



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:58 AM UTC

PDB ID : 7D5U / pdb_00007d5u
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 ⓘ 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

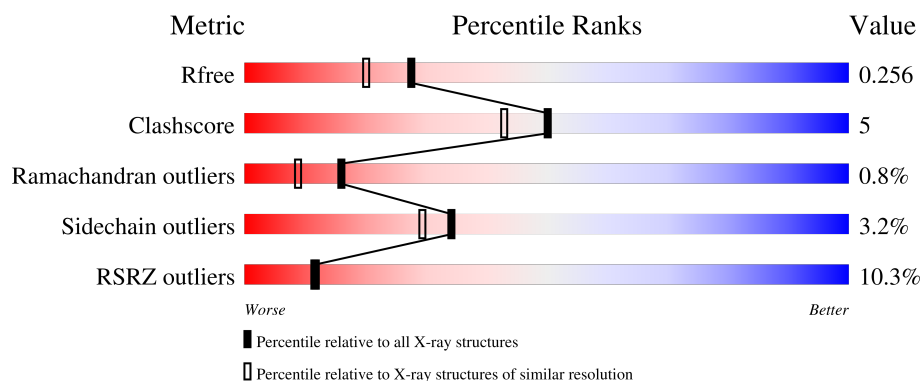
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (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 $\leq 5\%$. 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	10% 34% 53% 8% .
2	D	114	11% 38% 55% 5% .

Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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.

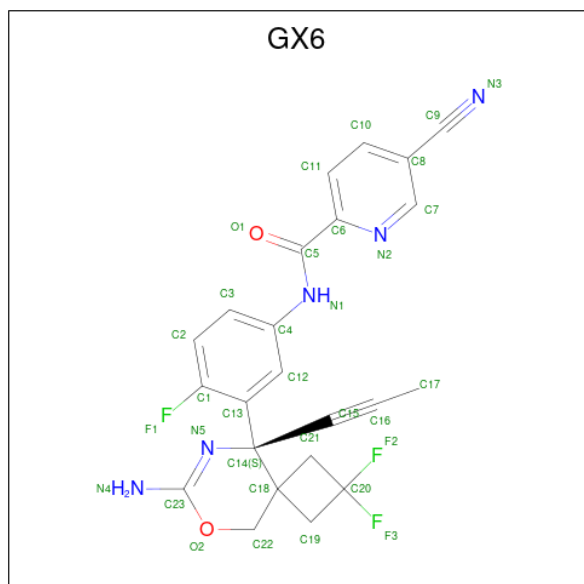
- Molecule 1 is a protein called Beta-secretase 2.

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

- Molecule 2 is a protein called xaperone.

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

- 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 (CCD ID: GX6) (formula: $C_{23}H_{18}F_3N_5O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is water.

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

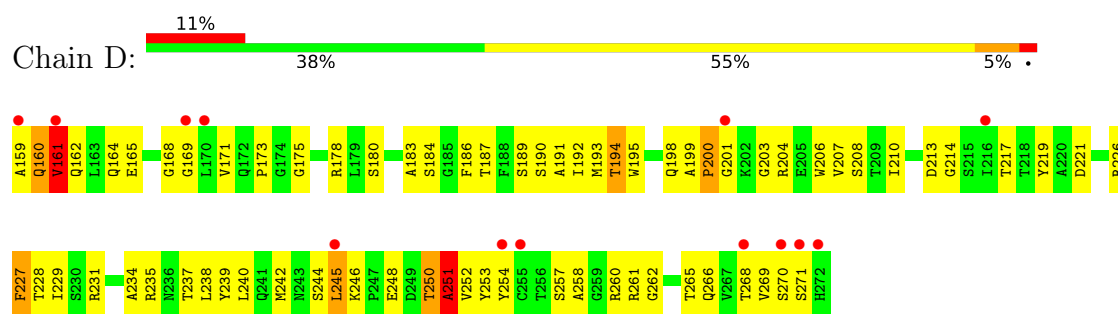
3 Residue-property plots

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 2: xaperone



4 Data and refinement statistics

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 61.31 – 2.04	Depositor EDS
% Data completeness (in resolution range)	96.0 (61.31-2.04) 96.0 (61.31-2.04)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (5.27%)	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 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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: 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	2.87	265/2886 (9.2%)	1.98	88/3935 (2.2%)
2	D	3.12	87/849 (10.2%)	1.99	22/1152 (1.9%)
All	All	2.93	352/3735 (9.4%)	1.98	110/5087 (2.2%)

