP	CB-CG-OD2	9.02	126.42	118.30
1	A	67	TYR	CB-CG-CD2	-8.22	116.07	121.00
1	A	158	THR	CA-CB-CG2	-8.09	101.08	112.40
1	A	322	MET	CG-SD-CE	7.97	112.96	100.20
1	A	248	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	A	193	GLU	OE1-CD-OE2	7.57	132.39	123.30
2	D	197	ARG	NE-CZ-NH2	-7.57	116.52	120.30
2	D	193	MET	CG-SD-CE	-7.20	88.68	100.20
1	A	302	ASP	CB-CG-OD1	7.15	124.73	118.30
1	A	247	LEU	CB-CG-CD1	7.10	123.07	111.00
1	A	319	ILE	N-CA-C	-6.96	92.22	111.00
1	A	353	PHE	CB-CG-CD2	-6.91	115.96	120.80
1	A	263	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	A	120	GLU	CA-CB-CG	6.51	127.71	113.40
2	D	178	ARG	NH1-CZ-NH2	6.38	126.41	119.40
1	A	373	GLU	OE1-CD-OE2	6.32	130.88	123.30
1	A	67	TYR	CB-CG-CD1	6.14	124.69	121.00
1	A	302	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	A	199	GLY	N-CA-C	-6.12	97.79	113.10
1	A	196	LEU	CB-CG-CD2	-6.08	100.67	111.00
1	A	149	LEU	CB-CG-CD1	6.04	121.26	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	120	GLU	OE1-CD-OE2	-5.93	116.18	123.30
2	D	163	LEU	CB-CG-CD1	-5.85	101.06	111.00
1	A	319	ILE	CA-CB-CG1	5.80	122.01	111.00
1	A	56	VAL	CA-CB-CG1	-5.77	102.24	110.90
1	A	225	SER	N-CA-CB	5.77	119.15	110.50
1	A	220	GLU	CA-CB-CG	5.71	125.96	113.40
1	A	350	MET	CG-SD-CE	5.71	109.33	100.20
1	A	128	GLY	N-CA-C	5.70	127.34	113.10
1	A	100	LEU	CB-CG-CD1	-5.68	101.34	111.00
1	A	48	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	241	ASP	CB-CG-OD2	5.67	123.40	118.30
1	A	254	PHE	CB-CG-CD1	-5.65	116.84	120.80
1	A	369	SER	N-CA-CB	5.63	118.95	110.50
1	A	211	TYR	CG-CD1-CE1	-5.61	116.81	121.30
1	A	196	LEU	CA-CB-CG	5.59	128.16	115.30
2	D	204	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	152	PHE	CB-CG-CD1	5.56	124.69	120.80
1	A	42	LYS	CG-CD-CE	5.56	128.58	111.90
2	D	204	ARG	CG-CD-NE	5.54	123.44	111.80
2	D	239	TYR	CD1-CE1-CZ	-5.54	114.81	119.80
1	A	351	GLU	CA-CB-CG	-5.53	101.23	113.40
1	A	307	ARG	CG-CD-NE	5.36	123.06	111.80
2	D	231	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	192	ILE	CG1-CB-CG2	5.32	123.10	111.40
1	A	267	ILE	CG1-CB-CG2	-5.26	99.83	111.40
1	A	69	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	146	SER	CB-CA-C	-5.17	100.29	110.10
2	D	260	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	116	ALA	CB-CA-C	5.10	117.76	110.10
1	A	122	GLU	CB-CA-C	5.09	120.59	110.40
1	A	101	VAL	CA-CB-CG1	5.09	118.54	110.90
1	A	281	ALA	N-CA-CB	-5.09	102.97	110.10
2	D	270	SER	N-CA-CB	5.07	118.11	110.50
1	A	34	MET	CG-SD-CE	-5.03	92.15	100.20
1	A	113	VAL	CG1-CB-CG2	5.01	118.92	110.90