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 (352) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	195	TRP	C-O	13.71	1.40	1.24
2	D	239	TYR	C-O	13.71	1.41	1.23
2	D	252	VAL	CA-CB	-12.31	1.39	1.54
1	A	342	ALA	N-CA	11.68	1.61	1.46
2	D	237	THR	C-O	11.37	1.37	1.23
2	D	193	MET	SD-CE	-10.86	1.52	1.79
1	A	78	SER	C-O	-10.75	1.10	1.24
2	D	175	GLY	C-O	10.57	1.33	1.23
1	A	63	TYR	CA-C	10.39	1.67	1.53
1	A	364	VAL	CA-CB	-10.23	1.42	1.54
1	A	275	TRP	NE1-CE2	-10.12	1.26	1.37
2	D	262	GLY	C-O	10.05	1.41	1.24
1	A	88	THR	CA-C	10.03	1.65	1.52
1	A	144	LYS	CA-C	10.00	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	THR	C-O	-9.96	1.12	1.24
1	A	222	GLY	N-CA	9.95	1.60	1.45
1	A	127	PRO	C-O	9.90	1.35	1.23
1	A	70	THR	C-O	-9.89	1.11	1.24
1	A	78	SER	CA-CB	9.67	1.67	1.53
1	A	218	LYS	N-CA	9.59	1.56	1.46
2	D	198	GLN	N-CA	9.57	1.58	1.46
2	D	165	GLU	N-CA	-9.52	1.34	1.45
1	A	158	THR	C-O	-9.49	1.13	1.24
1	A	266	LEU	N-CA	9.47	1.58	1.46
2	D	206	TRP	C-O	-9.47	1.12	1.23
1	A	146	SER	CA-C	-9.44	1.41	1.52
1	A	313	ILE	CA-C	9.38	1.63	1.52
1	A	245	THR	N-CA	9.37	1.57	1.46
1	A	350	MET	N-CA	9.34	1.58	1.46
2	D	164	GLN	N-CA	9.33	1.57	1.46
2	D	200	PRO	N-CA	-9.32	1.35	1.47
1	A	221	ILE	N-CA	9.30	1.58	1.46
1	A	311	ILE	C-O	9.28	1.36	1.24
1	A	142	LEU	C-O	9.24	1.36	1.24
1	A	255	ASP	C-O	-9.18	1.13	1.24
2	D	227	PHE	CA-C	-9.12	1.42	1.52
1	A	360	ALA	C-O	-9.11	1.12	1.24
1	A	95	PHE	CA-C	-9.11	1.41	1.52
1	A	263	ARG	C-O	-9.10	1.13	1.24
1	A	303	GLU	C-O	-9.08	1.13	1.24
1	A	303	GLU	N-CA	8.97	1.57	1.46
1	A	134	ILE	CA-C	-8.93	1.41	1.52
1	A	356	ILE	N-CA	8.92	1.57	1.46
2	D	183	ALA	N-CA	8.92	1.56	1.45
1	A	45	ILE	CA-CB	-8.77	1.43	1.54
1	A	98	GLU	N-CA	-8.75	1.34	1.45
1	A	55	ALA	CA-C	-8.67	1.42	1.52
1	A	103	ILE	N-CA	-8.66	1.38	1.46
1	A	42	LYS	CA-C	-8.61	1.42	1.52
1	A	101	VAL	C-O	-8.60	1.15	1.24
1	A	352	GLY	N-CA	8.55	1.56	1.45
1	A	138	ALA	C-O	-8.47	1.12	1.23
1	A	300	LEU	N-CA	8.38	1.56	1.46
1	A	329	TYR	CA-C	8.37	1.62	1.52
1	A	396	VAL	CA-C	8.37	1.59	1.53
1	A	47	VAL	N-CA	8.30	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	317	LEU	N-CA	8.27	1.56	1.46
1	A	125	PHE	CA-C	8.21	1.62	1.53
2	D	266	GLN	N-CA	8.15	1.56	1.46
2	D	168	GLY	N-CA	8.13	1.56	1.45
1	A	230	CYS	CA-C	8.11	1.64	1.52
1	A	354	TYR	CA-CB	-8.07	1.42	1.53
2	D	219	TYR	C-O	-8.07	1.14	1.23
1	A	121	SER	CA-CB	-8.07	1.41	1.53
1	A	347	ALA	C-O	-7.99	1.14	1.24
1	A	351	GLU	C-O	-7.98	1.13	1.24
1	A	154	ASP	CG-OD1	-7.95	1.10	1.25
2	D	226	ARG	CA-C	7.87	1.61	1.52
1	A	366	PHE	N-CA	7.85	1.55	1.46
1	A	41	GLN	CA-C	7.83	1.61	1.52
1	A	105	LYS	N-CA	7.80	1.57	1.46
1	A	118	ILE	N-CA	7.78	1.55	1.46
2	D	198	GLN	C-O	7.74	1.32	1.23
2	D	268	THR	C-O	-7.71	1.15	1.24
2	D	238	LEU	N-CA	7.71	1.55	1.45
2	D	200	PRO	C-O	-7.70	1.15	1.23
1	A	143	ALA	N-CA	7.68	1.55	1.46
1	A	289	PRO	CA-C	7.66	1.64	1.52
1	A	281	ALA	N-CA	7.65	1.54	1.45
1	A	357	PHE	C-O	-7.65	1.14	1.23
1	A	130	LYS	N-CA	7.63	1.56	1.46
1	A	276	THR	C-O	-7.59	1.13	1.24
1	A	295	LYS	N-CA	7.58	1.55	1.45
1	A	25	ASP	C-O	7.58	1.30	1.24
1	A	40	PRO	CA-C	7.55	1.62	1.52
1	A	171	CYS	CA-C	7.54	1.62	1.52
2	D	208	SER	C-O	-7.52	1.13	1.23
1	A	102	THR	N-CA	7.50	1.55	1.45
1	A	88	THR	C-O	7.49	1.33	1.24
1	A	279	GLN	N-CA	7.49	1.55	1.45
1	A	266	LEU	CA-C	7.44	1.62	1.52
1	A	65	ASP	N-CA	7.43	1.55	1.46
1	A	316	GLN	N-CA	-7.42	1.37	1.46
2	D	195	TRP	CA-C	-7.37	1.43	1.52
2	D	217	THR	C-O	-7.36	1.15	1.23
1	A	159	GLN	N-CA	-7.34	1.36	1.46
1	A	64	ILE	N-CA	7.31	1.55	1.46
1	A	310	ARG	N-CA	7.28	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	251	ALA	CA-C	-7.28	1.43	1.52
2	D	162	GLN	CA-CB	-7.28	1.43	1.53
1	A	77	ARG	C-O	-7.26	1.15	1.23
1	A	171	CYS	N-CA	-7.25	1.37	1.46
1	A	359	ARG	CA-C	7.24	1.62	1.52
2	D	253	TYR	CG-CD2	-7.23	1.24	1.39
1	A	51	SER	N-CA	7.20	1.55	1.46
1	A	241	ASP	N-CA	7.19	1.55	1.46
1	A	31	TYR	C-O	-7.18	1.14	1.23
1	A	198	LYS	C-O	7.18	1.32	1.23
1	A	19	VAL	N-CA	7.15	1.55	1.46
1	A	336	ILE	N-CA	7.12	1.54	1.46
2	D	160	GLN	N-CA	7.12	1.55	1.46
1	A	315	PRO	CA-CB	7.11	1.63	1.53
1	A	186	SER	C-O	-7.10	1.16	1.23
2	D	193	MET	CA-C	-7.10	1.44	1.52
1	A	347	ALA	N-CA	7.08	1.55	1.46
1	A	82	ASP	N-CA	7.05	1.54	1.45
1	A	282	CYS	N-CA	7.04	1.54	1.46
1	A	160	ALA	CA-C	-7.01	1.43	1.52
1	A	38	THR	CA-C	7.01	1.61	1.52
1	A	248	ARG	CZ-NH2	-7.01	1.24	1.33
2	D	204	ARG	C-O	7.00	1.32	1.23
1	A	59	THR	CA-C	6.99	1.59	1.52
2	D	190	SER	CB-OG	6.97	1.56	1.42
1	A	300	LEU	C-O	-6.95	1.15	1.24
1	A	35	LEU	N-CA	6.95	1.54	1.46
2	D	244	SER	C-O	6.95	1.32	1.23
1	A	396	VAL	C-O	-6.94	1.15	1.24
1	A	127	PRO	CA-C	6.93	1.60	1.52
1	A	304	ASN	N-CA	-6.92	1.37	1.46
1	A	213	GLN	C-O	6.91	1.32	1.24
1	A	82	ASP	CA-C	-6.91	1.44	1.52
1	A	359	ARG	NE-CZ	-6.90	1.25	1.33
1	A	379	VAL	CA-CB	6.89	1.63	1.54
1	A	349	VAL	N-CA	6.87	1.54	1.46
1	A	74	SER	CA-C	6.82	1.62	1.52
1	A	274	PHE	C-O	6.80	1.31	1.24
2	D	248	GLU	N-CA	6.80	1.54	1.46
2	D	231	ARG	N-CA	6.78	1.54	1.45
1	A	272	ASP	CA-CB	6.78	1.63	1.53
1	A	244	THR	CB-OG1	-6.74	1.32	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	169	GLY	N-CA	6.74	1.52	1.45
1	A	356	ILE	CA-C	6.72	1.61	1.52
1	A	210	TRP	NE1-CE2	-6.71	1.30	1.37
1	A	57	ALA	C-O	-6.66	1.16	1.24
1	A	263	ARG	N-CA	6.64	1.54	1.46
1	A	298	ILE	CA-CB	-6.62	1.46	1.54
1	A	172	GLY	N-CA	6.60	1.54	1.45
2	D	270	SER	CA-CB	6.59	1.63	1.53
1	A	207	LYS	C-O	-6.57	1.15	1.24
1	A	335	GLY	C-O	6.55	1.32	1.23
1	A	169	GLN	CD-OE1	6.54	1.35	1.23
2	D	184	SER	C-O	-6.51	1.15	1.23
1	A	254	PHE	C-O	-6.48	1.16	1.24
1	A	77	ARG	CD-NE	6.47	1.55	1.46
1	A	201	ILE	C-O	-6.46	1.17	1.24
1	A	87	TYR	C-O	6.46	1.32	1.24
1	A	30	TYR	N-CA	6.45	1.54	1.46
1	A	151	THR	CB-OG1	-6.44	1.33	1.43
1	A	226	LEU	C-O	6.43	1.32	1.23
1	A	15	PHE	N-CA	6.43	1.58	1.46
2	D	178	ARG	N-CA	-6.43	1.38	1.46
1	A	289	PRO	C-O	6.43	1.32	1.24
2	D	258	ALA	N-CA	-6.43	1.36	1.46
1	A	367	ALA	CA-C	6.41	1.60	1.52
2	D	164	GLN	CA-C	-6.41	1.45	1.52
1	A	187	LEU	CB-CG	6.41	1.66	1.53
2	D	258	ALA	CA-C	-6.40	1.44	1.53
1	A	73	SER	N-CA	6.39	1.54	1.46
1	A	110	SER	C-O	-6.39	1.16	1.23
1	A	320	GLN	CA-C	6.37	1.59	1.52
1	A	253	VAL	CA-CB	-6.35	1.46	1.54
1	A	338	PRO	N-CA	6.32	1.54	1.47
1	A	316	GLN	C-O	-6.32	1.16	1.24
1	A	122	GLU	C-O	6.31	1.31	1.23
1	A	253	VAL	C-O	-6.31	1.16	1.24
1	A	374	ILE	CA-CB	6.30	1.62	1.54
1	A	135	LEU	CA-CB	6.30	1.61	1.53
2	D	160	GLN	C-O	6.30	1.31	1.24
1	A	23	GLN	C-O	-6.27	1.15	1.23
1	A	55	ALA	N-CA	6.26	1.53	1.46
2	D	171	VAL	CA-CB	-6.23	1.45	1.54
2	D	201	GLY	C-O	-6.22	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	311	ILE	CA-C	6.21	1.60	1.52
1	A	142	LEU	N-CA	6.20	1.54	1.46
2	D	234	ALA	CA-CB	6.20	1.64	1.53
2	D	271	SER	CA-C	6.19	1.60	1.52
1	A	340	THR	CA-C	6.16	1.61	1.52
1	A	171	CYS	CA-CB	6.15	1.62	1.53
1	A	71	GLU	C-O	-6.14	1.16	1.24
1	A	124	PHE	CA-C	6.13	1.60	1.52
1	A	96	VAL	C-O	-6.10	1.17	1.24
1	A	192	ILE	C-O	-6.10	1.17	1.24
1	A	154	ASP	CA-CB	-6.10	1.43	1.53
2	D	250	THR	N-CA	6.09	1.53	1.46
2	D	261	ARG	CZ-NH2	6.09	1.41	1.33
1	A	83	VAL	CA-CB	-6.08	1.45	1.55
1	A	171	CYS	C-O	-6.08	1.15	1.24
1	A	337	SER	CA-C	-6.06	1.46	1.52
1	A	163	PRO	N-CA	-6.05	1.39	1.47
1	A	190	GLY	N-CA	-6.05	1.37	1.45
1	A	264	ALA	C-O	-6.04	1.16	1.24
1	A	161	ASN	CA-C	6.03	1.61	1.53
2	D	173	PRO	CA-C	6.02	1.60	1.52
1	A	270	PHE	C-O	6.01	1.31	1.23
1	A	359	ARG	CD-NE	-6.00	1.37	1.46
2	D	210	ILE	CA-CB	6.00	1.63	1.54
1	A	76	TYR	C-O	-5.96	1.16	1.23
1	A	155	SER	N-CA	5.96	1.53	1.46
1	A	215	GLU	CD-OE2	5.95	1.36	1.25
1	A	275	TRP	CD2-CE2	5.92	1.51	1.41
1	A	255	ASP	CA-C	-5.92	1.45	1.52
1	A	161	ASN	C-O	-5.90	1.15	1.23
2	D	194	THR	CB-CG2	5.90	1.72	1.52
1	A	237	LYS	CA-C	5.89	1.60	1.52
1	A	139	TYR	N-CA	-5.87	1.38	1.45
1	A	369	SER	CA-CB	5.87	1.62	1.52
1	A	371	CYS	CA-C	5.84	1.60	1.52
1	A	34	MET	N-CA	5.83	1.53	1.46
1	A	345	ILE	N-CA	-5.82	1.39	1.46
1	A	187	LEU	N-CA	-5.82	1.39	1.46
1	A	212	TYR	C-N	5.81	1.41	1.33
1	A	250	PRO	C-O	-5.80	1.16	1.23
1	A	272	ASP	CG-OD2	5.78	1.36	1.25
1	A	70	THR	N-CA	5.77	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	GLY	N-CA	5.77	1.53	1.45
2	D	261	ARG	CD-NE	5.76	1.54	1.46
1	A	361	GLN	CA-C	-5.75	1.45	1.52
1	A	130	LYS	CA-C	5.73	1.60	1.52
2	D	254	TYR	CA-CB	-5.73	1.42	1.54
1	A	216	ILE	CB-CG1	-5.73	1.42	1.53
1	A	62	SER	N-CA	5.72	1.53	1.46
1	A	107	PHE	C-O	-5.72	1.16	1.23
2	D	191	ALA	N-CA	5.72	1.52	1.46
2	D	261	ARG	N-CA	5.71	1.53	1.45