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	LEU	Mainchain
1	A	210	TRP	Peptide

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Mol	Chain	Res	Type	Group
1	A	23	GLN	Mainchain
1	A	302	ASP	Sidechain
1	A	345	ILE	Mainchain
2	D	199	ALA	Mainchain
2	D	227	PHE	Sidechain
2	D	251	ALA	Mainchain

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	2815	0	2648	32	0
2	D	835	0	794	5	0
3	A	33	0	0	1	0
4	A	85	0	0	1	0
4	D	47	0	0	1	0
All	All	3815	0	3442	35	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 5.

All (35) 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:A:270:PHE:CZ	1:A:293:PHE:HZ	2.02	0.77
1:A:288:THR:HG21	1:A:290:TRP:CE3	2.21	0.76
1:A:183:ASN:OD1	1:A:184:GLY:N	2.19	0.75
1:A:290:TRP:CD2	1:A:316:GLN:HG3	2.24	0.73
2:D:159:ALA:N	4:D:301:HOH:O	2.29	0.64
1:A:288:THR:HG22	1:A:290:TRP:H	1.68	0.59
1:A:340:THR:HG23	4:A:502:HOH:O	2.05	0.55
1:A:26:SER:O	1:A:245:THR:HG23	2.07	0.54
2:D:250:THR:O	2:D:251:ALA:HB2	2.06	0.54
1:A:26:SER:HA	3:A:401:GX6:N3	2.23	0.54
1:A:322:MET:HE3	1:A:333:ARG:CG	2.40	0.52
1:A:15:PHE:HA	1:A:18:MET:HE3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:PHE:CZ	1:A:293:PHE:CZ	2.93	0.49
1:A:267:ILE:O	1:A:268:PRO:C	2.46	0.49
1:A:284:THR:O	1:A:286:SER:N	2.46	0.48
1:A:288:THR:HG21	1:A:290:TRP:CD2	2.49	0.48
2:D:161:VAL:HA	2:D:186:PHE:CD1	2.50	0.47
1:A:320:GLN:HA	1:A:321:PRO:HD3	1.85	0.46
1:A:290:TRP:CE2	1:A:316:GLN:HG3	2.50	0.46
1:A:158:THR:HG21	2:D:194:THR:HG21	1.98	0.46
1:A:288:THR:CG2	1:A:290:TRP:CD2	2.99	0.46
1:A:270:PHE:N	1:A:270:PHE:CD1	2.84	0.45
1:A:265:SER:O	1:A:267:ILE:HG23	2.17	0.44
1:A:31:TYR:HA	1:A:45:ILE:O	2.18	0.43
1:A:288:THR:CG2	1:A:290:TRP:H	2.30	0.43
1:A:290:TRP:CG	1:A:316:GLN:HG3	2.54	0.43
1:A:238:ALA:HA	1:A:343:LEU:O	2.19	0.42
1:A:158:THR:CG2	2:D:194:THR:HG21	2.49	0.42
1:A:283:TRP:CZ3	1:A:289:PRO:HG3	2.55	0.42
1:A:322:MET:HE1	1:A:333:ARG:CZ	2.50	0.41
1:A:42:LYS:O	1:A:43:LEU:HD12	2.19	0.41
1:A:345:ILE:HG23	1:A:349:VAL:HB	2.03	0.41
1:A:249:LEU:HD23	1:A:343:LEU:HG	2.02	0.41
1:A:284:THR:C	1:A:286:SER:N	2.73	0.41
1:A:79:LYS:HE2	1:A:98:GLU:CG	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	366/386 (95%)	341 (93%)	23 (6%)	2 (0%)	29 18
2	D	113/114 (99%)	109 (96%)	2 (2%)	2 (2%)	8 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	479/500 (96%)	450 (94%)	25 (5%)	4 (1%)	19 10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	161	VAL
1	A	285	ASN
1	A	266	LEU
2	D	251	ALA