1	A	169	GLN	C-O	-5.70	1.17	1.24
2	D	192	ILE	N-CA	5.70	1.52	1.46
1	A	210	TRP	CE2-CZ2	-5.69	1.27	1.39
1	A	110	SER	N-CA	-5.67	1.39	1.45
2	D	266	GLN	CA-C	-5.66	1.45	1.52
1	A	353	PHE	CA-C	-5.64	1.45	1.52
1	A	367	ALA	C-O	5.64	1.30	1.23
2	D	192	ILE	C-O	-5.63	1.17	1.24
1	A	228	LEU	N-CA	5.62	1.53	1.46
1	A	31	TYR	C-N	-5.62	1.25	1.33
1	A	139	TYR	C-O	-5.61	1.16	1.23
1	A	337	SER	N-CA	5.60	1.50	1.45
1	A	249	LEU	CA-C	5.60	1.57	1.52
1	A	22	LEU	CB-CG	-5.58	1.42	1.53
1	A	164	ASN	CA-CB	5.57	1.59	1.52
1	A	235	ALA	C-O	5.56	1.30	1.24
2	D	254	TYR	CA-C	5.55	1.59	1.52
2	D	262	GLY	N-CA	-5.55	1.37	1.44
1	A	189	LEU	N-CA	5.54	1.53	1.46
1	A	92	TRP	NE1-CE2	-5.52	1.31	1.37
1	A	102	THR	C-N	-5.52	1.27	1.33
1	A	302	ASP	CA-CB	5.52	1.62	1.53
1	A	382	ILE	N-CA	5.51	1.52	1.46
1	A	386	PHE	C-N	-5.50	1.26	1.33
1	A	80	GLY	C-O	-5.50	1.15	1.23
1	A	163	PRO	CA-CB	5.49	1.61	1.53
2	D	221	ASP	N-CA	-5.49	1.39	1.46
1	A	334	PHE	CG-CD2	5.49	1.50	1.38
1	A	119	PHE	C-O	-5.49	1.16	1.24
2	D	187	THR	C-O	-5.49	1.16	1.23
1	A	210	TRP	CA-C	5.48	1.60	1.52
1	A	259	GLU	C-O	-5.48	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	260	ARG	C-N	-5.47	1.26	1.33
1	A	132	ASN	C-O	-5.47	1.15	1.24
1	A	84	THR	CA-CB	-5.47	1.45	1.53
1	A	184	GLY	C-N	-5.45	1.27	1.33
2	D	213	ASP	C-O	-5.45	1.16	1.24
1	A	35	LEU	CA-C	5.45	1.59	1.52
1	A	305	SER	C-O	-5.44	1.17	1.24
1	A	63	TYR	C-N	5.43	1.38	1.33
1	A	227	ASN	CA-CB	5.43	1.60	1.52
1	A	216	ILE	C-O	5.43	1.30	1.24
1	A	254	PHE	CE2-CZ	5.43	1.54	1.38
1	A	310	ARG	CA-C	-5.43	1.46	1.52
1	A	140	ALA	N-CA	-5.41	1.39	1.46
1	A	144	LYS	N-CA	-5.41	1.37	1.45
2	D	160	GLN	C-N	5.41	1.41	1.33
2	D	194	THR	C-O	-5.40	1.17	1.23
1	A	117	THR	C-O	5.39	1.30	1.24
2	D	168	GLY	C-N	-5.39	1.28	1.33
1	A	98	GLU	CA-CB	5.38	1.65	1.54
1	A	42	LYS	CB-CG	5.38	1.68	1.52
1	A	281	ALA	CA-CB	5.38	1.63	1.53
1	A	22	LEU	C-O	-5.38	1.17	1.24
1	A	85	VAL	CA-CB	-5.37	1.47	1.53
1	A	99	ASP	CA-CB	5.37	1.62	1.53
1	A	314	LEU	CA-C	5.37	1.60	1.52
1	A	113	VAL	CA-CB	5.37	1.64	1.54
1	A	349	VAL	C-O	-5.36	1.18	1.24
1	A	356	ILE	CB-CG1	5.36	1.64	1.53
2	D	161	VAL	CA-CB	5.36	1.61	1.54
1	A	92	TRP	C-O	5.35	1.30	1.23
1	A	357	PHE	CG-CD1	5.35	1.50	1.38
2	D	207	VAL	N-CA	-5.35	1.39	1.46
1	A	299	TYR	CA-CB	-5.34	1.45	1.53
1	A	304	ASN	CG-OD1	5.34	1.33	1.23
1	A	141	THR	N-CA	5.34	1.52	1.46
1	A	197	TYR	C-O	-5.33	1.17	1.23
2	D	231	ARG	CZ-NH2	5.31	1.40	1.33
1	A	241	ASP	CA-CB	-5.30	1.44	1.53
2	D	228	THR	C-O	5.30	1.30	1.24
2	D	206	TRP	CA-CB	-5.26	1.44	1.53
2	D	253	TYR	N-CA	5.23	1.52	1.46
1	A	266	LEU	C-O	5.23	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	257	SER	N-CA	-5.22	1.39	1.46
1	A	344	VAL	CA-C	5.22	1.59	1.52
2	D	187	THR	CA-CB	-5.21	1.46	1.52
1	A	379	VAL	C-O	5.20	1.31	1.24
2	D	178	ARG	CA-CB	-5.20	1.45	1.53
2	D	234	ALA	CA-C	5.20	1.59	1.52
1	A	60	PRO	CA-CB	-5.20	1.46	1.53
1	A	64	ILE	CA-C	5.20	1.58	1.52
2	D	198	GLN	CA-C	-5.19	1.46	1.52
1	A	98	GLU	CA-C	-5.19	1.46	1.52
1	A	303	GLU	CA-CB	-5.16	1.45	1.53
1	A	23	GLN	CA-C	5.16	1.59	1.52
1	A	188	VAL	C-O	-5.15	1.18	1.24
2	D	198	GLN	CA-CB	5.15	1.62	1.53
1	A	29	GLY	N-CA	5.14	1.50	1.45
2	D	203	GLY	N-CA	-5.12	1.38	1.45
2	D	227	PHE	C-O	-5.12	1.17	1.23
1	A	169	GLN	N-CA	-5.12	1.40	1.46
1	A	69	ASP	C-O	5.12	1.30	1.23
1	A	218	LYS	CA-CB	5.10	1.62	1.53
1	A	22	LEU	N-CA	5.10	1.52	1.46
2	D	245	LEU	C-O	-5.10	1.17	1.23
1	A	195	SER	N-CA	5.09	1.53	1.46
1	A	96	VAL	N-CA	5.09	1.52	1.46
1	A	75	THR	CB-CG2	5.09	1.69	1.52
1	A	313	ILE	N-CA	5.09	1.52	1.46
2	D	265	THR	CA-CB	5.09	1.64	1.53
1	A	373	GLU	CA-C	5.07	1.58	1.52
1	A	105	LYS	C-O	5.06	1.30	1.23
1	A	368	ALA	N-CA	5.06	1.52	1.46
1	A	150	GLU	N-CA	5.05	1.52	1.46
1	A	339	SER	N-CA	5.05	1.52	1.45
1	A	107	PHE	CA-C	5.05	1.58	1.52
2	D	270	SER	C-O	5.04	1.30	1.24
1	A	202	TRP	CA-C	-5.04	1.46	1.52
1	A	230	CYS	C-O	-5.04	1.17	1.24
1	A	275	TRP	C-O	-5.03	1.18	1.24
1	A	34	MET	CA-C	5.03	1.58	1.52
1	A	88	THR	CB-OG1	-5.03	1.35	1.43
1	A	183	ASN	C-N	5.02	1.38	1.33
1	A	372	ALA	C-N	-5.02	1.27	1.33
1	A	216	ILE	CA-CB	5.01	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	240	LEU	CA-C	-5.01	1.46	1.52
2	D	178	ARG	NE-CZ	-5.01	1.27	1.33

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	ILE	N-CA-C	-10.15	92.22	106.53
1	A	184	GLY	N-CA-C	9.37	122.64	110.45
2	D	178	ARG	NE-CZ-NH1	-8.51	112.99	121.50
1	A	199	GLY	N-CA-C	-8.38	97.79	112.53
1	A	320	GLN	N-CA-C	7.85	120.98	109.04
1	A	42	LYS	CG-CD-CE	7.51	128.58	111.30
1	A	265	SER	N-CA-C	7.50	120.52	111.82
1	A	360	ALA	N-CA-C	-7.29	103.36	111.82
2	D	258	ALA	CA-C-N	-7.26	112.25	122.86
2	D	258	ALA	C-N-CA	-7.26	112.25	122.86
2	D	261	ARG	NE-CZ-NH1	-7.22	114.28	121.50
1	A	338	PRO	CB-CA-C	-7.09	101.69	110.98
1	A	122	GLU	CB-CA-C	7.09	120.59	110.24
1	A	292	TYR	N-CA-C	7.09	121.53	113.02
2	D	214	GLY	N-CA-C	6.97	124.61	115.40
1	A	319	ILE	CA-CB-CG1	6.83	122.01	110.40
1	A	120	GLU	CA-CB-CG	6.81	127.71	114.10
1	A	88	THR	N-CA-C	6.80	118.78	111.36
1	A	126	LEU	CA-C-N	-6.71	112.74	119.92
1	A	126	LEU	C-N-CA	-6.71	112.74	119.92
1	A	62	SER	N-CA-C	6.70	120.08	110.10
1	A	369	SER	N-CA-CB	6.66	118.95	110.23
2	D	164	GLN	CB-CG-CD	6.62	123.86	112.60
1	A	88	THR	CB-CA-C	6.60	122.06	110.85
1	A	290	TRP	N-CA-C	6.46	119.14	111.71
1	A	172	GLY	N-CA-C	6.44	121.95	114.16
1	A	351	GLU	CA-CB-CG	-6.43	101.23	114.10
2	D	261	ARG	NE-CZ-NH2	6.41	124.97	119.20
1	A	165	VAL	CB-CA-C	-6.33	102.05	111.80
1	A	56	VAL	N-CA-C	6.29	118.95	109.20
1	A	239	ILE	N-CA-C	6.21	118.68	108.99
1	A	316	GLN	CA-C-O	-6.17	113.12	120.10
2	D	248	GLU	N-CA-C	6.17	120.36	112.34
1	A	281	ALA	N-CA-C	-6.15	100.17	109.95
1	A	227	ASN	CB-CA-C	6.14	118.77	111.22
1	A	148	SER	N-CA-C	-6.08	105.82	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	386	PHE	CA-C-N	6.07	129.48	120.87
1	A	386	PHE	C-N-CA	6.07	129.48	120.87
1	A	26	SER	CA-CB-OG	-6.04	99.01	111.10
1	A	146	SER	CB-CA-C	-6.04	100.29	110.43
1	A	128	GLY	N-CA-C	5.97	127.34	113.18
1	A	78	SER	CA-CB-OG	-5.96	99.18	111.10
1	A	261	VAL	N-CA-C	-5.93	104.72	110.42
1	A	220	GLU	CA-CB-CG	5.93	125.96	114.10
1	A	31	TYR	CA-C-N	5.92	131.17	123.00
1	A	31	TYR	C-N-CA	5.92	131.17	123.00
1	A	70	THR	N-CA-C	-5.89	104.99	111.82
2	D	206	TRP	CA-C-O	-5.88	114.72	121.19
1	A	198	LYS	N-CA-C	-5.87	100.23	109.50
1	A	225	SER	N-CA-CB	5.83	119.15	110.29
1	A	261	VAL	N-CA-CB	5.82	117.36	110.55
1	A	254	PHE	CA-C-N	5.82	128.07	120.28
1	A	254	PHE	C-N-CA	5.82	128.07	120.28
1	A	115	ILE	CB-CA-C	5.79	117.99	110.12
1	A	223	GLY	N-CA-C	5.78	123.22	115.59
1	A	95	PHE	CA-C-N	-5.73	115.71	123.10
1	A	95	PHE	C-N-CA	-5.73	115.71	123.10
1	A	396	VAL	CB-CA-C	5.70	116.24	110.94
1	A	54	PHE	N-CA-C	-5.68	99.26	108.41
2	D	229	ILE	CA-C-O	-5.67	113.82	121.02
2	D	184	SER	CA-CB-OG	5.58	122.26	111.10
1	A	244	THR	N-CA-C	-5.57	99.36	108.76
2	D	238	LEU	N-CA-C	-5.56	101.11	109.95
2	D	193	MET	CG-SD-CE	-5.55	88.68	100.90
1	A	158	THR	CA-CB-CG2	-5.54	101.08	110.50
1	A	284	THR	CB-CA-C	-5.52	102.38	110.06
1	A	252	LYS	N-CA-C	-5.51	105.36	111.36
1	A	284	THR	N-CA-C	-5.49	102.06	110.30
1	A	322	MET	CG-SD-CE	5.48	112.96	100.90
2	D	178	ARG	NH1-CZ-NH2	5.47	126.41	119.30
2	D	235	ARG	CB-CG-CD	5.46	123.86	111.30
1	A	102	THR	CA-C-N	5.45	129.25	123.25
1	A	102	THR	C-N-CA	5.45	129.25	123.25
1	A	245	THR	N-CA-C	5.45	116.90	111.07
1	A	57	ALA	CA-C-O	-5.41	114.31	120.58
1	A	190	GLY	N-CA-C	5.34	122.06	114.85
1	A	133	GLY	CA-C-N	5.33	130.40	122.99
1	A	133	GLY	C-N-CA	5.33	130.40	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	SER	CA-CB-OG	5.32	121.74	111.10
1	A	271	SER	CA-CB-OG	-5.31	100.48	111.10
1	A	154	ASP	CA-C-O	-5.29	114.94	120.55
2	D	219	TYR	CA-C-N	5.29	128.22	120.71
2	D	219	TYR	C-N-CA	5.29	128.22	120.71
1	A	192	ILE	N-CA-CB	-5.28	103.82	111.52
1	A	205	PRO	N-CA-C	5.26	119.44	111.19
2	D	191	ALA	CA-C-N	5.21	127.49	120.50
2	D	191	ALA	C-N-CA	5.21	127.49	120.50
1	A	189	LEU	CA-C-N	-5.21	115.28	122.63
1	A	189	LEU	C-N-CA	-5.21	115.28	122.63
2	D	204	ARG	CG-CD-NE	5.20	123.44	112.00
1	A	250	PRO	CA-C-O	-5.19	115.50	121.36
2	D	178	ARG	CB-CA-C	-5.18	102.17	110.14
1	A	359	ARG	N-CA-C	-5.15	105.84	111.82
1	A	256	ALA	N-CA-C	5.15	117.64	111.71
1	A	265	SER	CA-C-O	-5.14	114.06	119.97
1	A	274	PHE	N-CA-C	5.14	116.57	111.07
1	A	364	VAL	CA-C-N	-5.13	116.84	122.38
1	A	364	VAL	C-N-CA	-5.13	116.84	122.38
1	A	376	GLY	N-CA-C	-5.13	107.18	115.08
2	D	189	SER	CA-CB-OG	-5.10	100.90	111.10
1	A	310	ARG	CB-CG-CD	-5.05	99.68	111.30
1	A	218	LYS	CA-CB-CG	5.04	124.19	114.10
1	A	273	GLY	N-CA-C	5.04	118.78	112.73
1	A	112	LEU	CA-C-O	-5.04	114.97	120.36
1	A	272	ASP	N-CA-C	-5.04	105.79	111.28
1	A	307	ARG	CG-CD-NE	5.03	123.06	112.00
1	A	64	ILE	CB-CA-C	-5.03	104.81	111.80
1	A	363	ARG	N-CA-C	5.02	116.70	108.76
1	A	170	MET	CB-CG-SD	-5.02	97.65	112.70
1	A	275	TRP	N-CA-C	5.00	116.73	111.28