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	288/320 (90%)	277 (96%)	11 (4%)	33 26
2	D	85/91 (93%)	83 (98%)	2 (2%)	49 42
All	All	373/411 (91%)	360 (96%)	13 (4%)	39 29

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33[A]	GLU
1	A	33[B]	GLU
1	A	65	ASP
1	A	84	THR
1	A	210	TRP
1	A	250	PRO
1	A	263	ARG
1	A	278	SER
1	A	286	SER
1	A	333	ARG
1	A	391	VAL
2	D	160	GLN
2	D	180	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

1 ligand is 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	GX6	A	401	-	32,36,36	2.22	10 (31%)	34,55,55	1.52	7 (20%)

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	GX6	A	401	-	-	1/14/52/52	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	GX6	C21-C18	6.30	1.63	1.55
3	A	401	GX6	C18-C14	-5.05	1.48	1.59
3	A	401	GX6	C10-C8	3.82	1.47	1.39
3	A	401	GX6	C6-C5	-3.12	1.43	1.50
3	A	401	GX6	C14-C13	2.88	1.57	1.53
3	A	401	GX6	O1-C5	-2.86	1.17	1.23
3	A	401	GX6	C13-C1	2.65	1.42	1.38
3	A	401	GX6	C8-C9	-2.39	1.39	1.44
3	A	401	GX6	C6-N2	2.32	1.38	1.34
3	A	401	GX6	O2-C22	2.30	1.49	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	GX6	C18-C19-C20	3.26	92.31	76.59
3	A	401	GX6	C4-N1-C5	3.17	134.80	126.58
3	A	401	GX6	C7-N2-C6	2.82	121.75	117.36
3	A	401	GX6	C18-C21-C20	2.82	90.17	76.59
3	A	401	GX6	C2-C1-C13	-2.45	120.02	123.44
3	A	401	GX6	C12-C13-C1	2.34	120.05	116.79
3	A	401	GX6	F3-C20-F2	2.04	111.67	107.49

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	GX6	C12-C13-C14-C15

There are no ring outliers.