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
1	A	23	GLN	Mainchain
1	A	302	ASP	Sidechain
1	A	345	ILE	Mainchain

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Mol	Chain	Res	Type	Group
2	D	199	ALA	Mainchain
2	D	227	PHE	Sidechain
2	D	251	ALA	Mainchain

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	2815	0	2648	32	0
2	D	835	0	794	7	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	37	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 (37) 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:322:MET:HE3	1:A:333:ARG:CG	2.37	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:267:ILE:O	1:A:268:PRO:C	2.46	0.54
1:A:26:SER:HA	3:A:401:GX6:N3	2.23	0.54
1:A:15:PHE:HA	1:A:18:MET:HE3	1.93	0.51
1:A:270:PHE:CZ	1:A:293:PHE:CZ	2.93	0.49
1:A:284:THR:O	1:A:286:SER:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:242:MET:HE2	2:D:245:LEU:HD21	1.97	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:322:MET:HE3	1:A:333:ARG:HG2	1.96	0.46
1:A:284:THR:C	1:A:286:SER:N	2.73	0.45
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: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:79:LYS:HE2	1:A:98:GLU:CG	2.51	0.40
2:D:246:LYS:C	2:D:269:VAL:HG11	2.45	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%)	24	16
2	D	113/114 (99%)	109 (96%)	2 (2%)	2 (2%)	6	2
All	All	479/500 (96%)	450 (94%)	25 (5%)	4 (1%)	16	9