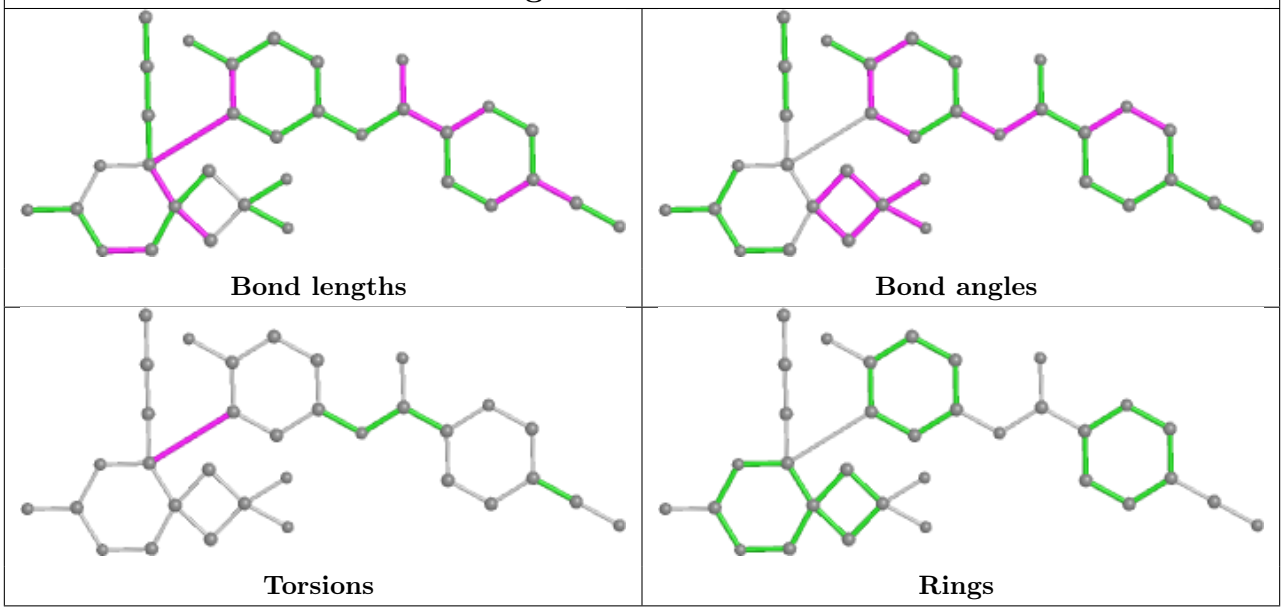
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	GX6	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 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 GX6 A 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	370/386 (95%)	0.37	19 (5%)	28	30	47, 69, 114, 190	0
2	D	114/114 (100%)	0.21	4 (3%)	44	48	46, 66, 100, 167	0
All	All	484/500 (96%)	0.33	23 (4%)	30	33	46, 68, 111, 190	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	63	TYR	5.2
2	D	272	HIS	4.7
1	A	329	TYR	4.0
1	A	62	SER	3.9
2	D	159	ALA	3.4
1	A	127	PRO	3.1
1	A	391	VAL	3.1
1	A	227	ASN	2.9
1	A	285	ASN	2.8
1	A	81	PHE	2.8
1	A	128	GLY	2.8
1	A	289	PRO	2.6
1	A	390	ASP	2.5
1	A	293	PHE	2.4
1	A	292	TYR	2.4
1	A	393	SER	2.4
1	A	61	HIS	2.3
1	A	283	TRP	2.2
1	A	124	PHE	2.2
2	D	170	LEU	2.1
1	A	59	THR	2.1
2	D	247	PRO	2.1
1	A	290	TRP	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 monosaccharides in this entry.

6.4 Ligands (i)

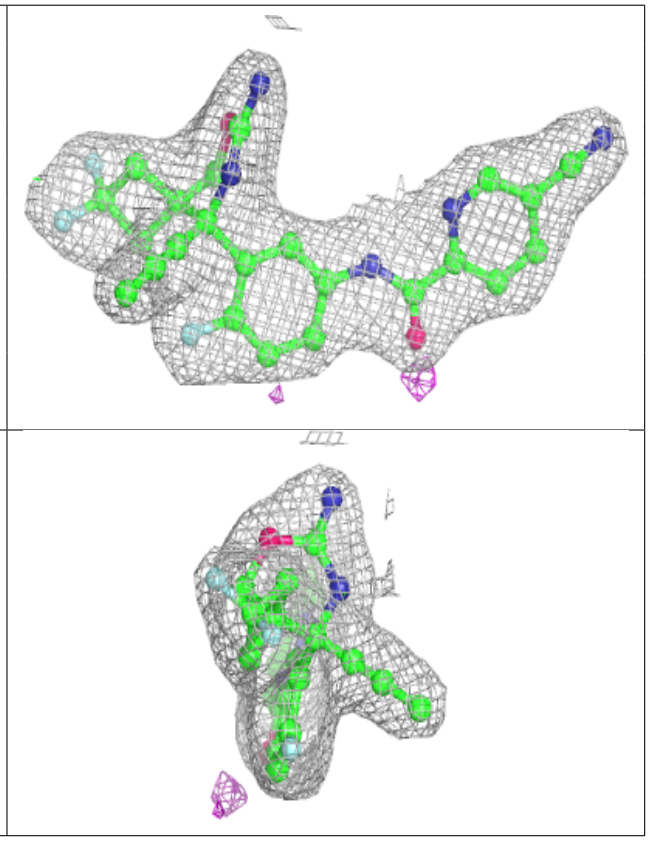
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GX6	A	401	33/33	0.97	0.12	45,59,73,86	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 GX6 A 401:

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.