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 ⓘ

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%)	278 (96%)	10 (4%)	32	27
2	D	85/91 (93%)	82 (96%)	3 (4%)	32	27
All	All	373/411 (91%)	360 (96%)	13 (4%)	34	27

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	250	PRO
1	A	263	ARG
1	A	278	SER
1	A	286	SER
1	A	288	THR
1	A	391	VAL
2	D	160	GLN
2	D	180	SER
2	D	200	PRO

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	132	ASN
2	D	241	GLN
2	D	243	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 [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	2.17	10 (31%)	37,55,55	1.41	6 (16%)

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	6.44	1.63	1.55
3	A	401	GX6	C19-C20	4.07	1.56	1.50
3	A	401	GX6	C10-C8	3.93	1.47	1.39
3	A	401	GX6	C14-C13	2.95	1.57	1.53
3	A	401	GX6	C13-C1	2.78	1.42	1.39
3	A	401	GX6	C6-C5	-2.73	1.43	1.50
3	A	401	GX6	C8-C9	-2.51	1.39	1.44
3	A	401	GX6	O1-C5	-2.51	1.17	1.23
3	A	401	GX6	O2-C22	2.40	1.49	1.45
3	A	401	GX6	C6-N2	2.30	1.38	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	GX6	C4-N1-C5	3.11	134.80	126.61
3	A	401	GX6	C7-N2-C6	2.74	121.75	117.46
3	A	401	GX6	C18-C19-C20	2.66	92.31	77.43
3	A	401	GX6	C2-C1-C13	-2.60	120.02	123.46
3	A	401	GX6	C12-C13-C1	2.34	120.05	116.82
3	A	401	GX6	C18-C21-C20	2.28	90.17	77.43

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

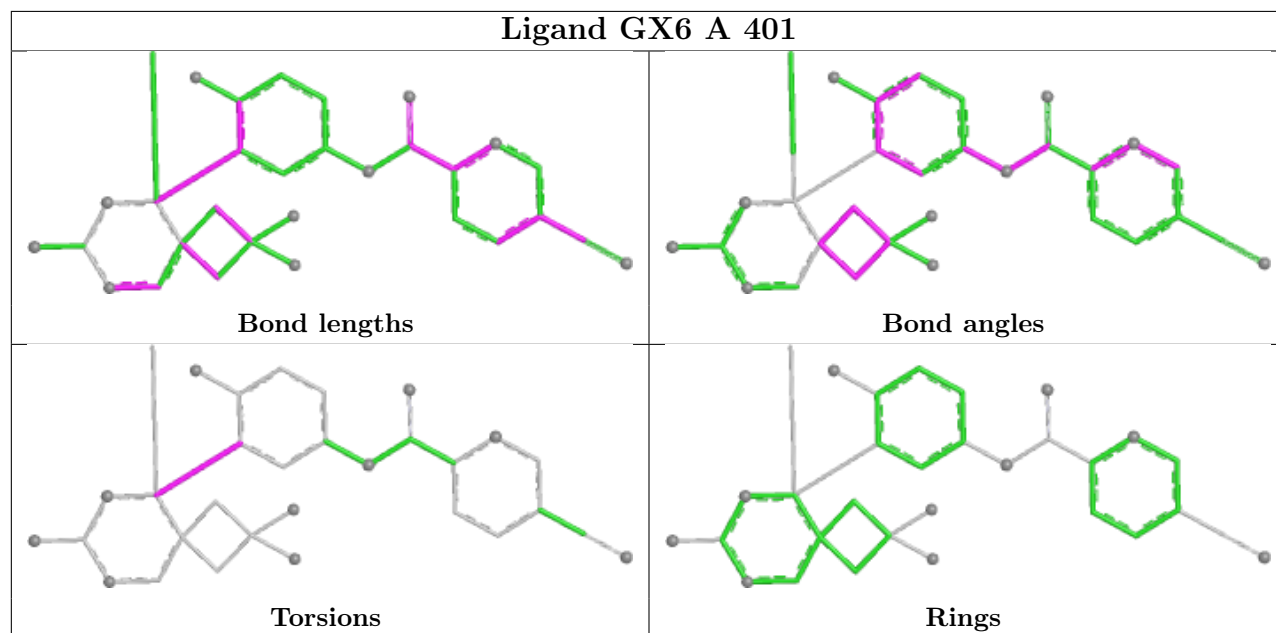
There are no ring outliers.

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 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	370/386 (95%)	0.93	37 (10%)	12 12	34, 69, 114, 190	2 (0%)
2	D	114/114 (100%)	0.92	13 (11%)	10 9	25, 66, 100, 167	1 (0%)
All	All	484/500 (96%)	0.93	50 (10%)	12 11	25, 68, 111, 190	3 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	341	ASN	4.6
2	D	272	HIS	4.6
1	A	328	ASN	3.9
1	A	292	TYR	3.7
1	A	63	TYR	3.7
1	A	289	PRO	3.5
2	D	216	ILE	3.4
2	D	270	SER	3.4
1	A	95	PHE	3.4
2	D	255	CYS	3.3
1	A	329	TYR	3.3
1	A	127	PRO	3.1
1	A	293	PHE	3.1
1	A	285	ASN	3.1
2	D	170	LEU	3.1
1	A	290	TRP	3.1
1	A	15	PHE	3.0
2	D	201	GLY	3.0
1	A	124	PHE	2.9
2	D	159	ALA	2.8
1	A	92	TRP	2.7
1	A	16	LEU	2.7
2	D	161	VAL	2.7
1	A	81	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	270	PHE	2.6
2	D	268	THR	2.5
1	A	252	LYS	2.4
1	A	235	ALA	2.4
2	D	169	GLY	2.4
1	A	88	THR	2.4
1	A	27	GLY	2.4
1	A	83	VAL	2.4
1	A	73	SER	2.4
1	A	283	TRP	2.4
1	A	386	PHE	2.3
1	A	267	ILE	2.3
1	A	385	PRO	2.3
2	D	254	TYR	2.3
1	A	376	GLY	2.3
2	D	271	SER	2.3
1	A	327	LEU	2.2
1	A	38	THR	2.2
1	A	119	PHE	2.1
1	A	69	ASP	2.1
1	A	125	PHE	2.1
1	A	223	GLY	2.1
1	A	68	PHE	2.1
1	A	74	SER	2.1
2	D	245	LEU	2.0
1	A	90	GLY	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 [\(i\)](#)

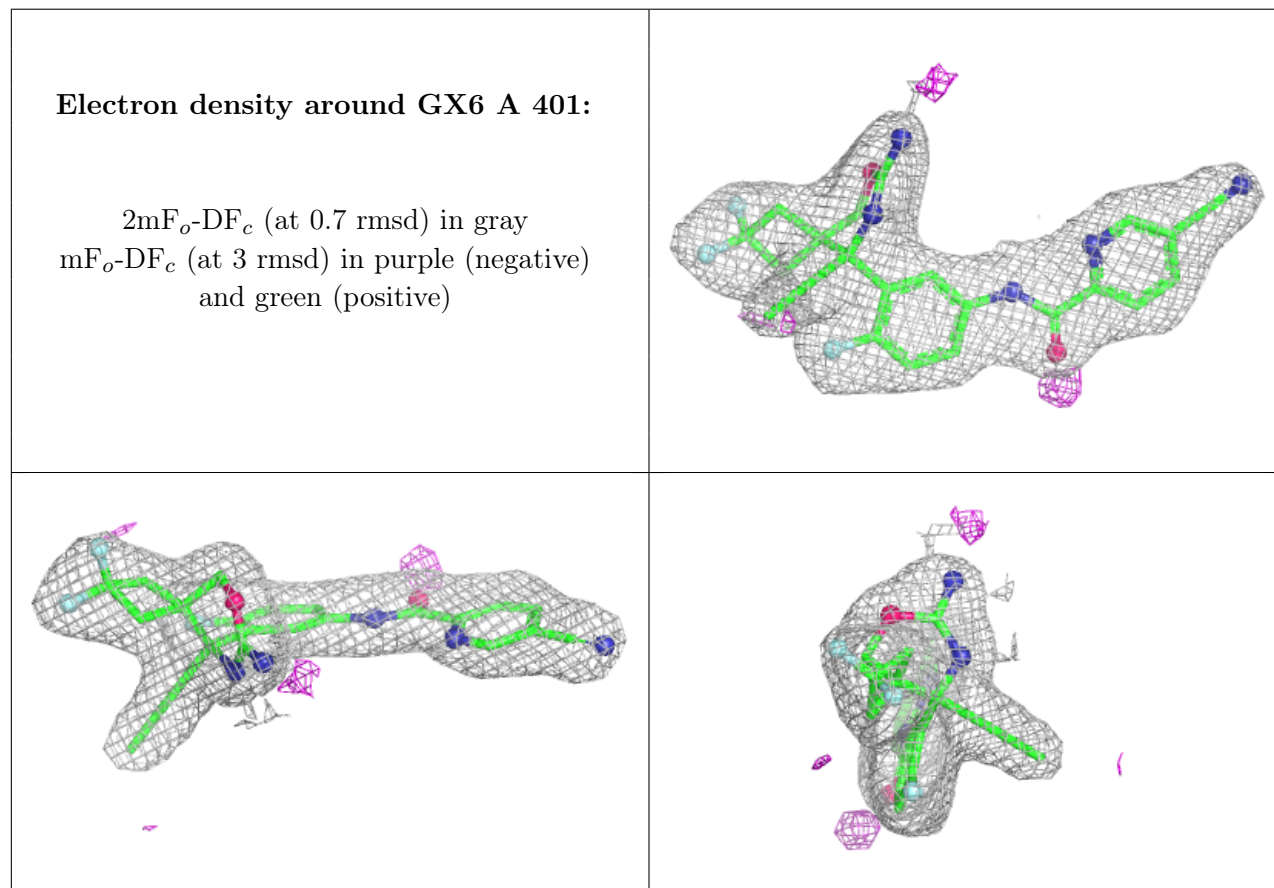
There are no oligosaccharides in this entry.

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
3	GX6	A	401	33/33	0.95	0.09	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.